



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 06:59 PM EST

PDB ID : 4NHH
Title : Structure of 2G12 IgG Dimer
Authors : Wu, Y.; West Jr., A.P.; Kim, H.J.; Thornton, M.E.; Ward, A.B.; Bjorkman, P.J.
Deposited on : 2013-11-05
Resolution : 6.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

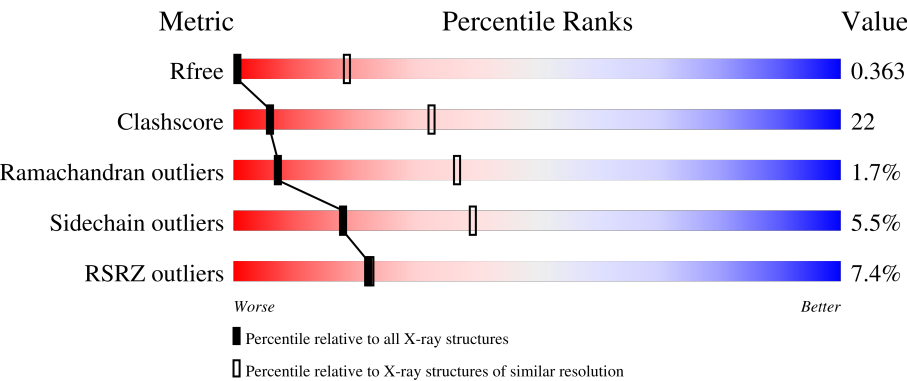
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1100 (9.00-4.00)
Clashscore	180529	1140 (9.00-4.00)
Ramachandran outliers	177936	1010 (9.00-4.00)
Sidechain outliers	177891	1032 (9.00-3.96)
RSRZ outliers	164620	1095 (9.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	F	213	<div><div>2%</div><div>81%</div><div>16%</div><div>..</div></div>
1	G	213	<div><div>8%</div><div>76%</div><div>21%</div><div>..</div></div>
1	K	213	<div><div>11%</div><div>82%</div><div>15%</div><div>..</div></div>
1	L	213	<div><div>10%</div><div>77%</div><div>20%</div><div>..</div></div>
1	P	213	<div><div>4%</div><div>82%</div><div>15%</div><div>..</div></div>
1	Q	213	<div><div>6%</div><div>76%</div><div>21%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
2	E	229	
2	H	229	
2	I	229	
2	M	229	
2	O	229	
2	R	229	
3	A	211	
3	B	211	
3	C	211	
3	D	211	
3	J	211	
3	N	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28972 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2G12 IgG dimer light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	K	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	G	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	F	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	Q	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
1	P	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			

- Molecule 2 is a protein called Hepatitis B virus receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	0	0	0
			1565	988	268	303	6			
2	M	206	Total	C	N	O	S	0	0	0
			1542	974	263	299	6			
2	E	210	Total	C	N	O	S	0	0	0
			1574	994	270	304	6			
2	I	206	Total	C	N	O	S	0	0	0
			1544	976	265	297	6			
2	O	208	Total	C	N	O	S	0	0	0
			1555	982	265	302	6			
2	R	206	Total	C	N	O	S	0	0	0
			1542	974	263	299	6			

There are 1158 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLU	SER	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	PHE	conflict	UNP Q6PYX1
H	5	VAL	-	expression tag	UNP Q6PYX1
H	6	GLU	-	expression tag	UNP Q6PYX1
H	7	SER	-	expression tag	UNP Q6PYX1
H	8	GLY	-	expression tag	UNP Q6PYX1
H	9	GLY	-	expression tag	UNP Q6PYX1
H	10	GLY	PHE	conflict	UNP Q6PYX1
H	11	LEU	PRO	conflict	UNP Q6PYX1
H	12	VAL	PRO	conflict	UNP Q6PYX1
H	14	ALA	PRO	conflict	UNP Q6PYX1
H	15	GLY	LYS	conflict	UNP Q6PYX1
H	16	GLY	ASP	conflict	UNP Q6PYX1
H	17	SER	THR	conflict	UNP Q6PYX1
H	19	ILE	MET	conflict	UNP Q6PYX1
H	20	LEU	ILE	conflict	UNP Q6PYX1
H	?	-	ARG	deletion	UNP Q6PYX1
H	?	-	THR	deletion	UNP Q6PYX1
H	?	-	PRO	deletion	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	?	-	VAL	deletion	UNP Q6PYX1
H	?	-	THR	deletion	UNP Q6PYX1
H	23	GLY	VAL	conflict	UNP Q6PYX1
H	25	SER	-	expression tag	UNP Q6PYX1
H	26	ASN	-	expression tag	UNP Q6PYX1
H	27	PHE	VAL	conflict	UNP Q6PYX1
H	28	ARG	ASP	conflict	UNP Q6PYX1
H	29	ILE	VAL	conflict	UNP Q6PYX1
H	31	ALA	-	expression tag	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	?	-	ASP	deletion	UNP Q6PYX1
H	?	-	PRO	deletion	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	?	-	VAL	deletion	UNP Q6PYX1
H	33	THR	LYS	conflict	UNP Q6PYX1
H	34	MET	PHE	conflict	UNP Q6PYX1
H	37	VAL	-	expression tag	UNP Q6PYX1
H	38	ARG	-	expression tag	UNP Q6PYX1
H	39	ARG	TYR	conflict	UNP Q6PYX1
H	41	PRO	-	expression tag	UNP Q6PYX1
H	42	GLY	-	expression tag	UNP Q6PYX1
H	43	GLY	ASP	conflict	UNP Q6PYX1
H	45	LEU	VAL	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	47	TRP	-	expression tag	UNP Q6PYX1
H	?	-	HIS	deletion	UNP Q6PYX1
H	?	-	ASN	deletion	UNP Q6PYX1
H	?	-	LYS	deletion	UNP Q6PYX1
H	?	-	THR	deletion	UNP Q6PYX1
H	?	-	LYS	deletion	UNP Q6PYX1
H	?	-	PRO	deletion	UNP Q6PYX1
H	?	-	ARG	deletion	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	50	SER	GLU	conflict	UNP Q6PYX1
H	51	ILE	GLN	conflict	UNP Q6PYX1
H	52	SER	TYR	conflict	UNP Q6PYX1
H	53	SER	ASN	conflict	UNP Q6PYX1
H	58	ASP	-	expression tag	UNP Q6PYX1
H	59	TYR	-	expression tag	UNP Q6PYX1
H	60	ALA	-	expression tag	UNP Q6PYX1
H	61	ASP	-	expression tag	UNP Q6PYX1
H	62	ALA	-	expression tag	UNP Q6PYX1
H	64	LYS	VAL	conflict	UNP Q6PYX1
H	65	GLY	SER	conflict	UNP Q6PYX1
H	66	ARG	VAL	conflict	UNP Q6PYX1
H	67	PHE	LEU	conflict	UNP Q6PYX1
H	70	SER	-	expression tag	UNP Q6PYX1
H	71	ARG	-	expression tag	UNP Q6PYX1
H	72	ASP	-	expression tag	UNP Q6PYX1
H	73	ASP	-	expression tag	UNP Q6PYX1
H	?	-	HIS	deletion	UNP Q6PYX1
H	75	GLU	GLN	conflict	UNP Q6PYX1
H	77	PHE	-	expression tag	UNP Q6PYX1
H	78	VAL	-	expression tag	UNP Q6PYX1
H	79	TYR	TRP	conflict	UNP Q6PYX1
H	81	GLN	-	expression tag	UNP Q6PYX1
H	82	MET	ASN	conflict	UNP Q6PYX1
H	83	HIS	GLY	conflict	UNP Q6PYX1
H	85	ARG	-	expression tag	UNP Q6PYX1
H	86	VAL	-	expression tag	UNP Q6PYX1
H	88	ASP	-	expression tag	UNP Q6PYX1
H	89	THR	-	expression tag	UNP Q6PYX1
H	90	ALA	-	expression tag	UNP Q6PYX1
H	91	ILE	-	expression tag	UNP Q6PYX1
H	93	TYR	LYS	conflict	UNP Q6PYX1
H	95	ALA	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	96	ARG	-	expression tag	UNP Q6PYX1
H	98	GLY	VAL	conflict	UNP Q6PYX1
H	?	-	ASN	deletion	UNP Q6PYX1
H	100	ASP	LYS	conflict	UNP Q6PYX1
H	101	ARG	ALA	conflict	UNP Q6PYX1
H	103	ASP	PRO	conflict	UNP Q6PYX1
H	105	TRP	-	expression tag	UNP Q6PYX1
H	106	GLY	-	expression tag	UNP Q6PYX1
H	108	GLY	-	expression tag	UNP Q6PYX1
H	109	THR	ILE	conflict	UNP Q6PYX1
H	110	VAL	GLU	conflict	UNP Q6PYX1
H	111	VAL	LYS	conflict	UNP Q6PYX1
H	113	VAL	ILE	conflict	UNP Q6PYX1
H	115	PRO	LYS	conflict	UNP Q6PYX1
H	117	SER	-	expression tag	UNP Q6PYX1
H	118	THR	-	expression tag	UNP Q6PYX1
H	?	-	GLN	deletion	UNP Q6PYX1
H	?	-	PRO	deletion	UNP Q6PYX1
H	?	-	ARG	deletion	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	122	SER	GLN	conflict	UNP Q6PYX1
H	124	PHE	TYR	conflict	UNP Q6PYX1
H	125	PRO	THR	conflict	UNP Q6PYX1
H	127	ALA	PRO	conflict	UNP Q6PYX1
H	?	-	ARG	deletion	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	130	GLY	MET	conflict	UNP Q6PYX1
H	?	-	LYS	deletion	UNP Q6PYX1
H	?	-	ASN	deletion	UNP Q6PYX1
H	?	-	GLN	deletion	UNP Q6PYX1
H	132	ALA	VAL	conflict	UNP Q6PYX1
H	133	ALA	SER	conflict	UNP Q6PYX1
H	135	GLY	THR	conflict	UNP Q6PYX1
H	140	ASP	GLY	conflict	UNP Q6PYX1
H	141	TYR	PHE	conflict	UNP Q6PYX1
H	142	PHE	TYR	conflict	UNP Q6PYX1
H	144	GLU	SER	conflict	UNP Q6PYX1
H	145	PRO	ASP	conflict	UNP Q6PYX1
H	146	VAL	ILE	conflict	UNP Q6PYX1
H	147	THR	ALA	conflict	UNP Q6PYX1
H	149	SER	GLU	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	151	ASN	GLU	conflict	UNP Q6PYX1
H	?	-	ASN	deletion	UNP Q6PYX1
H	154	ALA	GLN	conflict	UNP Q6PYX1
H	155	LEU	PRO	conflict	UNP Q6PYX1
H	156	THR	GLU	conflict	UNP Q6PYX1
H	157	SER	ASN	conflict	UNP Q6PYX1
H	158	GLY	ASN	conflict	UNP Q6PYX1
H	159	VAL	TYR	conflict	UNP Q6PYX1
H	160	HIS	LYS	conflict	UNP Q6PYX1
H	162	PHE	THR	conflict	UNP Q6PYX1
H	164	ALA	PRO	conflict	UNP Q6PYX1
H	167	GLN	ASP	conflict	UNP Q6PYX1
H	169	SER	ASP	conflict	UNP Q6PYX1
H	?	-	SER	deletion	UNP Q6PYX1
H	?	-	PHE	deletion	UNP Q6PYX1
H	?	-	PHE	deletion	UNP Q6PYX1
H	?	-	LYS	deletion	UNP Q6PYX1
H	175	SER	-	expression tag	UNP Q6PYX1
H	176	SER	-	expression tag	UNP Q6PYX1
H	177	VAL	-	expression tag	UNP Q6PYX1
H	178	VAL	-	expression tag	UNP Q6PYX1
H	181	PRO	ASP	conflict	UNP Q6PYX1
H	182	SER	LYS	conflict	UNP Q6PYX1
H	?	-	ARG	deletion	UNP Q6PYX1
H	?	-	TRP	deletion	UNP Q6PYX1
H	184	SER	GLN	conflict	UNP Q6PYX1
H	185	LEU	GLN	conflict	UNP Q6PYX1
H	187	THR	-	expression tag	UNP Q6PYX1
H	188	GLN	ASN	conflict	UNP Q6PYX1
H	189	THR	VAL	conflict	UNP Q6PYX1
H	190	TYR	PHE	conflict	UNP Q6PYX1
H	191	ILE	SER	conflict	UNP Q6PYX1
H	193	ASN	SER	conflict	UNP Q6PYX1
H	?	-	MET	deletion	UNP Q6PYX1
H	?	-	HIS	deletion	UNP Q6PYX1
H	?	-	GLU	deletion	UNP Q6PYX1
H	?	-	ALA	deletion	UNP Q6PYX1
H	?	-	LEU	deletion	UNP Q6PYX1
H	?	-	HIS	deletion	UNP Q6PYX1
H	197	LYS	-	expression tag	UNP Q6PYX1
H	198	PRO	-	expression tag	UNP Q6PYX1
H	199	SER	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	200	ASN	TYR	conflict	UNP Q6PYX1
H	202	LYS	-	expression tag	UNP Q6PYX1
H	203	VAL	-	expression tag	UNP Q6PYX1
H	204	ASP	-	expression tag	UNP Q6PYX1
H	205	LYS	-	expression tag	UNP Q6PYX1
H	206	LYS	-	expression tag	UNP Q6PYX1
H	207	VAL	-	expression tag	UNP Q6PYX1
H	208	GLU	-	expression tag	UNP Q6PYX1
H	209	PRO	GLN	conflict	UNP Q6PYX1
H	212	CYS	-	expression tag	UNP Q6PYX1
H	213	ASP	-	expression tag	UNP Q6PYX1
H	214	LYS	-	expression tag	UNP Q6PYX1
H	215	THR	LEU	conflict	UNP Q6PYX1
H	217	THR	LEU	conflict	UNP Q6PYX1
H	218	CYS	SER	conflict	UNP Q6PYX1
H	220	PRO	-	expression tag	UNP Q6PYX1
H	221	CYS	-	expression tag	UNP Q6PYX1
H	222	PRO	-	expression tag	UNP Q6PYX1
H	223	ALA	-	expression tag	UNP Q6PYX1
H	224	PRO	-	expression tag	UNP Q6PYX1
H	225	GLU	-	expression tag	UNP Q6PYX1
H	226	LEU	-	expression tag	UNP Q6PYX1
H	227	LEU	-	expression tag	UNP Q6PYX1
H	229	GLY	LYS	conflict	UNP Q6PYX1
M	1	GLU	SER	conflict	UNP Q6PYX1
M	3	GLN	PHE	conflict	UNP Q6PYX1
M	5	VAL	-	expression tag	UNP Q6PYX1
M	6	GLU	-	expression tag	UNP Q6PYX1
M	7	SER	-	expression tag	UNP Q6PYX1
M	8	GLY	-	expression tag	UNP Q6PYX1
M	9	GLY	-	expression tag	UNP Q6PYX1
M	10	GLY	PHE	conflict	UNP Q6PYX1
M	11	LEU	PRO	conflict	UNP Q6PYX1
M	12	VAL	PRO	conflict	UNP Q6PYX1
M	14	ALA	PRO	conflict	UNP Q6PYX1
M	15	GLY	LYS	conflict	UNP Q6PYX1
M	16	GLY	ASP	conflict	UNP Q6PYX1
M	17	SER	THR	conflict	UNP Q6PYX1
M	19	ILE	MET	conflict	UNP Q6PYX1
M	20	LEU	ILE	conflict	UNP Q6PYX1
M	?	-	ARG	deletion	UNP Q6PYX1
M	?	-	THR	deletion	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	PRO	deletion	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	?	-	VAL	deletion	UNP Q6PYX1
M	?	-	THR	deletion	UNP Q6PYX1
M	23	GLY	VAL	conflict	UNP Q6PYX1
M	25	SER	-	expression tag	UNP Q6PYX1
M	26	ASN	-	expression tag	UNP Q6PYX1
M	27	PHE	VAL	conflict	UNP Q6PYX1
M	28	ARG	ASP	conflict	UNP Q6PYX1
M	29	ILE	VAL	conflict	UNP Q6PYX1
M	31	ALA	-	expression tag	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	?	-	ASP	deletion	UNP Q6PYX1
M	?	-	PRO	deletion	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	?	-	VAL	deletion	UNP Q6PYX1
M	33	THR	LYS	conflict	UNP Q6PYX1
M	34	MET	PHE	conflict	UNP Q6PYX1
M	37	VAL	-	expression tag	UNP Q6PYX1
M	38	ARG	-	expression tag	UNP Q6PYX1
M	39	ARG	TYR	conflict	UNP Q6PYX1
M	41	PRO	-	expression tag	UNP Q6PYX1
M	42	GLY	-	expression tag	UNP Q6PYX1
M	43	GLY	ASP	conflict	UNP Q6PYX1
M	45	LEU	VAL	conflict	UNP Q6PYX1
M	47	TRP	-	expression tag	UNP Q6PYX1
M	?	-	HIS	deletion	UNP Q6PYX1
M	?	-	ASN	deletion	UNP Q6PYX1
M	?	-	LYS	deletion	UNP Q6PYX1
M	?	-	THR	deletion	UNP Q6PYX1
M	?	-	LYS	deletion	UNP Q6PYX1
M	?	-	PRO	deletion	UNP Q6PYX1
M	?	-	ARG	deletion	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	50	SER	GLU	conflict	UNP Q6PYX1
M	51	ILE	GLN	conflict	UNP Q6PYX1
M	52	SER	TYR	conflict	UNP Q6PYX1
M	53	SER	ASN	conflict	UNP Q6PYX1
M	58	ASP	-	expression tag	UNP Q6PYX1
M	59	TYR	-	expression tag	UNP Q6PYX1
M	60	ALA	-	expression tag	UNP Q6PYX1
M	61	ASP	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	62	ALA	-	expression tag	UNP Q6PYX1
M	64	LYS	VAL	conflict	UNP Q6PYX1
M	65	GLY	SER	conflict	UNP Q6PYX1
M	66	ARG	VAL	conflict	UNP Q6PYX1
M	67	PHE	LEU	conflict	UNP Q6PYX1
M	70	SER	-	expression tag	UNP Q6PYX1
M	71	ARG	-	expression tag	UNP Q6PYX1
M	72	ASP	-	expression tag	UNP Q6PYX1
M	73	ASP	-	expression tag	UNP Q6PYX1
M	?	-	HIS	deletion	UNP Q6PYX1
M	75	GLU	GLN	conflict	UNP Q6PYX1
M	77	PHE	-	expression tag	UNP Q6PYX1
M	78	VAL	-	expression tag	UNP Q6PYX1
M	79	TYR	TRP	conflict	UNP Q6PYX1
M	81	GLN	-	expression tag	UNP Q6PYX1
M	82	MET	ASN	conflict	UNP Q6PYX1
M	82A	HIS	GLY	conflict	UNP Q6PYX1
M	83	ARG	-	expression tag	UNP Q6PYX1
M	84	VAL	-	expression tag	UNP Q6PYX1
M	86	ASP	-	expression tag	UNP Q6PYX1
M	87	THR	-	expression tag	UNP Q6PYX1
M	88	ALA	-	expression tag	UNP Q6PYX1
M	89	ILE	-	expression tag	UNP Q6PYX1
M	91	TYR	LYS	conflict	UNP Q6PYX1
M	93	ALA	-	expression tag	UNP Q6PYX1
M	94	ARG	-	expression tag	UNP Q6PYX1
M	96	GLY	VAL	conflict	UNP Q6PYX1
M	?	-	ASN	deletion	UNP Q6PYX1
M	98	ASP	LYS	conflict	UNP Q6PYX1
M	99	ARG	ALA	conflict	UNP Q6PYX1
M	101	ASP	PRO	conflict	UNP Q6PYX1
M	103	TRP	-	expression tag	UNP Q6PYX1
M	104	GLY	-	expression tag	UNP Q6PYX1
M	106	GLY	-	expression tag	UNP Q6PYX1
M	107	THR	ILE	conflict	UNP Q6PYX1
M	108	VAL	GLU	conflict	UNP Q6PYX1
M	109	VAL	LYS	conflict	UNP Q6PYX1
M	111	VAL	ILE	conflict	UNP Q6PYX1
M	113	PRO	LYS	conflict	UNP Q6PYX1
M	115	SER	-	expression tag	UNP Q6PYX1
M	116	THR	-	expression tag	UNP Q6PYX1
M	?	-	GLN	deletion	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	PRO	deletion	UNP Q6PYX1
M	?	-	ARG	deletion	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	120	SER	GLN	conflict	UNP Q6PYX1
M	122	PHE	TYR	conflict	UNP Q6PYX1
M	123	PRO	THR	conflict	UNP Q6PYX1
M	125	ALA	PRO	conflict	UNP Q6PYX1
M	?	-	ARG	deletion	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	136	GLY	MET	conflict	UNP Q6PYX1
M	?	-	LYS	deletion	UNP Q6PYX1
M	?	-	ASN	deletion	UNP Q6PYX1
M	?	-	GLN	deletion	UNP Q6PYX1
M	138	ALA	VAL	conflict	UNP Q6PYX1
M	139	ALA	SER	conflict	UNP Q6PYX1
M	141	GLY	THR	conflict	UNP Q6PYX1
M	146	ASP	GLY	conflict	UNP Q6PYX1
M	147	TYR	PHE	conflict	UNP Q6PYX1
M	148	PHE	TYR	conflict	UNP Q6PYX1
M	150	GLU	SER	conflict	UNP Q6PYX1
M	151	PRO	ASP	conflict	UNP Q6PYX1
M	152	VAL	ILE	conflict	UNP Q6PYX1
M	153	THR	ALA	conflict	UNP Q6PYX1
M	156	SER	GLU	conflict	UNP Q6PYX1
M	162	ASN	GLU	conflict	UNP Q6PYX1
M	?	-	ASN	deletion	UNP Q6PYX1
M	165	ALA	GLN	conflict	UNP Q6PYX1
M	166	LEU	PRO	conflict	UNP Q6PYX1
M	167	THR	GLU	conflict	UNP Q6PYX1
M	168	SER	ASN	conflict	UNP Q6PYX1
M	169	GLY	ASN	conflict	UNP Q6PYX1
M	171	VAL	TYR	conflict	UNP Q6PYX1
M	172	HIS	LYS	conflict	UNP Q6PYX1
M	174	PHE	THR	conflict	UNP Q6PYX1
M	176	ALA	PRO	conflict	UNP Q6PYX1
M	179	GLN	ASP	conflict	UNP Q6PYX1
M	182	SER	ASP	conflict	UNP Q6PYX1
M	?	-	SER	deletion	UNP Q6PYX1
M	?	-	PHE	deletion	UNP Q6PYX1
M	?	-	PHE	deletion	UNP Q6PYX1
M	?	-	LYS	deletion	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	188	SER	-	expression tag	UNP Q6PYX1
M	189	SER	-	expression tag	UNP Q6PYX1
M	190	VAL	-	expression tag	UNP Q6PYX1
M	191	VAL	-	expression tag	UNP Q6PYX1
M	194	PRO	ASP	conflict	UNP Q6PYX1
M	195	SER	LYS	conflict	UNP Q6PYX1
M	?	-	ARG	deletion	UNP Q6PYX1
M	?	-	TRP	deletion	UNP Q6PYX1
M	197	SER	GLN	conflict	UNP Q6PYX1
M	198	LEU	GLN	conflict	UNP Q6PYX1
M	200	THR	-	expression tag	UNP Q6PYX1
M	203	GLN	ASN	conflict	UNP Q6PYX1
M	205	THR	VAL	conflict	UNP Q6PYX1
M	206	TYR	PHE	conflict	UNP Q6PYX1
M	207	ILE	SER	conflict	UNP Q6PYX1
M	209	ASN	SER	conflict	UNP Q6PYX1
M	?	-	MET	deletion	UNP Q6PYX1
M	?	-	HIS	deletion	UNP Q6PYX1
M	?	-	GLU	deletion	UNP Q6PYX1
M	?	-	ALA	deletion	UNP Q6PYX1
M	?	-	LEU	deletion	UNP Q6PYX1
M	?	-	HIS	deletion	UNP Q6PYX1
M	213	LYS	-	expression tag	UNP Q6PYX1
M	214	PRO	-	expression tag	UNP Q6PYX1
M	215	SER	-	expression tag	UNP Q6PYX1
M	216	ASN	TYR	conflict	UNP Q6PYX1
M	218	LYS	-	expression tag	UNP Q6PYX1
M	219	VAL	-	expression tag	UNP Q6PYX1
M	220	ASP	-	expression tag	UNP Q6PYX1
M	221	LYS	-	expression tag	UNP Q6PYX1
M	222	LYS	-	expression tag	UNP Q6PYX1
M	225	VAL	-	expression tag	UNP Q6PYX1
M	226	GLU	-	expression tag	UNP Q6PYX1
M	227	PRO	GLN	conflict	UNP Q6PYX1
M	230	CYS	-	expression tag	UNP Q6PYX1
M	231	ASP	-	expression tag	UNP Q6PYX1
M	232	LYS	-	expression tag	UNP Q6PYX1
M	233	THR	LEU	conflict	UNP Q6PYX1
M	235	THR	LEU	conflict	UNP Q6PYX1
M	236	CYS	SER	conflict	UNP Q6PYX1
M	238	PRO	-	expression tag	UNP Q6PYX1
M	239	CYS	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	240	PRO	-	expression tag	UNP Q6PYX1
M	241	ALA	-	expression tag	UNP Q6PYX1
M	242	PRO	-	expression tag	UNP Q6PYX1
M	243	GLU	-	expression tag	UNP Q6PYX1
M	244	LEU	-	expression tag	UNP Q6PYX1
M	245	LEU	-	expression tag	UNP Q6PYX1
M	247	GLY	LYS	conflict	UNP Q6PYX1
E	1	GLU	SER	conflict	UNP Q6PYX1
E	3	GLN	PHE	conflict	UNP Q6PYX1
E	5	VAL	-	expression tag	UNP Q6PYX1
E	6	GLU	-	expression tag	UNP Q6PYX1
E	7	SER	-	expression tag	UNP Q6PYX1
E	8	GLY	-	expression tag	UNP Q6PYX1
E	9	GLY	-	expression tag	UNP Q6PYX1
E	10	GLY	PHE	conflict	UNP Q6PYX1
E	11	LEU	PRO	conflict	UNP Q6PYX1
E	12	VAL	PRO	conflict	UNP Q6PYX1
E	14	ALA	PRO	conflict	UNP Q6PYX1
E	15	GLY	LYS	conflict	UNP Q6PYX1
E	16	GLY	ASP	conflict	UNP Q6PYX1
E	17	SER	THR	conflict	UNP Q6PYX1
E	19	ILE	MET	conflict	UNP Q6PYX1
E	20	LEU	ILE	conflict	UNP Q6PYX1
E	?	-	ARG	deletion	UNP Q6PYX1
E	?	-	THR	deletion	UNP Q6PYX1
E	?	-	PRO	deletion	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	?	-	VAL	deletion	UNP Q6PYX1
E	?	-	THR	deletion	UNP Q6PYX1
E	23	GLY	VAL	conflict	UNP Q6PYX1
E	25	SER	-	expression tag	UNP Q6PYX1
E	26	ASN	-	expression tag	UNP Q6PYX1
E	27	PHE	VAL	conflict	UNP Q6PYX1
E	28	ARG	ASP	conflict	UNP Q6PYX1
E	29	ILE	VAL	conflict	UNP Q6PYX1
E	31	ALA	-	expression tag	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	?	-	ASP	deletion	UNP Q6PYX1
E	?	-	PRO	deletion	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	?	-	VAL	deletion	UNP Q6PYX1
E	33	THR	LYS	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	34	MET	PHE	conflict	UNP Q6PYX1
E	37	VAL	-	expression tag	UNP Q6PYX1
E	38	ARG	-	expression tag	UNP Q6PYX1
E	39	ARG	TYR	conflict	UNP Q6PYX1
E	41	PRO	-	expression tag	UNP Q6PYX1
E	42	GLY	-	expression tag	UNP Q6PYX1
E	43	GLY	ASP	conflict	UNP Q6PYX1
E	45	LEU	VAL	conflict	UNP Q6PYX1
E	47	TRP	-	expression tag	UNP Q6PYX1
E	?	-	HIS	deletion	UNP Q6PYX1
E	?	-	ASN	deletion	UNP Q6PYX1
E	?	-	LYS	deletion	UNP Q6PYX1
E	?	-	THR	deletion	UNP Q6PYX1
E	?	-	LYS	deletion	UNP Q6PYX1
E	?	-	PRO	deletion	UNP Q6PYX1
E	?	-	ARG	deletion	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	50	SER	GLU	conflict	UNP Q6PYX1
E	51	ILE	GLN	conflict	UNP Q6PYX1
E	52	SER	TYR	conflict	UNP Q6PYX1
E	53	SER	ASN	conflict	UNP Q6PYX1
E	58	ASP	-	expression tag	UNP Q6PYX1
E	59	TYR	-	expression tag	UNP Q6PYX1
E	60	ALA	-	expression tag	UNP Q6PYX1
E	61	ASP	-	expression tag	UNP Q6PYX1
E	62	ALA	-	expression tag	UNP Q6PYX1
E	64	LYS	VAL	conflict	UNP Q6PYX1
E	65	GLY	SER	conflict	UNP Q6PYX1
E	66	ARG	VAL	conflict	UNP Q6PYX1
E	67	PHE	LEU	conflict	UNP Q6PYX1
E	70	SER	-	expression tag	UNP Q6PYX1
E	71	ARG	-	expression tag	UNP Q6PYX1
E	72	ASP	-	expression tag	UNP Q6PYX1
E	73	ASP	-	expression tag	UNP Q6PYX1
E	?	-	HIS	deletion	UNP Q6PYX1
E	75	GLU	GLN	conflict	UNP Q6PYX1
E	77	PHE	-	expression tag	UNP Q6PYX1
E	78	VAL	-	expression tag	UNP Q6PYX1
E	79	TYR	TRP	conflict	UNP Q6PYX1
E	81	GLN	-	expression tag	UNP Q6PYX1
E	82	MET	ASN	conflict	UNP Q6PYX1
E	83	HIS	GLY	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	85	ARG	-	expression tag	UNP Q6PYX1
E	86	VAL	-	expression tag	UNP Q6PYX1
E	88	ASP	-	expression tag	UNP Q6PYX1
E	89	THR	-	expression tag	UNP Q6PYX1
E	90	ALA	-	expression tag	UNP Q6PYX1
E	91	ILE	-	expression tag	UNP Q6PYX1
E	93	TYR	LYS	conflict	UNP Q6PYX1
E	95	ALA	-	expression tag	UNP Q6PYX1
E	96	ARG	-	expression tag	UNP Q6PYX1
E	98	GLY	VAL	conflict	UNP Q6PYX1
E	?	-	ASN	deletion	UNP Q6PYX1
E	100	ASP	LYS	conflict	UNP Q6PYX1
E	101	ARG	ALA	conflict	UNP Q6PYX1
E	103	ASP	PRO	conflict	UNP Q6PYX1
E	105	TRP	-	expression tag	UNP Q6PYX1
E	106	GLY	-	expression tag	UNP Q6PYX1
E	108	GLY	-	expression tag	UNP Q6PYX1
E	109	THR	ILE	conflict	UNP Q6PYX1
E	110	VAL	GLU	conflict	UNP Q6PYX1
E	111	VAL	LYS	conflict	UNP Q6PYX1
E	113	VAL	ILE	conflict	UNP Q6PYX1
E	115	PRO	LYS	conflict	UNP Q6PYX1
E	117	SER	-	expression tag	UNP Q6PYX1
E	118	THR	-	expression tag	UNP Q6PYX1
E	?	-	GLN	deletion	UNP Q6PYX1
E	?	-	PRO	deletion	UNP Q6PYX1
E	?	-	ARG	deletion	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	122	SER	GLN	conflict	UNP Q6PYX1
E	124	PHE	TYR	conflict	UNP Q6PYX1
E	125	PRO	THR	conflict	UNP Q6PYX1
E	127	ALA	PRO	conflict	UNP Q6PYX1
E	?	-	ARG	deletion	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	130	GLY	MET	conflict	UNP Q6PYX1
E	?	-	LYS	deletion	UNP Q6PYX1
E	?	-	ASN	deletion	UNP Q6PYX1
E	?	-	GLN	deletion	UNP Q6PYX1
E	132	ALA	VAL	conflict	UNP Q6PYX1
E	133	ALA	SER	conflict	UNP Q6PYX1
E	135	GLY	THR	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	140	ASP	GLY	conflict	UNP Q6PYX1
E	141	TYR	PHE	conflict	UNP Q6PYX1
E	142	PHE	TYR	conflict	UNP Q6PYX1
E	144	GLU	SER	conflict	UNP Q6PYX1
E	145	PRO	ASP	conflict	UNP Q6PYX1
E	146	VAL	ILE	conflict	UNP Q6PYX1
E	147	THR	ALA	conflict	UNP Q6PYX1
E	149	SER	GLU	conflict	UNP Q6PYX1
E	151	ASN	GLU	conflict	UNP Q6PYX1
E	?	-	ASN	deletion	UNP Q6PYX1
E	154	ALA	GLN	conflict	UNP Q6PYX1
E	155	LEU	PRO	conflict	UNP Q6PYX1
E	156	THR	GLU	conflict	UNP Q6PYX1
E	157	SER	ASN	conflict	UNP Q6PYX1
E	158	GLY	ASN	conflict	UNP Q6PYX1
E	159	VAL	TYR	conflict	UNP Q6PYX1
E	160	HIS	LYS	conflict	UNP Q6PYX1
E	162	PHE	THR	conflict	UNP Q6PYX1
E	164	ALA	PRO	conflict	UNP Q6PYX1
E	167	GLN	ASP	conflict	UNP Q6PYX1
E	169	SER	ASP	conflict	UNP Q6PYX1
E	?	-	SER	deletion	UNP Q6PYX1
E	?	-	PHE	deletion	UNP Q6PYX1
E	?	-	PHE	deletion	UNP Q6PYX1
E	?	-	LYS	deletion	UNP Q6PYX1
E	175	SER	-	expression tag	UNP Q6PYX1
E	176	SER	-	expression tag	UNP Q6PYX1
E	177	VAL	-	expression tag	UNP Q6PYX1
E	178	VAL	-	expression tag	UNP Q6PYX1
E	181	PRO	ASP	conflict	UNP Q6PYX1
E	182	SER	LYS	conflict	UNP Q6PYX1
E	?	-	ARG	deletion	UNP Q6PYX1
E	?	-	TRP	deletion	UNP Q6PYX1
E	184	SER	GLN	conflict	UNP Q6PYX1
E	185	LEU	GLN	conflict	UNP Q6PYX1
E	187	THR	-	expression tag	UNP Q6PYX1
E	188	GLN	ASN	conflict	UNP Q6PYX1
E	189	THR	VAL	conflict	UNP Q6PYX1
E	190	TYR	PHE	conflict	UNP Q6PYX1
E	191	ILE	SER	conflict	UNP Q6PYX1
E	193	ASN	SER	conflict	UNP Q6PYX1
E	?	-	MET	deletion	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	HIS	deletion	UNP Q6PYX1
E	?	-	GLU	deletion	UNP Q6PYX1
E	?	-	ALA	deletion	UNP Q6PYX1
E	?	-	LEU	deletion	UNP Q6PYX1
E	?	-	HIS	deletion	UNP Q6PYX1
E	197	LYS	-	expression tag	UNP Q6PYX1
E	198	PRO	-	expression tag	UNP Q6PYX1
E	199	SER	-	expression tag	UNP Q6PYX1
E	200	ASN	TYR	conflict	UNP Q6PYX1
E	202	LYS	-	expression tag	UNP Q6PYX1
E	203	VAL	-	expression tag	UNP Q6PYX1
E	204	ASP	-	expression tag	UNP Q6PYX1
E	205	LYS	-	expression tag	UNP Q6PYX1
E	206	LYS	-	expression tag	UNP Q6PYX1
E	207	VAL	-	expression tag	UNP Q6PYX1
E	208	GLU	-	expression tag	UNP Q6PYX1
E	209	PRO	GLN	conflict	UNP Q6PYX1
E	212	CYS	-	expression tag	UNP Q6PYX1
E	213	ASP	-	expression tag	UNP Q6PYX1
E	214	LYS	-	expression tag	UNP Q6PYX1
E	215	THR	LEU	conflict	UNP Q6PYX1
E	217	THR	LEU	conflict	UNP Q6PYX1
E	218	CYS	SER	conflict	UNP Q6PYX1
E	220	PRO	-	expression tag	UNP Q6PYX1
E	221	CYS	-	expression tag	UNP Q6PYX1
E	222	PRO	-	expression tag	UNP Q6PYX1
E	223	ALA	-	expression tag	UNP Q6PYX1
E	224	PRO	-	expression tag	UNP Q6PYX1
E	225	GLU	-	expression tag	UNP Q6PYX1
E	226	LEU	-	expression tag	UNP Q6PYX1
E	227	LEU	-	expression tag	UNP Q6PYX1
E	229	GLY	LYS	conflict	UNP Q6PYX1
I	1	GLU	SER	conflict	UNP Q6PYX1
I	3	GLN	PHE	conflict	UNP Q6PYX1
I	5	VAL	-	expression tag	UNP Q6PYX1
I	6	GLU	-	expression tag	UNP Q6PYX1
I	7	SER	-	expression tag	UNP Q6PYX1
I	8	GLY	-	expression tag	UNP Q6PYX1
I	9	GLY	-	expression tag	UNP Q6PYX1
I	10	GLY	PHE	conflict	UNP Q6PYX1
I	11	LEU	PRO	conflict	UNP Q6PYX1
I	12	VAL	PRO	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	14	ALA	PRO	conflict	UNP Q6PYX1
I	15	GLY	LYS	conflict	UNP Q6PYX1
I	16	GLY	ASP	conflict	UNP Q6PYX1
I	17	SER	THR	conflict	UNP Q6PYX1
I	19	ILE	MET	conflict	UNP Q6PYX1
I	20	LEU	ILE	conflict	UNP Q6PYX1
I	?	-	ARG	deletion	UNP Q6PYX1
I	?	-	THR	deletion	UNP Q6PYX1
I	?	-	PRO	deletion	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1
I	?	-	VAL	deletion	UNP Q6PYX1
I	?	-	THR	deletion	UNP Q6PYX1
I	23	GLY	VAL	conflict	UNP Q6PYX1
I	25	SER	-	expression tag	UNP Q6PYX1
I	26	ASN	-	expression tag	UNP Q6PYX1
I	27	PHE	VAL	conflict	UNP Q6PYX1
I	28	ARG	ASP	conflict	UNP Q6PYX1
I	29	ILE	VAL	conflict	UNP Q6PYX1
I	31	ALA	-	expression tag	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1
I	?	-	ASP	deletion	UNP Q6PYX1
I	?	-	PRO	deletion	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1
I	?	-	VAL	deletion	UNP Q6PYX1
I	33	THR	LYS	conflict	UNP Q6PYX1
I	34	MET	PHE	conflict	UNP Q6PYX1
I	37	VAL	-	expression tag	UNP Q6PYX1
I	38	ARG	-	expression tag	UNP Q6PYX1
I	39	ARG	TYR	conflict	UNP Q6PYX1
I	41	PRO	-	expression tag	UNP Q6PYX1
I	42	GLY	-	expression tag	UNP Q6PYX1
I	43	GLY	ASP	conflict	UNP Q6PYX1
I	45	LEU	VAL	conflict	UNP Q6PYX1
I	47	TRP	-	expression tag	UNP Q6PYX1
I	?	-	HIS	deletion	UNP Q6PYX1
I	?	-	ASN	deletion	UNP Q6PYX1
I	?	-	LYS	deletion	UNP Q6PYX1
I	?	-	THR	deletion	UNP Q6PYX1
I	?	-	LYS	deletion	UNP Q6PYX1
I	?	-	PRO	deletion	UNP Q6PYX1
I	?	-	ARG	deletion	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	50	SER	GLU	conflict	UNP Q6PYX1
I	51	ILE	GLN	conflict	UNP Q6PYX1
I	52	SER	TYR	conflict	UNP Q6PYX1
I	53	SER	ASN	conflict	UNP Q6PYX1
I	58	ASP	-	expression tag	UNP Q6PYX1
I	59	TYR	-	expression tag	UNP Q6PYX1
I	60	ALA	-	expression tag	UNP Q6PYX1
I	61	ASP	-	expression tag	UNP Q6PYX1
I	62	ALA	-	expression tag	UNP Q6PYX1
I	64	LYS	VAL	conflict	UNP Q6PYX1
I	65	GLY	SER	conflict	UNP Q6PYX1
I	66	ARG	VAL	conflict	UNP Q6PYX1
I	67	PHE	LEU	conflict	UNP Q6PYX1
I	70	SER	-	expression tag	UNP Q6PYX1
I	71	ARG	-	expression tag	UNP Q6PYX1
I	72	ASP	-	expression tag	UNP Q6PYX1
I	73	ASP	-	expression tag	UNP Q6PYX1
I	?	-	HIS	deletion	UNP Q6PYX1
I	75	GLU	GLN	conflict	UNP Q6PYX1
I	77	PHE	-	expression tag	UNP Q6PYX1
I	78	VAL	-	expression tag	UNP Q6PYX1
I	79	TYR	TRP	conflict	UNP Q6PYX1
I	81	GLN	-	expression tag	UNP Q6PYX1
I	82	MET	ASN	conflict	UNP Q6PYX1
I	83	HIS	GLY	conflict	UNP Q6PYX1
I	85	ARG	-	expression tag	UNP Q6PYX1
I	86	VAL	-	expression tag	UNP Q6PYX1
I	88	ASP	-	expression tag	UNP Q6PYX1
I	89	THR	-	expression tag	UNP Q6PYX1
I	90	ALA	-	expression tag	UNP Q6PYX1
I	91	ILE	-	expression tag	UNP Q6PYX1
I	93	TYR	LYS	conflict	UNP Q6PYX1
I	95	ALA	-	expression tag	UNP Q6PYX1
I	96	ARG	-	expression tag	UNP Q6PYX1
I	98	GLY	VAL	conflict	UNP Q6PYX1
I	?	-	ASN	deletion	UNP Q6PYX1
I	100	ASP	LYS	conflict	UNP Q6PYX1
I	101	ARG	ALA	conflict	UNP Q6PYX1
I	103	ASP	PRO	conflict	UNP Q6PYX1
I	105	TRP	-	expression tag	UNP Q6PYX1
I	106	GLY	-	expression tag	UNP Q6PYX1
I	108	GLY	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	109	THR	ILE	conflict	UNP Q6PYX1
I	110	VAL	GLU	conflict	UNP Q6PYX1
I	111	VAL	LYS	conflict	UNP Q6PYX1
I	113	VAL	ILE	conflict	UNP Q6PYX1
I	115	PRO	LYS	conflict	UNP Q6PYX1
I	117	SER	-	expression tag	UNP Q6PYX1
I	118	THR	-	expression tag	UNP Q6PYX1
I	?	-	GLN	deletion	UNP Q6PYX1
I	?	-	PRO	deletion	UNP Q6PYX1
I	?	-	ARG	deletion	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1
I	122	SER	GLN	conflict	UNP Q6PYX1
I	124	PHE	TYR	conflict	UNP Q6PYX1
I	125	PRO	THR	conflict	UNP Q6PYX1
I	127	ALA	PRO	conflict	UNP Q6PYX1
I	?	-	ARG	deletion	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1
I	130	GLY	MET	conflict	UNP Q6PYX1
I	?	-	LYS	deletion	UNP Q6PYX1
I	?	-	ASN	deletion	UNP Q6PYX1
I	?	-	GLN	deletion	UNP Q6PYX1
I	132	ALA	VAL	conflict	UNP Q6PYX1
I	133	ALA	SER	conflict	UNP Q6PYX1
I	135	GLY	THR	conflict	UNP Q6PYX1
I	140	ASP	GLY	conflict	UNP Q6PYX1
I	141	TYR	PHE	conflict	UNP Q6PYX1
I	142	PHE	TYR	conflict	UNP Q6PYX1
I	144	GLU	SER	conflict	UNP Q6PYX1
I	145	PRO	ASP	conflict	UNP Q6PYX1
I	146	VAL	ILE	conflict	UNP Q6PYX1
I	147	THR	ALA	conflict	UNP Q6PYX1
I	149	SER	GLU	conflict	UNP Q6PYX1
I	151	ASN	GLU	conflict	UNP Q6PYX1
I	?	-	ASN	deletion	UNP Q6PYX1
I	154	ALA	GLN	conflict	UNP Q6PYX1
I	155	LEU	PRO	conflict	UNP Q6PYX1
I	156	THR	GLU	conflict	UNP Q6PYX1
I	157	SER	ASN	conflict	UNP Q6PYX1
I	158	GLY	ASN	conflict	UNP Q6PYX1
I	159	VAL	TYR	conflict	UNP Q6PYX1
I	160	HIS	LYS	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	162	PHE	THR	conflict	UNP Q6PYX1
I	164	ALA	PRO	conflict	UNP Q6PYX1
I	167	GLN	ASP	conflict	UNP Q6PYX1
I	169	SER	ASP	conflict	UNP Q6PYX1
I	?	-	SER	deletion	UNP Q6PYX1
I	?	-	PHE	deletion	UNP Q6PYX1
I	?	-	PHE	deletion	UNP Q6PYX1
I	?	-	LYS	deletion	UNP Q6PYX1
I	175	SER	-	expression tag	UNP Q6PYX1
I	176	SER	-	expression tag	UNP Q6PYX1
I	177	VAL	-	expression tag	UNP Q6PYX1
I	178	VAL	-	expression tag	UNP Q6PYX1
I	181	PRO	ASP	conflict	UNP Q6PYX1
I	182	SER	LYS	conflict	UNP Q6PYX1
I	?	-	ARG	deletion	UNP Q6PYX1
I	?	-	TRP	deletion	UNP Q6PYX1
I	184	SER	GLN	conflict	UNP Q6PYX1
I	185	LEU	GLN	conflict	UNP Q6PYX1
I	187	THR	-	expression tag	UNP Q6PYX1
I	188	GLN	ASN	conflict	UNP Q6PYX1
I	189	THR	VAL	conflict	UNP Q6PYX1
I	190	TYR	PHE	conflict	UNP Q6PYX1
I	191	ILE	SER	conflict	UNP Q6PYX1
I	193	ASN	SER	conflict	UNP Q6PYX1
I	?	-	MET	deletion	UNP Q6PYX1
I	?	-	HIS	deletion	UNP Q6PYX1
I	?	-	GLU	deletion	UNP Q6PYX1
I	?	-	ALA	deletion	UNP Q6PYX1
I	?	-	LEU	deletion	UNP Q6PYX1
I	?	-	HIS	deletion	UNP Q6PYX1
I	197	LYS	-	expression tag	UNP Q6PYX1
I	198	PRO	-	expression tag	UNP Q6PYX1
I	199	SER	-	expression tag	UNP Q6PYX1
I	200	ASN	TYR	conflict	UNP Q6PYX1
I	202	LYS	-	expression tag	UNP Q6PYX1
I	203	VAL	-	expression tag	UNP Q6PYX1
I	204	ASP	-	expression tag	UNP Q6PYX1
I	205	LYS	-	expression tag	UNP Q6PYX1
I	206	LYS	-	expression tag	UNP Q6PYX1
I	207	VAL	-	expression tag	UNP Q6PYX1
I	208	GLU	-	expression tag	UNP Q6PYX1
I	209	PRO	GLN	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	212	CYS	-	expression tag	UNP Q6PYX1
I	213	ASP	-	expression tag	UNP Q6PYX1
I	214	LYS	-	expression tag	UNP Q6PYX1
I	215	THR	LEU	conflict	UNP Q6PYX1
I	217	THR	LEU	conflict	UNP Q6PYX1
I	218	CYS	SER	conflict	UNP Q6PYX1
I	220	PRO	-	expression tag	UNP Q6PYX1
I	221	CYS	-	expression tag	UNP Q6PYX1
I	222	PRO	-	expression tag	UNP Q6PYX1
I	223	ALA	-	expression tag	UNP Q6PYX1
I	224	PRO	-	expression tag	UNP Q6PYX1
I	225	GLU	-	expression tag	UNP Q6PYX1
I	226	LEU	-	expression tag	UNP Q6PYX1
I	227	LEU	-	expression tag	UNP Q6PYX1
I	229	GLY	LYS	conflict	UNP Q6PYX1
O	1	GLU	SER	conflict	UNP Q6PYX1
O	3	GLN	PHE	conflict	UNP Q6PYX1
O	5	VAL	-	expression tag	UNP Q6PYX1
O	6	GLU	-	expression tag	UNP Q6PYX1
O	7	SER	-	expression tag	UNP Q6PYX1
O	8	GLY	-	expression tag	UNP Q6PYX1
O	9	GLY	-	expression tag	UNP Q6PYX1
O	10	GLY	PHE	conflict	UNP Q6PYX1
O	11	LEU	PRO	conflict	UNP Q6PYX1
O	12	VAL	PRO	conflict	UNP Q6PYX1
O	14	ALA	PRO	conflict	UNP Q6PYX1
O	15	GLY	LYS	conflict	UNP Q6PYX1
O	16	GLY	ASP	conflict	UNP Q6PYX1
O	17	SER	THR	conflict	UNP Q6PYX1
O	19	ILE	MET	conflict	UNP Q6PYX1
O	20	LEU	ILE	conflict	UNP Q6PYX1
O	?	-	ARG	deletion	UNP Q6PYX1
O	?	-	THR	deletion	UNP Q6PYX1
O	?	-	PRO	deletion	UNP Q6PYX1
O	?	-	GLU	deletion	UNP Q6PYX1
O	?	-	VAL	deletion	UNP Q6PYX1
O	?	-	THR	deletion	UNP Q6PYX1
O	23	GLY	VAL	conflict	UNP Q6PYX1
O	25	SER	-	expression tag	UNP Q6PYX1
O	26	ASN	-	expression tag	UNP Q6PYX1
O	27	PHE	VAL	conflict	UNP Q6PYX1
O	28	ARG	ASP	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	29	ILE	VAL	conflict	UNP Q6PYX1
O	31	ALA	-	expression tag	UNP Q6PYX1
O	?	-	GLU	deletion	UNP Q6PYX1
O	?	-	ASP	deletion	UNP Q6PYX1
O	?	-	PRO	deletion	UNP Q6PYX1
O	?	-	GLU	deletion	UNP Q6PYX1
O	?	-	VAL	deletion	UNP Q6PYX1
O	33	THR	LYS	conflict	UNP Q6PYX1
O	34	MET	PHE	conflict	UNP Q6PYX1
O	37	VAL	-	expression tag	UNP Q6PYX1
O	38	ARG	-	expression tag	UNP Q6PYX1
O	39	ARG	TYR	conflict	UNP Q6PYX1
O	41	PRO	-	expression tag	UNP Q6PYX1
O	42	GLY	-	expression tag	UNP Q6PYX1
O	43	GLY	ASP	conflict	UNP Q6PYX1
O	45	LEU	VAL	conflict	UNP Q6PYX1
O	47	TRP	-	expression tag	UNP Q6PYX1
O	?	-	HIS	deletion	UNP Q6PYX1
O	?	-	ASN	deletion	UNP Q6PYX1
O	?	-	LYS	deletion	UNP Q6PYX1
O	?	-	THR	deletion	UNP Q6PYX1
O	?	-	LYS	deletion	UNP Q6PYX1
O	?	-	PRO	deletion	UNP Q6PYX1
O	?	-	ARG	deletion	UNP Q6PYX1
O	?	-	GLU	deletion	UNP Q6PYX1
O	50	SER	GLU	conflict	UNP Q6PYX1
O	51	ILE	GLN	conflict	UNP Q6PYX1
O	52	SER	TYR	conflict	UNP Q6PYX1
O	53	SER	ASN	conflict	UNP Q6PYX1
O	58	ASP	-	expression tag	UNP Q6PYX1
O	59	TYR	-	expression tag	UNP Q6PYX1
O	60	ALA	-	expression tag	UNP Q6PYX1
O	61	ASP	-	expression tag	UNP Q6PYX1
O	62	ALA	-	expression tag	UNP Q6PYX1
O	64	LYS	VAL	conflict	UNP Q6PYX1
O	65	GLY	SER	conflict	UNP Q6PYX1
O	66	ARG	VAL	conflict	UNP Q6PYX1
O	67	PHE	LEU	conflict	UNP Q6PYX1
O	70	SER	-	expression tag	UNP Q6PYX1
O	71	ARG	-	expression tag	UNP Q6PYX1
O	72	ASP	-	expression tag	UNP Q6PYX1
O	73	ASP	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	HIS	deletion	UNP Q6PYX1
O	75	GLU	GLN	conflict	UNP Q6PYX1
O	77	PHE	-	expression tag	UNP Q6PYX1
O	78	VAL	-	expression tag	UNP Q6PYX1
O	79	TYR	TRP	conflict	UNP Q6PYX1
O	81	GLN	-	expression tag	UNP Q6PYX1
O	82	MET	ASN	conflict	UNP Q6PYX1
O	82A	HIS	GLY	conflict	UNP Q6PYX1
O	83	ARG	-	expression tag	UNP Q6PYX1
O	84	VAL	-	expression tag	UNP Q6PYX1
O	86	ASP	-	expression tag	UNP Q6PYX1
O	87	THR	-	expression tag	UNP Q6PYX1
O	88	ALA	-	expression tag	UNP Q6PYX1
O	89	ILE	-	expression tag	UNP Q6PYX1
O	91	TYR	LYS	conflict	UNP Q6PYX1
O	93	ALA	-	expression tag	UNP Q6PYX1
O	94	ARG	-	expression tag	UNP Q6PYX1
O	96	GLY	VAL	conflict	UNP Q6PYX1
O	?	-	ASN	deletion	UNP Q6PYX1
O	98	ASP	LYS	conflict	UNP Q6PYX1
O	99	ARG	ALA	conflict	UNP Q6PYX1
O	101	ASP	PRO	conflict	UNP Q6PYX1
O	103	TRP	-	expression tag	UNP Q6PYX1
O	104	GLY	-	expression tag	UNP Q6PYX1
O	106	GLY	-	expression tag	UNP Q6PYX1
O	107	THR	ILE	conflict	UNP Q6PYX1
O	108	VAL	GLU	conflict	UNP Q6PYX1
O	109	VAL	LYS	conflict	UNP Q6PYX1
O	111	VAL	ILE	conflict	UNP Q6PYX1
O	113	PRO	LYS	conflict	UNP Q6PYX1
O	115	SER	-	expression tag	UNP Q6PYX1
O	116	THR	-	expression tag	UNP Q6PYX1
O	?	-	GLN	deletion	UNP Q6PYX1
O	?	-	PRO	deletion	UNP Q6PYX1
O	?	-	ARG	deletion	UNP Q6PYX1
O	?	-	GLU	deletion	UNP Q6PYX1
O	120	SER	GLN	conflict	UNP Q6PYX1
O	122	PHE	TYR	conflict	UNP Q6PYX1
O	123	PRO	THR	conflict	UNP Q6PYX1
O	125	ALA	PRO	conflict	UNP Q6PYX1
O	?	-	ARG	deletion	UNP Q6PYX1
O	?	-	GLU	deletion	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	GLU	deletion	UNP Q6PYX1
O	136	GLY	MET	conflict	UNP Q6PYX1
O	?	-	LYS	deletion	UNP Q6PYX1
O	?	-	ASN	deletion	UNP Q6PYX1
O	?	-	GLN	deletion	UNP Q6PYX1
O	138	ALA	VAL	conflict	UNP Q6PYX1
O	139	ALA	SER	conflict	UNP Q6PYX1
O	141	GLY	THR	conflict	UNP Q6PYX1
O	146	ASP	GLY	conflict	UNP Q6PYX1
O	147	TYR	PHE	conflict	UNP Q6PYX1
O	148	PHE	TYR	conflict	UNP Q6PYX1
O	150	GLU	SER	conflict	UNP Q6PYX1
O	151	PRO	ASP	conflict	UNP Q6PYX1
O	152	VAL	ILE	conflict	UNP Q6PYX1
O	153	THR	ALA	conflict	UNP Q6PYX1
O	156	SER	GLU	conflict	UNP Q6PYX1
O	162	ASN	GLU	conflict	UNP Q6PYX1
O	?	-	ASN	deletion	UNP Q6PYX1
O	165	ALA	GLN	conflict	UNP Q6PYX1
O	166	LEU	PRO	conflict	UNP Q6PYX1
O	167	THR	GLU	conflict	UNP Q6PYX1
O	168	SER	ASN	conflict	UNP Q6PYX1
O	169	GLY	ASN	conflict	UNP Q6PYX1
O	171	VAL	TYR	conflict	UNP Q6PYX1
O	172	HIS	LYS	conflict	UNP Q6PYX1
O	174	PHE	THR	conflict	UNP Q6PYX1
O	176	ALA	PRO	conflict	UNP Q6PYX1
O	179	GLN	ASP	conflict	UNP Q6PYX1
O	182	SER	ASP	conflict	UNP Q6PYX1
O	?	-	SER	deletion	UNP Q6PYX1
O	?	-	PHE	deletion	UNP Q6PYX1
O	?	-	PHE	deletion	UNP Q6PYX1
O	?	-	LYS	deletion	UNP Q6PYX1
O	188	SER	-	expression tag	UNP Q6PYX1
O	189	SER	-	expression tag	UNP Q6PYX1
O	190	VAL	-	expression tag	UNP Q6PYX1
O	191	VAL	-	expression tag	UNP Q6PYX1
O	194	PRO	ASP	conflict	UNP Q6PYX1
O	195	SER	LYS	conflict	UNP Q6PYX1
O	?	-	ARG	deletion	UNP Q6PYX1
O	?	-	TRP	deletion	UNP Q6PYX1
O	197	SER	GLN	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	198	LEU	GLN	conflict	UNP Q6PYX1
O	200	THR	-	expression tag	UNP Q6PYX1
O	203	GLN	ASN	conflict	UNP Q6PYX1
O	205	THR	VAL	conflict	UNP Q6PYX1
O	206	TYR	PHE	conflict	UNP Q6PYX1
O	207	ILE	SER	conflict	UNP Q6PYX1
O	209	ASN	SER	conflict	UNP Q6PYX1
O	?	-	MET	deletion	UNP Q6PYX1
O	?	-	HIS	deletion	UNP Q6PYX1
O	?	-	GLU	deletion	UNP Q6PYX1
O	?	-	ALA	deletion	UNP Q6PYX1
O	?	-	LEU	deletion	UNP Q6PYX1
O	?	-	HIS	deletion	UNP Q6PYX1
O	213	LYS	-	expression tag	UNP Q6PYX1
O	214	PRO	-	expression tag	UNP Q6PYX1
O	215	SER	-	expression tag	UNP Q6PYX1
O	216	ASN	TYR	conflict	UNP Q6PYX1
O	218	LYS	-	expression tag	UNP Q6PYX1
O	219	VAL	-	expression tag	UNP Q6PYX1
O	220	ASP	-	expression tag	UNP Q6PYX1
O	221	LYS	-	expression tag	UNP Q6PYX1
O	222	LYS	-	expression tag	UNP Q6PYX1
O	225	VAL	-	expression tag	UNP Q6PYX1
O	226	GLU	-	expression tag	UNP Q6PYX1
O	227	PRO	GLN	conflict	UNP Q6PYX1
O	230	CYS	-	expression tag	UNP Q6PYX1
O	231	ASP	-	expression tag	UNP Q6PYX1
O	232	LYS	-	expression tag	UNP Q6PYX1
O	233	THR	LEU	conflict	UNP Q6PYX1
O	235	THR	LEU	conflict	UNP Q6PYX1
O	236	CYS	SER	conflict	UNP Q6PYX1
O	238	PRO	-	expression tag	UNP Q6PYX1
O	239	CYS	-	expression tag	UNP Q6PYX1
O	240	PRO	-	expression tag	UNP Q6PYX1
O	241	ALA	-	expression tag	UNP Q6PYX1
O	242	PRO	-	expression tag	UNP Q6PYX1
O	243	GLU	-	expression tag	UNP Q6PYX1
O	244	LEU	-	expression tag	UNP Q6PYX1
O	245	LEU	-	expression tag	UNP Q6PYX1
O	247	GLY	LYS	conflict	UNP Q6PYX1
R	1	GLU	SER	conflict	UNP Q6PYX1
R	3	GLN	PHE	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	5	VAL	-	expression tag	UNP Q6PYX1
R	6	GLU	-	expression tag	UNP Q6PYX1
R	7	SER	-	expression tag	UNP Q6PYX1
R	8	GLY	-	expression tag	UNP Q6PYX1
R	9	GLY	-	expression tag	UNP Q6PYX1
R	10	GLY	PHE	conflict	UNP Q6PYX1
R	11	LEU	PRO	conflict	UNP Q6PYX1
R	12	VAL	PRO	conflict	UNP Q6PYX1
R	14	ALA	PRO	conflict	UNP Q6PYX1
R	15	GLY	LYS	conflict	UNP Q6PYX1
R	16	GLY	ASP	conflict	UNP Q6PYX1
R	17	SER	THR	conflict	UNP Q6PYX1
R	19	ILE	MET	conflict	UNP Q6PYX1
R	20	LEU	ILE	conflict	UNP Q6PYX1
R	?	-	ARG	deletion	UNP Q6PYX1
R	?	-	THR	deletion	UNP Q6PYX1
R	?	-	PRO	deletion	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	?	-	VAL	deletion	UNP Q6PYX1
R	?	-	THR	deletion	UNP Q6PYX1
R	23	GLY	VAL	conflict	UNP Q6PYX1
R	25	SER	-	expression tag	UNP Q6PYX1
R	26	ASN	-	expression tag	UNP Q6PYX1
R	27	PHE	VAL	conflict	UNP Q6PYX1
R	28	ARG	ASP	conflict	UNP Q6PYX1
R	29	ILE	VAL	conflict	UNP Q6PYX1
R	31	ALA	-	expression tag	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	?	-	ASP	deletion	UNP Q6PYX1
R	?	-	PRO	deletion	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	?	-	VAL	deletion	UNP Q6PYX1
R	33	THR	LYS	conflict	UNP Q6PYX1
R	34	MET	PHE	conflict	UNP Q6PYX1
R	37	VAL	-	expression tag	UNP Q6PYX1
R	38	ARG	-	expression tag	UNP Q6PYX1
R	39	ARG	TYR	conflict	UNP Q6PYX1
R	41	PRO	-	expression tag	UNP Q6PYX1
R	42	GLY	-	expression tag	UNP Q6PYX1
R	43	GLY	ASP	conflict	UNP Q6PYX1
R	45	LEU	VAL	conflict	UNP Q6PYX1
R	47	TRP	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	HIS	deletion	UNP Q6PYX1
R	?	-	ASN	deletion	UNP Q6PYX1
R	?	-	LYS	deletion	UNP Q6PYX1
R	?	-	THR	deletion	UNP Q6PYX1
R	?	-	LYS	deletion	UNP Q6PYX1
R	?	-	PRO	deletion	UNP Q6PYX1
R	?	-	ARG	deletion	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	50	SER	GLU	conflict	UNP Q6PYX1
R	51	ILE	GLN	conflict	UNP Q6PYX1
R	52	SER	TYR	conflict	UNP Q6PYX1
R	53	SER	ASN	conflict	UNP Q6PYX1
R	58	ASP	-	expression tag	UNP Q6PYX1
R	59	TYR	-	expression tag	UNP Q6PYX1
R	60	ALA	-	expression tag	UNP Q6PYX1
R	61	ASP	-	expression tag	UNP Q6PYX1
R	62	ALA	-	expression tag	UNP Q6PYX1
R	64	LYS	VAL	conflict	UNP Q6PYX1
R	65	GLY	SER	conflict	UNP Q6PYX1
R	66	ARG	VAL	conflict	UNP Q6PYX1
R	67	PHE	LEU	conflict	UNP Q6PYX1
R	70	SER	-	expression tag	UNP Q6PYX1
R	71	ARG	-	expression tag	UNP Q6PYX1
R	72	ASP	-	expression tag	UNP Q6PYX1
R	73	ASP	-	expression tag	UNP Q6PYX1
R	?	-	HIS	deletion	UNP Q6PYX1
R	75	GLU	GLN	conflict	UNP Q6PYX1
R	77	PHE	-	expression tag	UNP Q6PYX1
R	78	VAL	-	expression tag	UNP Q6PYX1
R	79	TYR	TRP	conflict	UNP Q6PYX1
R	81	GLN	-	expression tag	UNP Q6PYX1
R	82	MET	ASN	conflict	UNP Q6PYX1
R	82A	HIS	GLY	conflict	UNP Q6PYX1
R	83	ARG	-	expression tag	UNP Q6PYX1
R	84	VAL	-	expression tag	UNP Q6PYX1
R	86	ASP	-	expression tag	UNP Q6PYX1
R	87	THR	-	expression tag	UNP Q6PYX1
R	88	ALA	-	expression tag	UNP Q6PYX1
R	89	ILE	-	expression tag	UNP Q6PYX1
R	91	TYR	LYS	conflict	UNP Q6PYX1
R	93	ALA	-	expression tag	UNP Q6PYX1
R	94	ARG	-	expression tag	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	96	GLY	VAL	conflict	UNP Q6PYX1
R	?	-	ASN	deletion	UNP Q6PYX1
R	98	ASP	LYS	conflict	UNP Q6PYX1
R	99	ARG	ALA	conflict	UNP Q6PYX1
R	101	ASP	PRO	conflict	UNP Q6PYX1
R	103	TRP	-	expression tag	UNP Q6PYX1
R	104	GLY	-	expression tag	UNP Q6PYX1
R	106	GLY	-	expression tag	UNP Q6PYX1
R	107	THR	ILE	conflict	UNP Q6PYX1
R	108	VAL	GLU	conflict	UNP Q6PYX1
R	109	VAL	LYS	conflict	UNP Q6PYX1
R	111	VAL	ILE	conflict	UNP Q6PYX1
R	113	PRO	LYS	conflict	UNP Q6PYX1
R	115	SER	-	expression tag	UNP Q6PYX1
R	116	THR	-	expression tag	UNP Q6PYX1
R	?	-	GLN	deletion	UNP Q6PYX1
R	?	-	PRO	deletion	UNP Q6PYX1
R	?	-	ARG	deletion	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	120	SER	GLN	conflict	UNP Q6PYX1
R	122	PHE	TYR	conflict	UNP Q6PYX1
R	123	PRO	THR	conflict	UNP Q6PYX1
R	125	ALA	PRO	conflict	UNP Q6PYX1
R	?	-	ARG	deletion	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	136	GLY	MET	conflict	UNP Q6PYX1
R	?	-	LYS	deletion	UNP Q6PYX1
R	?	-	ASN	deletion	UNP Q6PYX1
R	?	-	GLN	deletion	UNP Q6PYX1
R	138	ALA	VAL	conflict	UNP Q6PYX1
R	139	ALA	SER	conflict	UNP Q6PYX1
R	141	GLY	THR	conflict	UNP Q6PYX1
R	146	ASP	GLY	conflict	UNP Q6PYX1
R	147	TYR	PHE	conflict	UNP Q6PYX1
R	148	PHE	TYR	conflict	UNP Q6PYX1
R	150	GLU	SER	conflict	UNP Q6PYX1
R	151	PRO	ASP	conflict	UNP Q6PYX1
R	152	VAL	ILE	conflict	UNP Q6PYX1
R	153	THR	ALA	conflict	UNP Q6PYX1
R	156	SER	GLU	conflict	UNP Q6PYX1
R	162	ASN	GLU	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	ASN	deletion	UNP Q6PYX1
R	165	ALA	GLN	conflict	UNP Q6PYX1
R	166	LEU	PRO	conflict	UNP Q6PYX1
R	167	THR	GLU	conflict	UNP Q6PYX1
R	168	SER	ASN	conflict	UNP Q6PYX1
R	169	GLY	ASN	conflict	UNP Q6PYX1
R	171	VAL	TYR	conflict	UNP Q6PYX1
R	172	HIS	LYS	conflict	UNP Q6PYX1
R	174	PHE	THR	conflict	UNP Q6PYX1
R	176	ALA	PRO	conflict	UNP Q6PYX1
R	179	GLN	ASP	conflict	UNP Q6PYX1
R	182	SER	ASP	conflict	UNP Q6PYX1
R	?	-	SER	deletion	UNP Q6PYX1
R	?	-	PHE	deletion	UNP Q6PYX1
R	?	-	PHE	deletion	UNP Q6PYX1
R	?	-	LYS	deletion	UNP Q6PYX1
R	188	SER	-	expression tag	UNP Q6PYX1
R	189	SER	-	expression tag	UNP Q6PYX1
R	190	VAL	-	expression tag	UNP Q6PYX1
R	191	VAL	-	expression tag	UNP Q6PYX1
R	194	PRO	ASP	conflict	UNP Q6PYX1
R	195	SER	LYS	conflict	UNP Q6PYX1
R	?	-	ARG	deletion	UNP Q6PYX1
R	?	-	TRP	deletion	UNP Q6PYX1
R	197	SER	GLN	conflict	UNP Q6PYX1
R	198	LEU	GLN	conflict	UNP Q6PYX1
R	200	THR	-	expression tag	UNP Q6PYX1
R	203	GLN	ASN	conflict	UNP Q6PYX1
R	205	THR	VAL	conflict	UNP Q6PYX1
R	206	TYR	PHE	conflict	UNP Q6PYX1
R	207	ILE	SER	conflict	UNP Q6PYX1
R	209	ASN	SER	conflict	UNP Q6PYX1
R	?	-	MET	deletion	UNP Q6PYX1
R	?	-	HIS	deletion	UNP Q6PYX1
R	?	-	GLU	deletion	UNP Q6PYX1
R	?	-	ALA	deletion	UNP Q6PYX1
R	?	-	LEU	deletion	UNP Q6PYX1
R	?	-	HIS	deletion	UNP Q6PYX1
R	213	LYS	-	expression tag	UNP Q6PYX1
R	214	PRO	-	expression tag	UNP Q6PYX1
R	215	SER	-	expression tag	UNP Q6PYX1
R	216	ASN	TYR	conflict	UNP Q6PYX1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	218	LYS	-	expression tag	UNP Q6PYX1
R	219	VAL	-	expression tag	UNP Q6PYX1
R	220	ASP	-	expression tag	UNP Q6PYX1
R	221	LYS	-	expression tag	UNP Q6PYX1
R	222	LYS	-	expression tag	UNP Q6PYX1
R	225	VAL	-	expression tag	UNP Q6PYX1
R	226	GLU	-	expression tag	UNP Q6PYX1
R	227	PRO	GLN	conflict	UNP Q6PYX1
R	230	CYS	-	expression tag	UNP Q6PYX1
R	231	ASP	-	expression tag	UNP Q6PYX1
R	232	LYS	-	expression tag	UNP Q6PYX1
R	233	THR	LEU	conflict	UNP Q6PYX1
R	235	THR	LEU	conflict	UNP Q6PYX1
R	236	CYS	SER	conflict	UNP Q6PYX1
R	238	PRO	-	expression tag	UNP Q6PYX1
R	239	CYS	-	expression tag	UNP Q6PYX1
R	240	PRO	-	expression tag	UNP Q6PYX1
R	241	ALA	-	expression tag	UNP Q6PYX1
R	242	PRO	-	expression tag	UNP Q6PYX1
R	243	GLU	-	expression tag	UNP Q6PYX1
R	244	LEU	-	expression tag	UNP Q6PYX1
R	245	LEU	-	expression tag	UNP Q6PYX1
R	247	GLY	LYS	conflict	UNP Q6PYX1

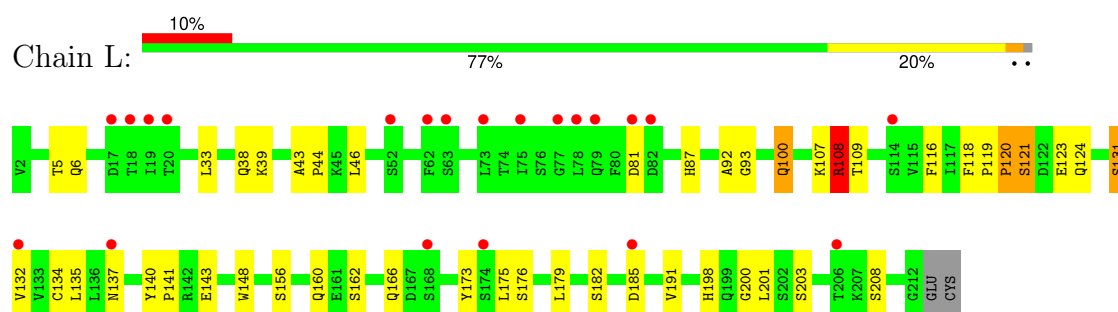
- Molecule 3 is a protein called 2G12 IgG dimer heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	B	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	C	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	D	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	J	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	N	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			

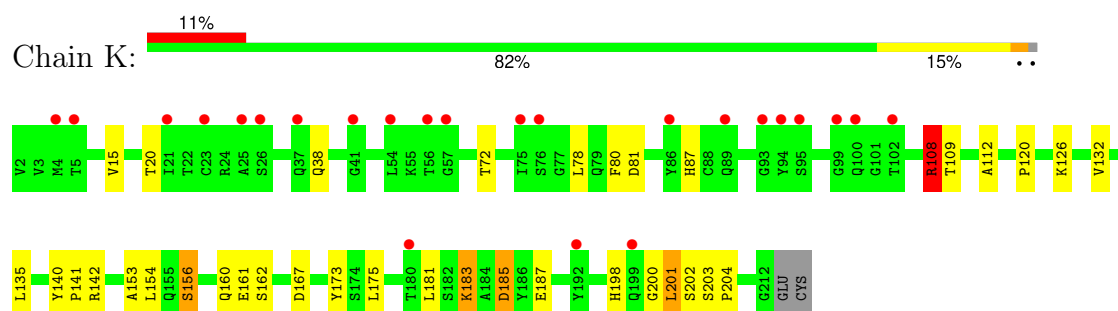
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

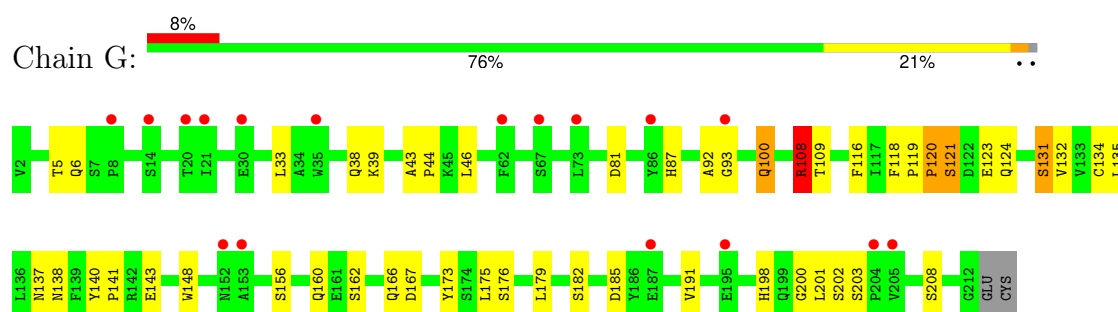
- Molecule 1: 2G12 IgG dimer light chain



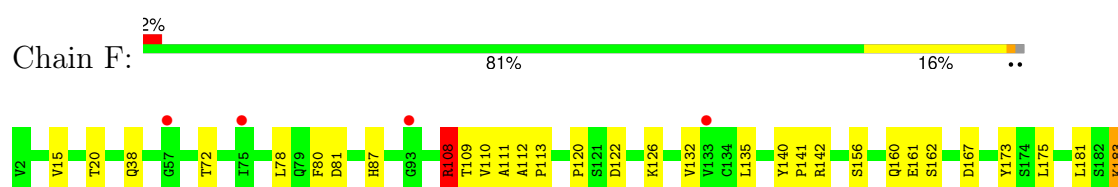
- Molecule 1: 2G12 IgG dimer light chain



- Molecule 1: 2G12 IgG dimer light chain

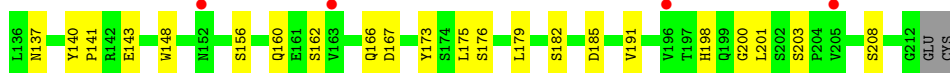
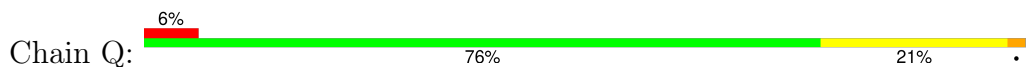


- Molecule 1: 2G12 IgG dimer light chain

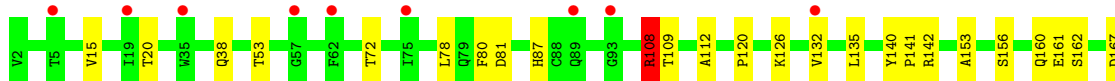
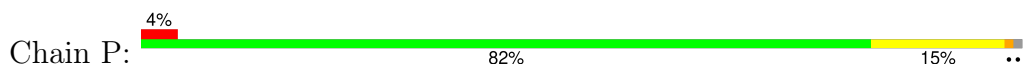




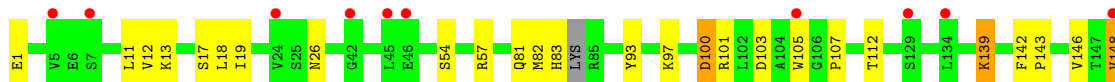
- Molecule 1: 2G12 IgG dimer light chain



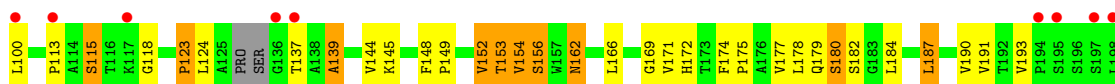
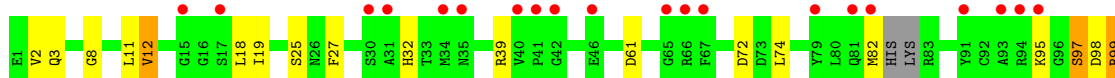
- Molecule 1: 2G12 IgG dimer light chain



- Molecule 2: Hepatitis B virus receptor binding protein

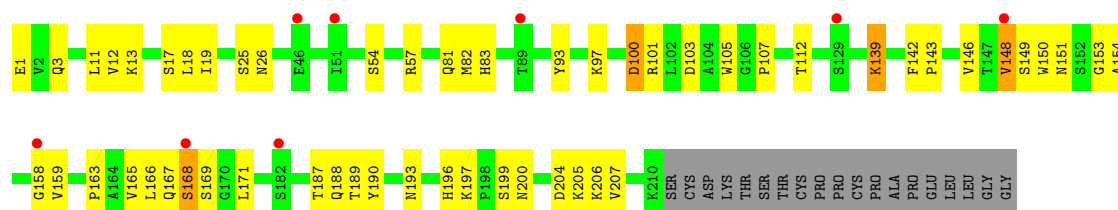


- Molecule 2: Hepatitis B virus receptor binding protein



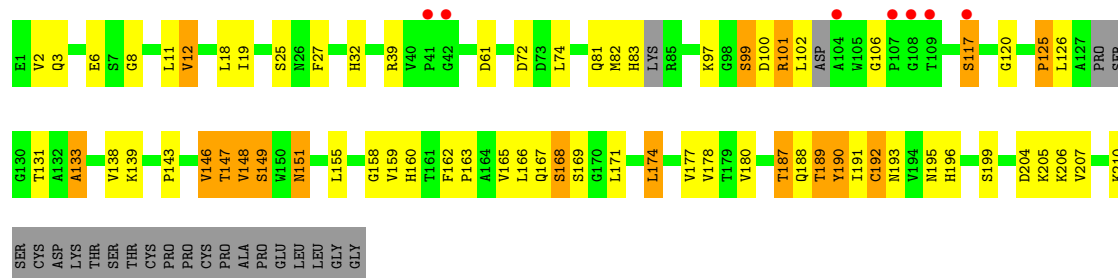
- Molecule 2: Hepatitis B virus receptor binding protein

Chain E: 



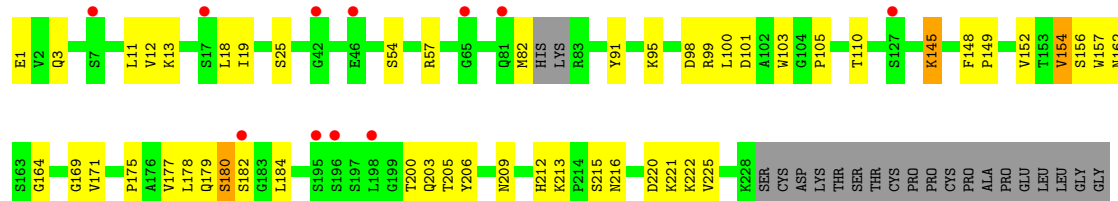
- Molecule 2: Hepatitis B virus receptor binding protein

Chain I: 



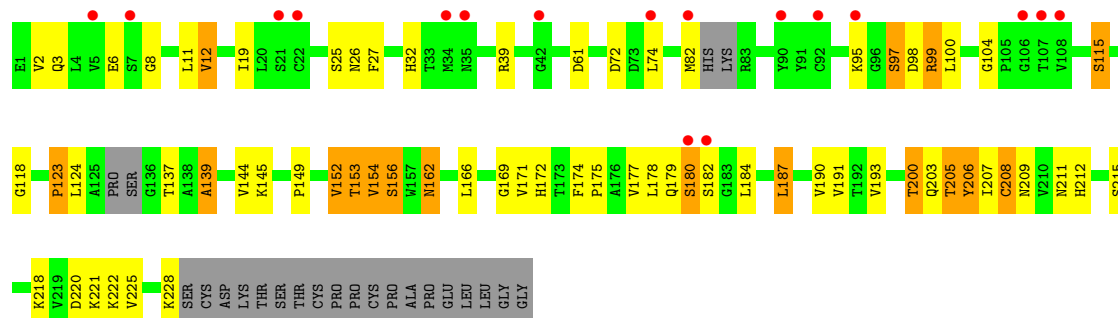
- Molecule 2: Hepatitis B virus receptor binding protein

Chain O: 

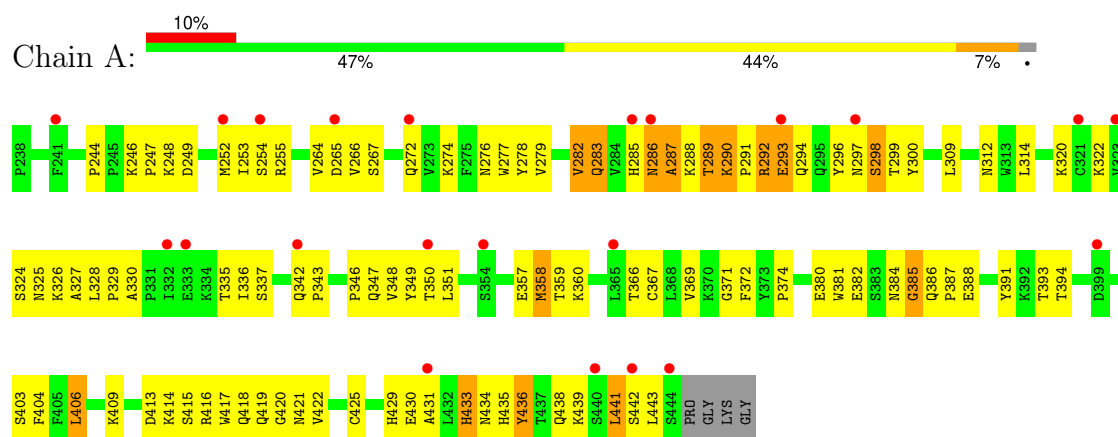


- Molecule 2: Hepatitis B virus receptor binding protein

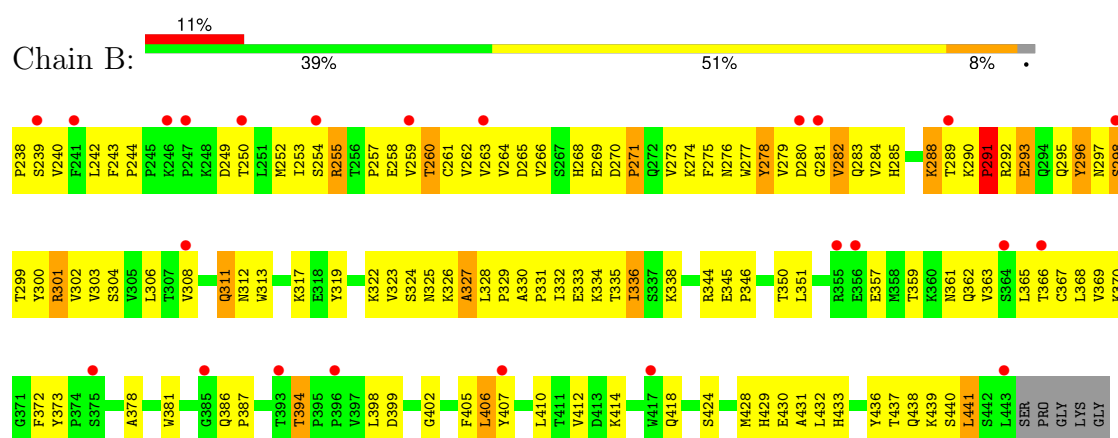
Chain R: 



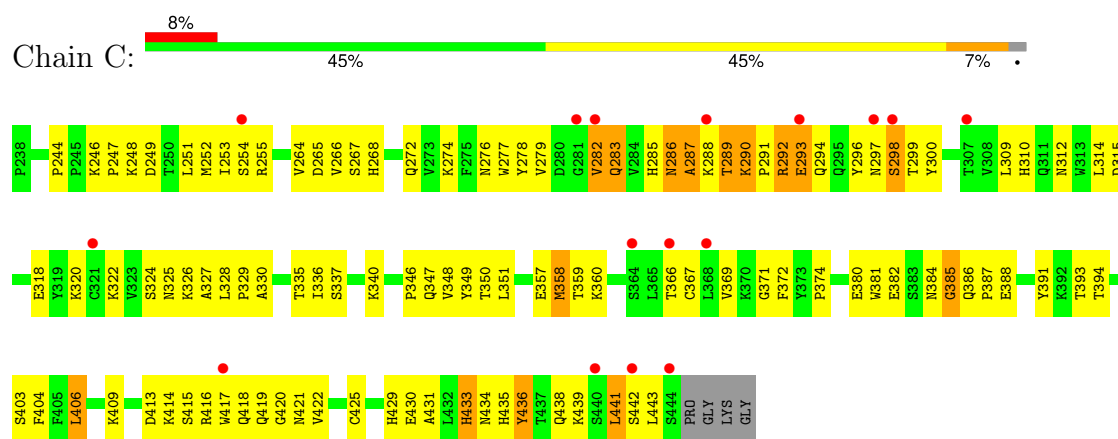
- Molecule 3: 2G12 IgG dimer heavy chain



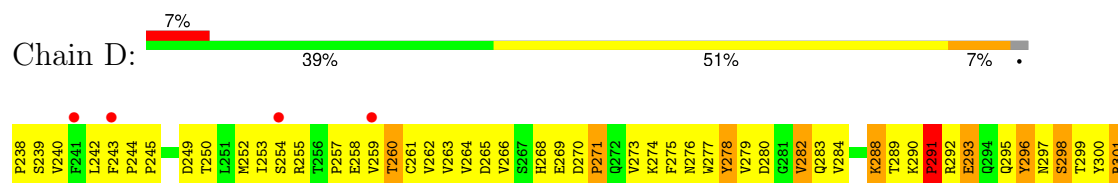
- Molecule 3: 2G12 IgG dimer heavy chain

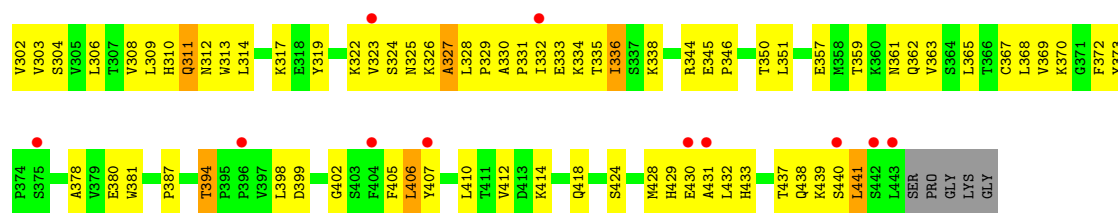


- Molecule 3: 2G12 IgG dimer heavy chain

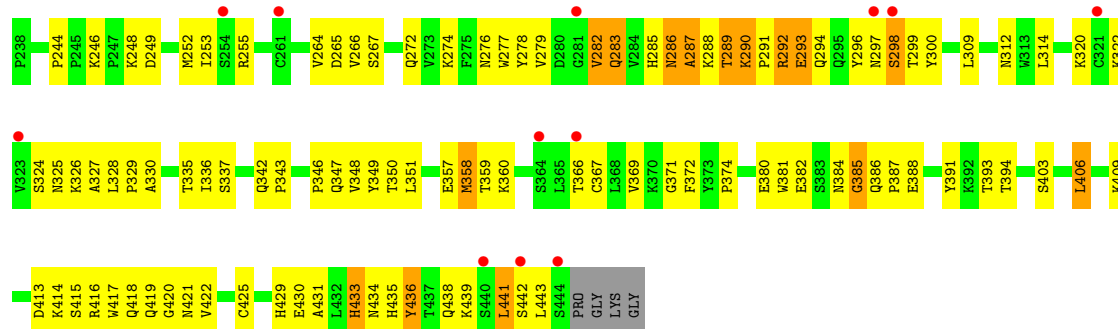


- Molecule 3: 2G12 IgG dimer heavy chain

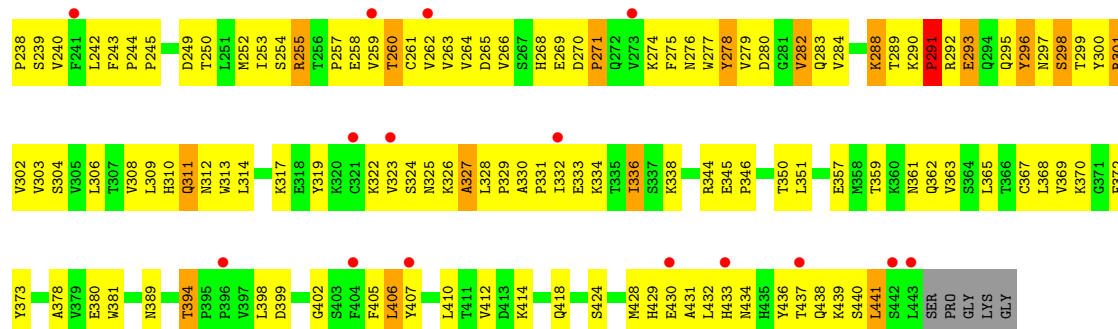




• Molecule 3: 2G12 IgG dimer heavy chain



• Molecule 3: 2G12 IgG dimer heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	374.73Å 374.73Å 64.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.91 – 6.50 64.91 – 6.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (64.91-6.50) 99.8 (64.91-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 6.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.381 , 0.366 0.382 , 0.363	Depositor DCC
R_{free} test set	519 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	243.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 600.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	28972	wwPDB-VP
Average B, all atoms (Å ²)	481.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4512e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	F	0.53	1/1654 (0.1%)	0.85	6/2246 (0.3%)
1	G	0.97	6/1654 (0.4%)	0.81	5/2246 (0.2%)
1	K	0.53	1/1654 (0.1%)	0.84	5/2246 (0.2%)
1	L	0.97	6/1654 (0.4%)	0.81	4/2246 (0.2%)
1	P	0.53	1/1654 (0.1%)	0.85	5/2246 (0.2%)
1	Q	0.97	6/1654 (0.4%)	0.81	6/2246 (0.3%)
2	E	0.89	2/1600 (0.1%)	0.78	3/2162 (0.1%)
2	H	0.89	2/1591 (0.1%)	0.78	3/2151 (0.1%)
2	I	1.18	9/1569 (0.6%)	0.83	5/2120 (0.2%)
2	M	1.18	9/1568 (0.6%)	0.84	5/2122 (0.2%)
2	O	0.89	2/1582 (0.1%)	0.79	3/2142 (0.1%)
2	R	1.18	9/1568 (0.6%)	0.84	5/2122 (0.2%)
3	A	0.42	0/1706	0.68	0/2323
3	B	0.37	0/1699	0.64	0/2312
3	C	0.43	0/1706	0.68	0/2323
3	D	0.37	0/1699	0.64	0/2312
3	J	0.42	0/1706	0.68	0/2323
3	N	0.37	0/1699	0.64	0/2312
All	All	0.78	54/29617 (0.2%)	0.77	55/40200 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	1
3	D	0	1
3	N	0	1
All	All	0	3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	180	SER	C-N	27.91	1.98	1.34
2	I	168	SER	C-N	27.90	1.98	1.34
2	R	180	SER	C-N	27.85	1.98	1.34
1	G	121	SER	CB-OG	24.55	1.74	1.42
1	Q	121	SER	CB-OG	24.55	1.74	1.42
1	L	121	SER	CB-OG	24.52	1.74	1.42
2	E	168	SER	C-N	23.32	1.87	1.34
2	O	180	SER	C-N	23.31	1.87	1.34
2	H	168	SER	C-N	23.29	1.87	1.34
2	I	148	VAL	C-N	22.64	1.86	1.34
2	R	154	VAL	C-N	22.64	1.86	1.34
2	M	154	VAL	C-N	22.59	1.86	1.34
2	E	148	VAL	C-N	16.81	1.72	1.34
2	O	154	VAL	C-N	16.81	1.72	1.34
2	H	148	VAL	C-N	16.78	1.72	1.34
1	L	119	PRO	C-O	12.54	1.48	1.23
1	Q	119	PRO	C-O	12.46	1.48	1.23
1	G	119	PRO	C-O	12.46	1.48	1.23
1	L	131	SER	CB-OG	12.04	1.57	1.42
1	Q	131	SER	CB-OG	11.99	1.57	1.42
1	G	131	SER	CB-OG	11.98	1.57	1.42
1	L	182	SER	CB-OG	8.19	1.52	1.42
1	Q	182	SER	CB-OG	8.19	1.52	1.42
1	G	182	SER	CB-OG	8.14	1.52	1.42
2	I	131	THR	C-O	6.95	1.36	1.23
2	M	137	THR	C-O	6.90	1.36	1.23
2	R	137	THR	C-O	6.90	1.36	1.23
2	I	133	ALA	C-O	6.80	1.36	1.23
2	R	139	ALA	C-O	6.75	1.36	1.23
2	M	139	ALA	C-O	6.75	1.36	1.23
1	Q	119	PRO	C-N	6.27	1.46	1.34
1	P	183	LYS	C-O	6.20	1.35	1.23
1	K	183	LYS	C-O	6.16	1.35	1.23
1	G	119	PRO	C-N	6.16	1.46	1.34
1	F	183	LYS	C-O	6.15	1.35	1.23
1	L	119	PRO	C-N	6.15	1.46	1.34
1	Q	120	PRO	N-CD	5.95	1.56	1.47
2	R	208	CYS	CB-SG	5.92	1.92	1.82
1	L	120	PRO	N-CD	5.90	1.56	1.47
1	G	120	PRO	N-CD	5.89	1.56	1.47
2	M	208	CYS	CB-SG	5.88	1.92	1.82
2	I	192	CYS	CB-SG	5.88	1.92	1.82
2	M	206	TYR	CE1-CZ	5.57	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	206	TYR	CG-CD2	5.57	1.46	1.39
2	M	206	TYR	CG-CD2	5.53	1.46	1.39
2	I	190	TYR	CG-CD2	5.51	1.46	1.39
2	I	190	TYR	CE1-CZ	5.51	1.45	1.38
2	R	206	TYR	CE1-CZ	5.50	1.45	1.38
2	I	125	PRO	C-O	5.48	1.34	1.23
2	R	123	PRO	C-O	5.46	1.34	1.23
2	M	123	PRO	C-O	5.44	1.34	1.23
2	M	137	THR	C-N	5.26	1.46	1.34
2	I	131	THR	C-N	5.25	1.46	1.34
2	R	137	THR	C-N	5.22	1.46	1.34

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	108	ARG	NE-CZ-NH2	-13.67	113.46	120.30
1	P	108	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	K	108	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	L	108	ARG	NE-CZ-NH2	-12.31	114.15	120.30
1	L	108	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	Q	108	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	Q	108	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	G	108	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	G	108	ARG	NE-CZ-NH1	12.02	126.31	120.30
1	F	108	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	P	108	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	K	108	ARG	NE-CZ-NH1	10.28	125.44	120.30
2	E	168	SER	O-C-N	-8.46	109.17	122.70
2	H	168	SER	O-C-N	-8.43	109.21	122.70
2	O	180	SER	O-C-N	-8.43	109.22	122.70
2	R	154	VAL	C-N-CA	-6.45	105.57	121.70
2	I	148	VAL	C-N-CA	-6.42	105.64	121.70
2	M	154	VAL	C-N-CA	-6.42	105.66	121.70
2	I	168	SER	O-C-N	-6.36	112.53	122.70
2	M	180	SER	O-C-N	-6.35	112.54	122.70
2	R	180	SER	O-C-N	-6.34	112.55	122.70
1	K	81	ASP	CB-CG-OD2	6.26	123.93	118.30
1	P	81	ASP	CB-CG-OD2	6.24	123.92	118.30
1	F	81	ASP	CB-CG-OD2	6.19	123.87	118.30
1	Q	81	ASP	CB-CG-OD2	6.15	123.83	118.30
1	G	81	ASP	CB-CG-OD2	6.14	123.83	118.30
1	L	81	ASP	CB-CG-OD2	6.13	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	100	ASP	CB-CG-OD2	5.81	123.53	118.30
2	R	98	ASP	CB-CG-OD2	5.79	123.51	118.30
2	M	98	ASP	CB-CG-OD2	5.76	123.48	118.30
2	I	204	ASP	CB-CG-OD2	5.63	123.37	118.30
2	M	220	ASP	CB-CG-OD2	5.61	123.35	118.30
2	R	220	ASP	CB-CG-OD2	5.54	123.29	118.30
2	E	204	ASP	CB-CG-OD2	5.50	123.25	118.30
2	H	204	ASP	CB-CG-OD2	5.50	123.25	118.30
2	O	220	ASP	CB-CG-OD2	5.50	123.25	118.30
1	L	185	ASP	CB-CG-OD2	5.32	123.09	118.30
1	Q	185	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	185	ASP	CB-CG-OD2	5.18	122.97	118.30
2	E	100	ASP	CB-CG-OD2	5.17	122.95	118.30
2	R	61	ASP	CB-CG-OD2	5.17	122.95	118.30
1	P	185	ASP	CB-CG-OD2	5.16	122.94	118.30
2	M	61	ASP	CB-CG-OD2	5.15	122.93	118.30
2	I	61	ASP	CB-CG-OD2	5.12	122.91	118.30
2	H	100	ASP	CB-CG-OD2	5.11	122.90	118.30
1	G	167	ASP	CB-CG-OD2	5.09	122.89	118.30
1	F	167	ASP	CB-CG-OD2	5.09	122.89	118.30
1	F	185	ASP	CB-CG-OD2	5.08	122.88	118.30
1	P	167	ASP	CB-CG-OD2	5.05	122.85	118.30
1	Q	167	ASP	CB-CG-OD2	5.05	122.85	118.30
1	K	167	ASP	CB-CG-OD2	5.05	122.84	118.30
1	Q	17	ASP	CB-CG-OD2	5.04	122.84	118.30
1	K	185	ASP	CB-CG-OD2	5.04	122.84	118.30
2	O	98	ASP	CB-CG-OD2	5.03	122.82	118.30
1	F	122	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	373	TYR	Sidechain
3	D	373	TYR	Sidechain
3	N	373	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1618	0	1580	69	0
1	G	1618	0	1580	60	1
1	K	1618	0	1579	47	2
1	L	1618	0	1580	59	1
1	P	1618	0	1580	39	3
1	Q	1618	0	1580	63	0
2	E	1574	0	1546	53	41
2	H	1565	0	1533	51	38
2	I	1544	0	1517	89	3
2	M	1542	0	1516	103	0
2	O	1555	0	1525	82	1
2	R	1542	0	1516	87	1
3	A	1660	0	1632	102	79
3	B	1654	0	1627	151	43
3	C	1660	0	1626	182	1
3	D	1654	0	1627	122	34
3	J	1660	0	1632	101	60
3	N	1654	0	1627	190	2
All	All	28972	0	28403	1283	155

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:ILE:HG21	3:N:310:HIS:CE1	1.27	1.67
1:F:201:LEU:CD1	2:O:99:ARG:CG	1.80	1.57
1:F:112:ALA:HB3	2:O:99:ARG:CB	1.23	1.56
1:F:112:ALA:CB	2:O:99:ARG:CB	1.81	1.55
1:F:201:LEU:HD11	2:O:99:ARG:CD	1.45	1.46
1:F:112:ALA:CB	2:O:99:ARG:HB3	1.39	1.45
3:C:310:HIS:CD2	3:N:253:ILE:HD12	1.50	1.42
2:O:154:VAL:C	2:O:156:SER:N	1.72	1.42
2:E:148:VAL:C	2:E:149:SER:N	1.72	1.41
3:C:253:ILE:CG2	3:N:310:HIS:CE1	2.03	1.41
2:H:148:VAL:C	2:H:149:SER:N	1.72	1.39
3:C:253:ILE:HG21	3:N:310:HIS:NE2	1.40	1.36
1:Q:121:SER:CB	1:Q:121:SER:OG	1.74	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:121:SER:CB	1:L:121:SER:OG	1.74	1.35
1:G:121:SER:CB	1:G:121:SER:OG	1.74	1.35
1:F:112:ALA:HB1	2:O:99:ARG:CG	1.56	1.33
2:M:115:SER:N	3:B:282:VAL:HG12	1.36	1.33
2:R:154:VAL:C	2:R:156:SER:N	1.86	1.29
2:M:154:VAL:C	2:M:156:SER:N	1.86	1.28
2:O:180:SER:C	2:O:182:SER:N	1.87	1.28
1:F:201:LEU:HD13	2:O:99:ARG:CG	1.48	1.27
2:I:148:VAL:C	2:I:149:SER:N	1.86	1.27
2:H:168:SER:C	2:H:169:SER:N	1.87	1.27
2:E:168:SER:C	2:E:169:SER:N	1.87	1.25
3:C:252:MET:C	3:N:253:ILE:HD13	1.58	1.23
1:F:112:ALA:CB	2:O:99:ARG:CG	2.14	1.20
1:F:202:SER:O	3:C:297:ASN:CA	1.89	1.20
2:E:11:LEU:HD11	2:I:166:LEU:HD21	1.24	1.17
1:F:202:SER:O	3:C:297:ASN:HA	1.39	1.17
2:I:168:SER:C	2:I:169:SER:N	1.98	1.17
2:R:180:SER:C	2:R:182:SER:N	1.98	1.16
1:P:203:SER:CB	3:J:298:SER:HB3	1.76	1.16
2:M:180:SER:C	2:M:182:SER:N	1.98	1.16
1:P:203:SER:HB2	3:J:298:SER:HB3	1.20	1.15
1:K:156:SER:CB	3:B:333:GLU:OE2	1.95	1.15
1:F:112:ALA:CB	2:O:99:ARG:HG2	1.74	1.14
2:O:11:LEU:HD11	2:R:178:LEU:HD21	1.24	1.14
2:M:115:SER:HB2	3:B:282:VAL:CG1	1.77	1.14
1:F:201:LEU:CD1	2:O:99:ARG:CD	2.17	1.13
2:H:11:LEU:HD11	2:M:178:LEU:HD21	1.24	1.13
1:K:202:SER:HB2	3:A:296:TYR:O	1.47	1.12
1:F:112:ALA:HB2	2:O:99:ARG:HA	1.22	1.12
3:C:310:HIS:CD2	3:N:253:ILE:CD1	2.33	1.12
2:H:11:LEU:CD1	2:M:178:LEU:HD21	1.79	1.11
1:K:202:SER:CB	3:A:296:TYR:O	1.99	1.11
2:O:11:LEU:CD1	2:R:178:LEU:HD21	1.79	1.11
2:E:11:LEU:CD1	2:I:166:LEU:HD21	1.79	1.10
1:F:201:LEU:HD12	2:O:99:ARG:HG3	1.21	1.09
1:F:201:LEU:CD1	2:O:99:ARG:HG3	1.58	1.08
3:C:310:HIS:HD2	3:N:253:ILE:CD1	1.64	1.08
2:I:117:SER:HB2	3:D:282:VAL:HG12	1.30	1.07
1:P:203:SER:HB2	3:J:298:SER:CB	1.84	1.07
1:F:112:ALA:CB	2:O:99:ARG:CA	2.30	1.06
2:M:115:SER:CB	3:B:282:VAL:CG1	2.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ALA:HB2	2:O:99:ARG:CA	1.86	1.05
2:O:178:LEU:HD21	2:R:11:LEU:HD11	1.07	1.05
1:F:203:SER:CB	3:C:298:SER:HB3	1.87	1.04
3:C:436:TYR:CE2	3:N:434:ASN:HB2	1.91	1.04
1:F:110:VAL:HB	2:O:100:LEU:HD12	1.34	1.04
2:H:166:LEU:HD21	2:M:11:LEU:HD11	1.07	1.03
1:F:201:LEU:CD1	2:O:99:ARG:HG2	1.66	1.02
2:E:166:LEU:HD21	2:I:11:LEU:HD11	1.07	1.02
2:M:115:SER:CB	3:B:282:VAL:HG11	1.90	1.01
2:I:117:SER:HB2	3:D:282:VAL:CG1	1.90	1.01
2:H:166:LEU:HD21	2:M:11:LEU:CD1	1.91	1.01
2:E:166:LEU:HD21	2:I:11:LEU:CD1	1.91	1.01
1:F:203:SER:HB2	3:C:298:SER:CB	1.90	1.01
3:C:252:MET:C	3:N:253:ILE:CD1	2.29	1.01
3:C:294:GLN:HG2	2:O:1:GLU:O	1.21	0.99
2:O:178:LEU:HD21	2:R:11:LEU:CD1	1.91	0.99
3:B:266:VAL:HB	3:B:300:TYR:HB2	1.44	0.99
3:C:294:GLN:CG	2:O:1:GLU:O	2.08	0.99
3:D:266:VAL:HB	3:D:300:TYR:HB2	1.44	0.98
1:F:201:LEU:CD1	2:O:99:ARG:HD3	1.87	0.98
2:H:158:GLY:C	2:H:159:VAL:N	2.17	0.98
2:O:169:GLY:C	2:O:171:VAL:N	2.17	0.98
3:N:266:VAL:HB	3:N:300:TYR:HB2	1.45	0.98
1:F:203:SER:HB2	3:C:298:SER:HB3	0.99	0.97
3:C:254:SER:HA	3:N:311:GLN:OE1	1.65	0.97
2:M:113:PRO:HB2	3:B:281:GLY:HA3	1.47	0.96
1:K:156:SER:HB3	3:B:333:GLU:OE2	1.63	0.96
2:E:158:GLY:C	2:E:159:VAL:N	2.17	0.96
1:K:156:SER:CB	3:B:333:GLU:CD	2.34	0.96
3:C:252:MET:O	3:N:253:ILE:HD13	1.66	0.96
1:K:156:SER:HB2	3:B:333:GLU:OE2	1.64	0.95
3:C:436:TYR:CE2	3:N:434:ASN:CB	2.50	0.94
1:K:156:SER:OG	3:B:333:GLU:OE1	1.86	0.94
3:C:253:ILE:HD13	3:N:310:HIS:HE2	1.29	0.94
3:C:382:GLU:OE1	3:N:433:HIS:CD2	2.20	0.94
1:F:20:THR:HG23	1:F:72:THR:HG23	1.48	0.94
2:O:11:LEU:HD11	2:R:178:LEU:CD2	1.97	0.93
1:P:20:THR:HG23	1:P:72:THR:HG23	1.48	0.93
2:H:11:LEU:HD11	2:M:178:LEU:CD2	1.97	0.93
1:Q:120:PRO:HD3	1:Q:132:VAL:HG12	1.50	0.93
2:E:11:LEU:HD11	2:I:166:LEU:CD2	1.97	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:115:SER:HB2	3:B:282:VAL:CB	1.99	0.92
1:L:120:PRO:HD3	1:L:132:VAL:HG12	1.50	0.92
1:K:20:THR:HG23	1:K:72:THR:HG23	1.48	0.92
1:F:112:ALA:HB1	2:O:99:ARG:HG2	0.92	0.91
2:M:115:SER:OG	3:B:282:VAL:HG11	1.69	0.91
2:M:115:SER:H	3:B:282:VAL:CG1	1.82	0.91
1:F:201:LEU:HD11	2:O:99:ARG:HD3	0.92	0.91
2:M:115:SER:H	3:B:282:VAL:HG12	1.00	0.91
1:G:120:PRO:HD3	1:G:132:VAL:HG12	1.50	0.91
3:C:434:ASN:ND2	3:N:428:MET:HE1	1.85	0.90
3:A:272:GLN:HE22	3:A:326:LYS:HD2	1.35	0.90
1:K:202:SER:HB2	3:A:296:TYR:C	1.90	0.90
1:F:201:LEU:HD13	2:O:99:ARG:HG2	0.90	0.90
3:J:272:GLN:HE22	3:J:326:LYS:HD2	1.35	0.90
2:M:115:SER:N	3:B:282:VAL:CG1	2.33	0.89
3:C:282:VAL:O	3:C:283:GLN:HB2	1.72	0.89
1:Q:118:PHE:CE1	2:R:139:ALA:O	2.25	0.89
1:G:118:PHE:CE1	2:I:133:ALA:O	2.25	0.89
2:H:166:LEU:CD2	2:M:11:LEU:HD11	2.01	0.89
3:C:436:TYR:HE2	3:N:434:ASN:OD1	1.56	0.89
1:L:118:PHE:CE1	2:M:139:ALA:O	2.25	0.89
1:P:203:SER:CB	3:J:298:SER:CB	2.44	0.89
1:K:108:ARG:HD3	1:K:109:THR:O	1.74	0.88
3:J:282:VAL:O	3:J:283:GLN:HB2	1.72	0.88
2:M:115:SER:CA	3:B:282:VAL:HG12	2.04	0.88
3:C:272:GLN:HE22	3:C:326:LYS:HD2	1.35	0.88
1:F:108:ARG:HD3	1:F:109:THR:O	1.74	0.88
2:O:178:LEU:CD2	2:R:11:LEU:HD11	2.01	0.88
1:K:20:THR:HG23	1:K:72:THR:CG2	2.04	0.87
1:P:20:THR:HG23	1:P:72:THR:CG2	2.04	0.87
3:B:311:GLN:H	3:B:311:GLN:NE2	1.71	0.87
3:A:282:VAL:O	3:A:283:GLN:HB2	1.72	0.87
1:F:20:THR:HG23	1:F:72:THR:CG2	2.04	0.87
2:M:115:SER:HB2	3:B:282:VAL:HB	1.56	0.86
3:D:311:GLN:H	3:D:311:GLN:NE2	1.71	0.86
3:N:311:GLN:NE2	3:N:311:GLN:H	1.71	0.86
1:F:110:VAL:O	2:O:100:LEU:HB2	1.75	0.86
3:C:436:TYR:CD2	3:N:434:ASN:CB	2.59	0.86
2:E:81:GLN:HE21	2:E:83:HIS:HE1	1.23	0.85
1:P:108:ARG:HD3	1:P:109:THR:O	1.74	0.85
2:H:81:GLN:HE21	2:H:83:HIS:HE1	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:LEU:CD2	2:I:11:LEU:HD11	2.01	0.85
3:N:328:LEU:HD21	3:N:332:ILE:HG13	1.59	0.85
3:C:436:TYR:CE2	3:N:434:ASN:OD1	2.30	0.85
3:B:328:LEU:HD21	3:B:332:ILE:HG13	1.59	0.84
2:M:217:THR:OG1	3:B:285:HIS:CD2	2.31	0.84
3:C:253:ILE:HD13	3:N:310:HIS:NE2	1.93	0.84
3:C:253:ILE:HG22	3:N:310:HIS:CE1	2.13	0.83
3:D:328:LEU:HD21	3:D:332:ILE:HG13	1.59	0.83
3:C:346:PRO:HB3	3:C:372:PHE:HB3	1.60	0.83
2:R:115:SER:HB2	3:N:282:VAL:CG1	2.07	0.83
3:N:291:PRO:HB3	3:N:304:SER:HA	1.60	0.82
3:A:346:PRO:HB3	3:A:372:PHE:HB3	1.60	0.82
1:Q:6:GLN:H	1:Q:100:GLN:HE22	1.27	0.82
1:F:202:SER:O	3:C:297:ASN:C	2.17	0.82
3:D:291:PRO:HB3	3:D:304:SER:HA	1.60	0.82
3:A:314:LEU:HD22	3:A:430:GLU:HG3	1.62	0.82
3:B:243:PHE:HB2	3:B:260:THR:HG23	1.60	0.81
2:H:206:LYS:HA	2:H:207:VAL:N	1.95	0.81
3:B:291:PRO:HB3	3:B:304:SER:HA	1.60	0.81
2:O:222:LYS:HA	2:O:225:VAL:N	1.94	0.81
3:N:243:PHE:HB2	3:N:260:THR:HG23	1.60	0.81
3:C:314:LEU:HD22	3:C:430:GLU:HG3	1.62	0.81
3:J:314:LEU:HD22	3:J:430:GLU:HG3	1.62	0.81
3:J:346:PRO:HB3	3:J:372:PHE:HB3	1.60	0.81
1:G:6:GLN:H	1:G:100:GLN:HE22	1.27	0.80
3:D:243:PHE:HB2	3:D:260:THR:HG23	1.60	0.80
2:E:206:LYS:HA	2:E:207:VAL:N	1.95	0.80
3:C:252:MET:N	3:N:253:ILE:HD11	1.97	0.80
1:L:6:GLN:H	1:L:100:GLN:HE22	1.27	0.80
1:L:118:PHE:HE1	2:M:139:ALA:O	1.65	0.80
3:D:289:THR:HG22	3:D:290:LYS:H	1.48	0.79
3:D:346:PRO:HB3	3:D:372:PHE:HB3	1.63	0.79
2:R:115:SER:HB2	3:N:282:VAL:HG11	1.64	0.79
3:N:346:PRO:HB3	3:N:372:PHE:HB3	1.63	0.79
1:G:92:ALA:O	2:E:97:LYS:NZ	2.16	0.79
3:B:346:PRO:HB3	3:B:372:PHE:HB3	1.63	0.79
3:B:289:THR:HG22	3:B:290:LYS:H	1.48	0.79
3:A:291:PRO:C	3:A:292:ARG:HD2	2.03	0.79
1:G:118:PHE:HE1	2:I:133:ALA:O	1.65	0.79
1:G:108:ARG:HD3	1:G:109:THR:O	1.83	0.79
1:Q:108:ARG:HD3	1:Q:109:THR:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:92:ALA:O	2:O:95:LYS:NZ	2.16	0.78
3:J:291:PRO:C	3:J:292:ARG:HD2	2.03	0.78
3:N:289:THR:HG22	3:N:290:LYS:H	1.48	0.78
3:N:429:HIS:HD2	3:N:431:ALA:H	1.31	0.78
1:L:108:ARG:HD3	1:L:109:THR:O	1.83	0.78
1:Q:118:PHE:HE1	2:R:139:ALA:O	1.65	0.78
3:B:263:VAL:O	3:B:301:ARG:HA	1.84	0.78
3:C:291:PRO:C	3:C:292:ARG:HD2	2.03	0.78
3:A:292:ARG:O	3:A:293:GLU:HB3	1.84	0.78
3:D:429:HIS:HD2	3:D:431:ALA:H	1.31	0.78
1:L:92:ALA:O	2:H:97:LYS:NZ	2.16	0.77
3:B:429:HIS:HD2	3:B:431:ALA:H	1.31	0.77
3:C:268:HIS:HB3	1:Q:57:GLY:HA2	1.66	0.77
1:G:160:GLN:NE2	2:I:165:VAL:CG1	2.48	0.77
3:C:436:TYR:CD2	3:N:434:ASN:HB3	2.20	0.77
3:N:263:VAL:O	3:N:301:ARG:HA	1.84	0.77
3:C:252:MET:C	3:N:253:ILE:CG1	2.46	0.77
3:D:263:VAL:O	3:D:301:ARG:HA	1.84	0.77
3:D:429:HIS:CD2	3:D:431:ALA:H	2.03	0.77
2:M:113:PRO:CB	3:B:281:GLY:HA3	2.15	0.76
3:B:429:HIS:CD2	3:B:431:ALA:H	2.03	0.76
3:C:253:ILE:CD1	3:N:310:HIS:HE2	1.98	0.76
1:Q:160:GLN:NE2	2:R:177:VAL:CG1	2.48	0.76
3:N:429:HIS:CD2	3:N:431:ALA:H	2.03	0.76
1:L:160:GLN:NE2	2:M:177:VAL:CG1	2.48	0.76
3:C:292:ARG:O	3:C:293:GLU:HB3	1.84	0.76
3:C:253:ILE:CG2	3:N:310:HIS:ND1	2.47	0.76
2:I:81:GLN:HE21	2:I:83:HIS:HE1	1.33	0.76
3:N:252:MET:SD	3:N:428:MET:HE1	2.26	0.76
1:L:198:HIS:CD2	1:L:200:GLY:H	2.04	0.75
3:B:266:VAL:HB	3:B:300:TYR:CB	2.15	0.75
3:C:272:GLN:NE2	3:C:326:LYS:HD2	2.01	0.75
1:Q:198:HIS:CD2	1:Q:200:GLY:H	2.04	0.75
3:B:328:LEU:HD12	3:B:329:PRO:HD2	1.69	0.75
3:C:253:ILE:CD1	3:N:310:HIS:NE2	2.49	0.75
3:C:252:MET:N	3:N:253:ILE:CD1	2.49	0.75
3:D:266:VAL:HB	3:D:300:TYR:CB	2.15	0.75
3:J:272:GLN:NE2	3:J:326:LYS:HD2	2.01	0.75
3:D:365:LEU:HD12	3:D:410:LEU:HD23	1.69	0.74
3:B:365:LEU:HD12	3:B:410:LEU:HD23	1.69	0.74
1:G:198:HIS:CD2	1:G:200:GLY:H	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:328:LEU:HD12	3:D:329:PRO:HD2	1.69	0.74
3:J:292:ARG:O	3:J:293:GLU:HB3	1.85	0.74
3:N:328:LEU:HD12	3:N:329:PRO:HD2	1.69	0.74
3:N:365:LEU:HD12	3:N:410:LEU:HD23	1.69	0.74
3:J:429:HIS:CD2	3:J:431:ALA:H	2.05	0.74
3:N:266:VAL:HB	3:N:300:TYR:CB	2.16	0.74
3:A:272:GLN:NE2	3:A:326:LYS:HD2	2.01	0.74
3:A:429:HIS:CD2	3:A:431:ALA:H	2.05	0.74
1:F:112:ALA:HB3	2:O:99:ARG:CA	2.03	0.74
3:C:429:HIS:CD2	3:C:431:ALA:H	2.05	0.74
3:C:434:ASN:ND2	3:N:428:MET:CE	2.51	0.74
3:C:310:HIS:HD2	3:N:253:ILE:HD12	0.93	0.72
3:N:288:LYS:H	3:N:288:LYS:HD3	1.54	0.72
2:E:81:GLN:HE21	2:E:83:HIS:CE1	2.07	0.72
3:B:288:LYS:H	3:B:288:LYS:HD3	1.54	0.72
2:M:113:PRO:HB2	3:B:281:GLY:CA	2.19	0.72
1:P:153:ALA:HA	3:N:330:ALA:CB	2.20	0.72
1:F:198:HIS:CD2	1:F:200:GLY:H	2.08	0.71
1:P:198:HIS:CD2	1:P:200:GLY:H	2.08	0.71
3:D:288:LYS:H	3:D:288:LYS:HD3	1.54	0.71
1:G:43:ALA:HB2	2:E:107:PRO:HA	1.72	0.71
1:K:198:HIS:HD2	1:K:200:GLY:H	1.39	0.71
1:L:43:ALA:HB2	2:H:107:PRO:HA	1.72	0.71
1:K:198:HIS:CD2	1:K:200:GLY:H	2.08	0.71
2:H:11:LEU:HD12	2:M:178:LEU:HD21	1.70	0.70
1:F:110:VAL:O	2:O:100:LEU:CB	2.39	0.70
2:H:81:GLN:HE21	2:H:83:HIS:CE1	2.07	0.70
1:L:160:GLN:HB3	2:M:177:VAL:HG11	1.74	0.70
3:C:253:ILE:HG21	3:N:310:HIS:CD2	2.26	0.70
3:C:251:LEU:C	3:N:253:ILE:HD11	2.11	0.70
1:Q:43:ALA:HB2	2:O:105:PRO:HA	1.72	0.70
1:P:112:ALA:HB1	1:P:201:LEU:HD13	1.73	0.69
2:M:215:SER:O	3:B:285:HIS:HB2	1.91	0.69
3:A:422:VAL:HG22	3:A:442:SER:OG	1.92	0.69
3:C:253:ILE:HG22	3:N:310:HIS:ND1	2.06	0.69
3:C:422:VAL:HG22	3:C:442:SER:OG	1.92	0.69
2:M:115:SER:CB	3:B:282:VAL:HG12	2.13	0.69
2:M:145:LYS:HE2	2:M:179:GLN:HE22	1.58	0.69
2:H:143:PRO:O	2:H:196:HIS:HE1	1.75	0.69
1:G:137:ASN:OD1	2:I:160:HIS:CD2	2.46	0.69
1:F:112:ALA:CB	2:O:99:ARG:HA	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:422:VAL:HG22	3:J:442:SER:OG	1.92	0.69
3:C:434:ASN:HA	3:N:252:MET:CE	2.23	0.69
2:O:149:PRO:O	2:O:212:HIS:HE1	1.75	0.69
3:A:252:MET:HB2	3:A:255:ARG:HG3	1.75	0.69
3:C:436:TYR:CD1	3:N:436:TYR:HD1	2.11	0.69
1:P:198:HIS:HD2	1:P:200:GLY:H	1.39	0.69
1:L:137:ASN:OD1	2:M:172:HIS:CD2	2.46	0.68
1:K:112:ALA:HB1	1:K:201:LEU:HD13	1.73	0.68
2:E:143:PRO:O	2:E:196:HIS:HE1	1.75	0.68
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.58	0.68
2:R:145:LYS:HE2	2:R:179:GLN:HE22	1.58	0.68
1:F:110:VAL:CB	2:O:100:LEU:HD12	2.19	0.68
1:G:160:GLN:HB3	2:I:165:VAL:HG11	1.74	0.68
1:F:198:HIS:HD2	1:F:200:GLY:H	1.39	0.68
3:C:253:ILE:CG2	3:N:310:HIS:NE2	2.32	0.68
1:K:202:SER:OG	3:A:296:TYR:O	2.12	0.68
1:Q:137:ASN:OD1	2:R:172:HIS:CD2	2.46	0.68
3:J:325:ASN:HD21	3:J:327:ALA:HB3	1.58	0.68
2:H:81:GLN:NE2	2:H:83:HIS:HE1	1.91	0.68
3:B:270:ASP:N	3:B:271:PRO:HD3	2.09	0.68
2:I:139:LYS:HE2	2:I:167:GLN:HE22	1.58	0.68
1:K:156:SER:OG	3:B:333:GLU:CD	2.31	0.68
1:F:111:ALA:HA	2:O:100:LEU:O	1.93	0.68
2:E:81:GLN:NE2	2:E:83:HIS:HE1	1.91	0.68
3:J:252:MET:HB2	3:J:255:ARG:HG3	1.75	0.68
3:C:436:TYR:CD1	3:N:436:TYR:CD1	2.82	0.68
3:N:270:ASP:N	3:N:271:PRO:HD3	2.09	0.67
3:C:252:MET:HB2	3:C:255:ARG:HG3	1.75	0.67
3:J:429:HIS:HD2	3:J:431:ALA:H	1.43	0.67
3:D:270:ASP:N	3:D:271:PRO:HD3	2.09	0.67
1:Q:160:GLN:HB3	2:R:177:VAL:HG11	1.74	0.67
2:E:11:LEU:HD12	2:I:166:LEU:HD21	1.70	0.67
3:C:429:HIS:HD2	3:C:431:ALA:H	1.42	0.67
1:F:20:THR:CG2	1:F:72:THR:HG23	2.24	0.67
1:F:112:ALA:HB1	1:F:201:LEU:HD13	1.73	0.67
2:O:11:LEU:HD12	2:R:178:LEU:HD21	1.70	0.67
1:P:20:THR:CG2	1:P:72:THR:HG23	2.24	0.67
3:J:418:GLN:HA	3:J:443:LEU:CD2	2.24	0.67
3:A:325:ASN:ND2	3:A:327:ALA:HB3	2.10	0.66
3:A:418:GLN:HA	3:A:443:LEU:CD2	2.24	0.66
3:C:418:GLN:HA	3:C:443:LEU:CD2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:THR:HB	3:C:441:LEU:HG	1.77	0.66
3:A:325:ASN:HD21	3:A:327:ALA:HB3	1.58	0.66
3:B:290:LYS:HE3	3:B:292:ARG:HH22	1.61	0.66
3:J:350:THR:HB	3:J:441:LEU:HG	1.77	0.66
3:A:350:THR:HB	3:A:441:LEU:HG	1.77	0.65
2:M:154:VAL:C	2:M:156:SER:CA	2.65	0.65
2:E:12:VAL:HG11	2:E:82:MET:CE	2.26	0.65
2:I:81:GLN:HE21	2:I:83:HIS:CE1	2.13	0.65
2:O:12:VAL:HG11	2:O:82:MET:CE	2.26	0.65
2:H:12:VAL:HG11	2:H:82:MET:CE	2.26	0.65
1:K:20:THR:CG2	1:K:72:THR:HG23	2.24	0.65
1:Q:160:GLN:CD	2:R:177:VAL:HG11	2.17	0.65
3:J:325:ASN:ND2	3:J:327:ALA:HB3	2.10	0.65
3:A:429:HIS:HD2	3:A:431:ALA:H	1.43	0.65
2:E:11:LEU:HD11	2:I:166:LEU:CG	2.27	0.65
1:L:160:GLN:CD	2:M:177:VAL:HG11	2.17	0.65
2:O:11:LEU:HD11	2:R:178:LEU:CG	2.27	0.65
1:P:153:ALA:HA	3:N:330:ALA:HB2	1.77	0.65
1:F:203:SER:HB3	3:C:298:SER:CA	2.26	0.65
3:A:279:VAL:O	3:A:282:VAL:HG13	1.97	0.64
3:A:328:LEU:HG	3:A:330:ALA:O	1.98	0.64
3:D:290:LYS:HE3	3:D:292:ARG:HH22	1.61	0.64
3:J:328:LEU:HG	3:J:330:ALA:O	1.98	0.64
1:G:160:GLN:CD	2:I:165:VAL:HG11	2.17	0.64
3:C:325:ASN:ND2	3:C:327:ALA:HB3	2.10	0.64
3:C:328:LEU:HG	3:C:330:ALA:O	1.98	0.64
3:D:330:ALA:HB1	3:D:331:PRO:HD2	1.79	0.64
3:N:290:LYS:HE3	3:N:292:ARG:HH22	1.61	0.64
3:C:433:HIS:NE2	3:N:380:GLU:OE1	2.29	0.64
2:I:148:VAL:C	2:I:149:SER:CA	2.65	0.64
2:R:169:GLY:C	2:R:171:VAL:N	2.51	0.64
3:J:279:VAL:O	3:J:282:VAL:HG13	1.97	0.64
3:B:330:ALA:HB1	3:B:331:PRO:HD2	1.79	0.64
1:Q:132:VAL:HG22	1:Q:179:LEU:HB3	1.80	0.64
2:O:12:VAL:HG11	2:O:82:MET:HE3	1.79	0.64
1:L:137:ASN:OD1	2:M:172:HIS:HD2	1.81	0.64
1:P:203:SER:OG	3:J:298:SER:HB3	1.96	0.64
1:G:132:VAL:HG22	1:G:179:LEU:HB3	1.79	0.63
2:R:154:VAL:C	2:R:156:SER:CA	2.64	0.63
1:L:132:VAL:HG22	1:L:179:LEU:HB3	1.79	0.63
2:H:11:LEU:HD11	2:M:178:LEU:CG	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:169:GLY:C	2:M:171:VAL:N	2.52	0.63
3:A:288:LYS:H	3:A:288:LYS:HD2	1.63	0.63
1:G:162:SER:OG	2:I:163:PRO:HD2	1.99	0.63
3:N:330:ALA:HB1	3:N:331:PRO:HD2	1.80	0.63
3:B:332:ILE:HG22	3:B:333:GLU:N	2.13	0.63
3:C:279:VAL:O	3:C:282:VAL:HG13	1.97	0.63
1:Q:162:SER:OG	2:R:175:PRO:HD2	1.99	0.63
1:F:202:SER:O	3:C:296:TYR:O	2.17	0.63
2:I:158:GLY:C	2:I:159:VAL:N	2.52	0.63
1:L:162:SER:OG	2:M:175:PRO:HD2	1.99	0.63
3:J:288:LYS:H	3:J:288:LYS:HD2	1.63	0.63
1:L:100:GLN:H	1:L:100:GLN:CD	2.02	0.63
1:G:5:THR:HA	1:G:100:GLN:HE22	1.64	0.63
1:Q:137:ASN:OD1	2:R:172:HIS:HD2	1.81	0.63
3:N:332:ILE:HG22	3:N:333:GLU:N	2.13	0.62
1:G:118:PHE:CZ	2:I:133:ALA:O	2.52	0.62
2:I:81:GLN:NE2	2:I:83:HIS:HE1	1.98	0.62
1:Q:100:GLN:H	1:Q:100:GLN:CD	2.02	0.62
1:L:118:PHE:CZ	2:M:139:ALA:O	2.52	0.62
2:M:12:VAL:HG11	2:M:82:MET:HE3	1.81	0.62
1:G:137:ASN:OD1	2:I:160:HIS:HD2	1.82	0.62
3:C:288:LYS:H	3:C:288:LYS:HD2	1.63	0.62
3:D:332:ILE:HG22	3:D:333:GLU:N	2.13	0.62
1:Q:118:PHE:CZ	2:R:139:ALA:O	2.52	0.62
2:I:12:VAL:HG11	2:I:82:MET:HE3	1.82	0.62
1:L:5:THR:HA	1:L:100:GLN:HE22	1.64	0.62
2:R:115:SER:HB2	3:N:282:VAL:HG12	1.81	0.62
2:I:12:VAL:HG11	2:I:82:MET:CE	2.30	0.62
2:R:12:VAL:HG11	2:R:82:MET:CE	2.30	0.61
1:Q:5:THR:HA	1:Q:100:GLN:HE22	1.64	0.61
1:G:100:GLN:H	1:G:100:GLN:CD	2.02	0.61
3:C:436:TYR:CE2	3:N:434:ASN:CG	2.74	0.61
1:F:202:SER:O	3:C:297:ASN:N	2.33	0.61
3:B:394:THR:HG23	3:B:407:TYR:O	2.01	0.61
3:C:434:ASN:HA	3:N:252:MET:HE1	1.82	0.61
2:M:12:VAL:HG11	2:M:82:MET:CE	2.30	0.61
2:M:113:PRO:O	3:B:282:VAL:N	2.33	0.61
1:G:118:PHE:HB2	2:I:126:LEU:HD22	1.83	0.61
1:Q:118:PHE:HB2	2:R:124:LEU:HD22	1.83	0.61
3:C:435:HIS:CE1	3:N:254:SER:OG	2.53	0.60
1:Q:121:SER:CB	2:R:123:PRO:HD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:MET:CA	3:N:253:ILE:CD1	2.79	0.60
1:G:160:GLN:CD	2:I:165:VAL:CG1	2.70	0.60
3:C:434:ASN:CG	3:N:428:MET:CE	2.70	0.60
3:B:406:LEU:C	3:B:406:LEU:HD12	2.22	0.60
3:N:274:LYS:HE2	3:N:276:ASN:HD21	1.67	0.60
3:N:406:LEU:C	3:N:406:LEU:HD12	2.22	0.60
2:H:150:TRP:C	2:H:151:ASN:N	2.55	0.60
3:J:384:ASN:O	3:J:386:GLN:N	2.31	0.60
3:D:394:THR:HG23	3:D:407:TYR:O	2.01	0.60
1:G:121:SER:CB	2:I:125:PRO:HD2	2.32	0.60
3:C:417:TRP:CH2	3:C:441:LEU:HD22	2.37	0.60
3:N:394:THR:HG23	3:N:407:TYR:O	2.01	0.60
1:L:121:SER:CB	2:M:123:PRO:HD2	2.31	0.60
2:O:157:TRP:C	2:O:162:ASN:N	2.55	0.60
3:C:382:GLU:OE1	3:N:433:HIS:CG	2.56	0.59
3:C:382:GLU:OE1	3:N:433:HIS:NE2	2.35	0.59
3:D:274:LYS:HE2	3:D:276:ASN:HD21	1.67	0.59
3:D:406:LEU:C	3:D:406:LEU:HD12	2.22	0.59
1:Q:160:GLN:CD	2:R:177:VAL:CG1	2.70	0.59
1:L:135:LEU:HD22	2:M:190:VAL:HG21	1.84	0.59
1:L:160:GLN:CD	2:M:177:VAL:CG1	2.70	0.59
2:M:203:GLN:OE1	2:M:205:THR:N	2.36	0.59
3:B:274:LYS:HE2	3:B:276:ASN:HD21	1.67	0.59
1:G:135:LEU:HD22	2:I:177:VAL:HG21	1.84	0.59
2:E:150:TRP:C	2:E:151:ASN:N	2.55	0.59
3:C:417:TRP:HH2	3:C:441:LEU:HD22	1.67	0.59
3:C:433:HIS:ND1	3:C:434:ASN:OD1	2.35	0.59
3:J:433:HIS:ND1	3:J:434:ASN:OD1	2.35	0.59
1:L:46:LEU:HD22	2:H:103:ASP:HA	1.84	0.59
3:C:436:TYR:CE1	3:N:436:TYR:HD1	2.20	0.59
3:D:257:PRO:HB2	3:D:308:VAL:HB	1.85	0.59
2:R:203:GLN:OE1	2:R:205:THR:N	2.36	0.59
3:A:417:TRP:CH2	3:A:441:LEU:HD22	2.37	0.59
3:A:417:TRP:HH2	3:A:441:LEU:HD22	1.68	0.59
3:B:257:PRO:HB2	3:B:308:VAL:HB	1.85	0.59
1:G:176:SER:HB3	2:I:162:PHE:CE1	2.37	0.59
2:I:188:GLN:OE1	2:I:189:THR:N	2.36	0.59
3:C:252:MET:CA	3:N:253:ILE:HG12	2.33	0.59
2:E:139:LYS:HE2	2:E:167:GLN:OE1	2.03	0.59
1:Q:176:SER:HB3	2:R:174:PHE:CE1	2.37	0.59
3:J:421:ASN:N	3:J:421:ASN:HD22	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:118:PHE:HB2	2:M:124:LEU:HD22	1.83	0.59
1:L:176:SER:HB3	2:M:174:PHE:CE1	2.37	0.59
3:B:266:VAL:CB	3:B:300:TYR:HB2	2.28	0.59
1:G:46:LEU:HD22	2:E:103:ASP:HA	1.84	0.59
1:F:202:SER:O	3:C:297:ASN:O	2.17	0.59
3:J:417:TRP:CH2	3:J:441:LEU:HD22	2.37	0.59
3:J:417:TRP:HH2	3:J:441:LEU:HD22	1.67	0.59
1:L:118:PHE:CD1	2:M:124:LEU:HB3	2.38	0.58
3:A:286:ASN:O	3:A:287:ALA:HB2	2.03	0.58
3:C:436:TYR:HD1	3:N:436:TYR:CD1	2.20	0.58
1:Q:132:VAL:CG2	1:Q:179:LEU:HB3	2.34	0.58
1:Q:135:LEU:HD22	2:R:190:VAL:HG21	1.84	0.58
3:N:269:GLU:O	3:N:269:GLU:HG2	2.03	0.58
3:C:421:ASN:N	3:C:421:ASN:HD22	2.00	0.58
1:Q:118:PHE:CD1	2:R:124:LEU:HB3	2.38	0.58
3:N:279:VAL:HG23	3:N:279:VAL:O	2.03	0.58
1:L:160:GLN:CB	2:M:177:VAL:HG11	2.33	0.58
1:G:166:GLN:HG3	1:G:173:TYR:CZ	2.39	0.58
3:D:296:TYR:CE1	3:D:301:ARG:HD3	2.38	0.58
3:N:296:TYR:CE1	3:N:301:ARG:HD3	2.38	0.58
1:L:132:VAL:CG2	1:L:179:LEU:HB3	2.33	0.58
1:Q:46:LEU:HD22	2:O:101:ASP:HA	1.84	0.58
3:N:424:SER:OG	3:N:438:GLN:HG2	2.04	0.58
3:A:384:ASN:O	3:A:386:GLN:N	2.31	0.58
3:A:433:HIS:ND1	3:A:434:ASN:OD1	2.36	0.58
2:O:145:LYS:HE2	2:O:179:GLN:OE1	2.03	0.58
1:P:183:LYS:O	1:P:187:GLU:HG3	2.04	0.58
1:K:154:LEU:N	3:B:330:ALA:HB3	2.19	0.58
3:B:279:VAL:HG23	3:B:279:VAL:O	2.04	0.58
3:D:288:LYS:HE2	3:D:306:LEU:HD11	1.86	0.58
1:L:166:GLN:HG3	1:L:173:TYR:CZ	2.38	0.57
3:B:296:TYR:CE1	3:B:301:ARG:HD3	2.38	0.57
3:D:279:VAL:HG23	3:D:279:VAL:O	2.04	0.57
3:J:415:SER:O	3:J:419:GLN:HG3	2.04	0.57
3:N:257:PRO:HB2	3:N:308:VAL:HB	1.85	0.57
1:G:118:PHE:CD1	2:I:126:LEU:HB3	2.38	0.57
1:G:132:VAL:CG2	1:G:179:LEU:HB3	2.33	0.57
1:G:160:GLN:CB	2:I:165:VAL:HG11	2.33	0.57
3:N:265:ASP:HA	3:N:299:THR:HB	1.86	0.57
1:K:183:LYS:O	1:K:187:GLU:HG3	2.04	0.57
3:B:325:ASN:HD22	3:B:326:LYS:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:5:THR:HA	1:Q:100:GLN:NE2	2.19	0.57
1:Q:166:GLN:HG3	1:Q:173:TYR:CZ	2.39	0.57
3:A:421:ASN:HD22	3:A:421:ASN:N	2.00	0.57
1:F:203:SER:CB	3:C:298:SER:CB	2.66	0.57
3:C:276:ASN:HB2	3:C:322:LYS:HB3	1.86	0.57
3:C:286:ASN:O	3:C:287:ALA:HB2	2.03	0.57
3:J:286:ASN:O	3:J:287:ALA:HB2	2.03	0.57
3:B:269:GLU:O	3:B:269:GLU:HG2	2.03	0.57
3:B:424:SER:OG	3:B:438:GLN:HG2	2.04	0.57
3:D:424:SER:OG	3:D:438:GLN:HG2	2.04	0.57
2:H:12:VAL:HG11	2:H:82:MET:HE3	1.85	0.57
3:D:265:ASP:HA	3:D:299:THR:HB	1.85	0.57
1:Q:160:GLN:CB	2:R:177:VAL:HG11	2.33	0.57
2:H:139:LYS:HE2	2:H:167:GLN:OE1	2.03	0.57
1:G:5:THR:HA	1:G:100:GLN:NE2	2.18	0.57
1:F:183:LYS:O	1:F:187:GLU:HG3	2.04	0.57
1:L:5:THR:HA	1:L:100:GLN:NE2	2.19	0.57
2:I:120:GLY:HA2	2:I:196:HIS:CD2	2.40	0.57
2:R:118:GLY:HA2	2:R:212:HIS:CD2	2.40	0.57
3:C:415:SER:O	3:C:419:GLN:HG3	2.04	0.57
1:K:156:SER:CB	3:B:333:GLU:OE1	2.46	0.56
2:M:162:ASN:OD1	2:M:162:ASN:N	2.38	0.56
3:D:325:ASN:HD22	3:D:326:LYS:H	1.50	0.56
3:N:288:LYS:HE2	3:N:306:LEU:HD11	1.86	0.56
1:K:38:GLN:NE2	2:M:39:ARG:HD2	2.20	0.56
3:A:276:ASN:HB2	3:A:322:LYS:HB3	1.86	0.56
3:B:328:LEU:HG	3:B:330:ALA:O	2.05	0.56
3:B:439:LYS:HE3	3:B:440:SER:O	2.05	0.56
3:C:384:ASN:O	3:C:386:GLN:N	2.31	0.56
2:M:118:GLY:HA2	2:M:212:HIS:CD2	2.40	0.56
2:M:153:THR:HG22	2:M:211:ASN:HB3	1.87	0.56
3:A:415:SER:O	3:A:419:GLN:HG3	2.04	0.56
3:B:311:GLN:H	3:B:311:GLN:CD	2.08	0.56
3:D:269:GLU:HG2	3:D:269:GLU:O	2.03	0.56
3:D:328:LEU:HG	3:D:330:ALA:O	2.05	0.56
2:R:166:LEU:HD21	2:R:191:VAL:HG21	1.86	0.56
3:J:276:ASN:HB2	3:J:322:LYS:HB3	1.86	0.56
3:N:311:GLN:H	3:N:311:GLN:CD	2.08	0.56
3:N:325:ASN:HD22	3:N:326:LYS:H	1.50	0.56
3:N:328:LEU:HG	3:N:330:ALA:O	2.06	0.56
3:B:265:ASP:HA	3:B:299:THR:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:439:LYS:HE3	3:D:440:SER:O	2.05	0.56
1:P:38:GLN:NE2	2:R:39:ARG:HD2	2.20	0.56
1:Q:118:PHE:CB	2:R:124:LEU:HD22	2.36	0.56
3:N:301:ARG:HE	3:N:303:VAL:CG2	2.18	0.56
2:H:206:LYS:CA	2:H:207:VAL:N	2.67	0.56
3:D:311:GLN:H	3:D:311:GLN:CD	2.08	0.56
3:D:325:ASN:ND2	3:D:326:LYS:H	2.03	0.56
3:A:328:LEU:HD12	3:A:329:PRO:HD2	1.88	0.56
3:B:288:LYS:HE2	3:B:306:LEU:HD11	1.86	0.56
2:E:158:GLY:O	2:E:159:VAL:N	2.38	0.56
3:C:320:LYS:HG3	3:C:335:THR:HG22	1.87	0.56
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
2:M:166:LEU:HD21	2:M:191:VAL:HG21	1.87	0.56
3:A:288:LYS:O	3:A:289:THR:O	2.24	0.56
3:A:320:LYS:HG3	3:A:335:THR:HG22	1.87	0.56
3:B:301:ARG:HE	3:B:303:VAL:CG2	2.18	0.56
1:G:118:PHE:CB	2:I:126:LEU:HD22	2.36	0.56
1:F:38:GLN:NE2	2:I:39:ARG:HD2	2.20	0.56
1:F:203:SER:CB	3:C:298:SER:CA	2.84	0.56
2:I:155:LEU:HD21	2:I:178:VAL:HG21	1.87	0.56
3:D:301:ARG:HE	3:D:303:VAL:CG2	2.18	0.56
1:Q:135:LEU:CD2	2:R:190:VAL:HG21	2.36	0.56
3:N:325:ASN:ND2	3:N:326:LYS:H	2.04	0.56
1:G:135:LEU:CD2	2:I:177:VAL:HG21	2.36	0.56
1:P:203:SER:HA	3:J:297:ASN:CB	2.33	0.56
2:R:12:VAL:HG11	2:R:82:MET:HE3	1.87	0.56
1:L:135:LEU:CD2	2:M:190:VAL:HG21	2.36	0.56
2:E:12:VAL:HG11	2:E:82:MET:HE3	1.88	0.56
3:C:288:LYS:O	3:C:289:THR:O	2.24	0.56
3:D:270:ASP:OD2	3:D:327:ALA:HB2	2.06	0.56
2:H:165:VAL:HG11	1:K:160:GLN:CD	2.27	0.55
1:G:6:GLN:N	1:G:100:GLN:HE22	2.02	0.55
3:C:434:ASN:CG	3:N:428:MET:HE3	2.27	0.55
2:R:162:ASN:OD1	2:R:162:ASN:N	2.38	0.55
2:E:188:GLN:HB2	2:E:190:TYR:CZ	2.42	0.55
2:I:147:THR:HG22	2:I:195:ASN:HB3	1.87	0.55
2:O:177:VAL:HG11	1:P:160:GLN:CD	2.27	0.55
2:O:203:GLN:HB2	2:O:206:TYR:CZ	2.42	0.55
2:R:153:THR:HG22	2:R:211:ASN:HB3	1.87	0.55
3:N:439:LYS:HE3	3:N:440:SER:O	2.05	0.55
1:L:118:PHE:CB	2:M:124:LEU:HD22	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:GLN:HB2	2:H:190:TYR:CZ	2.42	0.55
2:E:12:VAL:HG11	2:E:82:MET:HE1	1.89	0.55
2:O:169:GLY:O	2:O:171:VAL:N	2.38	0.55
2:I:151:ASN:OD1	2:I:151:ASN:N	2.38	0.55
1:K:204:PRO:HD3	3:A:297:ASN:HB2	1.88	0.55
3:B:325:ASN:ND2	3:B:326:LYS:H	2.04	0.55
1:F:202:SER:O	3:C:296:TYR:C	2.45	0.55
3:J:320:LYS:HG3	3:J:335:THR:HG22	1.87	0.55
3:B:270:ASP:OD2	3:B:327:ALA:HB2	2.06	0.55
3:C:328:LEU:HD12	3:C:329:PRO:HD2	1.88	0.55
1:P:15:VAL:HG21	1:P:80:PHE:CZ	2.42	0.55
3:N:270:ASP:OD2	3:N:327:ALA:HB2	2.06	0.55
1:K:153:ALA:HB1	3:B:331:PRO:HD2	1.89	0.54
3:A:289:THR:O	3:A:290:LYS:HB2	2.07	0.54
2:E:165:VAL:HG11	1:F:160:GLN:CD	2.27	0.54
1:F:38:GLN:HE22	2:I:39:ARG:HD2	1.72	0.54
2:O:13:LYS:HD3	2:O:148:PHE:CE1	2.42	0.54
3:J:328:LEU:HD12	3:J:329:PRO:HD2	1.88	0.54
2:H:158:GLY:O	2:H:159:VAL:N	2.38	0.54
2:I:180:VAL:HG11	2:I:190:TYR:CE1	2.43	0.54
1:P:38:GLN:HE22	2:R:39:ARG:HD2	1.72	0.54
2:M:193:VAL:HG11	2:M:206:TYR:CE1	2.43	0.54
3:B:275:PHE:HE1	3:B:302:VAL:HG12	1.72	0.54
3:C:414:LYS:HE2	3:C:418:GLN:NE2	2.22	0.54
3:D:238:PRO:CG	3:D:328:LEU:HD13	2.37	0.54
3:D:262:VAL:HG13	3:D:303:VAL:HG22	1.90	0.54
3:J:289:THR:O	3:J:290:LYS:HB2	2.07	0.54
3:J:414:LYS:O	3:J:418:GLN:HG3	2.07	0.54
3:N:238:PRO:CG	3:N:328:LEU:HD13	2.37	0.54
2:H:13:LYS:HD3	2:H:142:PHE:CE1	2.42	0.54
3:A:414:LYS:HE2	3:A:418:GLN:NE2	2.22	0.54
3:A:414:LYS:O	3:A:418:GLN:HG3	2.08	0.54
1:F:15:VAL:HG21	1:F:80:PHE:CZ	2.42	0.54
3:C:253:ILE:CG2	3:N:310:HIS:CD2	2.88	0.54
1:Q:198:HIS:HD2	1:Q:200:GLY:H	1.53	0.54
3:B:238:PRO:CG	3:B:328:LEU:HD13	2.37	0.54
3:B:322:LYS:HE3	3:B:333:GLU:OE2	2.08	0.54
2:E:13:LYS:HD3	2:E:142:PHE:CE1	2.42	0.54
3:C:253:ILE:HD13	3:N:255:ARG:O	2.08	0.54
3:B:240:VAL:O	3:B:334:LYS:HE3	2.08	0.54
3:D:322:LYS:HE3	3:D:333:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:193:VAL:HG11	2:R:206:TYR:CE1	2.43	0.54
3:B:351:LEU:C	3:B:441:LEU:HD11	2.28	0.54
2:E:190:TYR:O	2:E:207:VAL:N	2.41	0.54
2:E:206:LYS:CA	2:E:207:VAL:N	2.67	0.54
3:N:240:VAL:O	3:N:334:LYS:HE3	2.08	0.54
3:N:322:LYS:HE3	3:N:333:GLU:OE2	2.08	0.54
3:B:262:VAL:HG13	3:B:303:VAL:HG22	1.90	0.54
2:O:222:LYS:CA	2:O:225:VAL:N	2.67	0.54
1:P:203:SER:HA	3:J:297:ASN:HB2	1.90	0.54
3:J:414:LYS:HE2	3:J:418:GLN:NE2	2.22	0.54
3:N:351:LEU:C	3:N:441:LEU:HD11	2.28	0.54
3:A:418:GLN:HA	3:A:443:LEU:HD22	1.90	0.54
2:I:117:SER:HB2	3:D:282:VAL:HG11	1.85	0.54
1:K:38:GLN:HE22	2:M:39:ARG:HD2	1.72	0.53
2:R:149:PRO:O	2:R:212:HIS:HE1	1.92	0.53
1:G:6:GLN:H	1:G:100:GLN:NE2	2.03	0.53
3:C:418:GLN:HA	3:C:443:LEU:HD22	1.90	0.53
3:J:418:GLN:HA	3:J:443:LEU:HD22	1.90	0.53
3:C:414:LYS:O	3:C:418:GLN:HG3	2.08	0.53
1:K:15:VAL:HG21	1:K:80:PHE:CZ	2.42	0.53
3:N:275:PHE:HE1	3:N:302:VAL:HG12	1.72	0.53
2:H:190:TYR:O	2:H:207:VAL:N	2.41	0.53
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.91	0.53
3:C:289:THR:O	3:C:290:LYS:HB2	2.07	0.53
3:D:351:LEU:C	3:D:441:LEU:HD11	2.28	0.53
2:O:212:HIS:HD2	2:O:215:SER:OG	1.92	0.53
1:L:93:GLY:O	2:H:97:LYS:HE2	2.09	0.53
2:H:57:ARG:NH1	2:M:72:ASP:OD2	2.37	0.53
3:C:285:HIS:O	3:C:286:ASN:HB2	2.08	0.53
3:D:275:PHE:HE1	3:D:302:VAL:HG12	1.72	0.53
3:D:291:PRO:HB3	3:D:304:SER:CA	2.37	0.53
1:G:93:GLY:O	2:E:97:LYS:HE2	2.09	0.53
2:E:196:HIS:HD2	2:E:199:SER:OG	1.92	0.53
3:D:240:VAL:O	3:D:334:LYS:HE3	2.08	0.53
2:O:206:TYR:O	2:O:225:VAL:N	2.41	0.53
1:L:198:HIS:HD2	1:L:200:GLY:H	1.53	0.53
1:K:202:SER:C	3:A:296:TYR:O	2.42	0.53
2:H:188:GLN:HA	2:H:189:THR:N	2.24	0.53
2:I:143:PRO:O	2:I:196:HIS:HE1	1.91	0.53
3:C:351:LEU:HB2	3:C:366:THR:HB	1.90	0.53
2:O:57:ARG:NH1	2:R:72:ASP:OD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:LEU:C	2:M:174:PHE:CE2	2.82	0.52
2:H:196:HIS:HD2	2:H:199:SER:OG	1.92	0.52
3:A:351:LEU:HB2	3:A:366:THR:HB	1.90	0.52
3:J:285:HIS:O	3:J:286:ASN:HB2	2.09	0.52
1:Q:116:PHE:CG	2:R:139:ALA:HB3	2.44	0.52
3:A:393:THR:HG22	3:A:394:THR:O	2.10	0.52
1:F:110:VAL:HB	2:O:100:LEU:CD1	2.23	0.52
1:G:116:PHE:CG	2:I:133:ALA:HB3	2.44	0.52
3:D:312:ASN:ND2	3:D:317:LYS:HD2	2.24	0.52
1:Q:175:LEU:C	2:R:174:PHE:CE2	2.82	0.52
3:N:262:VAL:HG13	3:N:303:VAL:HG22	1.90	0.52
1:F:203:SER:HB3	3:C:298:SER:HA	1.90	0.52
3:J:393:THR:HG22	3:J:394:THR:O	2.10	0.52
3:N:312:ASN:ND2	3:N:317:LYS:HD2	2.24	0.52
1:L:116:PHE:CG	2:M:139:ALA:HB3	2.44	0.52
3:C:393:THR:HG22	3:C:394:THR:O	2.10	0.52
2:O:203:GLN:HA	2:O:205:THR:N	2.24	0.52
3:N:291:PRO:HB3	3:N:304:SER:CA	2.37	0.52
1:L:175:LEU:CA	2:M:174:PHE:HE2	2.23	0.52
3:J:351:LEU:HB2	3:J:366:THR:HB	1.90	0.52
3:N:297:ASN:O	3:N:298:SER:HB3	2.09	0.52
2:M:149:PRO:O	2:M:212:HIS:HE1	1.91	0.52
3:B:297:ASN:O	3:B:298:SER:HB3	2.09	0.52
3:B:312:ASN:ND2	3:B:317:LYS:HD2	2.24	0.52
3:D:297:ASN:O	3:D:298:SER:HB3	2.09	0.52
1:Q:93:GLY:O	2:O:95:LYS:HE2	2.09	0.52
1:L:44:PRO:HG2	2:H:105:TRP:CE3	2.45	0.52
3:C:294:GLN:NE2	2:O:1:GLU:O	2.43	0.52
3:D:378:ALA:HB3	3:D:428:MET:HB2	1.92	0.52
1:Q:121:SER:HB2	2:R:123:PRO:HD2	1.92	0.52
1:P:120:PRO:HD3	1:P:132:VAL:HG22	1.91	0.52
1:L:121:SER:HB2	2:M:123:PRO:HD2	1.92	0.52
3:A:285:HIS:O	3:A:286:ASN:HB2	2.08	0.52
3:A:436:TYR:CD1	3:A:436:TYR:C	2.84	0.52
3:D:249:ASP:O	3:D:257:PRO:HG3	2.10	0.52
3:B:378:ALA:HB3	3:B:428:MET:HB2	1.92	0.51
3:J:436:TYR:CD1	3:J:436:TYR:C	2.84	0.51
3:N:296:TYR:HE1	3:N:301:ARG:HD3	1.74	0.51
1:G:44:PRO:HG2	2:E:105:TRP:CE3	2.45	0.51
1:G:175:LEU:C	2:I:162:PHE:CE2	2.82	0.51
1:Q:175:LEU:CA	2:R:174:PHE:HE2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:196:HIS:CD2	2:I:199:SER:OG	2.64	0.51
3:C:436:TYR:CD1	3:C:436:TYR:C	2.84	0.51
3:D:289:THR:HG22	3:D:290:LYS:N	2.21	0.51
3:D:325:ASN:ND2	3:D:326:LYS:N	2.58	0.51
3:N:325:ASN:ND2	3:N:326:LYS:N	2.59	0.51
2:M:212:HIS:CD2	2:M:215:SER:OG	2.64	0.51
3:N:378:ALA:HB3	3:N:428:MET:HB2	1.92	0.51
3:B:325:ASN:ND2	3:B:326:LYS:N	2.59	0.51
1:G:175:LEU:CA	2:I:162:PHE:HE2	2.23	0.51
3:J:350:THR:HB	3:J:441:LEU:CG	2.40	0.51
3:B:296:TYR:HE1	3:B:301:ARG:HD3	1.74	0.51
3:C:350:THR:HB	3:C:441:LEU:CG	2.40	0.51
1:Q:44:PRO:HG2	2:O:103:TRP:CE3	2.45	0.51
1:G:198:HIS:HD2	1:G:200:GLY:H	1.53	0.51
1:F:120:PRO:HD3	1:F:132:VAL:HG22	1.91	0.51
3:D:332:ILE:CG2	3:D:333:GLU:N	2.74	0.51
1:G:162:SER:OG	2:I:163:PRO:CD	2.59	0.51
3:C:283:GLN:C	3:C:285:HIS:N	2.63	0.51
3:D:266:VAL:CB	3:D:300:TYR:HB2	2.28	0.51
3:N:249:ASP:O	3:N:257:PRO:HG3	2.11	0.51
3:C:443:LEU:HG	3:C:443:LEU:O	2.11	0.51
3:D:278:TYR:N	3:D:278:TYR:CD1	2.79	0.51
3:D:296:TYR:HE1	3:D:301:ARG:HD3	1.74	0.51
2:H:12:VAL:HG11	2:H:82:MET:HE1	1.91	0.51
2:M:144:VAL:HG11	2:M:152:VAL:HG11	1.93	0.51
2:M:203:GLN:O	2:M:205:THR:HA	2.11	0.51
3:A:418:GLN:C	3:A:420:GLY:H	2.15	0.51
2:E:188:GLN:HA	2:E:189:THR:N	2.24	0.51
3:C:429:HIS:O	3:C:435:HIS:HA	2.11	0.51
3:J:418:GLN:C	3:J:420:GLY:H	2.15	0.51
3:J:443:LEU:O	3:J:443:LEU:HG	2.11	0.51
3:N:266:VAL:CB	3:N:300:TYR:HB2	2.28	0.50
1:L:162:SER:OG	2:M:175:PRO:CD	2.59	0.50
3:B:291:PRO:CB	3:B:304:SER:HA	2.37	0.50
3:D:261:CYS:HB2	3:D:277:TRP:CZ2	2.47	0.50
2:R:212:HIS:CD2	2:R:215:SER:OG	2.64	0.50
3:B:261:CYS:HB2	3:B:277:TRP:CZ2	2.47	0.50
3:C:357:GLU:C	3:C:359:THR:H	2.15	0.50
3:N:278:TYR:N	3:N:278:TYR:CD1	2.79	0.50
3:B:291:PRO:HB3	3:B:304:SER:CA	2.37	0.50
3:B:332:ILE:CG2	3:B:333:GLU:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:ILE:HD12	3:N:310:HIS:CD2	2.47	0.50
3:C:360:LYS:O	3:C:414:LYS:HD2	2.11	0.50
3:J:360:LYS:O	3:J:414:LYS:HD2	2.11	0.50
3:N:261:CYS:HB2	3:N:277:TRP:CZ2	2.47	0.50
3:A:429:HIS:O	3:A:435:HIS:HA	2.11	0.50
3:B:249:ASP:O	3:B:257:PRO:HG3	2.11	0.50
2:I:138:VAL:HG11	2:I:146:VAL:HG11	1.93	0.50
3:C:268:HIS:HB3	1:Q:57:GLY:CA	2.39	0.50
3:C:409:LYS:HB2	3:D:407:TYR:OH	2.12	0.50
1:Q:162:SER:OG	2:R:175:PRO:CD	2.59	0.50
3:J:357:GLU:C	3:J:359:THR:H	2.15	0.50
1:K:154:LEU:N	3:B:330:ALA:CB	2.70	0.50
3:B:249:ASP:C	3:B:257:PRO:HG3	2.32	0.50
3:B:432:LEU:CD1	3:B:437:THR:HG22	2.42	0.50
3:D:406:LEU:HD12	3:D:406:LEU:O	2.12	0.50
1:L:124:GLN:NE2	1:L:131:SER:OG	2.40	0.50
1:G:124:GLN:NE2	1:G:131:SER:OG	2.40	0.50
1:Q:6:GLN:N	1:Q:100:GLN:HE22	2.02	0.50
3:A:246:LYS:HB2	3:A:249:ASP:OD2	2.12	0.50
3:A:283:GLN:C	3:A:285:HIS:N	2.62	0.50
3:C:253:ILE:HD11	3:N:255:ARG:H	1.76	0.50
3:C:380:GLU:O	3:C:425:CYS:HA	2.12	0.50
3:C:418:GLN:C	3:C:420:GLY:H	2.15	0.50
3:A:294:GLN:O	3:A:300:TYR:CD1	2.65	0.50
3:A:409:LYS:HB2	3:B:407:TYR:OH	2.12	0.50
3:B:250:THR:HG22	3:B:257:PRO:HB3	1.94	0.50
3:C:253:ILE:HB	3:N:310:HIS:CD2	2.47	0.50
3:C:294:GLN:O	3:C:300:TYR:CD1	2.65	0.50
3:D:250:THR:HG22	3:D:257:PRO:HB3	1.94	0.50
3:J:380:GLU:O	3:J:425:CYS:HA	2.12	0.50
3:J:429:HIS:O	3:J:435:HIS:HA	2.11	0.50
1:G:121:SER:HB2	2:I:125:PRO:HD2	1.92	0.49
2:R:203:GLN:O	2:R:205:THR:HA	2.11	0.49
3:N:250:THR:HG22	3:N:257:PRO:HB3	1.94	0.49
3:N:406:LEU:HD12	3:N:406:LEU:O	2.12	0.49
3:D:292:ARG:O	3:D:293:GLU:HB3	2.12	0.49
3:D:432:LEU:CD1	3:D:437:THR:HG22	2.42	0.49
3:J:283:GLN:C	3:J:285:HIS:N	2.62	0.49
3:N:292:ARG:O	3:N:293:GLU:HB3	2.12	0.49
3:A:357:GLU:C	3:A:359:THR:H	2.15	0.49
3:A:380:GLU:O	3:A:425:CYS:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:278:TYR:CD1	3:B:278:TYR:N	2.79	0.49
3:B:289:THR:HG22	3:B:290:LYS:N	2.21	0.49
2:I:188:GLN:O	2:I:189:THR:HA	2.11	0.49
2:R:144:VAL:HG11	2:R:152:VAL:HG11	1.93	0.49
3:N:249:ASP:C	3:N:257:PRO:HG3	2.32	0.49
3:N:432:LEU:CD1	3:N:437:THR:HG22	2.42	0.49
3:A:350:THR:HB	3:A:441:LEU:CG	2.40	0.49
3:A:360:LYS:O	3:A:414:LYS:HD2	2.11	0.49
3:B:292:ARG:O	3:B:293:GLU:HB3	2.12	0.49
3:D:369:VAL:O	3:D:405:PHE:HA	2.12	0.49
2:O:203:GLN:O	2:O:205:THR:HA	2.13	0.49
3:J:246:LYS:HB2	3:J:249:ASP:OD2	2.12	0.49
3:J:294:GLN:O	3:J:300:TYR:CD1	2.65	0.49
3:N:332:ILE:CG2	3:N:333:GLU:N	2.74	0.49
3:A:277:TRP:O	3:A:283:GLN:HB3	2.13	0.49
3:A:443:LEU:HG	3:A:443:LEU:O	2.11	0.49
3:C:246:LYS:HB2	3:C:249:ASP:OD2	2.12	0.49
3:C:266:VAL:O	3:C:300:TYR:HB2	2.13	0.49
3:D:249:ASP:C	3:D:257:PRO:HG3	2.32	0.49
3:B:369:VAL:O	3:B:405:PHE:HA	2.12	0.49
3:J:409:LYS:HB2	3:N:407:TYR:OH	2.12	0.49
3:J:277:TRP:O	3:J:283:GLN:HB3	2.13	0.49
3:C:252:MET:HA	3:N:253:ILE:HG12	1.94	0.49
3:D:398:LEU:HD11	3:D:402:GLY:HA2	1.95	0.49
1:P:20:THR:CG2	1:P:72:THR:CG2	2.86	0.49
3:A:248:LYS:O	3:A:255:ARG:HD3	2.13	0.49
3:A:266:VAL:O	3:A:300:TYR:HB2	2.13	0.49
3:B:406:LEU:HD12	3:B:406:LEU:O	2.12	0.49
3:C:277:TRP:O	3:C:283:GLN:HB3	2.13	0.49
3:J:266:VAL:O	3:J:300:TYR:HB2	2.13	0.49
3:J:278:TYR:HB2	3:J:320:LYS:HB3	1.95	0.49
3:N:244:PRO:HB3	3:N:336:ILE:HD11	1.95	0.49
3:A:278:TYR:HB2	3:A:320:LYS:HB3	1.95	0.49
3:A:384:ASN:OD1	3:A:385:GLY:N	2.41	0.48
2:E:188:GLN:O	2:E:189:THR:HA	2.12	0.48
1:Q:124:GLN:NE2	1:Q:131:SER:OG	2.40	0.48
3:N:369:VAL:O	3:N:405:PHE:HA	2.12	0.48
3:C:278:TYR:HB2	3:C:320:LYS:HB3	1.94	0.48
3:C:283:GLN:CD	3:C:287:ALA:HB2	2.34	0.48
2:O:11:LEU:HD11	2:R:178:LEU:HD11	1.95	0.48
3:N:398:LEU:HD11	3:N:402:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:108:ARG:HD2	1:K:140:TYR:CB	2.43	0.48
1:Q:176:SER:N	2:R:174:PHE:CE2	2.81	0.48
1:P:108:ARG:HD2	1:P:140:TYR:CB	2.43	0.48
3:N:259:VAL:HG23	3:N:308:VAL:CG2	2.43	0.48
3:A:282:VAL:O	3:A:283:GLN:CB	2.52	0.48
3:A:283:GLN:CD	3:A:287:ALA:HB2	2.34	0.48
2:E:57:ARG:HH22	2:I:72:ASP:CG	2.16	0.48
3:A:358:MET:O	3:A:414:LYS:HE3	2.14	0.48
3:B:350:THR:HB	3:B:441:LEU:HG	1.95	0.48
1:F:108:ARG:HD2	1:F:140:TYR:CB	2.43	0.48
3:C:248:LYS:O	3:C:255:ARG:HD3	2.13	0.48
3:C:346:PRO:CB	3:C:372:PHE:HB3	2.39	0.48
3:J:248:LYS:O	3:J:255:ARG:HD3	2.13	0.48
3:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	0.48
3:J:346:PRO:CB	3:J:372:PHE:HB3	2.39	0.48
3:B:259:VAL:HG23	3:B:308:VAL:CG2	2.43	0.48
3:D:259:VAL:HG23	3:D:308:VAL:CG2	2.43	0.48
3:J:358:MET:O	3:J:414:LYS:HE3	2.14	0.48
1:K:156:SER:HB3	3:B:333:GLU:CD	2.22	0.48
1:G:176:SER:N	2:I:162:PHE:CE2	2.81	0.48
2:E:57:ARG:NH1	2:I:72:ASP:OD2	2.37	0.48
3:D:350:THR:HB	3:D:441:LEU:HG	1.95	0.48
2:R:118:GLY:HA2	2:R:212:HIS:HD2	1.77	0.48
1:L:176:SER:N	2:M:174:PHE:CE2	2.81	0.48
3:D:291:PRO:CB	3:D:304:SER:HA	2.37	0.48
2:O:57:ARG:HH22	2:R:72:ASP:CG	2.16	0.48
2:H:57:ARG:HH22	2:M:72:ASP:CG	2.16	0.48
3:B:312:ASN:HB3	3:B:319:TYR:OH	2.14	0.48
3:C:252:MET:CA	3:N:253:ILE:HD13	2.36	0.48
3:D:244:PRO:HB3	3:D:336:ILE:HD11	1.95	0.48
3:B:398:LEU:HD11	3:B:402:GLY:HA2	1.95	0.48
2:E:11:LEU:HD11	2:I:166:LEU:HD11	1.95	0.47
1:Q:6:GLN:H	1:Q:100:GLN:NE2	2.03	0.47
3:N:289:THR:HG22	3:N:290:LYS:N	2.21	0.47
1:L:6:GLN:N	1:L:100:GLN:HE22	2.02	0.47
3:B:368:LEU:HD12	3:B:369:VAL:H	1.79	0.47
1:G:162:SER:OG	2:I:163:PRO:O	2.28	0.47
3:C:253:ILE:CG2	3:N:310:HIS:CG	2.96	0.47
2:H:188:GLN:O	2:H:189:THR:HA	2.13	0.47
2:M:2:VAL:HG13	2:M:27:PHE:CD2	2.49	0.47
3:A:292:ARG:O	3:A:293:GLU:CB	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:388:GLU:OE2	3:A:416:ARG:NH2	2.42	0.47
3:D:368:LEU:HD12	3:D:369:VAL:H	1.79	0.47
3:J:414:LYS:HG2	3:J:418:GLN:NE2	2.29	0.47
3:N:350:THR:HB	3:N:441:LEU:HG	1.95	0.47
3:B:244:PRO:HB3	3:B:336:ILE:HD11	1.95	0.47
2:I:120:GLY:HA2	2:I:196:HIS:HD2	1.77	0.47
3:C:358:MET:O	3:C:414:LYS:HE3	2.14	0.47
3:D:432:LEU:HD22	3:D:437:THR:HB	1.97	0.47
2:H:11:LEU:HD11	2:M:178:LEU:HD11	1.95	0.47
2:M:212:HIS:HD2	2:M:215:SER:OG	1.97	0.47
3:J:384:ASN:OD1	3:J:385:GLY:N	2.41	0.47
2:M:32:HIS:HD2	2:M:95:LYS:O	1.97	0.47
2:M:118:GLY:HA2	2:M:212:HIS:HD2	1.77	0.47
3:A:414:LYS:HG2	3:A:418:GLN:NE2	2.29	0.47
3:A:438:GLN:O	3:A:439:LYS:HD3	2.15	0.47
1:G:176:SER:HB3	2:I:162:PHE:CD1	2.50	0.47
3:C:289:THR:CG2	3:C:290:LYS:N	2.78	0.47
3:C:384:ASN:OD1	3:C:385:GLY:N	2.41	0.47
3:C:414:LYS:HG2	3:C:418:GLN:NE2	2.29	0.47
3:D:275:PHE:HZ	3:D:302:VAL:O	1.98	0.47
3:D:312:ASN:HB3	3:D:319:TYR:OH	2.14	0.47
2:R:2:VAL:HG13	2:R:27:PHE:CD2	2.49	0.47
3:J:371:GLY:HA2	3:J:403:SER:OG	2.14	0.47
3:J:438:GLN:O	3:J:439:LYS:HD3	2.15	0.47
3:N:368:LEU:HD12	3:N:369:VAL:H	1.80	0.47
3:N:432:LEU:HD22	3:N:437:THR:HB	1.97	0.47
3:A:388:GLU:OE1	3:A:388:GLU:HA	2.14	0.47
3:B:432:LEU:HD22	3:B:437:THR:HB	1.97	0.47
2:I:196:HIS:HD2	2:I:199:SER:OG	1.97	0.47
2:R:208:CYS:SG	2:R:221:LYS:HB3	2.55	0.47
3:J:388:GLU:HA	3:J:388:GLU:OE1	2.14	0.47
3:N:312:ASN:HB3	3:N:319:TYR:OH	2.14	0.47
3:B:278:TYR:CE2	3:B:284:VAL:HG22	2.50	0.47
2:I:2:VAL:HG13	2:I:27:PHE:CD2	2.49	0.47
3:C:371:GLY:HA2	3:C:403:SER:OG	2.14	0.47
3:N:275:PHE:HZ	3:N:302:VAL:O	1.97	0.47
3:B:261:CYS:HB2	3:B:277:TRP:CH2	2.50	0.47
3:D:278:TYR:CE2	3:D:284:VAL:HG22	2.50	0.47
1:K:154:LEU:H	3:B:330:ALA:HB3	1.77	0.46
2:I:32:HIS:HD2	2:I:97:LYS:O	1.97	0.46
3:C:288:LYS:H	3:C:288:LYS:CD	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:388:GLU:HA	3:C:388:GLU:OE1	2.14	0.46
3:C:438:GLN:O	3:C:439:LYS:HD3	2.15	0.46
2:R:212:HIS:HD2	2:R:215:SER:OG	1.97	0.46
3:N:261:CYS:HB2	3:N:277:TRP:CH2	2.50	0.46
3:N:291:PRO:CB	3:N:304:SER:HA	2.37	0.46
1:L:6:GLN:H	1:L:100:GLN:NE2	2.03	0.46
3:C:286:ASN:O	3:C:287:ALA:CB	2.63	0.46
1:P:153:ALA:CB	3:N:330:ALA:HB1	2.45	0.46
1:P:202:SER:HB2	3:J:296:TYR:O	2.14	0.46
3:J:289:THR:CG2	3:J:290:LYS:N	2.78	0.46
3:A:371:GLY:HA2	3:A:403:SER:OG	2.15	0.46
3:B:300:TYR:O	3:B:301:ARG:HB2	2.16	0.46
2:E:17:SER:OG	2:E:83:HIS:HD2	1.99	0.46
3:B:308:VAL:HG11	3:B:313:TRP:HB2	1.97	0.46
3:B:432:LEU:HD11	3:B:437:THR:HG22	1.98	0.46
2:E:18:LEU:N	2:E:82:MET:HE2	2.30	0.46
3:N:322:LYS:HG3	3:N:333:GLU:HG2	1.97	0.46
3:A:288:LYS:H	3:A:288:LYS:CD	2.27	0.46
3:A:289:THR:CG2	3:A:290:LYS:N	2.78	0.46
3:D:361:ASN:ND2	3:D:362:GLN:HG3	2.31	0.46
1:Q:176:SER:HB3	2:R:174:PHE:CD1	2.50	0.46
3:J:286:ASN:O	3:J:287:ALA:CB	2.63	0.46
2:M:208:CYS:SG	2:M:221:LYS:HB3	2.55	0.46
3:B:275:PHE:HZ	3:B:302:VAL:O	1.98	0.46
3:B:311:GLN:NE2	3:B:311:GLN:N	2.53	0.46
3:B:344:ARG:O	3:B:372:PHE:HA	2.16	0.46
3:D:311:GLN:NE2	3:D:311:GLN:N	2.53	0.46
3:N:279:VAL:O	3:N:282:VAL:HG22	2.15	0.46
3:N:300:TYR:O	3:N:301:ARG:HB2	2.16	0.46
2:H:17:SER:OG	2:H:83:HIS:HD2	1.99	0.46
2:O:19:ILE:HD13	2:R:19:ILE:O	2.16	0.46
2:H:163:PRO:HD2	1:K:162:SER:OG	2.16	0.46
3:D:261:CYS:HB2	3:D:277:TRP:CH2	2.50	0.46
2:R:32:HIS:HD2	2:R:95:LYS:O	1.97	0.46
2:R:97:SER:C	2:R:99:ARG:H	2.19	0.46
3:N:344:ARG:O	3:N:372:PHE:HA	2.16	0.46
3:A:346:PRO:CB	3:A:372:PHE:HB3	2.39	0.46
2:I:99:SER:C	2:I:101:ARG:H	2.19	0.46
3:D:242:LEU:HD13	3:D:336:ILE:HG22	1.98	0.46
3:D:279:VAL:O	3:D:282:VAL:HG22	2.15	0.46
2:O:12:VAL:HG11	2:O:82:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:406:LEU:C	3:N:406:LEU:CD1	2.85	0.46
3:A:265:ASP:HA	3:A:299:THR:HB	1.98	0.46
3:A:296:TYR:HB3	3:A:297:ASN:H	1.56	0.46
3:B:279:VAL:O	3:B:282:VAL:HG22	2.15	0.46
3:D:300:TYR:O	3:D:301:ARG:HB2	2.16	0.46
3:D:322:LYS:HG3	3:D:333:GLU:HG2	1.97	0.46
1:P:153:ALA:CB	3:N:330:ALA:CB	2.94	0.46
3:N:278:TYR:CE2	3:N:284:VAL:HG22	2.50	0.46
1:L:121:SER:CB	1:L:121:SER:HG	2.17	0.45
3:A:266:VAL:HB	3:A:300:TYR:HB2	1.98	0.45
3:B:242:LEU:HD13	3:B:336:ILE:HG22	1.98	0.45
3:B:279:VAL:O	3:B:280:ASP:HB2	2.17	0.45
3:B:322:LYS:HG3	3:B:333:GLU:HG2	1.97	0.45
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	0.45
3:N:279:VAL:O	3:N:280:ASP:HB2	2.16	0.45
3:N:361:ASN:ND2	3:N:362:GLN:HG3	2.31	0.45
3:N:439:LYS:HA	3:N:439:LYS:HD2	1.81	0.45
1:L:176:SER:HB3	2:M:174:PHE:CD1	2.50	0.45
2:H:11:LEU:HD21	2:M:179:GLN:O	2.16	0.45
2:M:97:SER:C	2:M:99:ARG:H	2.19	0.45
3:A:421:ASN:N	3:A:421:ASN:ND2	2.64	0.45
1:F:141:PRO:O	1:F:198:HIS:HE1	2.00	0.45
3:C:253:ILE:CB	3:N:310:HIS:CD2	3.00	0.45
3:D:406:LEU:C	3:D:406:LEU:CD1	2.84	0.45
1:Q:92:ALA:O	2:O:95:LYS:CE	2.64	0.45
3:J:296:TYR:HB3	3:J:297:ASN:H	1.56	0.45
3:N:345:GLU:HA	3:N:431:ALA:HB3	1.98	0.45
1:G:160:GLN:NE2	2:I:165:VAL:HG12	2.31	0.45
3:D:344:ARG:O	3:D:372:PHE:HA	2.16	0.45
1:Q:121:SER:CB	1:Q:121:SER:HG	2.17	0.45
1:K:141:PRO:O	1:K:198:HIS:HE1	2.00	0.45
3:A:286:ASN:O	3:A:287:ALA:CB	2.63	0.45
1:G:118:PHE:CG	2:I:126:LEU:HB3	2.52	0.45
2:I:192:CYS:SG	2:I:205:LYS:HB3	2.55	0.45
3:C:374:PRO:O	3:C:429:HIS:HE1	2.00	0.45
3:D:308:VAL:HG11	3:D:313:TRP:HB2	1.97	0.45
3:D:326:LYS:C	3:D:328:LEU:H	2.20	0.45
3:N:308:VAL:HG11	3:N:313:TRP:HB2	1.97	0.45
3:N:432:LEU:HD11	3:N:437:THR:HG22	1.98	0.45
3:C:265:ASP:HA	3:C:299:THR:HB	1.98	0.45
3:C:292:ARG:O	3:C:293:GLU:CB	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:175:PRO:HD2	1:P:162:SER:OG	2.16	0.45
2:M:18:LEU:HB2	2:M:82:MET:HE1	1.99	0.45
3:B:361:ASN:ND2	3:B:362:GLN:HG3	2.31	0.45
1:G:92:ALA:O	2:E:97:LYS:CE	2.64	0.45
3:C:278:TYR:CD1	3:C:278:TYR:N	2.85	0.45
3:D:269:GLU:C	3:D:271:PRO:HD3	2.36	0.45
3:D:345:GLU:HA	3:D:431:ALA:HB3	1.99	0.45
3:J:374:PRO:O	3:J:429:HIS:HE1	2.00	0.45
3:N:238:PRO:CB	3:N:328:LEU:HD13	2.47	0.45
3:B:323:VAL:HG12	3:B:324:SER:N	2.32	0.45
3:D:238:PRO:CB	3:D:328:LEU:HD13	2.47	0.45
3:J:278:TYR:CD1	3:J:278:TYR:N	2.85	0.45
2:M:200:THR:HB	2:M:203:GLN:N	2.32	0.45
3:B:300:TYR:O	3:B:301:ARG:CB	2.64	0.45
3:B:406:LEU:C	3:B:406:LEU:CD1	2.84	0.45
3:D:432:LEU:HD11	3:D:437:THR:HG22	1.98	0.45
1:Q:118:PHE:CG	2:R:124:LEU:HB3	2.52	0.45
1:L:92:ALA:O	2:H:97:LYS:CE	2.64	0.45
2:H:165:VAL:CG1	1:K:160:GLN:CD	2.86	0.45
3:A:244:PRO:HB3	3:A:336:ILE:HD13	1.99	0.45
3:B:238:PRO:CB	3:B:328:LEU:HD13	2.47	0.45
3:B:269:GLU:C	3:B:271:PRO:HD3	2.36	0.45
3:B:301:ARG:HG2	3:B:303:VAL:HG23	1.99	0.45
3:C:244:PRO:HB3	3:C:336:ILE:HD13	1.99	0.45
3:D:279:VAL:O	3:D:280:ASP:HB2	2.17	0.45
3:D:300:TYR:O	3:D:301:ARG:CB	2.65	0.45
3:D:323:VAL:HG12	3:D:324:SER:N	2.32	0.45
1:Q:116:PHE:CG	2:R:139:ALA:CB	3.00	0.45
3:B:265:ASP:HA	3:B:299:THR:CB	2.47	0.45
2:E:19:ILE:HD13	2:I:19:ILE:O	2.16	0.45
3:D:290:LYS:HE3	3:D:292:ARG:HH12	1.82	0.45
3:D:301:ARG:HG2	3:D:303:VAL:HG23	1.99	0.45
1:P:204:PRO:HD3	3:J:297:ASN:HB2	1.99	0.45
3:J:292:ARG:O	3:J:293:GLU:CB	2.58	0.45
3:J:388:GLU:OE2	3:J:416:ARG:NH2	2.42	0.45
3:J:421:ASN:N	3:J:421:ASN:ND2	2.64	0.45
2:E:163:PRO:HD2	1:F:162:SER:OG	2.16	0.44
3:C:347:GLN:NE2	3:C:349:TYR:OH	2.50	0.44
3:J:265:ASP:HA	3:J:299:THR:HB	1.98	0.44
3:J:266:VAL:HB	3:J:300:TYR:HB2	1.98	0.44
3:N:300:TYR:O	3:N:301:ARG:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:326:LYS:C	3:N:328:LEU:H	2.20	0.44
3:B:239:SER:HB3	3:B:264:VAL:CG2	2.48	0.44
1:F:112:ALA:HB3	2:O:99:ARG:HB3	0.48	0.44
3:D:296:TYR:HB3	3:D:297:ASN:H	1.34	0.44
2:O:11:LEU:HD21	2:R:179:GLN:O	2.17	0.44
1:P:141:PRO:O	1:P:198:HIS:HE1	2.00	0.44
1:P:153:ALA:CA	3:N:330:ALA:HB2	2.45	0.44
2:R:115:SER:H	3:N:282:VAL:HG12	1.82	0.44
2:H:19:ILE:HD13	2:M:19:ILE:O	2.16	0.44
3:A:291:PRO:O	3:A:292:ARG:HD2	2.17	0.44
3:B:326:LYS:C	3:B:328:LEU:H	2.20	0.44
1:G:116:PHE:CG	2:I:133:ALA:CB	3.00	0.44
3:C:296:TYR:HB3	3:C:297:ASN:H	1.56	0.44
2:O:177:VAL:CG1	1:P:160:GLN:CD	2.86	0.44
3:N:265:ASP:HA	3:N:299:THR:CB	2.47	0.44
3:N:290:LYS:HE3	3:N:292:ARG:HH12	1.82	0.44
3:N:311:GLN:NE2	3:N:311:GLN:N	2.53	0.44
1:L:118:PHE:CG	2:M:124:LEU:HB3	2.52	0.44
2:H:18:LEU:N	2:H:82:MET:HE2	2.32	0.44
3:B:258:GLU:HA	3:B:308:VAL:HG23	1.99	0.44
2:E:11:LEU:HD21	2:I:167:GLN:O	2.16	0.44
3:C:266:VAL:HB	3:C:300:TYR:HB2	1.98	0.44
2:R:200:THR:HB	2:R:203:GLN:N	2.32	0.44
3:N:242:LEU:HD13	3:N:336:ILE:HG22	1.97	0.44
3:A:278:TYR:CD1	3:A:278:TYR:N	2.85	0.44
3:B:296:TYR:HB3	3:B:297:ASN:H	1.34	0.44
3:C:309:LEU:O	3:C:312:ASN:N	2.51	0.44
3:C:318:GLU:OE1	3:C:340:LYS:NZ	2.45	0.44
3:D:239:SER:HB3	3:D:264:VAL:CG2	2.47	0.44
3:D:258:GLU:HA	3:D:308:VAL:HG23	1.99	0.44
3:J:288:LYS:H	3:J:288:LYS:CD	2.27	0.44
3:J:347:GLN:NE2	3:J:349:TYR:OH	2.50	0.44
3:N:239:SER:HB3	3:N:264:VAL:CG2	2.47	0.44
3:D:265:ASP:HA	3:D:299:THR:CB	2.47	0.44
3:B:345:GLU:HA	3:B:431:ALA:HB3	1.98	0.44
2:I:18:LEU:HB2	2:I:82:MET:HE1	1.99	0.44
3:D:439:LYS:HA	3:D:439:LYS:HD2	1.82	0.44
1:Q:38:GLN:NE2	2:O:91:TYR:OH	2.48	0.44
2:R:206:TYR:O	2:R:225:VAL:N	2.51	0.44
3:N:323:VAL:HG12	3:N:324:SER:N	2.32	0.44
1:K:153:ALA:HB2	3:B:329:PRO:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:VAL:CG1	1:F:160:GLN:CD	2.86	0.44
2:I:187:THR:HB	2:I:188:GLN:N	2.32	0.44
2:I:190:TYR:O	2:I:207:VAL:N	2.51	0.44
3:C:436:TYR:CD2	3:N:434:ASN:OD1	2.71	0.44
3:N:258:GLU:HA	3:N:308:VAL:HG23	1.99	0.44
3:C:291:PRO:O	3:C:292:ARG:HD2	2.17	0.44
3:C:421:ASN:N	3:C:421:ASN:ND2	2.64	0.44
2:M:115:SER:HB2	3:B:282:VAL:HG11	1.58	0.43
3:A:278:TYR:HA	3:A:282:VAL:O	2.18	0.43
3:A:287:ALA:O	3:A:288:LYS:C	2.56	0.43
3:D:363:VAL:HG22	3:D:412:VAL:O	2.18	0.43
3:J:244:PRO:HB3	3:J:336:ILE:HD13	1.99	0.43
1:L:38:GLN:NE2	2:H:93:TYR:OH	2.48	0.43
1:L:116:PHE:CG	2:M:139:ALA:CB	3.00	0.43
3:A:374:PRO:O	3:A:429:HIS:HE1	2.00	0.43
3:A:348:VAL:O	3:A:439:LYS:HG3	2.19	0.43
2:E:19:ILE:CD1	2:I:19:ILE:O	2.67	0.43
3:C:294:GLN:HG3	2:O:1:GLU:HB2	1.65	0.43
3:C:310:HIS:CG	3:N:253:ILE:HD12	2.33	0.43
3:C:436:TYR:CD2	3:N:434:ASN:CG	2.90	0.43
1:Q:160:GLN:NE2	2:R:177:VAL:HG12	2.31	0.43
3:A:347:GLN:NE2	3:A:349:TYR:OH	2.51	0.43
3:C:278:TYR:HA	3:C:282:VAL:O	2.18	0.43
3:C:293:GLU:OE1	2:O:1:GLU:CG	2.66	0.43
3:C:388:GLU:OE2	3:C:416:ARG:NH2	2.42	0.43
1:P:142:ARG:HD3	1:P:173:TYR:CE2	2.54	0.43
3:J:278:TYR:HA	3:J:282:VAL:O	2.18	0.43
3:N:301:ARG:HG2	3:N:303:VAL:HG23	1.99	0.43
3:N:363:VAL:HG22	3:N:412:VAL:O	2.18	0.43
3:N:414:LYS:O	3:N:418:GLN:HG3	2.19	0.43
3:B:266:VAL:HB	3:B:300:TYR:CD2	2.54	0.43
3:B:386:GLN:HA	3:B:387:PRO:HD3	1.76	0.43
1:F:113:PRO:O	2:O:99:ARG:HD2	2.17	0.43
3:N:296:TYR:HB3	3:N:297:ASN:H	1.34	0.43
3:A:264:VAL:O	3:A:265:ASP:HB2	2.18	0.43
3:B:363:VAL:HG22	3:B:412:VAL:O	2.18	0.43
3:C:282:VAL:O	3:C:283:GLN:CB	2.52	0.43
3:C:436:TYR:CE1	3:N:436:TYR:O	2.72	0.43
2:O:11:LEU:HD11	2:R:178:LEU:CD1	2.49	0.43
2:M:206:TYR:O	2:M:225:VAL:N	2.51	0.43
3:C:287:ALA:O	3:C:288:LYS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:338:LYS:NZ	3:D:430:GLU:OE2	2.52	0.43
3:D:414:LYS:O	3:D:418:GLN:HG3	2.18	0.43
2:H:19:ILE:CD1	2:M:19:ILE:O	2.66	0.43
1:K:202:SER:CB	3:A:296:TYR:C	2.66	0.43
3:B:278:TYR:HE2	3:B:284:VAL:HG22	1.83	0.43
3:C:348:VAL:O	3:C:439:LYS:HG3	2.19	0.43
3:N:338:LYS:NZ	3:N:430:GLU:OE2	2.52	0.43
2:H:11:LEU:HD11	2:M:178:LEU:CD1	2.49	0.43
2:M:115:SER:H	3:B:282:VAL:CB	2.30	0.43
3:B:290:LYS:HE3	3:B:292:ARG:HH12	1.82	0.43
3:C:253:ILE:CD1	3:N:310:HIS:CD2	3.02	0.43
3:D:368:LEU:HD12	3:D:369:VAL:N	2.34	0.43
2:I:192:CYS:SG	2:I:192:CYS:O	2.77	0.43
2:O:19:ILE:CD1	2:R:19:ILE:O	2.67	0.43
2:R:222:LYS:HA	2:R:225:VAL:N	2.34	0.43
3:J:291:PRO:O	3:J:292:ARG:HD2	2.17	0.43
3:N:238:PRO:HB2	3:N:328:LEU:HD13	2.01	0.43
3:N:278:TYR:HE2	3:N:284:VAL:HG22	1.83	0.43
1:K:203:SER:HA	3:A:297:ASN:HB2	1.15	0.42
2:M:208:CYS:SG	2:M:208:CYS:O	2.77	0.42
3:C:391:TYR:CD2	3:C:391:TYR:C	2.92	0.42
1:P:161:GLU:HG2	1:P:175:LEU:HD21	2.01	0.42
1:K:15:VAL:HG21	1:K:80:PHE:CE2	2.54	0.42
2:M:222:LYS:HA	2:M:225:VAL:N	2.34	0.42
3:B:368:LEU:HD12	3:B:369:VAL:N	2.34	0.42
1:G:108:ARG:CD	1:G:109:THR:O	2.62	0.42
3:C:328:LEU:HA	3:C:329:PRO:HD3	1.94	0.42
3:J:248:LYS:NZ	3:J:380:GLU:OE2	2.47	0.42
3:D:278:TYR:HE2	3:D:284:VAL:HG22	1.83	0.42
1:Q:108:ARG:HD2	1:Q:140:TYR:CB	2.50	0.42
3:J:287:ALA:O	3:J:288:LYS:C	2.56	0.42
3:N:368:LEU:HD12	3:N:369:VAL:N	2.34	0.42
1:K:38:GLN:OE1	1:K:87:HIS:HE1	2.03	0.42
1:K:156:SER:HB2	3:B:333:GLU:CD	2.18	0.42
3:A:391:TYR:C	3:A:391:TYR:CD2	2.92	0.42
3:B:414:LYS:O	3:B:418:GLN:HG3	2.19	0.42
1:G:38:GLN:NE2	2:E:93:TYR:OH	2.48	0.42
2:E:11:LEU:HD11	2:I:166:LEU:CD1	2.49	0.42
3:C:283:GLN:C	3:C:285:HIS:H	2.23	0.42
3:D:252:MET:SD	3:D:428:MET:HE3	2.59	0.42
3:D:357:GLU:C	3:D:359:THR:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:266:VAL:HB	3:N:300:TYR:CD2	2.54	0.42
3:N:357:GLU:C	3:N:359:THR:H	2.23	0.42
3:B:350:THR:HB	3:B:441:LEU:CD1	2.50	0.42
3:C:264:VAL:O	3:C:265:ASP:HB2	2.18	0.42
1:P:153:ALA:HB1	3:N:330:ALA:HB1	2.02	0.42
2:H:19:ILE:CD1	2:M:8:GLY:HA3	2.49	0.42
1:K:161:GLU:HG2	1:K:175:LEU:HD21	2.01	0.42
3:B:357:GLU:C	3:B:359:THR:H	2.23	0.42
1:G:138:ASN:OD1	2:I:160:HIS:NE2	2.48	0.42
1:F:15:VAL:HG21	1:F:80:PHE:CE2	2.54	0.42
1:F:142:ARG:HD3	1:F:173:TYR:CE2	2.54	0.42
3:C:433:HIS:CE1	3:N:380:GLU:OE1	2.73	0.42
3:D:266:VAL:HB	3:D:300:TYR:CD2	2.54	0.42
2:O:19:ILE:CD1	2:R:8:GLY:HA3	2.49	0.42
1:P:15:VAL:HG21	1:P:80:PHE:CE2	2.54	0.42
2:R:208:CYS:SG	2:R:208:CYS:O	2.77	0.42
3:J:386:GLN:HG3	3:J:387:PRO:HD2	2.02	0.42
1:K:142:ARG:HD3	1:K:173:TYR:CE2	2.54	0.42
2:M:3:GLN:HB2	2:M:25:SER:HB2	2.02	0.42
2:I:206:LYS:HA	2:I:207:VAL:N	2.34	0.42
3:D:291:PRO:O	3:D:292:ARG:HB3	2.19	0.42
2:R:12:VAL:HG11	2:R:82:MET:HE1	1.99	0.42
3:J:264:VAL:O	3:J:265:ASP:HB2	2.18	0.42
3:N:291:PRO:O	3:N:292:ARG:HB3	2.19	0.42
1:L:100:GLN:CD	1:L:100:GLN:N	2.71	0.42
2:M:162:ASN:N	2:M:207:ILE:O	2.53	0.42
3:B:291:PRO:O	3:B:292:ARG:HB3	2.19	0.42
3:B:338:LYS:NZ	3:B:430:GLU:OE2	2.52	0.42
1:G:141:PRO:O	1:G:198:HIS:HE1	2.02	0.42
1:P:38:GLN:OE1	1:P:87:HIS:HE1	2.03	0.42
3:J:391:TYR:CD2	3:J:391:TYR:C	2.93	0.42
1:K:108:ARG:HD2	1:K:140:TYR:CG	2.55	0.42
3:A:328:LEU:HD12	3:A:329:PRO:CD	2.50	0.42
3:A:367:CYS:HB2	3:A:381:TRP:CH2	2.55	0.42
3:B:238:PRO:HB2	3:B:328:LEU:HD13	2.01	0.42
3:C:372:PHE:O	3:C:404:PHE:N	2.44	0.42
3:D:350:THR:HB	3:D:441:LEU:CD1	2.50	0.42
1:Q:141:PRO:O	1:Q:198:HIS:HE1	2.02	0.42
3:A:283:GLN:C	3:A:285:HIS:H	2.23	0.41
1:F:20:THR:CG2	1:F:72:THR:CG2	2.86	0.41
3:A:372:PHE:O	3:A:404:PHE:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:268:HIS:O	3:B:271:PRO:CG	2.68	0.41
2:E:54:SER:HB2	2:I:74:LEU:HD12	2.02	0.41
1:F:161:GLU:HG2	1:F:175:LEU:HD21	2.01	0.41
3:C:384:ASN:CG	3:C:385:GLY:H	2.22	0.41
3:J:348:VAL:O	3:J:439:LYS:HG3	2.19	0.41
3:A:336:ILE:HG12	3:A:337:SER:N	2.35	0.41
3:A:369:VAL:HB	3:A:406:LEU:HD12	2.02	0.41
1:G:100:GLN:CD	1:G:100:GLN:N	2.71	0.41
3:D:238:PRO:HB2	3:D:328:LEU:HD13	2.01	0.41
3:D:300:TYR:HB3	3:D:301:ARG:H	1.37	0.41
1:Q:100:GLN:CD	1:Q:100:GLN:N	2.72	0.41
1:L:141:PRO:O	1:L:198:HIS:HE1	2.02	0.41
1:L:160:GLN:NE2	2:M:177:VAL:HG12	2.31	0.41
2:M:217:THR:HG1	3:B:285:HIS:CD2	2.36	0.41
3:A:342:GLN:HA	3:A:343:PRO:HD3	1.83	0.41
1:F:108:ARG:HD2	1:F:140:TYR:CG	2.55	0.41
2:I:151:ASN:N	2:I:191:ILE:O	2.53	0.41
3:C:434:ASN:HA	3:N:252:MET:HE3	2.00	0.41
3:D:325:ASN:HD22	3:D:326:LYS:N	2.15	0.41
1:P:108:ARG:HD2	1:P:140:TYR:CG	2.55	0.41
3:N:325:ASN:HD22	3:N:326:LYS:N	2.15	0.41
1:L:38:GLN:OE1	1:L:87:HIS:HE1	2.04	0.41
1:L:108:ARG:HD2	1:L:140:TYR:CB	2.50	0.41
3:A:246:LYS:HA	3:A:247:PRO:HD3	1.94	0.41
3:B:325:ASN:HD22	3:B:326:LYS:N	2.15	0.41
2:E:19:ILE:CD1	2:I:8:GLY:HA3	2.49	0.41
3:C:328:LEU:HD12	3:C:329:PRO:CD	2.50	0.41
3:C:367:CYS:HB2	3:C:381:TRP:CH2	2.55	0.41
1:Q:108:ARG:CD	1:Q:109:THR:O	2.62	0.41
3:J:274:LYS:HE2	3:J:324:SER:HB2	2.02	0.41
3:J:309:LEU:O	3:J:312:ASN:N	2.51	0.41
3:J:328:LEU:HD12	3:J:329:PRO:CD	2.50	0.41
3:J:367:CYS:HB2	3:J:381:TRP:CH2	2.55	0.41
3:A:274:LYS:HE2	3:A:324:SER:HB2	2.02	0.41
3:B:276:ASN:HB3	3:B:278:TYR:CE1	2.56	0.41
1:G:38:GLN:OE1	1:G:87:HIS:HE1	2.04	0.41
1:G:108:ARG:HD2	1:G:140:TYR:CB	2.49	0.41
2:O:54:SER:HB2	2:R:74:LEU:HD12	2.02	0.41
1:P:108:ARG:HD2	1:P:140:TYR:HB3	2.03	0.41
2:R:3:GLN:HB2	2:R:25:SER:HB2	2.02	0.41
1:L:143:GLU:CD	1:L:143:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:20:THR:CG2	1:K:72:THR:CG2	2.86	0.41
3:B:273:VAL:HB	3:B:302:VAL:HG21	2.03	0.41
1:G:134:CYS:HB2	1:G:148:TRP:CH2	2.56	0.41
1:G:175:LEU:CA	2:I:162:PHE:CE2	3.03	0.41
3:C:386:GLN:HG3	3:C:387:PRO:HD2	2.02	0.41
1:Q:38:GLN:OE1	1:Q:87:HIS:HE1	2.04	0.41
3:J:283:GLN:C	3:J:285:HIS:H	2.23	0.41
3:J:369:VAL:HB	3:J:406:LEU:HD12	2.02	0.41
2:M:148:PHE:HA	2:M:149:PRO:HA	1.92	0.41
3:B:252:MET:SD	3:B:428:MET:HE3	2.60	0.41
1:G:143:GLU:H	1:G:143:GLU:CD	2.24	0.41
2:I:3:GLN:HB2	2:I:25:SER:HB2	2.02	0.41
3:D:335:THR:O	3:D:336:ILE:HB	2.21	0.41
3:N:268:HIS:O	3:N:271:PRO:CG	2.68	0.41
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.56	0.41
1:L:175:LEU:CA	2:M:174:PHE:CE2	3.03	0.41
1:K:204:PRO:HD2	3:A:298:SER:OG	2.21	0.41
2:M:154:VAL:CA	2:M:156:SER:N	2.79	0.41
3:A:328:LEU:HA	3:A:329:PRO:HD3	1.94	0.41
3:B:367:CYS:HB2	3:B:381:TRP:CZ2	2.56	0.41
1:F:38:GLN:OE1	1:F:87:HIS:HE1	2.03	0.41
1:F:108:ARG:HD2	1:F:140:TYR:HB3	2.03	0.41
3:C:274:LYS:HE2	3:C:324:SER:HB2	2.02	0.41
3:C:286:ASN:HB3	3:C:287:ALA:H	1.63	0.41
3:C:382:GLU:OE1	3:N:433:HIS:CE1	2.74	0.41
3:D:268:HIS:O	3:D:271:PRO:CG	2.68	0.41
1:Q:134:CYS:HB2	1:Q:148:TRP:CH2	2.56	0.41
1:Q:143:GLU:CD	1:Q:143:GLU:H	2.24	0.41
1:Q:175:LEU:CA	2:R:174:PHE:CE2	3.03	0.41
2:R:162:ASN:N	2:R:207:ILE:O	2.53	0.41
3:J:336:ILE:HG12	3:J:337:SER:N	2.35	0.41
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.41
3:N:350:THR:HB	3:N:441:LEU:CD1	2.50	0.41
2:H:54:SER:HB2	2:M:74:LEU:HD12	2.02	0.41
3:A:309:LEU:O	3:A:312:ASN:N	2.51	0.41
3:B:350:THR:HB	3:B:441:LEU:HD12	2.03	0.41
2:I:205:LYS:HA	2:I:205:LYS:HD3	1.97	0.41
1:Q:162:SER:OG	2:R:175:PRO:O	2.28	0.41
2:O:18:LEU:N	2:O:82:MET:HE2	2.36	0.41
2:R:154:VAL:CA	2:R:156:SER:N	2.79	0.41
3:J:386:GLN:HA	3:J:387:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:367:CYS:HB2	3:N:381:TRP:CZ2	2.56	0.41
2:M:187:LEU:HD12	2:M:187:LEU:C	2.41	0.40
3:A:386:GLN:HG3	3:A:387:PRO:HD2	2.02	0.40
2:I:6:GLU:OE1	2:I:106:GLY:HA3	2.22	0.40
3:C:248:LYS:NZ	3:C:380:GLU:OE2	2.47	0.40
2:R:187:LEU:C	2:R:187:LEU:HD12	2.41	0.40
3:J:342:GLN:HA	3:J:343:PRO:HD3	1.83	0.40
3:N:308:VAL:HG12	3:N:309:LEU:N	2.36	0.40
3:N:310:HIS:O	3:N:314:LEU:HG	2.22	0.40
3:N:350:THR:HB	3:N:441:LEU:CG	2.51	0.40
3:B:350:THR:HB	3:B:441:LEU:CG	2.51	0.40
3:C:336:ILE:HG12	3:C:337:SER:N	2.35	0.40
3:D:270:ASP:N	3:D:271:PRO:CD	2.82	0.40
3:D:273:VAL:HB	3:D:302:VAL:HG21	2.03	0.40
3:D:276:ASN:HB3	3:D:278:TYR:CE1	2.56	0.40
3:D:350:THR:HB	3:D:441:LEU:HD12	2.03	0.40
3:D:350:THR:HB	3:D:441:LEU:CG	2.51	0.40
3:N:276:ASN:HB3	3:N:278:TYR:CE1	2.56	0.40
3:B:274:LYS:HG2	3:B:275:PHE:N	2.37	0.40
2:E:3:GLN:HB2	2:E:25:SER:HB2	2.04	0.40
3:D:308:VAL:HG12	3:D:309:LEU:N	2.36	0.40
3:D:367:CYS:HB2	3:D:381:TRP:CZ2	2.56	0.40
1:Q:176:SER:HB3	2:R:174:PHE:CZ	2.57	0.40
2:R:6:GLU:OE1	2:R:104:GLY:HA3	2.22	0.40
3:J:282:VAL:O	3:J:283:GLN:CB	2.52	0.40
3:A:252:MET:HB2	3:A:255:ARG:CG	2.49	0.40
3:B:335:THR:O	3:B:336:ILE:HB	2.21	0.40
3:B:351:LEU:HB2	3:B:366:THR:HB	2.03	0.40
2:E:206:LYS:O	2:E:207:VAL:HA	2.22	0.40
2:I:174:LEU:C	2:I:174:LEU:HD12	2.41	0.40
3:C:246:LYS:HA	3:C:247:PRO:HD3	1.94	0.40
3:C:310:HIS:CD2	3:N:253:ILE:HD13	2.44	0.40
3:D:245:PRO:HB3	3:D:258:GLU:H	1.87	0.40
1:L:176:SER:HB3	2:M:174:PHE:CZ	2.57	0.40
2:H:165:VAL:HG11	1:K:160:GLN:OE1	2.21	0.40
2:E:165:VAL:HG11	1:F:160:GLN:OE1	2.21	0.40
3:C:369:VAL:HB	3:C:406:LEU:HD12	2.02	0.40
3:D:310:HIS:O	3:D:314:LEU:HG	2.22	0.40
2:O:3:GLN:HB2	2:O:25:SER:HB2	2.04	0.40
3:N:245:PRO:HB3	3:N:258:GLU:H	1.87	0.40

All (155) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:GLU:N	3:J:294:GLN:CB[3_565]	0.39	1.81
2:H:1:GLU:N	3:A:294:GLN:CB[5_555]	0.53	1.67
3:A:253:ILE:N	3:B:253:ILE:CB[6_555]	0.53	1.67
3:A:382:GLU:OE1	3:B:433:HIS:CD2[6_555]	0.60	1.60
3:D:253:ILE:CG2	3:J:253:ILE:CA[3_565]	0.68	1.52
2:H:1:GLU:CG	3:A:294:GLN:N[5_555]	0.70	1.50
3:A:253:ILE:CG1	3:B:253:ILE:C[6_555]	0.72	1.48
3:A:252:MET:C	3:B:253:ILE:CG1[6_555]	0.74	1.46
2:E:1:GLU:CD	3:J:293:GLU:CG[3_565]	0.76	1.44
3:D:253:ILE:CA	3:J:253:ILE:CG1[3_565]	0.77	1.43
2:H:26:ASN:ND2	3:A:294:GLN:NE2[5_555]	0.86	1.34
2:E:1:GLU:CA	3:J:294:GLN:CA[3_565]	0.90	1.30
2:H:1:GLU:CA	3:A:294:GLN:CA[5_555]	0.93	1.27
3:D:252:MET:O	3:J:253:ILE:CD1[3_565]	0.98	1.22
2:H:1:GLU:CA	3:A:294:GLN:CB[5_555]	1.03	1.17
3:A:254:SER:N	3:B:253:ILE:CG2[6_555]	1.07	1.13
2:H:1:GLU:CB	3:A:294:GLN:CA[5_555]	1.11	1.09
2:E:1:GLU:CG	3:J:294:GLN:N[3_565]	1.13	1.07
3:A:253:ILE:CA	3:B:253:ILE:CB[6_555]	1.14	1.06
2:E:1:GLU:OE2	3:J:293:GLU:CG[3_565]	1.14	1.06
2:H:1:GLU:CB	3:A:294:GLN:N[5_555]	1.15	1.05
3:D:253:ILE:CG2	3:J:253:ILE:N[3_565]	1.18	1.02
2:E:1:GLU:OE2	3:J:293:GLU:CB[3_565]	1.20	1.00
2:H:1:GLU:OE1	3:A:293:GLU:CG[5_555]	1.21	0.99
2:E:153:GLY:C	3:D:269:GLU:OE2[1_556]	1.22	0.98
3:A:382:GLU:OE1	3:B:433:HIS:NE2[6_555]	1.24	0.96
3:A:253:ILE:N	3:B:253:ILE:CG1[6_555]	1.25	0.95
2:E:1:GLU:CB	3:J:293:GLU:C[3_565]	1.26	0.94
2:E:26:ASN:CG	3:J:294:GLN:NE2[3_565]	1.26	0.94
3:A:253:ILE:CG1	3:B:253:ILE:O[6_555]	1.27	0.93
2:E:1:GLU:OE1	3:J:293:GLU:CG[3_565]	1.28	0.92
3:A:252:MET:O	3:B:253:ILE:CD1[6_555]	1.31	0.89
2:H:1:GLU:CD	3:A:293:GLU:CG[5_555]	1.32	0.88
2:E:26:ASN:ND2	3:J:294:GLN:NE2[3_565]	1.32	0.88
3:A:252:MET:C	3:B:253:ILE:CD1[6_555]	1.34	0.86
3:A:252:MET:CA	3:B:253:ILE:CG1[6_555]	1.34	0.86
2:E:1:GLU:CB	3:J:293:GLU:O[3_565]	1.34	0.86
3:A:252:MET:C	3:B:253:ILE:CB[6_555]	1.35	0.85
3:D:253:ILE:N	3:J:253:ILE:CG1[3_565]	1.35	0.85
3:A:253:ILE:N	3:B:253:ILE:CA[6_555]	1.36	0.84
2:E:1:GLU:CB	3:J:294:GLN:N[3_565]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:GLU:OE2	3:A:293:GLU:OE1[5_555]	1.38	0.82
2:E:1:GLU:CD	3:J:293:GLU:CB[3_565]	1.40	0.80
2:E:1:GLU:OE2	3:J:293:GLU:CD[3_565]	1.41	0.79
3:A:253:ILE:CB	3:B:253:ILE:CA[6_555]	1.42	0.78
3:A:253:ILE:CD1	3:B:255:ARG:N[6_555]	1.42	0.78
3:D:253:ILE:CB	3:J:253:ILE:CA[3_565]	1.42	0.78
2:H:1:GLU:OE2	3:A:293:GLU:CD[5_555]	1.44	0.76
2:E:1:GLU:N	3:J:294:GLN:CA[3_565]	1.46	0.74
2:E:1:GLU:CA	3:J:294:GLN:CB[3_565]	1.47	0.73
3:A:253:ILE:CA	3:B:253:ILE:CA[6_555]	1.48	0.72
2:E:154:ALA:N	3:D:269:GLU:OE2[1_556]	1.48	0.72
3:D:253:ILE:CG2	3:J:253:ILE:C[3_565]	1.48	0.72
2:E:1:GLU:N	3:J:294:GLN:CG[3_565]	1.50	0.70
2:H:26:ASN:CG	3:A:294:GLN:NE2[5_555]	1.52	0.68
2:H:1:GLU:OE2	3:A:293:GLU:CB[5_555]	1.54	0.66
2:H:1:GLU:OE2	3:A:293:GLU:CG[5_555]	1.55	0.65
2:H:1:GLU:CB	3:A:293:GLU:C[5_555]	1.55	0.65
2:E:1:GLU:CG	3:J:293:GLU:C[3_565]	1.55	0.65
3:D:253:ILE:CB	3:J:253:ILE:N[3_565]	1.55	0.65
3:D:252:MET:SD	3:J:434:ASN:ND2[3_565]	1.56	0.64
3:D:253:ILE:CA	3:J:253:ILE:CB[3_565]	1.58	0.62
3:A:253:ILE:CG1	3:B:254:SER:N[6_555]	1.60	0.60
3:A:253:ILE:C	3:B:253:ILE:CG2[6_555]	1.60	0.60
3:A:382:GLU:CD	3:B:433:HIS:CD2[6_555]	1.63	0.57
3:D:310:HIS:CE1	3:J:253:ILE:CG2[3_565]	1.64	0.56
1:P:53:THR:OG1	3:N:389:ASN:OD1[1_556]	1.66	0.54
2:E:153:GLY:O	3:D:269:GLU:OE2[1_556]	1.67	0.53
2:H:1:GLU:O	3:A:294:GLN:CG[5_555]	1.68	0.52
3:A:253:ILE:CB	3:B:253:ILE:C[6_555]	1.68	0.52
2:H:1:GLU:CG	3:A:293:GLU:C[5_555]	1.69	0.51
2:E:1:GLU:CB	3:J:294:GLN:CA[3_565]	1.69	0.51
3:D:253:ILE:C	3:J:253:ILE:CG1[3_565]	1.69	0.51
3:A:382:GLU:OE1	3:B:433:HIS:CG[6_555]	1.70	0.50
2:H:1:GLU:CG	3:A:294:GLN:CA[5_555]	1.71	0.49
3:A:252:MET:CA	3:B:253:ILE:CD1[6_555]	1.72	0.48
2:E:26:ASN:CB	3:J:294:GLN:NE2[3_565]	1.73	0.47
2:E:153:GLY:O	3:D:269:GLU:CD[1_556]	1.73	0.47
2:H:1:GLU:CB	3:A:293:GLU:O[5_555]	1.75	0.45
2:H:1:GLU:CD	3:A:293:GLU:CB[5_555]	1.75	0.45
2:H:1:GLU:CD	3:A:293:GLU:C[5_555]	1.75	0.45
3:A:253:ILE:CB	3:B:253:ILE:O[6_555]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:433:HIS:CD2	3:J:382:GLU:OE1[3_565]	1.76	0.44
3:A:253:ILE:CG1	3:B:253:ILE:CA[6_555]	1.77	0.43
2:H:1:GLU:N	3:A:294:GLN:CG[5_555]	1.80	0.40
2:H:26:ASN:ND2	3:A:294:GLN:CD[5_555]	1.80	0.40
2:H:100:ASP:O	1:K:200:GLY:O[5_555]	1.80	0.40
3:A:252:MET:N	3:B:253:ILE:CD1[6_555]	1.80	0.40
2:E:1:GLU:CD	3:J:293:GLU:CD[3_565]	1.80	0.40
2:H:1:GLU:OE2	3:A:293:GLU:CA[5_555]	1.81	0.39
2:H:1:GLU:OE1	3:A:293:GLU:CB[5_555]	1.81	0.39
3:D:310:HIS:NE2	3:J:253:ILE:CG2[3_565]	1.82	0.38
2:H:1:GLU:CD	3:A:293:GLU:CD[5_555]	1.83	0.37
3:D:252:MET:C	3:J:253:ILE:CD1[3_565]	1.84	0.36
2:E:1:GLU:OE2	3:J:293:GLU:OE1[3_565]	1.85	0.35
3:D:380:GLU:OE1	3:J:433:HIS:NE2[3_565]	1.85	0.35
1:L:107:LYS:CE	1:G:202:SER:OG[5_555]	1.86	0.34
2:H:1:GLU:CD	3:A:293:GLU:CA[5_555]	1.86	0.34
3:D:253:ILE:CG2	3:J:252:MET:C[3_565]	1.86	0.34
2:H:1:GLU:N	3:A:294:GLN:CA[5_555]	1.87	0.33
2:E:1:GLU:O	3:J:294:GLN:CG[3_565]	1.87	0.33
2:E:1:GLU:OE1	3:J:293:GLU:CB[3_565]	1.87	0.33
3:A:252:MET:O	3:B:253:ILE:CG1[6_555]	1.88	0.32
3:A:253:ILE:N	3:B:253:ILE:CG2[6_555]	1.89	0.31
2:E:100:ASP:O	1:P:200:GLY:O[3_565]	1.89	0.31
3:D:252:MET:C	3:J:253:ILE:CG1[3_565]	1.89	0.31
3:A:253:ILE:CD1	3:B:255:ARG:O[6_555]	1.91	0.29
2:H:1:GLU:CD	3:A:294:GLN:N[5_555]	1.92	0.28
2:I:101:ARG:NE	3:D:387:PRO:CD[1_556]	1.92	0.28
2:H:1:GLU:CD	3:A:293:GLU:OE1[5_555]	1.93	0.27
3:D:253:ILE:CG1	3:J:253:ILE:N[3_565]	1.93	0.27
2:E:26:ASN:ND2	3:J:294:GLN:CD[3_565]	1.94	0.26
3:A:252:MET:C	3:B:253:ILE:CG2[6_555]	1.96	0.24
3:A:254:SER:O	3:B:311:GLN:OE1[6_555]	1.96	0.24
2:E:1:GLU:CA	3:J:294:GLN:N[3_565]	1.97	0.23
3:A:253:ILE:C	3:B:253:ILE:CB[6_555]	1.99	0.21
2:E:153:GLY:C	3:D:269:GLU:CD[1_556]	1.99	0.21
2:H:1:GLU:CA	3:A:294:GLN:CG[5_555]	2.01	0.19
3:A:252:MET:O	3:B:253:ILE:CB[6_555]	2.01	0.19
3:A:436:TYR:CE1	3:B:436:TYR:CD1[6_555]	2.01	0.19
3:A:434:ASN:ND2	3:B:252:MET:SD[6_555]	2.02	0.18
3:D:252:MET:O	3:J:253:ILE:CG1[3_565]	2.02	0.18
2:H:1:GLU:C	3:A:294:GLN:CB[5_555]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:GLU:CA	3:A:294:GLN:C[5_555]	2.03	0.17
2:E:1:GLU:CD	3:J:293:GLU:CA[3_565]	2.03	0.17
2:H:1:GLU:C	3:A:294:GLN:CG[5_555]	2.05	0.15
3:A:253:ILE:CG2	3:B:253:ILE:O[6_555]	2.05	0.15
2:I:101:ARG:NE	3:D:387:PRO:CG[1_556]	2.05	0.15
3:D:253:ILE:CA	3:J:253:ILE:CA[3_565]	2.05	0.15
2:H:1:GLU:CB	3:A:294:GLN:CB[5_555]	2.06	0.14
3:A:253:ILE:CA	3:B:253:ILE:CG2[6_555]	2.06	0.14
2:E:1:GLU:OE2	3:J:293:GLU:CA[3_565]	2.06	0.14
3:A:252:MET:O	3:B:253:ILE:CG2[6_555]	2.07	0.13
2:E:1:GLU:CA	3:J:294:GLN:CG[3_565]	2.07	0.13
3:D:253:ILE:CG1	3:J:252:MET:C[3_565]	2.08	0.12
2:O:164:GLY:O	3:N:269:GLU:OE2[1_556]	2.08	0.12
3:D:254:SER:OG	3:J:435:HIS:CE1[3_565]	2.09	0.11
2:E:1:GLU:C	3:J:294:GLN:CG[3_565]	2.12	0.08
3:D:253:ILE:CG2	3:J:252:MET:O[3_565]	2.12	0.08
2:H:26:ASN:CB	3:A:294:GLN:NE2[5_555]	2.14	0.06
2:E:1:GLU:CD	3:J:293:GLU:C[3_565]	2.14	0.06
2:H:101:ARG:CG	1:K:112:ALA:CB[5_555]	2.15	0.05
3:A:253:ILE:CD1	3:B:252:MET:O[6_555]	2.15	0.05
3:A:253:ILE:N	3:B:253:ILE:N[6_555]	2.16	0.04
3:A:253:ILE:CA	3:B:253:ILE:C[6_555]	2.16	0.04
3:C:315:ASP:OD2	2:R:26:ASN:O[1_554]	2.16	0.04
3:D:380:GLU:OE1	3:J:433:HIS:CE1[3_565]	2.16	0.04
3:A:252:MET:N	3:B:253:ILE:CG1[6_555]	2.17	0.03
3:A:382:GLU:OE1	3:B:433:HIS:CE1[6_555]	2.17	0.03
2:E:1:GLU:CG	3:J:294:GLN:CA[3_565]	2.17	0.03
2:E:1:GLU:CG	3:J:293:GLU:CG[3_565]	2.17	0.03
2:E:101:ARG:CG	1:P:201:LEU:CD1[3_565]	2.17	0.03
2:E:1:GLU:N	3:J:294:GLN:N[3_565]	2.19	0.01
2:I:101:ARG:NH2	3:D:387:PRO:CG[1_556]	2.19	0.01
3:D:253:ILE:CG2	3:J:253:ILE:CB[3_565]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	209/213 (98%)	202 (97%)	7 (3%)	0	100	100
1	G	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
1	K	209/213 (98%)	202 (97%)	7 (3%)	0	100	100
1	L	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
1	P	209/213 (98%)	202 (97%)	7 (3%)	0	100	100
1	Q	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
2	E	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
2	H	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
2	I	185/229 (81%)	177 (96%)	8 (4%)	0	100	100
2	M	187/229 (82%)	179 (96%)	8 (4%)	0	100	100
2	O	189/229 (82%)	186 (98%)	3 (2%)	0	100	100
2	R	187/229 (82%)	179 (96%)	8 (4%)	0	100	100
3	A	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	1	15
3	B	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	16
3	C	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	1	15
3	D	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	16
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	1	15
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	16
All	All	3605/3918 (92%)	3348 (93%)	194 (5%)	63 (2%)	7	37

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	283	GLN
3	A	287	ALA
3	A	289	THR
3	A	433	HIS
3	B	298	SER
3	B	301	ARG
3	C	283	GLN
3	C	287	ALA
3	C	289	THR
3	C	433	HIS
3	D	298	SER
3	D	301	ARG

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Mol	Chain	Res	Type
3	J	283	GLN
3	J	287	ALA
3	J	289	THR
3	J	433	HIS
3	N	298	SER
3	N	301	ARG
3	A	267	SER
3	A	298	SER
3	B	271	PRO
3	C	267	SER
3	C	298	SER
3	D	271	PRO
3	J	267	SER
3	J	298	SER
3	N	271	PRO
3	A	293	GLU
3	A	385	GLY
3	B	282	VAL
3	B	291	PRO
3	B	293	GLU
3	C	293	GLU
3	C	385	GLY
3	D	282	VAL
3	D	291	PRO
3	D	293	GLU
3	J	293	GLU
3	J	385	GLY
3	N	282	VAL
3	N	291	PRO
3	N	293	GLU
3	A	286	ASN
3	A	358	MET
3	B	283	GLN
3	B	295	GLN
3	C	286	ASN
3	C	358	MET
3	D	283	GLN
3	D	295	GLN
3	J	286	ASN
3	J	358	MET
3	N	283	GLN
3	N	295	GLN

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Mol	Chain	Res	Type
3	B	336	ILE
3	D	327	ALA
3	D	336	ILE
3	N	327	ALA
3	N	336	ILE
3	B	327	ALA
3	A	290	LYS
3	C	290	LYS
3	J	290	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	182/184 (99%)	174 (96%)	8 (4%)	24	45
1	G	182/184 (99%)	172 (94%)	10 (6%)	18	39
1	K	182/184 (99%)	174 (96%)	8 (4%)	24	45
1	L	182/184 (99%)	172 (94%)	10 (6%)	18	39
1	P	182/184 (99%)	174 (96%)	8 (4%)	24	45
1	Q	182/184 (99%)	172 (94%)	10 (6%)	18	39
2	E	176/192 (92%)	167 (95%)	9 (5%)	20	41
2	H	175/192 (91%)	166 (95%)	9 (5%)	20	41
2	I	172/192 (90%)	157 (91%)	15 (9%)	8	25
2	M	172/192 (90%)	157 (91%)	15 (9%)	8	25
2	O	174/192 (91%)	165 (95%)	9 (5%)	19	40
2	R	172/192 (90%)	156 (91%)	16 (9%)	7	23
3	A	193/196 (98%)	187 (97%)	6 (3%)	35	54
3	B	192/196 (98%)	180 (94%)	12 (6%)	15	36
3	C	193/196 (98%)	187 (97%)	6 (3%)	35	54
3	D	192/196 (98%)	180 (94%)	12 (6%)	15	36
3	J	193/196 (98%)	187 (97%)	6 (3%)	35	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	192/196 (98%)	180 (94%)	12 (6%)	15	36
All	All	3288/3432 (96%)	3107 (94%)	181 (6%)	18	39

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	33	LEU
1	L	39	LYS
1	L	100	GLN
1	L	108	ARG
1	L	123	GLU
1	L	156	SER
1	L	191	VAL
1	L	201	LEU
1	L	203	SER
1	L	208	SER
2	H	112	THR
2	H	139	LYS
2	H	146	VAL
2	H	171	LEU
2	H	187	THR
2	H	193	ASN
2	H	197	LYS
2	H	200	ASN
2	H	205	LYS
1	K	78	LEU
1	K	108	ARG
1	K	126	LYS
1	K	135	LEU
1	K	156	SER
1	K	181	LEU
1	K	185	ASP
1	K	201	LEU
2	M	12	VAL
2	M	97	SER
2	M	99	ARG
2	M	100	LEU
2	M	115	SER
2	M	152	VAL
2	M	153	THR
2	M	156	SER
2	M	162	ASN

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Mol	Chain	Res	Type
2	M	184	LEU
2	M	187	LEU
2	M	200	THR
2	M	205	THR
2	M	209	ASN
2	M	228	LYS
3	A	282	VAL
3	A	292	ARG
3	A	406	LEU
3	A	413	ASP
3	A	436	TYR
3	A	441	LEU
3	B	255	ARG
3	B	260	THR
3	B	278	TYR
3	B	288	LYS
3	B	291	PRO
3	B	296	TYR
3	B	311	GLN
3	B	370	LYS
3	B	394	THR
3	B	399	ASP
3	B	406	LEU
3	B	441	LEU
1	G	33	LEU
1	G	39	LYS
1	G	100	GLN
1	G	108	ARG
1	G	123	GLU
1	G	156	SER
1	G	191	VAL
1	G	201	LEU
1	G	203	SER
1	G	208	SER
2	E	112	THR
2	E	139	LYS
2	E	146	VAL
2	E	171	LEU
2	E	187	THR
2	E	193	ASN
2	E	197	LYS
2	E	200	ASN

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Mol	Chain	Res	Type
2	E	205	LYS
1	F	78	LEU
1	F	108	ARG
1	F	126	LYS
1	F	135	LEU
1	F	156	SER
1	F	181	LEU
1	F	185	ASP
1	F	201	LEU
2	I	12	VAL
2	I	99	SER
2	I	101	ARG
2	I	102	LEU
2	I	117	SER
2	I	146	VAL
2	I	147	THR
2	I	149	SER
2	I	151	ASN
2	I	171	LEU
2	I	174	LEU
2	I	187	THR
2	I	189	THR
2	I	193	ASN
2	I	210	LYS
3	C	282	VAL
3	C	292	ARG
3	C	406	LEU
3	C	413	ASP
3	C	436	TYR
3	C	441	LEU
3	D	255	ARG
3	D	260	THR
3	D	278	TYR
3	D	288	LYS
3	D	291	PRO
3	D	296	TYR
3	D	311	GLN
3	D	370	LYS
3	D	394	THR
3	D	399	ASP
3	D	406	LEU
3	D	441	LEU

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Mol	Chain	Res	Type
1	Q	33	LEU
1	Q	39	LYS
1	Q	100	GLN
1	Q	108	ARG
1	Q	123	GLU
1	Q	156	SER
1	Q	191	VAL
1	Q	201	LEU
1	Q	203	SER
1	Q	208	SER
2	O	110	THR
2	O	145	LYS
2	O	152	VAL
2	O	184	LEU
2	O	200	THR
2	O	209	ASN
2	O	213	LYS
2	O	216	ASN
2	O	221	LYS
1	P	78	LEU
1	P	108	ARG
1	P	126	LYS
1	P	135	LEU
1	P	156	SER
1	P	181	LEU
1	P	185	ASP
1	P	201	LEU
2	R	12	VAL
2	R	97	SER
2	R	99	ARG
2	R	100	LEU
2	R	115	SER
2	R	152	VAL
2	R	153	THR
2	R	156	SER
2	R	162	ASN
2	R	184	LEU
2	R	187	LEU
2	R	200	THR
2	R	205	THR
2	R	209	ASN
2	R	218	LYS

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Mol	Chain	Res	Type
2	R	228	LYS
3	J	282	VAL
3	J	292	ARG
3	J	406	LEU
3	J	413	ASP
3	J	436	TYR
3	J	441	LEU
3	N	255	ARG
3	N	260	THR
3	N	278	TYR
3	N	288	LYS
3	N	291	PRO
3	N	296	TYR
3	N	311	GLN
3	N	370	LYS
3	N	394	THR
3	N	399	ASP
3	N	406	LEU
3	N	441	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	87	HIS
1	L	89	GLN
1	L	100	GLN
1	L	198	HIS
2	H	32	HIS
2	H	81	GLN
2	H	83	HIS
2	H	196	HIS
1	K	87	HIS
1	K	89	GLN
1	K	90	HIS
1	K	198	HIS
1	K	210	ASN
2	M	32	HIS
2	M	81	GLN
2	M	179	GLN
2	M	212	HIS
3	A	272	GLN

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Mol	Chain	Res	Type
3	A	283	GLN
3	A	311	GLN
3	A	325	ASN
3	A	347	GLN
3	A	361	ASN
3	A	390	ASN
3	A	418	GLN
3	A	419	GLN
3	A	421	ASN
3	A	429	HIS
3	B	272	GLN
3	B	276	ASN
3	B	283	GLN
3	B	285	HIS
3	B	311	GLN
3	B	312	ASN
3	B	325	ASN
3	B	342	GLN
3	B	361	ASN
3	B	389	ASN
3	B	390	ASN
3	B	419	GLN
3	B	429	HIS
3	B	434	ASN
3	B	438	GLN
1	G	38	GLN
1	G	87	HIS
1	G	89	GLN
1	G	100	GLN
1	G	198	HIS
2	E	32	HIS
2	E	81	GLN
2	E	83	HIS
2	E	196	HIS
1	F	87	HIS
1	F	89	GLN
1	F	90	HIS
1	F	198	HIS
1	F	210	ASN
2	I	32	HIS
2	I	81	GLN
2	I	83	HIS

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Mol	Chain	Res	Type
2	I	167	GLN
2	I	196	HIS
3	C	272	GLN
3	C	283	GLN
3	C	311	GLN
3	C	325	ASN
3	C	347	GLN
3	C	361	ASN
3	C	390	ASN
3	C	418	GLN
3	C	419	GLN
3	C	421	ASN
3	C	429	HIS
3	C	435	HIS
3	D	272	GLN
3	D	276	ASN
3	D	283	GLN
3	D	286	ASN
3	D	311	GLN
3	D	312	ASN
3	D	325	ASN
3	D	342	GLN
3	D	361	ASN
3	D	389	ASN
3	D	390	ASN
3	D	419	GLN
3	D	429	HIS
3	D	434	ASN
3	D	438	GLN
1	Q	38	GLN
1	Q	87	HIS
1	Q	89	GLN
1	Q	100	GLN
1	Q	198	HIS
2	O	32	HIS
2	O	212	HIS
1	P	87	HIS
1	P	89	GLN
1	P	90	HIS
1	P	198	HIS
1	P	210	ASN
2	R	32	HIS

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Mol	Chain	Res	Type
2	R	179	GLN
2	R	212	HIS
3	J	272	GLN
3	J	283	GLN
3	J	311	GLN
3	J	325	ASN
3	J	347	GLN
3	J	361	ASN
3	J	390	ASN
3	J	418	GLN
3	J	419	GLN
3	J	421	ASN
3	J	429	HIS
3	N	272	GLN
3	N	276	ASN
3	N	283	GLN
3	N	286	ASN
3	N	312	ASN
3	N	325	ASN
3	N	342	GLN
3	N	361	ASN
3	N	389	ASN
3	N	390	ASN
3	N	419	GLN
3	N	429	HIS
3	N	434	ASN
3	N	438	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	13
2	H	12
2	O	11
2	M	10
2	R	10
2	I	10

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	102:LEU	C	103:ASP	N	11.62
1	E	102:LEU	C	103:ASP	N	11.62
1	O	100:LEU	C	101:ASP	N	11.62
1	H	129:SER	C	130:GLY	N	11.41
1	E	129:SER	C	130:GLY	N	11.41
1	O	127:SER	C	136:GLY	N	11.41
1	M	100:LEU	C	101:ASP	N	11.16
1	R	100:LEU	C	101:ASP	N	11.16
1	H	81:GLN	C	82:MET	N	8.84
1	E	81:GLN	C	82:MET	N	8.84
1	O	81:GLN	C	82:MET	N	8.84
1	M	81:GLN	C	82:MET	N	8.78
1	I	81:GLN	C	82:MET	N	8.78
1	R	81:GLN	C	82:MET	N	8.78
1	I	82:MET	C	83:HIS	N	7.02
1	H	82:MET	C	83:HIS	N	6.99
1	E	82:MET	C	83:HIS	N	6.99
1	E	84:LYS	C	85:ARG	N	4.06
1	H	52:SER	C	53:SER	N	3.91
1	E	52:SER	C	53:SER	N	3.91

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	52:SER	C	53:SER	N	3.91
1	M	52:SER	C	53:SER	N	3.88
1	I	52:SER	C	53:SER	N	3.88
1	R	52:SER	C	53:SER	N	3.88
1	M	203:GLN	C	205:THR	N	3.66
1	I	188:GLN	C	189:THR	N	3.66
1	R	203:GLN	C	205:THR	N	3.66
1	H	188:GLN	C	189:THR	N	3.28
1	E	188:GLN	C	189:THR	N	3.28
1	O	203:GLN	C	205:THR	N	3.28
1	M	200:THR	C	203:GLN	N	3.26
1	I	187:THR	C	188:GLN	N	3.26
1	R	200:THR	C	203:GLN	N	3.26
1	M	222:LYS	C	225:VAL	N	3.05
1	I	206:LYS	C	207:VAL	N	3.05
1	R	222:LYS	C	225:VAL	N	3.05
1	H	187:THR	C	188:GLN	N	2.93
1	E	187:THR	C	188:GLN	N	2.93
1	O	200:THR	C	203:GLN	N	2.93
1	M	157:TRP	C	162:ASN	N	2.89
1	I	150:TRP	C	151:ASN	N	2.89
1	R	157:TRP	C	162:ASN	N	2.89
1	H	206:LYS	C	207:VAL	N	2.78
1	E	206:LYS	C	207:VAL	N	2.78
1	O	222:LYS	C	225:VAL	N	2.78
1	H	150:TRP	C	151:ASN	N	2.55
1	E	150:TRP	C	151:ASN	N	2.55
1	O	157:TRP	C	162:ASN	N	2.55
1	M	169:GLY	C	171:VAL	N	2.52
1	I	158:GLY	C	159:VAL	N	2.52
1	R	169:GLY	C	171:VAL	N	2.51
1	H	158:GLY	C	159:VAL	N	2.17
1	E	158:GLY	C	159:VAL	N	2.17
1	O	169:GLY	C	171:VAL	N	2.17
1	M	180:SER	C	182:SER	N	1.98
1	I	168:SER	C	169:SER	N	1.98
1	R	180:SER	C	182:SER	N	1.98
1	H	168:SER	C	169:SER	N	1.87
1	E	168:SER	C	169:SER	N	1.87
1	O	180:SER	C	182:SER	N	1.87
1	M	154:VAL	C	156:SER	N	1.86
1	I	148:VAL	C	149:SER	N	1.86

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	154:VAL	C	156:SER	N	1.86
1	H	148:VAL	C	149:SER	N	1.72
1	E	148:VAL	C	149:SER	N	1.72
1	O	154:VAL	C	156:SER	N	1.72

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.447, which does not match the depositor's R factor of 0.3813. Please interpret the results in this section carefully.

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	F	211/213 (99%)	0.50	4 (1%) 66 54	467, 467, 467, 467	0
1	G	211/213 (99%)	0.72	17 (8%) 19 20	526, 526, 526, 526	0
1	K	211/213 (99%)	0.77	24 (11%) 11 15	487, 487, 487, 487	0
1	L	211/213 (99%)	0.77	21 (9%) 14 16	547, 547, 547, 547	0
1	P	211/213 (99%)	0.56	9 (4%) 40 34	467, 467, 467, 467	0
1	Q	211/213 (99%)	0.64	12 (5%) 30 28	527, 527, 527, 527	0
2	E	210/229 (91%)	0.44	8 (3%) 44 37	406, 406, 406, 406	0
2	H	209/229 (91%)	0.60	12 (5%) 30 28	427, 427, 427, 427	0
2	I	206/229 (89%)	0.59	7 (3%) 48 39	456, 456, 456, 456	0
2	M	206/229 (89%)	0.79	30 (14%) 7 12	477, 477, 477, 477	0
2	O	208/229 (90%)	0.55	11 (5%) 33 29	407, 407, 407, 407	0
2	R	206/229 (89%)	0.72	17 (8%) 19 20	457, 457, 457, 457	0
3	A	207/211 (98%)	0.70	22 (10%) 13 16	516, 516, 516, 516	0
3	B	206/211 (97%)	0.97	24 (11%) 10 15	520, 520, 520, 520	0
3	C	207/211 (98%)	0.68	16 (7%) 21 21	485, 485, 485, 485	0
3	D	206/211 (97%)	0.71	15 (7%) 22 22	489, 489, 489, 489	0
3	J	207/211 (98%)	0.71	12 (5%) 30 28	490, 490, 490, 490	0
3	N	206/211 (97%)	0.75	15 (7%) 22 22	494, 494, 494, 494	0
All	All	3750/3918 (95%)	0.68	276 (7%) 22 22	406, 487, 547, 547	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	254	SER	5.5
3	J	364	SER	4.9
1	Q	60	SER	4.8
3	D	396	PRO	4.8
2	H	168	SER	4.7
1	L	19	ILE	4.5
2	M	113	PRO	4.4
2	R	90	TYR	3.9
3	B	259	VAL	3.8
2	M	34	MET	3.7
1	K	23	CYS	3.7
1	L	78	LEU	3.7
3	J	366	THR	3.7
3	B	396	PRO	3.7
3	B	281	GLY	3.7
2	E	129	SER	3.6
3	C	444	SER	3.6
3	J	440	SER	3.6
2	O	46	GLU	3.6
2	H	169	SER	3.6
3	D	332	ILE	3.5
1	L	132	VAL	3.5
3	J	444	SER	3.5
3	C	440	SER	3.4
3	C	307	THR	3.4
3	D	323	VAL	3.4
1	F	75	ILE	3.3
3	N	323	VAL	3.3
3	B	239	SER	3.3
3	A	440	SER	3.2
2	M	30	SER	3.2
3	A	350	THR	3.2
1	L	62	PHE	3.2
1	G	205	VAL	3.2
2	M	41	PRO	3.2
3	C	442	SER	3.2
2	M	65	GLY	3.2
2	R	108	VAL	3.2
3	C	364	SER	3.2
3	N	442	SER	3.2
1	L	137	ASN	3.2
3	J	298	SER	3.2
3	B	263	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	89	THR	3.1
3	D	241	PHE	3.1
1	P	5	THR	3.1
3	B	250	THR	3.0
3	B	241	PHE	3.0
2	O	81	GLN	3.0
1	L	206	THR	3.0
3	C	366	THR	3.0
3	A	265	ASP	3.0
1	L	174	SER	3.0
1	L	185	ASP	2.9
1	G	73	LEU	2.9
1	K	102	THR	2.9
3	B	366	THR	2.9
2	M	17	SER	2.9
3	C	254	SER	2.9
1	G	20	THR	2.9
2	R	22	CYS	2.9
3	J	323	VAL	2.9
1	K	41	GLY	2.9
1	K	199	GLN	2.9
2	I	117	SER	2.9
1	P	62	PHE	2.9
2	E	148	VAL	2.8
3	D	442	SER	2.8
3	J	254	SER	2.8
2	I	42	GLY	2.8
1	Q	205	VAL	2.8
1	G	14	SER	2.8
2	M	15	GLY	2.8
3	D	375	SER	2.8
2	H	7	SER	2.8
1	K	180	THR	2.8
2	M	42	GLY	2.8
2	R	107	THR	2.8
1	G	62	PHE	2.8
3	B	393	THR	2.7
2	M	198	LEU	2.7
2	R	180	SER	2.7
1	Q	196	VAL	2.7
3	A	342	GLN	2.7
1	G	204	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	B	289	THR	2.7
1	P	19	ILE	2.7
2	M	46	GLU	2.7
1	K	89	GLN	2.7
1	P	89	GLN	2.7
2	R	182	SER	2.7
2	M	31	ALA	2.7
2	R	34	MET	2.7
2	R	92	CYS	2.7
3	N	332	ILE	2.7
2	O	195	SER	2.7
3	J	261	CYS	2.7
2	M	136	GLY	2.7
3	J	281	GLY	2.7
1	G	21	ILE	2.7
3	N	241	PHE	2.6
1	F	93	GLY	2.6
2	M	195	SER	2.6
3	D	259	VAL	2.6
2	M	79	TYR	2.6
2	O	42	GLY	2.6
2	H	148	VAL	2.6
2	M	67	PHE	2.6
2	O	127	SER	2.6
3	N	262	VAL	2.6
3	A	254	SER	2.6
3	B	375	SER	2.6
3	J	442	SER	2.6
2	R	5	VAL	2.6
3	J	321	CYS	2.6
3	A	272	GLN	2.6
1	G	8	PRO	2.6
1	K	5	THR	2.6
2	H	129	SER	2.6
2	E	168	SER	2.6
3	A	286	ASN	2.6
2	M	206	TYR	2.6
2	O	182	SER	2.6
2	E	46	GLU	2.6
1	P	75	ILE	2.5
2	O	196	SER	2.5
1	G	86	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	N	407	TYR	2.5
1	K	25	ALA	2.5
2	M	197	SER	2.5
3	A	442	SER	2.5
2	I	107	PRO	2.5
1	L	63	SER	2.5
1	L	75	ILE	2.5
2	R	95	LYS	2.5
3	A	323	VAL	2.5
1	L	73	LEU	2.4
1	P	57	GLY	2.4
1	K	76	SER	2.4
2	M	94	ARG	2.4
1	K	100	GLN	2.4
1	G	195	GLU	2.4
1	K	56	THR	2.4
2	M	137	THR	2.4
1	K	86	TYR	2.4
3	B	355	ARG	2.4
1	Q	10	THR	2.4
1	L	114	SER	2.4
3	C	321	CYS	2.4
2	R	21	SER	2.4
1	Q	163	VAL	2.4
3	C	288	LYS	2.4
1	L	81	ASP	2.4
1	F	57	GLY	2.4
1	Q	86	TYR	2.4
1	G	152	ASN	2.4
3	N	259	VAL	2.4
2	R	42	GLY	2.4
3	D	443	LEU	2.4
1	F	133	VAL	2.4
3	C	282	VAL	2.4
1	L	168	SER	2.4
3	B	364	SER	2.4
3	C	281	GLY	2.4
3	D	431	ALA	2.3
2	M	100	LEU	2.3
3	N	437	THR	2.3
2	R	82	MET	2.3
2	R	106	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	246	LYS	2.3
3	B	443	LEU	2.3
3	D	440	SER	2.3
3	B	407	TYR	2.3
3	B	247	PRO	2.3
3	B	417	TRP	2.3
3	N	430	GLU	2.3
3	B	308	VAL	2.3
1	P	93	GLY	2.3
1	L	18	THR	2.3
2	R	7	SER	2.3
2	M	81	GLN	2.3
3	J	297	ASN	2.3
3	A	321	CYS	2.2
2	M	194	PRO	2.2
1	G	153	ALA	2.2
1	Q	21	ILE	2.2
2	H	5	VAL	2.2
2	O	17	SER	2.2
3	A	365	LEU	2.2
1	L	82	ASP	2.2
3	D	407	TYR	2.2
1	K	95	SER	2.2
1	G	67	SER	2.2
1	L	20	THR	2.2
3	D	243	PHE	2.2
2	H	134	LEU	2.2
3	B	254	SER	2.2
3	N	443	LEU	2.2
1	Q	104	VAL	2.2
1	P	132	VAL	2.2
2	M	66	ARG	2.2
2	I	108	GLY	2.2
1	G	30	GLU	2.2
1	G	187	GLU	2.2
2	H	46	GLU	2.2
3	A	444	SER	2.2
1	K	4	MET	2.2
3	A	332	ILE	2.2
3	N	273	VAL	2.2
3	A	241	PHE	2.2
3	C	297	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	94	TYR	2.2
3	C	368	LEU	2.2
3	B	356	GLU	2.2
3	C	293	GLU	2.2
3	N	433	HIS	2.2
1	K	26	SER	2.1
1	K	75	ILE	2.1
1	Q	152	ASN	2.1
2	M	95	LYS	2.1
2	E	182	SER	2.1
2	I	41	PRO	2.1
1	K	57	GLY	2.1
1	Q	30	GLU	2.1
3	A	399	ASP	2.1
1	Q	9	SER	2.1
2	O	65	GLY	2.1
3	B	385	GLY	2.1
3	C	298	SER	2.1
3	N	404	PHE	2.1
1	G	35	TRP	2.1
3	A	293	GLU	2.1
3	A	252	MET	2.1
1	K	21	ILE	2.1
1	K	37	GLN	2.1
2	O	198	LEU	2.1
2	R	35	ASN	2.1
2	I	109	THR	2.1
3	D	430	GLU	2.1
2	M	82	MET	2.1
1	L	77	GLY	2.1
1	K	93	GLY	2.1
2	M	93	ALA	2.1
2	O	7	SER	2.1
2	H	24	VAL	2.1
3	B	280	ASP	2.1
2	H	45	LEU	2.1
3	A	431	ALA	2.1
3	N	321	CYS	2.1
1	K	192	TYR	2.1
2	M	40	VAL	2.1
1	K	54	LEU	2.1
1	G	93	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	42	GLY	2.1
2	R	74	LEU	2.0
3	B	298	SER	2.0
1	P	35	TRP	2.0
2	M	35	ASN	2.0
3	A	333	GLU	2.0
1	L	17	ASP	2.0
2	M	91	TYR	2.0
3	A	285	HIS	2.0
3	A	354	SER	2.0
1	Q	113	PRO	2.0
2	I	104	ALA	2.0
3	C	417	TRP	2.0
3	A	297	ASN	2.0
1	L	79	GLN	2.0
2	E	51	ILE	2.0
2	M	117	LYS	2.0
3	D	404	PHE	2.0
1	L	52	SER	2.0
1	K	99	GLY	2.0
2	H	105	TRP	2.0
2	E	158	GLY	2.0
3	N	396	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.