



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 08:28 AM EDT

PDB ID : 3TCF
Title : Crystal structure of E. coli OppA complexed with endogenous ligands
Authors : Klepsch, M.M.; Kovermann, M.; Low, C.; Balbach, J.; de Gier, J.W.; Slotboom, D.J.; Berntsson, R.P.-A.
Deposited on : 2011-08-09
Resolution : 2.00 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)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

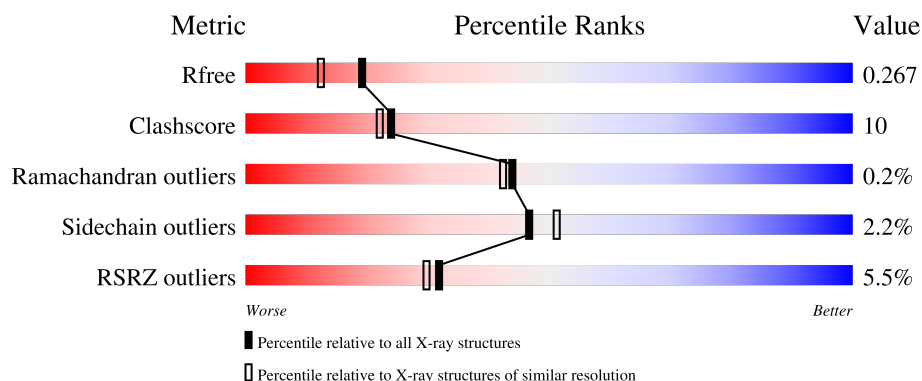
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.








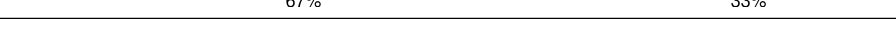



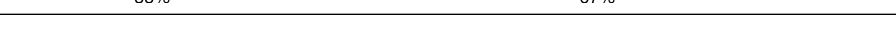
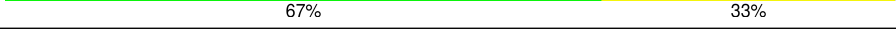
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	524	<div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	524	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	C	524	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	524	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	E	524	<div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	524	
1	G	524	
1	H	524	
2	I	3	
2	J	3	
2	K	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35615 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 Periplasmic oligopeptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	2	0
			4137	2636	695	796	10			
1	B	517	Total	C	N	O	S	0	2	0
			4136	2636	694	796	10			
1	C	517	Total	C	N	O	S	0	1	0
			4129	2632	693	794	10			
1	D	517	Total	C	N	O	S	0	1	0
			4129	2632	693	794	10			
1	E	517	Total	C	N	O	S	0	2	0
			4137	2636	694	797	10			
1	F	517	Total	C	N	O	S	0	4	0
			4155	2649	696	800	10			
1	G	517	Total	C	N	O	S	0	2	0
			4135	2635	694	796	10			
1	H	517	Total	C	N	O	S	0	1	0
			4129	2632	693	794	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP P23843
A	544	HIS	-	expression tag	UNP P23843
A	545	HIS	-	expression tag	UNP P23843
A	546	HIS	-	expression tag	UNP P23843
A	547	HIS	-	expression tag	UNP P23843
A	548	HIS	-	expression tag	UNP P23843
A	549	HIS	-	expression tag	UNP P23843
B	26	MET	-	expression tag	UNP P23843
B	544	HIS	-	expression tag	UNP P23843
B	545	HIS	-	expression tag	UNP P23843
B	546	HIS	-	expression tag	UNP P23843
B	547	HIS	-	expression tag	UNP P23843
B	548	HIS	-	expression tag	UNP P23843

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Chain	Residue	Modelled	Actual	Comment	Reference
B	549	HIS	-	expression tag	UNP P23843
C	26	MET	-	expression tag	UNP P23843
C	544	HIS	-	expression tag	UNP P23843
C	545	HIS	-	expression tag	UNP P23843
C	546	HIS	-	expression tag	UNP P23843
C	547	HIS	-	expression tag	UNP P23843
C	548	HIS	-	expression tag	UNP P23843
C	549	HIS	-	expression tag	UNP P23843
D	26	MET	-	expression tag	UNP P23843
D	544	HIS	-	expression tag	UNP P23843
D	545	HIS	-	expression tag	UNP P23843
D	546	HIS	-	expression tag	UNP P23843
D	547	HIS	-	expression tag	UNP P23843
D	548	HIS	-	expression tag	UNP P23843
D	549	HIS	-	expression tag	UNP P23843
E	26	MET	-	expression tag	UNP P23843
E	544	HIS	-	expression tag	UNP P23843
E	545	HIS	-	expression tag	UNP P23843
E	546	HIS	-	expression tag	UNP P23843
E	547	HIS	-	expression tag	UNP P23843
E	548	HIS	-	expression tag	UNP P23843
E	549	HIS	-	expression tag	UNP P23843
F	26	MET	-	expression tag	UNP P23843
F	544	HIS	-	expression tag	UNP P23843
F	545	HIS	-	expression tag	UNP P23843
F	546	HIS	-	expression tag	UNP P23843
F	547	HIS	-	expression tag	UNP P23843
F	548	HIS	-	expression tag	UNP P23843
F	549	HIS	-	expression tag	UNP P23843
G	26	MET	-	expression tag	UNP P23843
G	544	HIS	-	expression tag	UNP P23843
G	545	HIS	-	expression tag	UNP P23843
G	546	HIS	-	expression tag	UNP P23843
G	547	HIS	-	expression tag	UNP P23843
G	548	HIS	-	expression tag	UNP P23843
G	549	HIS	-	expression tag	UNP P23843
H	26	MET	-	expression tag	UNP P23843
H	544	HIS	-	expression tag	UNP P23843
H	545	HIS	-	expression tag	UNP P23843
H	546	HIS	-	expression tag	UNP P23843
H	547	HIS	-	expression tag	UNP P23843
H	548	HIS	-	expression tag	UNP P23843

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Chain	Residue	Modelled	Actual	Comment	Reference
H	549	HIS	-	expression tag	UNP P23843

- Molecule 2 is a protein called Endogenous peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	J	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	K	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	L	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	M	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	N	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	O	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	P	3	Total	C	N	O	0	0	0
			15	9	3	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	360	Total	O	0	0
			360	360		
3	B	268	Total	O	0	0
			268	268		
3	C	285	Total	O	0	0
			285	285		
3	D	265	Total	O	0	0
			265	265		
3	E	351	Total	O	0	0
			351	351		
3	F	344	Total	O	0	0
			344	344		
3	G	305	Total	O	0	0
			305	305		
3	H	221	Total	O	0	0
			221	221		
3	I	2	Total	O	0	0
			2	2		

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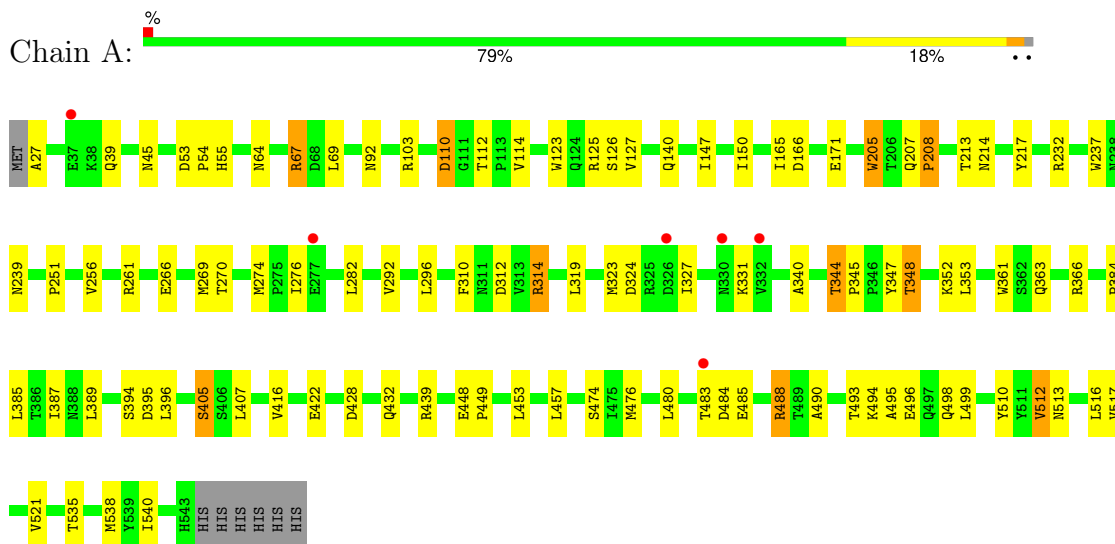
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	O	0	0
			2	2		
3	K	1	Total	O	0	0
			1	1		
3	M	2	Total	O	0	0
			2	2		
3	P	2	Total	O	0	0
			2	2		

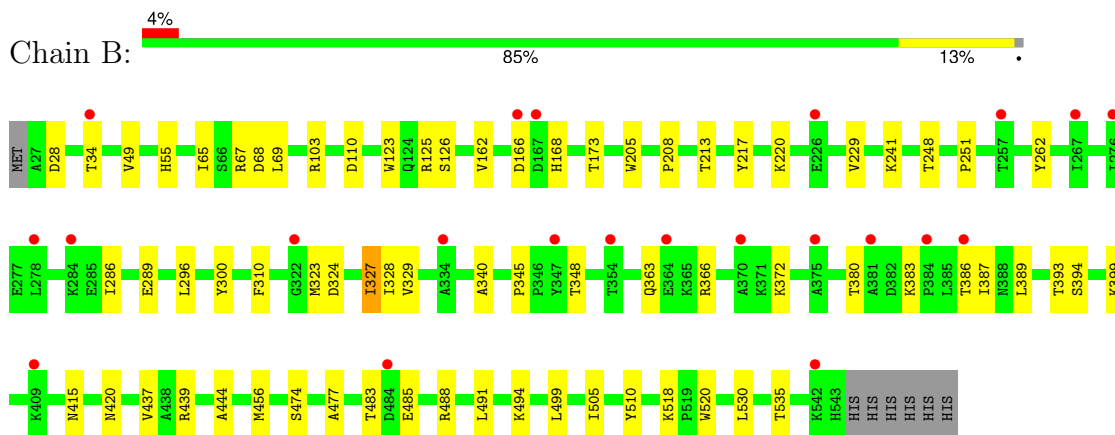
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

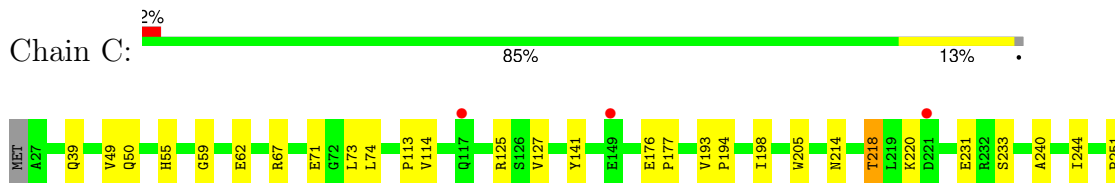
- Molecule 1: Periplasmic oligopeptide-binding protein



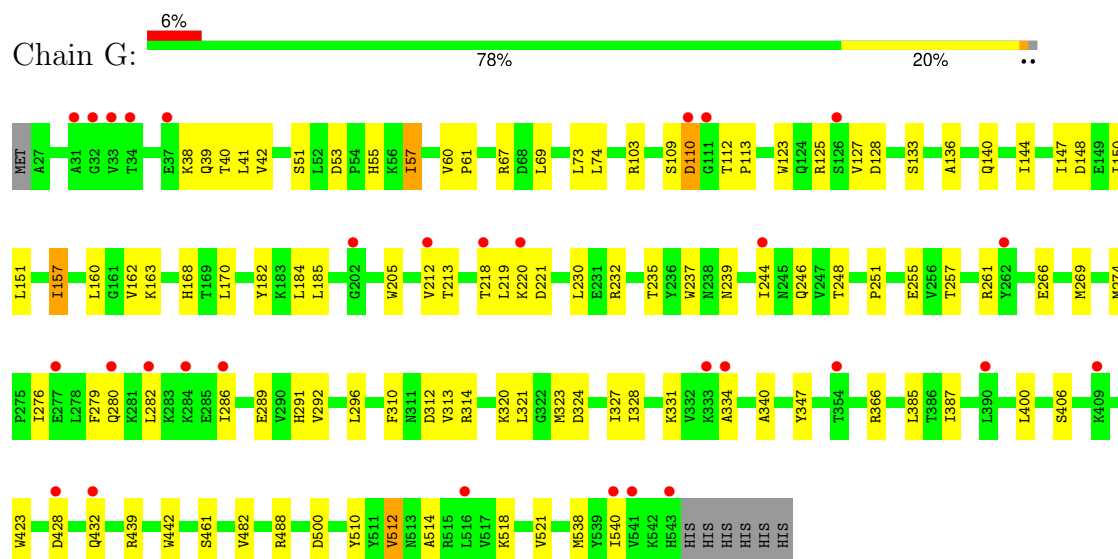
- Molecule 1: Periplasmic oligopeptide-binding protein



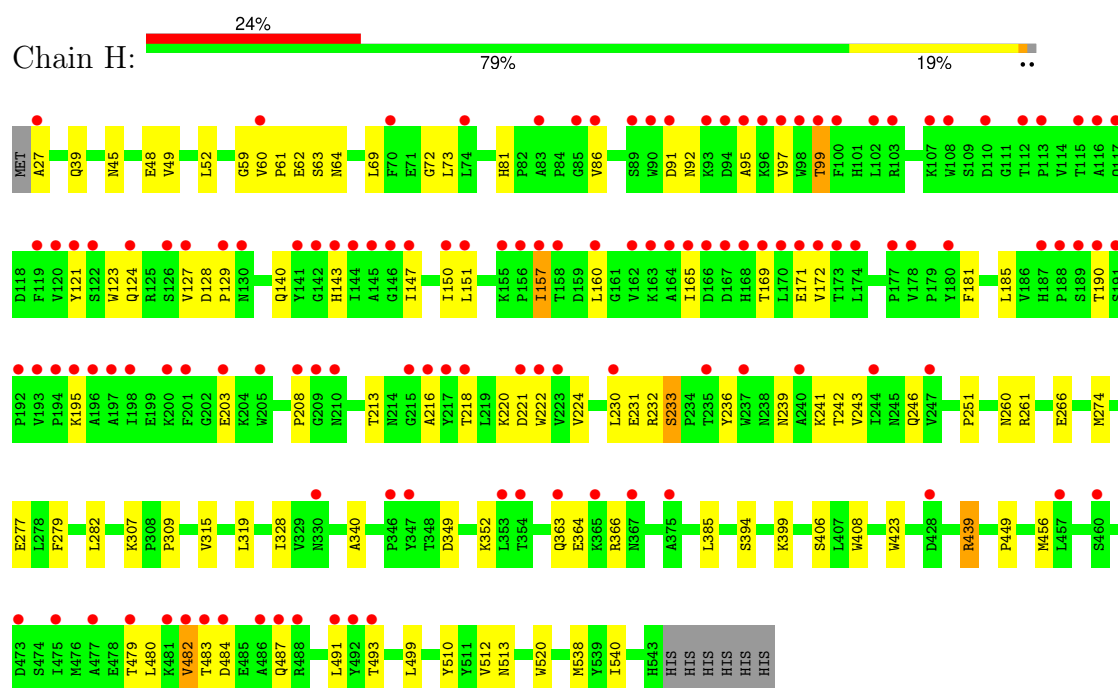
- Molecule 1: Periplasmic oligopeptide-binding protein



- Molecule 1: Periplasmic oligopeptide-binding protein



- Molecule 1: Periplasmic oligopeptide-binding protein



- Molecule 2: Endogenous peptide



- Molecule 2: Endogenous peptide





- Molecule 2: Endogenous peptide



- Molecule 2: Endogenous peptide



- Molecule 2: Endogenous peptide



- Molecule 2: Endogenous peptide



- Molecule 2: Endogenous peptide



There are no outlier residues recorded for this chain.

- Molecule 2: Endogenous peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.62Å 202.60Å 208.95Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	48.37 – 2.00 48.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.37-2.00) 99.2 (48.37-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.267 0.230 , 0.267	Depositor DCC
R_{free} test set	17261 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35615	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 33.69 % 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 7.6804e-04. 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	A	0.77	2/4245 (0.0%)	0.80	6/5790 (0.1%)
1	B	0.68	2/4244 (0.0%)	0.71	4/5789 (0.1%)
1	C	0.68	4/4237 (0.1%)	0.68	2/5779 (0.0%)
1	D	0.66	3/4237 (0.1%)	0.69	2/5779 (0.0%)
1	E	0.71	2/4245 (0.0%)	0.74	5/5790 (0.1%)
1	F	0.72	4/4264 (0.1%)	0.71	3/5817 (0.1%)
1	G	0.69	5/4243 (0.1%)	0.70	3/5788 (0.1%)
1	H	0.66	2/4237 (0.0%)	0.64	1/5779 (0.0%)
All	All	0.70	24/33952 (0.1%)	0.71	26/46311 (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
1	B	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	TRP	CD2-CE2	5.75	1.48	1.41
1	A	205	TRP	CD2-CE2	5.72	1.48	1.41
1	F	237	TRP	CD2-CE2	5.70	1.48	1.41
1	G	205	TRP	CD2-CE2	5.63	1.48	1.41
1	D	98	TRP	CD2-CE2	5.58	1.48	1.41
1	E	520	TRP	CD2-CE2	5.51	1.48	1.41
1	F	205	TRP	CD2-CE2	5.46	1.48	1.41
1	H	520	TRP	CD2-CE2	5.34	1.47	1.41
1	A	361	TRP	CD2-CE2	5.32	1.47	1.41
1	C	520	TRP	CD2-CE2	5.29	1.47	1.41
1	F	90	TRP	CD2-CE2	5.29	1.47	1.41
1	E	90	TRP	CD2-CE2	5.28	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	408	TRP	CD2-CE2	5.23	1.47	1.41
1	C	205	TRP	CD2-CE2	5.21	1.47	1.41
1	D	358	TRP	CD2-CE2	5.11	1.47	1.41
1	D	408	TRP	CD2-CE2	5.10	1.47	1.41
1	G	442	TRP	CD2-CE2	5.07	1.47	1.41
1	B	520	TRP	CD2-CE2	5.06	1.47	1.41
1	F	222	TRP	CD2-CE2	5.06	1.47	1.41
1	G	123	TRP	CD2-CE2	5.05	1.47	1.41
1	G	237	TRP	CD2-CE2	5.04	1.47	1.41
1	C	361	TRP	CD2-CE2	5.04	1.47	1.41
1	G	423	TRP	CD2-CE2	5.00	1.47	1.41
1	H	423	TRP	CD2-CE2	5.00	1.47	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ARG	NE-CZ-NH2	-12.89	113.86	120.30
1	A	67	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	103	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	A	67	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	B	103	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	D	67	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	E	67	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	C	67	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	F	67	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	F	67	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	D	67	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	67	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	F	488	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	67	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	G	103	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	488	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	488	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	G	103	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	B	67	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	E	232	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	G	67	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	E	232	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	103	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	E	261	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	H	439	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	110	ASP	CB-CA-C	-5.19	100.02	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	483	THR	Peptide

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	A	4137	0	4046	92	0
1	B	4136	0	4047	59	0
1	C	4129	0	4041	73	0
1	D	4129	0	4041	55	0
1	E	4137	0	4044	69	0
1	F	4155	0	4061	89	0
1	G	4135	0	4046	107	0
1	H	4129	0	4041	99	0
2	I	15	0	5	2	0
2	J	15	0	5	1	0
2	K	15	0	5	1	0
2	L	15	0	5	1	0
2	M	15	0	5	2	0
2	N	15	0	5	1	0
2	O	15	0	5	0	0
2	P	15	0	5	1	0
3	A	360	0	0	35	0
3	B	268	0	0	12	0
3	C	285	0	0	25	0
3	D	265	0	0	9	0
3	E	351	0	0	20	0
3	F	344	0	0	38	0
3	G	305	0	0	33	0
3	H	221	0	0	41	0
3	I	2	0	0	1	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
3	M	2	0	0	0	0
3	P	2	0	0	1	0
All	All	35615	0	32407	650	0

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 10.

All (650) 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)
1:H:147:ILE:HG21	3:H:3221:HOH:O	1.16	1.33
1:E:158:THR:HG23	3:E:3234:HOH:O	1.21	1.30
1:G:184:LEU:HD22	3:G:3263:HOH:O	1.27	1.29
1:A:457:LEU:HD13	3:A:3253:HOH:O	1.11	1.27
1:F:65:ILE:HG22	3:F:3274:HOH:O	1.26	1.26
1:F:403:ALA:HB3	3:F:2122:HOH:O	1.05	1.23
1:C:193:VAL:CG1	1:C:198:ILE:HD11	1.70	1.21
1:G:185:LEU:HD12	3:G:3189:HOH:O	1.38	1.20
1:A:323:MET:SD	3:A:3197:HOH:O	1.95	1.19
1:C:218:THR:HB	3:C:3250:HOH:O	1.39	1.18
1:C:472:PHE:CE2	3:C:3252:HOH:O	1.97	1.17
1:H:385:LEU:HD12	3:H:3237:HOH:O	1.44	1.16
1:G:269:MET:CE	1:G:538:MET:HE3	1.76	1.15
1:H:185:LEU:HD23	3:H:2390:HOH:O	1.47	1.14
3:E:3220:HOH:O	2:M:3:UNK:C	1.93	1.12
1:G:269:MET:HE1	1:G:538:MET:CE	1.79	1.12
1:G:127:VAL:HG22	3:G:3275:HOH:O	1.49	1.08
1:E:232:ARG:HD3	1:E:239:ASN:HD21	1.18	1.07
1:B:173:THR:HG23	3:B:1116:HOH:O	1.53	1.05
1:B:535:THR:HG22	3:B:1831:HOH:O	1.57	1.05
1:C:319:LEU:HD12	3:C:2520:HOH:O	1.56	1.05
1:A:274:MET:SD	3:A:3172:HOH:O	2.13	1.04
1:A:453:LEU:HB3	1:A:476:MET:HE3	1.38	1.03
1:G:41:LEU:HD21	1:G:269:MET:HE3	1.40	1.03
1:E:206:THR:HG21	3:E:3239:HOH:O	1.62	1.00
1:B:393:THR:HG22	1:B:420:ASN:HD22	1.27	1.00
1:C:193:VAL:HG11	1:C:198:ILE:HD11	1.39	0.98
1:D:220:LYS:NZ	1:D:246:GLN:NE2	2.12	0.98
1:B:323:MET:SD	3:B:3160:HOH:O	2.22	0.97
1:F:353:LEU:HD11	3:F:3264:HOH:O	1.62	0.97
1:H:456:MET:HE3	1:H:499:LEU:HD11	1.46	0.97
1:A:428:ASP:OD2	1:A:432:GLN:NE2	1.98	0.96
1:B:477:ALA:HB1	3:B:3251:HOH:O	1.65	0.96
1:G:269:MET:HE1	1:G:538:MET:HE3	0.96	0.95
1:G:151:LEU:HD21	3:G:3275:HOH:O	1.64	0.95
1:H:242:THR:HG22	3:H:561:HOH:O	1.66	0.94
1:H:160:LEU:HD21	3:H:3244:HOH:O	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:428:ASP:OD2	1:F:432:GLN:NE2	2.00	0.94
1:D:220:LYS:HZ1	1:D:246:GLN:NE2	1.64	0.94
1:B:386:THR:HG22	1:B:415:ASN:HB2	1.49	0.94
1:E:232:ARG:HD3	1:E:239:ASN:ND2	1.82	0.93
1:A:319:LEU:HD23	3:A:3257:HOH:O	1.68	0.93
1:F:387:ILE:CG2	3:F:3261:HOH:O	2.16	0.93
1:H:456:MET:CE	1:H:499:LEU:HD11	2.00	0.92
1:G:324:ASP:O	1:G:328:ILE:HD12	1.70	0.92
1:C:193:VAL:CG1	1:C:198:ILE:CD1	2.47	0.92
1:G:220:LYS:NZ	1:G:246:GLN:NE2	2.18	0.92
1:D:220:LYS:NZ	1:D:246:GLN:HE21	1.67	0.92
3:A:3286:HOH:O	2:I:1:UNK:CB	2.18	0.90
1:G:220:LYS:HZ1	1:G:246:GLN:HE21	1.16	0.90
1:D:220:LYS:HZ3	1:D:246:GLN:HE21	1.15	0.90
1:E:232:ARG:CD	1:E:239:ASN:HD21	1.84	0.89
1:H:315:VAL:HG21	3:H:3206:HOH:O	1.71	0.89
1:H:538:MET:CE	3:H:3292:HOH:O	2.20	0.89
1:H:160:LEU:CD2	3:H:3244:HOH:O	2.20	0.89
1:C:456:MET:HB2	3:C:3252:HOH:O	1.73	0.89
1:E:428:ASP:OD2	1:E:432:GLN:NE2	2.05	0.88
1:E:39:GLN:HE22	1:E:540:ILE:H	1.18	0.88
1:F:387:ILE:HG22	3:F:3261:HOH:O	1.68	0.88
1:D:540:ILE:HG12	3:D:3217:HOH:O	1.74	0.88
1:F:400:LEU:HD23	3:F:3267:HOH:O	1.74	0.87
1:D:127:VAL:HG13	1:D:151:LEU:CD2	2.05	0.86
1:C:276:ILE:HD12	1:C:399:LYS:HD3	1.58	0.86
1:H:406:SER:HB2	3:H:2605:HOH:O	1.76	0.86
1:C:319:LEU:HB2	3:C:2520:HOH:O	1.75	0.85
1:D:39:GLN:HE22	1:D:540:ILE:H	1.23	0.85
2:I:1:UNK:CB	3:I:3280:HOH:O	2.25	0.85
1:A:282:LEU:HD12	3:A:2233:HOH:O	1.74	0.85
3:C:3176:HOH:O	2:K:1:UNK:CB	2.25	0.85
1:G:220:LYS:NZ	1:G:246:GLN:HE21	1.72	0.85
1:A:493:THR:HG23	3:A:666:HOH:O	1.77	0.85
1:B:380:THR:HG22	3:B:3213:HOH:O	1.77	0.85
1:G:274:MET:SD	3:G:3205:HOH:O	2.35	0.85
1:G:140:GLN:HG3	1:G:147:ILE:HD13	1.59	0.84
1:G:40:THR:O	1:G:540:ILE:HD11	1.77	0.84
1:D:143:HIS:CD2	1:D:480:LEU:HD11	2.11	0.84
1:F:344:THR:HG22	3:F:3264:HOH:O	1.76	0.84
1:A:39:GLN:HE22	1:A:540:ILE:H	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:MET:CE	1:G:538:MET:CE	2.47	0.83
1:G:220:LYS:HZ2	1:G:246:GLN:NE2	1.77	0.83
1:G:182:TYR:HA	3:G:3189:HOH:O	1.78	0.82
1:G:57:ILE:HG23	3:G:2129:HOH:O	1.79	0.82
1:G:39:GLN:HE22	1:G:540:ILE:H	1.26	0.81
1:H:213:THR:OG1	1:H:218:THR:HG22	1.80	0.81
1:F:535[A]:THR:HG22	3:F:1234:HOH:O	1.80	0.81
1:E:493:THR:HG23	3:E:949:HOH:O	1.81	0.81
1:H:140:GLN:HA	3:H:3221:HOH:O	1.81	0.80
1:F:213:THR:OG1	1:F:218:THR:HG22	1.82	0.80
1:C:317:THR:HG22	1:C:503:SER:OG	1.82	0.79
1:A:476:MET:CE	1:A:495:ALA:HB1	2.12	0.79
1:C:39:GLN:HA	1:C:540:ILE:HD13	1.62	0.79
1:A:476:MET:HE2	1:A:495:ALA:HB1	1.62	0.79
1:C:193:VAL:HG12	1:C:198:ILE:CD1	2.13	0.79
1:A:453:LEU:HD13	1:A:476:MET:HE1	1.65	0.78
1:C:456:MET:C	3:C:3252:HOH:O	2.22	0.78
1:F:220:LYS:HZ3	1:F:246:GLN:HE21	1.29	0.78
1:G:53:ASP:O	1:G:57:ILE:HD13	1.84	0.78
1:E:53:ASP:N	3:E:3239:HOH:O	2.16	0.77
1:H:482:VAL:HG22	1:H:487:GLN:NE2	1.99	0.77
1:F:65:ILE:CG2	3:F:3274:HOH:O	2.01	0.77
1:C:193:VAL:HG13	1:C:194:PRO:HD2	1.66	0.77
1:A:483:THR:HG22	1:A:484:ASP:OD1	1.85	0.77
1:C:456:MET:CB	3:C:3252:HOH:O	2.32	0.77
1:A:237:TRP:CZ2	3:A:3207:HOH:O	2.35	0.76
1:G:69:LEU:HD21	1:G:230:LEU:HD22	1.66	0.76
1:B:34:THR:HG23	3:B:2193:HOH:O	1.85	0.76
3:E:2276:HOH:O	2:M:1:UNK:CB	2.32	0.75
1:G:296:LEU:HD23	1:G:347:TYR:CE2	2.20	0.75
1:H:185:LEU:HA	3:H:2390:HOH:O	1.86	0.74
1:C:482:VAL:HG12	1:C:484:ASP:H	1.52	0.74
1:C:176:GLU:HG2	1:C:480:LEU:HB3	1.71	0.73
1:D:40:THR:O	1:D:540:ILE:HD11	1.87	0.73
1:D:274:MET:SD	3:D:3195:HOH:O	2.46	0.73
1:G:286:ILE:HG21	1:G:289:GLU:CD	2.08	0.73
1:F:480:LEU:HD23	1:F:488:ARG:HH21	1.54	0.73
1:C:316:ARG:HA	3:C:2520:HOH:O	1.89	0.72
1:F:127:VAL:HG12	1:F:150:ILE:HG22	1.70	0.72
1:H:49:VAL:HG22	3:H:2458:HOH:O	1.89	0.72
1:E:128:ASP:HA	1:E:157:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:ILE:HG23	1:H:157:ILE:HD12	1.72	0.72
1:F:385:LEU:HG	1:F:387:ILE:HD13	1.72	0.72
1:A:476:MET:CE	1:A:495:ALA:CB	2.68	0.71
1:A:53:ASP:HA	3:A:3229:HOH:O	1.90	0.71
1:G:127:VAL:HG12	1:G:150:ILE:HG22	1.72	0.71
1:D:274:MET:HE2	1:D:279:PHE:CD2	2.26	0.70
1:A:476:MET:HE1	1:A:495:ALA:CB	2.21	0.70
1:B:286:ILE:HG22	1:B:286:ILE:O	1.90	0.70
1:C:218:THR:CB	3:C:3250:HOH:O	2.13	0.70
1:H:190:THR:HG21	3:H:2390:HOH:O	1.90	0.70
1:H:232:ARG:HE	1:H:239:ASN:HD21	1.38	0.70
1:B:248:THR:HG23	3:B:828:HOH:O	1.91	0.70
1:E:428:ASP:OD1	1:E:432:GLN:NE2	2.23	0.70
1:F:69:LEU:HG	3:F:3274:HOH:O	1.90	0.70
1:A:205:TRP:CH2	3:A:3229:HOH:O	2.44	0.70
1:F:453:LEU:HB2	3:F:3223:HOH:O	1.90	0.70
1:A:261:ARG:HD3	1:A:266:GLU:OE2	1.92	0.70
1:F:416:VAL:HG13	3:F:3261:HOH:O	1.92	0.70
1:G:127:VAL:HG13	3:G:3275:HOH:O	1.92	0.70
1:A:205:TRP:CZ2	3:A:3229:HOH:O	2.44	0.69
1:E:428:ASP:CG	1:E:432:GLN:NE2	2.46	0.69
1:F:286:ILE:O	1:F:286:ILE:HG22	1.90	0.69
1:E:157:ILE:HG22	3:E:3234:HOH:O	1.92	0.69
1:G:257:THR:HG21	3:G:1413:HOH:O	1.92	0.69
1:B:456:MET:CE	1:B:499:LEU:HD11	2.23	0.69
1:F:344:THR:CG2	3:F:3264:HOH:O	2.36	0.69
1:G:136:ALA:HB3	3:G:2204:HOH:O	1.93	0.69
1:F:39:GLN:HE22	1:F:540:ILE:H	1.38	0.69
1:B:323:MET:HE1	1:B:328:ILE:CD1	2.23	0.69
1:F:493[A]:THR:HG23	3:F:1094:HOH:O	1.91	0.69
1:G:162:VAL:HG12	1:G:170:LEU:HD11	1.74	0.68
1:H:52:LEU:HD12	1:H:222:TRP:CZ3	2.29	0.68
1:G:41:LEU:CD2	1:G:269:MET:HE3	2.22	0.68
1:D:274:MET:HE2	1:D:279:PHE:HD2	1.59	0.68
1:H:538:MET:HE2	3:H:3292:HOH:O	1.83	0.68
1:E:456:MET:HE2	1:E:499:LEU:HD11	1.76	0.67
1:A:310:PHE:HE1	3:A:3257:HOH:O	1.77	0.67
1:C:317:THR:OG1	1:C:373:LEU:HD13	1.94	0.67
1:H:236:TYR:CZ	3:H:3291:HOH:O	2.47	0.67
1:E:428:ASP:CG	1:E:432:GLN:HE21	1.98	0.67
1:D:127:VAL:HG13	1:D:151:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LEU:HD22	1:B:348[A]:THR:HG22	1.77	0.67
1:D:218:THR:HG21	3:D:2464:HOH:O	1.93	0.67
1:H:73:LEU:HD12	1:H:185:LEU:HD13	1.76	0.67
1:H:352:LYS:O	1:H:493:THR:HG21	1.95	0.67
1:C:493:THR:HG23	3:C:2120:HOH:O	1.93	0.67
1:B:456:MET:HE3	1:B:499:LEU:HD11	1.75	0.66
1:A:39:GLN:HE22	1:A:540:ILE:N	1.92	0.66
1:F:335:GLN:NE2	3:F:3260:HOH:O	2.28	0.66
1:H:127:VAL:HG13	1:H:151:LEU:CD2	2.26	0.66
1:A:312:ASP:OD2	1:A:314:ARG:HD3	1.95	0.66
1:F:386:THR:HG22	1:F:415:ASN:HD22	1.60	0.66
1:A:110:ASP:HB3	1:A:112:THR:HG23	1.78	0.66
1:G:428:ASP:OD2	1:G:432:GLN:NE2	2.29	0.66
1:C:349:ASP:HB3	3:C:3228:HOH:O	1.95	0.66
1:F:220:LYS:NZ	1:F:246:GLN:HE21	1.94	0.66
1:B:220:LYS:HD2	3:B:3283:HOH:O	1.95	0.65
1:G:518:LYS:HB2	3:G:3259:HOH:O	1.96	0.65
1:E:39:GLN:HA	1:E:540:ILE:HD13	1.77	0.65
1:F:127:VAL:CG1	1:F:150:ILE:HG22	2.25	0.65
1:B:393:THR:CG2	1:B:420:ASN:HD22	2.06	0.65
1:E:165:ILE:HD11	1:E:171:GLU:HB2	1.78	0.65
1:H:48:GLU:HG2	3:H:2455:HOH:O	1.97	0.65
1:H:309:PRO:HB2	3:H:3206:HOH:O	1.96	0.65
1:F:386:THR:HG22	1:F:415:ASN:HB2	1.78	0.65
1:D:92:ASN:HD22	1:D:95:ALA:H	1.45	0.64
1:A:123:TRP:O	1:A:126[B]:SER:OG	2.16	0.64
1:H:69:LEU:HD21	1:H:230:LEU:HD22	1.79	0.64
1:D:173:THR:HG23	3:D:1678:HOH:O	1.98	0.64
1:G:128:ASP:HA	1:G:157:ILE:HD11	1.78	0.64
1:A:480:LEU:HD23	1:A:488:ARG:HH21	1.62	0.64
1:A:165:ILE:HD11	1:A:171:GLU:HB2	1.80	0.64
1:B:386:THR:HG22	1:B:415:ASN:HD22	1.63	0.63
1:H:39:GLN:HE22	1:H:540:ILE:H	1.46	0.63
1:H:147:ILE:HD13	3:H:3221:HOH:O	1.97	0.63
1:E:456:MET:CE	1:E:499:LEU:HD11	2.29	0.63
1:E:124:GLN:HB3	1:E:157:ILE:HG23	1.80	0.63
1:A:296:LEU:HD23	1:A:347:TYR:CE2	2.34	0.63
1:F:220:LYS:NZ	1:F:246:GLN:NE2	2.47	0.63
1:G:185:LEU:CD1	3:G:3189:HOH:O	2.17	0.63
1:D:310:PHE:HZ	1:D:387:ILE:HG21	1.63	0.62
3:A:1774:HOH:O	1:C:313:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:CD1	3:A:2233:HOH:O	2.38	0.62
1:E:488:ARG:NH2	3:E:2202:HOH:O	2.27	0.62
3:B:2264:HOH:O	2:J:1:UNK:CB	2.48	0.62
1:F:220:LYS:NZ	3:F:2779:HOH:O	2.32	0.62
1:G:144:ILE:O	1:G:147:ILE:HG13	1.99	0.62
1:D:220:LYS:HZ1	1:D:246:GLN:HE22	1.42	0.62
1:F:480:LEU:HD23	1:F:488:ARG:NH2	2.15	0.62
1:C:218:THR:HG23	1:C:233:SER:HB2	1.81	0.62
1:D:45:ASN:ND2	1:D:64:ASN:HD22	1.97	0.61
1:E:269:MET:CG	3:E:1154:HOH:O	2.47	0.61
1:C:71:GLU:O	1:C:214:ASN:ND2	2.33	0.61
1:F:410:LYS:HD2	3:F:3294:HOH:O	2.00	0.61
1:H:128:ASP:HA	1:H:157:ILE:HD11	1.81	0.61
3:F:3269:HOH:O	2:N:1:UNK:CB	2.47	0.61
1:G:324:ASP:O	1:G:328:ILE:CD1	2.45	0.61
1:H:143:HIS:NE2	3:H:3262:HOH:O	2.23	0.61
1:E:269:MET:SD	3:E:1154:HOH:O	2.56	0.61
1:F:220:LYS:HZ3	1:F:246:GLN:NE2	1.98	0.61
1:C:193:VAL:HG11	1:C:198:ILE:CD1	2.22	0.60
1:A:54:PRO:HD3	3:A:3229:HOH:O	2.00	0.60
1:C:310:PHE:HZ	1:C:387:ILE:HG21	1.66	0.60
1:G:41:LEU:HD11	1:G:269:MET:HE2	1.84	0.60
1:G:220:LYS:HZ2	1:G:246:GLN:HE22	1.49	0.60
1:H:39:GLN:NE2	1:H:243:VAL:HG12	2.16	0.60
1:A:385:LEU:HG	1:A:387:ILE:HD13	1.83	0.60
1:E:124:GLN:HB3	1:E:157:ILE:CG2	2.31	0.60
1:H:480:LEU:HD11	3:H:3262:HOH:O	2.01	0.60
1:H:127:VAL:HG12	1:H:150:ILE:HG22	1.83	0.60
1:A:345:PRO:O	1:A:348:THR:CG2	2.49	0.60
1:C:313:VAL:O	1:C:317:THR:HG23	2.01	0.60
1:A:319:LEU:CD2	3:A:3257:HOH:O	2.38	0.60
1:A:499:LEU:HG	3:A:3293:HOH:O	1.99	0.60
1:D:71:GLU:O	1:D:214:ASN:ND2	2.35	0.60
1:F:128:ASP:HA	1:F:157:ILE:HD11	1.84	0.60
1:H:220:LYS:HZ1	1:H:246:GLN:NE2	1.99	0.60
1:C:286:ILE:O	1:C:286:ILE:HD12	2.03	0.59
1:E:352:LYS:O	1:E:493:THR:HG21	2.03	0.59
1:C:310:PHE:CD2	3:C:2179:HOH:O	2.52	0.59
1:G:147:ILE:HD11	3:G:599:HOH:O	2.02	0.59
1:H:232:ARG:HE	1:H:239:ASN:ND2	2.02	0.58
1:B:262:TYR:CZ	1:B:518:LYS:HD3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:MET:HE3	1:E:467:TYR:CD1	2.39	0.58
1:H:309:PRO:CG	3:H:3206:HOH:O	2.51	0.58
1:A:232:ARG:HE	1:A:239:ASN:HD21	1.52	0.58
1:A:345:PRO:O	1:A:348:THR:HG23	2.03	0.58
1:C:193:VAL:HG12	1:C:198:ILE:HD12	1.83	0.58
1:A:344:THR:HG23	1:A:496:GLU:OE2	2.04	0.58
1:F:476:MET:CE	3:F:3223:HOH:O	2.52	0.58
1:F:514:ALA:HB3	3:F:3186:HOH:O	2.04	0.58
1:G:269:MET:HE2	1:G:521:VAL:HG11	1.86	0.58
1:A:256:VAL:HG23	1:A:395:ASP:OD2	2.04	0.57
1:A:453:LEU:HB3	1:A:476:MET:CE	2.26	0.57
1:B:380:THR:HA	3:B:3213:HOH:O	2.04	0.57
1:C:482:VAL:CG1	1:C:487:GLN:HB2	2.34	0.57
1:H:274:MET:HE1	1:H:282:LEU:HD13	1.85	0.57
1:A:217:TYR:OH	1:A:535:THR:HG22	2.04	0.57
1:C:310:PHE:HE1	1:C:319:LEU:HD11	1.69	0.57
1:H:99:THR:HG23	3:H:1470:HOH:O	2.04	0.57
1:D:274:MET:CE	1:D:279:PHE:HD2	2.17	0.57
1:G:113:PRO:HG2	3:G:2745:HOH:O	2.05	0.57
2:P:3:UNK:C	3:P:455:HOH:O	2.52	0.57
1:G:312:ASP:OD2	1:G:314:ARG:HD3	2.04	0.57
1:B:323:MET:HE1	1:B:328:ILE:HG12	1.86	0.57
1:G:147:ILE:HG23	1:G:160:LEU:HD11	1.86	0.57
1:H:127:VAL:HG13	1:H:151:LEU:HD23	1.87	0.56
1:G:323:MET:SD	1:G:328:ILE:HD11	2.45	0.56
1:B:363:GLN:NE2	1:B:366:ARG:NH2	2.53	0.56
1:F:286:ILE:HG22	1:F:289:GLU:HB2	1.86	0.56
1:H:220:LYS:NZ	1:H:246:GLN:NE2	2.53	0.56
1:D:312:ASP:OD2	1:D:314:ARG:HD3	2.06	0.56
1:D:353:LEU:HA	1:D:493:THR:CG2	2.36	0.56
1:H:456:MET:HE2	1:H:499:LEU:HD11	1.84	0.56
1:C:317:THR:HG22	1:C:503:SER:HG	1.71	0.56
1:F:330:ASN:O	1:F:333:LYS:NZ	2.39	0.56
1:H:456:MET:HE3	1:H:499:LEU:CD1	2.30	0.56
1:G:232:ARG:HE	1:G:239:ASN:HD21	1.52	0.56
1:E:261:ARG:HD3	1:E:266:GLU:OE2	2.05	0.56
1:G:279:PHE:N	3:G:3231:HOH:O	2.38	0.56
1:B:123:TRP:HE3	1:B:162:VAL:HG21	1.71	0.56
1:C:296:LEU:HD23	1:C:347:TYR:CE1	2.40	0.56
1:A:345:PRO:HB2	1:A:348:THR:HG22	1.88	0.55
1:F:385:LEU:HG	1:F:387:ILE:CD1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:HIS:NE2	1:D:480:LEU:HD11	2.21	0.55
1:H:216:ALA:HB2	3:H:3291:HOH:O	2.06	0.55
1:B:491:LEU:HD23	1:B:494:LYS:HE3	1.89	0.55
1:F:491:LEU:HD23	3:F:1702:HOH:O	2.07	0.55
1:H:129:PRO:HD3	3:H:2123:HOH:O	2.06	0.55
1:A:55:HIS:HE1	3:A:736:HOH:O	1.90	0.55
1:B:363:GLN:NE2	1:B:366:ARG:HH21	2.05	0.54
1:C:240:ALA:HB3	3:C:2465:HOH:O	2.05	0.54
1:G:269:MET:CE	1:G:521:VAL:HG11	2.38	0.54
1:D:127:VAL:HG13	1:D:151:LEU:HD23	1.89	0.54
1:D:37:GLU:HB3	3:D:2127:HOH:O	2.07	0.54
1:A:363:GLN:NE2	1:A:366:ARG:HE	2.06	0.54
1:D:232:ARG:HE	1:D:239:ASN:HD21	1.54	0.54
1:F:320:LYS:HA	1:F:506:VAL:HG13	1.90	0.54
1:B:323:MET:CE	1:B:328:ILE:HD13	2.38	0.54
1:D:45:ASN:HD21	1:D:64:ASN:HD22	1.56	0.54
1:G:296:LEU:HD23	1:G:347:TYR:CD2	2.43	0.53
1:A:324:ASP:OD2	1:A:327:ILE:HD12	2.07	0.53
1:A:55:HIS:CD2	1:A:125:ARG:HH11	2.27	0.53
1:B:286:ILE:HG22	1:B:289:GLU:HB2	1.91	0.53
1:E:55:HIS:HE1	3:E:1549:HOH:O	1.90	0.53
1:H:143:HIS:NE2	1:H:480:LEU:HD11	2.23	0.53
1:A:498:GLN:NE2	3:A:3152:HOH:O	2.40	0.53
1:E:55:HIS:CD2	1:E:125:ARG:HH11	2.26	0.53
1:G:127:VAL:HG12	1:G:150:ILE:CG2	2.39	0.53
1:H:27:ALA:N	1:H:241:LYS:O	2.41	0.53
1:A:276:ILE:HG23	1:A:331:LYS:O	2.08	0.53
1:B:55:HIS:HE1	3:B:1032:HOH:O	1.90	0.53
1:A:407:LEU:HD13	3:A:3197:HOH:O	2.08	0.53
1:C:73:LEU:C	1:C:74:LEU:HD23	2.29	0.53
1:C:349:ASP:CB	3:C:3228:HOH:O	2.54	0.53
1:A:407:LEU:CD1	3:A:3197:HOH:O	2.56	0.53
1:E:353:LEU:HD23	1:E:493:THR:HG22	1.91	0.53
1:A:270:THR:HG23	1:A:516:LEU:HB2	1.91	0.53
1:A:389:LEU:HD22	3:A:3282:HOH:O	2.09	0.53
1:D:482:VAL:CG1	1:D:484:ASP:O	2.57	0.53
1:H:309:PRO:CB	3:H:3206:HOH:O	2.55	0.52
1:B:386:THR:HG22	1:B:415:ASN:CB	2.33	0.52
1:E:130:ASN:HB3	3:E:2203:HOH:O	2.10	0.52
1:A:319:LEU:CG	3:A:3257:HOH:O	2.56	0.52
1:A:499:LEU:CG	3:A:3293:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:PHE:HZ	1:G:387:ILE:CG1	2.23	0.52
1:H:220:LYS:NZ	1:H:246:GLN:HE21	2.07	0.52
1:C:218:THR:CG2	1:C:233:SER:HB2	2.40	0.52
1:F:217:TYR:CE2	1:F:535[A]:THR:OG1	2.61	0.52
1:H:364:GLU:CD	1:H:364:GLU:H	2.13	0.52
1:D:162:VAL:HG13	1:D:172:VAL:HG22	1.92	0.52
1:H:363:GLN:HE21	1:H:366:ARG:HH21	1.57	0.52
1:A:165:ILE:HD11	1:A:171:GLU:CB	2.39	0.52
1:G:162:VAL:CG1	1:G:170:LEU:HD11	2.38	0.52
1:G:328:ILE:HG23	1:G:400:LEU:HD22	1.91	0.52
1:H:479:THR:HA	3:H:3242:HOH:O	2.10	0.52
1:C:349:ASP:O	1:C:449:PRO:HD3	2.10	0.52
1:F:389:LEU:HB2	3:F:3261:HOH:O	2.10	0.52
1:B:399:LYS:NZ	3:B:2260:HOH:O	2.43	0.51
1:F:324:ASP:O	1:F:328:ILE:HD13	2.09	0.51
1:H:491:LEU:HD12	3:H:3242:HOH:O	2.10	0.51
1:A:276:ILE:HD11	1:A:396:LEU:CD1	2.40	0.51
1:C:350:GLY:O	1:C:489:THR:HG22	2.11	0.51
1:F:69:LEU:CD1	3:F:3274:HOH:O	2.59	0.51
1:G:218:THR:HG22	1:G:219:LEU:H	1.75	0.51
1:H:218:THR:HG23	1:H:233:SER:HB2	1.92	0.51
1:E:363:GLN:NE2	1:E:366:ARG:HE	2.09	0.51
1:H:319:LEU:HD12	1:H:408:TRP:CE2	2.45	0.51
1:H:340:ALA:HA	1:H:510:TYR:CE2	2.45	0.51
1:B:386:THR:CG2	1:B:415:ASN:HD22	2.24	0.51
1:G:127:VAL:HG13	1:G:151:LEU:CD2	2.40	0.51
1:A:387:ILE:HG22	1:A:416:VAL:HG13	1.92	0.51
1:F:127:VAL:HG12	1:F:150:ILE:CG2	2.39	0.51
1:C:482:VAL:HG13	1:C:487:GLN:HB2	1.93	0.51
1:F:476:MET:HE2	3:F:3223:HOH:O	2.10	0.51
1:A:384:PRO:HA	3:A:2492:HOH:O	2.09	0.51
1:B:55:HIS:CD2	1:B:125:ARG:HH11	2.28	0.51
1:F:127:VAL:CG1	1:F:127:VAL:O	2.58	0.50
1:G:310:PHE:HZ	1:G:387:ILE:HG13	1.76	0.50
1:C:310:PHE:CE2	3:C:2179:HOH:O	2.64	0.50
1:D:213:THR:OG1	1:D:218:THR:HG23	2.11	0.50
1:E:52:LEU:C	3:E:3239:HOH:O	2.48	0.50
1:E:292:VAL:HG13	1:E:512:VAL:CG1	2.41	0.50
1:G:244:ILE:HD12	1:G:538:MET:HB2	1.94	0.50
1:E:55:HIS:HD2	1:E:125:ARG:HH11	1.59	0.50
1:G:521:VAL:CG2	3:G:3259:HOH:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:482:VAL:HG21	3:H:3242:HOH:O	2.11	0.50
1:C:218:THR:HG21	3:C:1599:HOH:O	2.12	0.50
1:D:38:LYS:O	1:D:540:ILE:HD12	2.11	0.50
1:D:55:HIS:CD2	1:D:125:ARG:HH11	2.30	0.50
1:E:207:GLN:HG3	1:E:208:PRO:HD2	1.93	0.50
1:G:55:HIS:CD2	1:G:125:ARG:HH11	2.30	0.50
1:G:128:ASP:CA	1:G:157:ILE:HD11	2.42	0.50
1:E:261:ARG:CD	1:E:266:GLU:OE2	2.60	0.49
1:H:220:LYS:HZ3	1:H:231:GLU:HG2	1.77	0.49
1:B:323:MET:HE1	1:B:328:ILE:CG1	2.42	0.49
1:E:162:VAL:HG12	1:E:170:LEU:HD11	1.95	0.49
1:H:224:VAL:HG13	3:H:2455:HOH:O	2.12	0.49
1:H:72:GLY:O	1:H:86:VAL:HG23	2.13	0.49
1:H:242:THR:HG21	3:H:1088:HOH:O	2.11	0.49
1:A:69:LEU:O	1:A:213:THR:HB	2.13	0.49
1:D:232:ARG:HE	1:D:239:ASN:ND2	2.10	0.49
1:F:55:HIS:HE1	3:F:1079:HOH:O	1.94	0.49
1:E:67:ARG:NH2	3:E:827:HOH:O	2.45	0.49
1:F:283:LYS:HA	1:F:290:VAL:HG21	1.95	0.49
1:C:55:HIS:CD2	1:C:125:ARG:HH11	2.29	0.49
1:C:59:GLY:HA3	1:C:62:GLU:OE1	2.13	0.49
1:D:274:MET:HE1	1:D:282:LEU:HD13	1.94	0.49
1:G:324:ASP:OD2	1:G:327:ILE:HD12	2.12	0.49
1:C:114:VAL:HG21	1:C:214:ASN:OD1	2.13	0.49
1:C:307:LYS:NZ	3:C:1868:HOH:O	2.38	0.49
1:C:482:VAL:HG11	1:C:484:ASP:O	2.13	0.49
1:G:280:GLN:HE21	1:G:334:ALA:HB2	1.78	0.49
1:A:476:MET:HE2	1:A:495:ALA:CB	2.34	0.48
1:B:345:PRO:HB2	1:B:348[A]:THR:HG23	1.95	0.48
1:C:244:ILE:CD1	1:C:539:TYR:HA	2.43	0.48
3:E:3240:HOH:O	1:F:37:GLU:HG2	2.13	0.48
1:F:400:LEU:HA	3:F:3267:HOH:O	2.12	0.48
1:G:127:VAL:CG2	3:G:3275:HOH:O	2.29	0.48
1:D:261:ARG:HD2	1:D:266:GLU:OE2	2.13	0.48
1:H:73:LEU:CD1	1:H:185:LEU:HD13	2.43	0.48
1:C:310:PHE:CE1	1:C:319:LEU:HD11	2.47	0.48
1:G:53:ASP:O	1:G:57:ILE:CD1	2.59	0.48
1:B:300:TYR:CE1	1:B:505:ILE:HD12	2.49	0.48
1:B:323:MET:CE	1:B:328:ILE:CD1	2.91	0.48
1:C:220:LYS:HB2	1:C:231:GLU:HG3	1.95	0.48
1:G:244:ILE:CD1	1:G:538:MET:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:GLN:HB3	1:H:157:ILE:HG23	1.95	0.48
1:B:69:LEU:O	1:B:213:THR:HB	2.14	0.48
1:H:482:VAL:HG13	1:H:483:THR:N	2.28	0.48
1:G:232:ARG:HE	1:G:239:ASN:ND2	2.12	0.48
1:G:274:MET:HE2	1:G:279:PHE:HD2	1.78	0.48
1:A:521:VAL:CG1	1:A:538:MET:CE	2.92	0.48
1:E:39:GLN:NE2	1:E:540:ILE:HD12	2.29	0.47
1:E:383:LYS:CE	3:G:2188:HOH:O	2.61	0.47
1:G:69:LEU:O	1:G:213:THR:HB	2.14	0.47
1:F:242:THR:HG21	3:F:858:HOH:O	2.12	0.47
1:H:363:GLN:NE2	1:H:366:ARG:HH21	2.12	0.47
1:A:296:LEU:HD23	1:A:347:TYR:CD2	2.49	0.47
1:H:482:VAL:CG2	3:H:3242:HOH:O	2.62	0.47
1:A:269:MET:HG2	1:A:517:VAL:HG13	1.96	0.47
1:C:491:LEU:HD23	1:C:494:LYS:HD2	1.96	0.47
1:E:124:GLN:CB	1:E:157:ILE:HG23	2.42	0.47
1:E:292:VAL:HG13	1:E:512:VAL:HG13	1.95	0.47
1:A:353:LEU:HA	1:A:493:THR:HG22	1.96	0.47
1:B:340:ALA:HA	1:B:510:TYR:CE2	2.50	0.47
1:H:92:ASN:HD22	1:H:95:ALA:H	1.62	0.47
1:G:73:LEU:C	1:G:74:LEU:HD23	2.34	0.47
1:D:127:VAL:HG12	1:D:127:VAL:O	2.15	0.47
1:E:383:LYS:HE2	3:G:2188:HOH:O	2.13	0.47
1:B:323:MET:CE	1:B:328:ILE:HG12	2.44	0.47
1:C:49:VAL:HG22	3:C:3216:HOH:O	2.15	0.47
1:E:409:LYS:HB2	3:E:2517:HOH:O	2.14	0.47
1:G:41:LEU:HD11	1:G:269:MET:CE	2.45	0.47
1:G:73:LEU:O	1:G:74:LEU:HD23	2.15	0.47
1:H:45:ASN:ND2	1:H:64:ASN:HD22	2.13	0.47
1:F:525:THR:O	1:F:527:LYS:NZ	2.38	0.46
1:A:448:GLU:CD	1:A:449:PRO:HD2	2.35	0.46
1:E:277:GLU:HG3	1:E:399:LYS:HZ1	1.80	0.46
1:F:91:ASP:C	3:F:3255:HOH:O	2.52	0.46
1:H:165:ILE:HD12	1:H:165:ILE:N	2.31	0.46
1:A:217:TYR:CZ	1:A:535:THR:HG22	2.51	0.46
1:B:485:GLU:OE2	1:B:488:ARG:NH1	2.49	0.46
1:D:55:HIS:HD2	1:D:125:ARG:HH11	1.63	0.46
1:E:399:LYS:NZ	3:E:2097:HOH:O	2.35	0.46
1:A:405:SER:N	3:A:3282:HOH:O	2.48	0.46
1:H:39:GLN:HA	1:H:540:ILE:HD13	1.98	0.46
1:H:482:VAL:HG21	1:H:487:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HD12	1:A:165:ILE:H	1.81	0.46
1:D:117:GLN:HG3	3:D:2160:HOH:O	2.16	0.46
1:F:123:TRP:HE3	1:F:162:VAL:HG21	1.81	0.46
1:G:127:VAL:CG1	3:G:3275:HOH:O	2.60	0.46
1:A:207:GLN:HG3	1:A:208:PRO:HD2	1.98	0.46
1:E:52:LEU:HD13	1:E:219:LEU:HD22	1.98	0.46
1:E:330:ASN:HB3	3:E:3278:HOH:O	2.15	0.46
1:C:310:PHE:HE1	1:C:319:LEU:CD1	2.28	0.46
1:H:171:GLU:HB3	3:H:2194:HOH:O	2.15	0.46
1:E:165:ILE:CD1	1:E:171:GLU:HB2	2.44	0.46
1:E:363:GLN:HE21	1:E:366:ARG:HH21	1.64	0.46
1:G:428:ASP:HB2	3:G:2431:HOH:O	2.14	0.46
1:B:323:MET:HE3	1:B:328:ILE:HD13	1.98	0.45
1:E:141:TYR:CE2	1:E:454:ASN:HB3	2.51	0.45
1:G:55:HIS:HE1	3:G:2761:HOH:O	1.99	0.45
1:G:276:ILE:HG23	1:G:331:LYS:O	2.17	0.45
1:A:114:VAL:HG21	1:A:214[A]:ASN:OD1	2.16	0.45
1:D:482:VAL:HG22	1:D:487:GLN:HB3	1.97	0.45
1:F:286:ILE:CG2	1:F:289:GLU:CD	2.84	0.45
1:B:49:VAL:HG11	1:B:65:ILE:HD12	1.98	0.45
1:D:319:LEU:HD12	1:D:408:TRP:CE2	2.51	0.45
1:E:482:VAL:CG1	1:E:484:ASP:O	2.64	0.45
1:A:352:LYS:O	1:A:493:THR:HG21	2.17	0.45
1:D:482:VAL:HG11	1:D:484:ASP:O	2.16	0.45
1:A:67:ARG:NH2	3:A:3030:HOH:O	2.49	0.45
1:C:456:MET:CA	3:C:3252:HOH:O	2.59	0.45
1:F:45:ASN:ND2	1:F:64:ASN:HD22	2.13	0.45
1:F:232:ARG:HE	1:F:239:ASN:HD21	1.65	0.45
1:F:340:ALA:HA	1:F:510:TYR:CE2	2.52	0.45
1:A:385:LEU:HG	1:A:387:ILE:CD1	2.46	0.45
1:F:428:ASP:CG	1:F:432:GLN:HE21	2.19	0.45
1:G:220:LYS:HZ1	1:G:246:GLN:NE2	1.87	0.45
1:B:444:ALA:HB3	1:B:530:LEU:CD2	2.47	0.45
1:C:193:VAL:HG13	1:C:198:ILE:HD11	1.86	0.45
1:G:147:ILE:HD12	1:G:148:ASP:N	2.32	0.45
1:G:261:ARG:HD3	1:G:266:GLU:OE2	2.16	0.45
1:G:320:LYS:NZ	1:G:500:ASP:O	2.50	0.45
1:C:141:TYR:CE1	1:C:454:ASN:HB3	2.51	0.45
1:D:409:LYS:HZ3	1:D:415:ASN:HA	1.82	0.45
1:F:127:VAL:CG1	1:F:150:ILE:CG2	2.92	0.45
1:G:212:VAL:HG11	3:G:2550:HOH:O	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:VAL:HG11	1:H:181:PHE:CZ	2.51	0.45
1:A:422:GLU:HG2	3:A:2751:HOH:O	2.17	0.44
1:F:310:PHE:HZ	1:F:387:ILE:CG1	2.29	0.44
1:B:229:VAL:HG22	1:B:248:THR:HG22	1.99	0.44
1:C:50:GLN:HA	1:C:424:LYS:HD3	1.99	0.44
1:D:59:GLY:HA3	1:D:62:GLU:OE2	2.17	0.44
1:F:27:ALA:HB3	1:F:243:VAL:HG23	1.99	0.44
1:G:292:VAL:HG13	1:G:512:VAL:CG1	2.46	0.44
1:G:385:LEU:HG	1:G:387:ILE:CD1	2.47	0.44
1:G:540:ILE:HG12	3:G:3201:HOH:O	2.16	0.44
1:B:166:ASP:HB3	1:B:168:HIS:H	1.82	0.44
1:D:310:PHE:HZ	1:D:387:ILE:CG2	2.29	0.44
1:F:476:MET:HE1	3:F:3223:HOH:O	2.17	0.44
1:D:350:GLY:O	1:D:489:THR:HG23	2.18	0.44
1:F:127:VAL:HG12	1:F:127:VAL:O	2.17	0.44
1:F:453:LEU:CB	3:F:3223:HOH:O	2.57	0.44
1:G:110:ASP:HB3	1:G:112:THR:HG23	2.00	0.44
1:H:81:HIS:HD2	3:H:2341:HOH:O	2.01	0.44
1:H:352:LYS:O	1:H:493:THR:CG2	2.65	0.44
1:E:103:ARG:HD3	1:E:237:TRP:CD2	2.52	0.44
1:H:39:GLN:NE2	1:H:540:ILE:HD12	2.33	0.44
1:H:349:ASP:O	1:H:449:PRO:HD3	2.17	0.44
1:D:69:LEU:O	1:D:213:THR:HB	2.18	0.44
1:G:109:SER:HA	1:G:235:THR:OG1	2.17	0.44
1:H:123:TRP:HB3	3:H:3244:HOH:O	2.18	0.44
1:B:389:LEU:CD1	1:B:437:VAL:HG12	2.47	0.44
1:F:69:LEU:CG	3:F:3274:HOH:O	2.58	0.44
1:G:218:THR:HG22	1:G:219:LEU:N	2.32	0.44
1:G:321:LEU:HD22	1:G:366:ARG:HG2	1.99	0.44
1:A:147:ILE:HA	1:A:150:ILE:HD12	1.99	0.44
1:B:456:MET:HE2	1:B:499:LEU:HD11	1.98	0.44
1:C:482:VAL:CG1	1:C:484:ASP:O	2.66	0.44
1:G:296:LEU:CD2	1:G:347:TYR:CD2	3.00	0.44
1:A:27:ALA:N	3:A:1804:HOH:O	2.51	0.43
1:A:405:SER:CA	3:A:3282:HOH:O	2.66	0.43
1:G:128:ASP:HA	1:G:157:ILE:CD1	2.47	0.43
1:H:63:SER:HB2	3:H:1280:HOH:O	2.18	0.43
1:A:345:PRO:O	1:A:348:THR:HG22	2.17	0.43
1:F:242:THR:HG22	1:F:536:ARG:HB2	2.00	0.43
1:G:291:HIS:O	1:G:514:ALA:HA	2.18	0.43
1:H:195:LYS:HB3	3:H:1528:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:TYR:CD1	1:B:505:ILE:HG23	2.53	0.43
1:C:310:PHE:HD2	3:C:2179:HOH:O	1.93	0.43
1:D:296:LEU:HD23	1:D:347:TYR:CE2	2.53	0.43
1:F:347[A]:TYR:CD1	1:F:347[A]:TYR:N	2.85	0.43
1:E:296:LEU:HD12	1:E:530:LEU:CD1	2.49	0.43
1:G:521:VAL:HG22	3:G:3201:HOH:O	2.17	0.43
1:H:165:ILE:N	1:H:165:ILE:CD1	2.81	0.43
1:E:124:GLN:CG	1:E:157:ILE:HG23	2.48	0.43
1:E:349:ASP:O	1:E:449:PRO:HD3	2.17	0.43
1:G:340:ALA:HA	1:G:510:TYR:CE2	2.54	0.43
1:C:176:GLU:HG3	1:C:177:PRO:HD2	2.00	0.43
1:E:109:SER:HA	1:E:235:THR:OG1	2.18	0.43
1:G:136:ALA:O	3:G:3275:HOH:O	2.21	0.43
1:E:269:MET:HG3	3:E:1154:HOH:O	2.17	0.43
1:G:127:VAL:CB	3:G:3275:HOH:O	2.61	0.43
1:A:485:GLU:OE2	1:A:488:ARG:NH1	2.52	0.43
1:F:256:VAL:HG13	1:F:278:LEU:HD11	2.00	0.43
1:F:278:LEU:O	1:F:282:LEU:HG	2.19	0.43
1:F:500:ASP:HB3	3:F:1241:HOH:O	2.19	0.43
1:H:60:VAL:N	1:H:61:PRO:CD	2.82	0.43
1:H:277:GLU:HG3	1:H:399:LYS:NZ	2.34	0.43
1:A:405:SER:HA	3:A:3282:HOH:O	2.19	0.42
1:B:68:ASP:OD2	1:B:535:THR:HG23	2.19	0.42
1:C:472:PHE:CZ	3:C:3252:HOH:O	2.52	0.42
1:D:69:LEU:HD21	1:D:230:LEU:HD22	2.00	0.42
1:H:143:HIS:CE1	1:H:480:LEU:HD11	2.53	0.42
1:H:261:ARG:HD2	1:H:266:GLU:OE2	2.18	0.42
1:F:409:LYS:HG3	3:F:2305:HOH:O	2.18	0.42
1:G:488:ARG:NH2	3:G:2501:HOH:O	2.52	0.42
1:H:59:GLY:HA3	1:H:62:GLU:OE1	2.20	0.42
1:H:97:VAL:HG13	3:H:2194:HOH:O	2.18	0.42
1:A:207:GLN:O	1:A:208:PRO:C	2.57	0.42
1:A:490:ALA:O	1:A:493:THR:OG1	2.28	0.42
1:C:310:PHE:CE1	1:C:319:LEU:CD1	3.03	0.42
1:F:68:ASP:OD2	1:F:535[A]:THR:HG23	2.19	0.42
1:G:163:LYS:HD3	3:G:2241:HOH:O	2.18	0.42
1:H:121:TYR:CB	1:H:195:LYS:HZ2	2.33	0.42
1:E:313:VAL:HG11	1:G:314:ARG:HD2	2.02	0.42
1:F:387:ILE:HG22	1:F:416:VAL:HG13	2.00	0.42
1:C:127:VAL:HG12	1:C:127:VAL:O	2.19	0.42
1:C:193:VAL:HG13	1:C:194:PRO:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ARG:HG3	1:E:242:THR:HG21	2.01	0.42
1:F:279:PHE:HB2	3:F:3260:HOH:O	2.19	0.42
1:H:128:ASP:HA	1:H:157:ILE:CD1	2.46	0.42
3:A:2316:HOH:O	1:C:313:VAL:HG22	2.19	0.42
1:B:300:TYR:HD1	1:B:505:ILE:HG23	1.85	0.42
1:F:277:GLU:HB2	3:F:2128:HOH:O	2.19	0.42
1:F:386:THR:HG22	1:F:415:ASN:ND2	2.31	0.42
1:A:140:GLN:NE2	3:A:558:HOH:O	2.52	0.42
1:A:296:LEU:CD2	1:A:347:TYR:CD2	3.03	0.42
1:D:110:ASP:HB3	1:D:112:THR:H	1.85	0.42
3:D:3300:HOH:O	2:L:2:UNK:CB	2.68	0.42
1:E:310:PHE:HZ	1:E:387:ILE:CG2	2.33	0.42
1:E:310:PHE:HZ	1:E:387:ILE:HG21	1.84	0.42
1:F:213:THR:HG1	1:F:218:THR:HG22	1.78	0.42
1:H:127:VAL:HG21	1:H:147:ILE:CD1	2.50	0.42
1:B:300:TYR:CD1	1:B:505:ILE:HD12	2.55	0.42
1:F:329:VAL:HG23	1:F:509:TYR:HB3	2.01	0.42
1:A:485:GLU:OE1	1:A:488:ARG:HD2	2.20	0.42
1:C:261:ARG:HB2	1:C:267:ILE:HD12	2.02	0.42
1:D:37:GLU:CB	3:D:2127:HOH:O	2.68	0.42
1:G:127:VAL:HA	3:G:3275:HOH:O	2.19	0.42
1:G:385:LEU:HD11	1:G:387:ILE:HD11	2.02	0.42
1:A:292:VAL:HG13	1:A:512:VAL:HG13	2.01	0.41
1:D:55:HIS:O	1:D:133:SER:HB2	2.19	0.41
1:E:92:ASN:HD22	1:E:95:ALA:H	1.68	0.41
1:E:399:LYS:CE	3:E:2255:HOH:O	2.68	0.41
1:F:117:GLN:NE2	3:F:2475:HOH:O	2.53	0.41
1:G:538:MET:HE1	3:G:2372:HOH:O	2.19	0.41
1:A:323:MET:HE2	1:A:323:MET:HA	2.02	0.41
1:F:386:THR:O	1:F:387:ILE:HD12	2.20	0.41
1:G:51:SER:C	1:G:57:ILE:HD11	2.40	0.41
1:G:60:VAL:N	1:G:61:PRO:CD	2.83	0.41
1:G:385:LEU:HG	1:G:387:ILE:HD13	2.02	0.41
1:H:274:MET:CE	1:H:279:PHE:HD2	2.33	0.41
1:A:310:PHE:CE1	3:A:3257:HOH:O	2.57	0.41
1:B:310:PHE:HZ	1:B:387:ILE:HG21	1.85	0.41
1:D:273:SER:HB3	3:D:600:HOH:O	2.21	0.41
1:E:69:LEU:O	1:E:213:THR:HB	2.20	0.41
1:A:127:VAL:O	1:A:127:VAL:HG12	2.20	0.41
1:F:55:HIS:CD2	1:F:125:ARG:HH21	2.38	0.41
1:F:367:ASN:O	1:F:370:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:454:ASN:N	3:F:3223:HOH:O	2.54	0.41
1:H:52:LEU:HD12	1:H:222:TRP:CE3	2.56	0.41
1:H:260:ASN:ND2	3:H:1449:HOH:O	2.46	0.41
1:E:363:GLN:NE2	1:E:366:ARG:HH21	2.19	0.41
1:G:461:SER:HB3	3:G:2204:HOH:O	2.20	0.41
1:B:123:TRP:CE3	1:B:162:VAL:HG21	2.52	0.41
1:C:424:LYS:HD2	3:C:756:HOH:O	2.20	0.41
1:F:286:ILE:O	1:F:286:ILE:CG2	2.63	0.41
1:F:330:ASN:HB3	1:F:333:LYS:HZ2	1.86	0.41
1:A:45:ASN:ND2	1:A:64:ASN:HD22	2.19	0.41
1:A:166:ASP:HB2	3:A:1863:HOH:O	2.21	0.41
1:B:123:TRP:O	1:B:126[A]:SER:HB3	2.20	0.41
1:C:50:GLN:HG2	1:C:424:LYS:HD2	2.03	0.41
1:D:276:ILE:HG12	1:D:332:VAL:HG12	2.03	0.41
1:G:274:MET:HE3	1:G:282:LEU:CD1	2.51	0.41
1:H:92:ASN:HD22	1:H:95:ALA:HA	1.85	0.41
1:F:196:ALA:HB3	3:F:1857:HOH:O	2.21	0.41
1:G:168:HIS:CD2	3:G:958:HOH:O	2.74	0.41
1:H:150:ILE:CG2	1:H:157:ILE:HD12	2.44	0.41
1:H:236:TYR:CE1	3:H:3291:HOH:O	2.71	0.41
1:A:165:ILE:CD1	1:A:171:GLU:HB2	2.47	0.40
1:B:324:ASP:CG	1:B:327:ILE:HD13	2.41	0.40
1:C:280:GLN:NE2	3:C:3302:HOH:O	2.51	0.40
1:C:350:GLY:O	1:C:489:THR:CG2	2.69	0.40
1:E:127:VAL:HG13	1:E:150:ILE:CG2	2.52	0.40
1:A:340:ALA:HA	1:A:510:TYR:CE2	2.56	0.40
1:B:28:ASP:OD1	1:B:241:LYS:NZ	2.44	0.40
1:C:317:THR:HG21	3:C:621:HOH:O	2.21	0.40
1:E:340:ALA:HA	1:E:510:TYR:CE2	2.56	0.40
1:B:286:ILE:CG2	1:B:289:GLU:HB2	2.51	0.40
1:B:386:THR:HG22	1:B:415:ASN:ND2	2.33	0.40
1:E:313:VAL:HG12	1:G:313:VAL:HG12	2.04	0.40
1:F:540:ILE:N	1:F:540:ILE:HD12	2.36	0.40
1:H:352:LYS:HG3	3:H:2487:HOH:O	2.21	0.40
1:B:217:TYR:CE2	1:B:535:THR:OG1	2.75	0.40
1:B:286:ILE:HG21	1:B:289:GLU:CD	2.42	0.40
1:D:55:HIS:O	1:D:133:SER:CB	2.69	0.40
1:G:42:VAL:HG22	1:G:248:THR:HB	2.02	0.40
1:H:195:LYS:HG3	3:H:2094:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	A	517/524 (99%)	500 (97%)	15 (3%)	2 (0%)	30	27
1	B	517/524 (99%)	504 (98%)	12 (2%)	1 (0%)	44	42
1	C	516/524 (98%)	497 (96%)	18 (4%)	1 (0%)	44	42
1	D	516/524 (98%)	501 (97%)	14 (3%)	1 (0%)	44	42
1	E	517/524 (99%)	500 (97%)	16 (3%)	1 (0%)	44	42
1	F	519/524 (99%)	503 (97%)	15 (3%)	1 (0%)	44	42
1	G	517/524 (99%)	503 (97%)	13 (2%)	1 (0%)	44	42
1	H	516/524 (98%)	498 (96%)	16 (3%)	2 (0%)	30	27
All	All	4135/4192 (99%)	4006 (97%)	119 (3%)	10 (0%)	44	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	PRO
1	F	251	PRO
1	G	251	PRO
1	A	251	PRO
1	A	394	SER
1	C	251	PRO
1	E	251	PRO
1	H	251	PRO
1	H	394	SER
1	D	251	PRO

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	A	453/458 (99%)	442 (98%)	11 (2%)	44	47
1	B	453/458 (99%)	444 (98%)	9 (2%)	50	55
1	C	452/458 (99%)	447 (99%)	5 (1%)	70	76
1	D	452/458 (99%)	437 (97%)	15 (3%)	33	33
1	E	453/458 (99%)	446 (98%)	7 (2%)	60	66
1	F	455/458 (99%)	447 (98%)	8 (2%)	54	59
1	G	453/458 (99%)	441 (97%)	12 (3%)	41	44
1	H	452/458 (99%)	437 (97%)	15 (3%)	33	33
All	All	3623/3664 (99%)	3541 (98%)	82 (2%)	47	49

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	208	PRO
1	A	314	ARG
1	A	344	THR
1	A	348	THR
1	A	405	SER
1	A	439	ARG
1	A	474	SER
1	A	494	LYS
1	A	512	VAL
1	A	513	ASN
1	B	110	ASP
1	B	208	PRO
1	B	327	ILE
1	B	329	VAL
1	B	372	LYS
1	B	383	LYS
1	B	394	SER
1	B	439	ARG
1	B	474	SER
1	C	113	PRO
1	C	218	THR
1	C	346	PRO
1	C	439	ARG

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Mol	Chain	Res	Type
1	C	481	LYS
1	D	38	LYS
1	D	91	ASP
1	D	110	ASP
1	D	162	VAL
1	D	165	ILE
1	D	176	GLU
1	D	177	PRO
1	D	218	THR
1	D	233	SER
1	D	314	ARG
1	D	439	ARG
1	D	482	VAL
1	D	484	ASP
1	D	493	THR
1	D	513	ASN
1	E	91	ASP
1	E	127	VAL
1	E	176	GLU
1	E	220	LYS
1	E	357	GLU
1	E	439	ARG
1	E	513	ASN
1	F	38	LYS
1	F	157	ILE
1	F	329	VAL
1	F	347[A]	TYR
1	F	347[B]	TYR
1	F	396	LEU
1	F	439	ARG
1	F	512	VAL
1	G	38	LYS
1	G	57	ILE
1	G	110	ASP
1	G	133[A]	SER
1	G	133[B]	SER
1	G	157	ILE
1	G	221	ASP
1	G	255	GLU
1	G	406	SER
1	G	439	ARG
1	G	482	VAL

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Mol	Chain	Res	Type
1	G	512	VAL
1	H	91	ASP
1	H	99	THR
1	H	157	ILE
1	H	169	THR
1	H	203	GLU
1	H	208	PRO
1	H	221	ASP
1	H	233	SER
1	H	307	LYS
1	H	328	ILE
1	H	439	ARG
1	H	482	VAL
1	H	484	ASP
1	H	512	VAL
1	H	513	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	45	ASN
1	A	55	HIS
1	A	140	GLN
1	A	239	ASN
1	A	337	ASN
1	A	363	GLN
1	A	513	ASN
1	B	55	HIS
1	B	271	ASN
1	B	305	ASN
1	B	363	GLN
1	B	415	ASN
1	B	420	ASN
1	C	55	HIS
1	C	280	GLN
1	C	305	ASN
1	C	335	GLN
1	D	39	GLN
1	D	45	ASN
1	D	55	HIS
1	D	92	ASN

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Mol	Chain	Res	Type
1	D	140	GLN
1	D	239	ASN
1	D	246	GLN
1	D	363	GLN
1	D	513	ASN
1	E	39	GLN
1	E	45	ASN
1	E	55	HIS
1	E	92	ASN
1	E	239	ASN
1	E	305	ASN
1	E	363	GLN
1	E	432	GLN
1	E	487	GLN
1	E	513	ASN
1	F	39	GLN
1	F	45	ASN
1	F	55	HIS
1	F	117	GLN
1	F	140	GLN
1	F	239	ASN
1	F	246	GLN
1	F	305	ASN
1	F	363	GLN
1	F	432	GLN
1	F	513	ASN
1	G	39	GLN
1	G	45	ASN
1	G	55	HIS
1	G	140	GLN
1	G	207	GLN
1	G	239	ASN
1	G	246	GLN
1	G	280	GLN
1	G	363	GLN
1	G	432	GLN
1	G	513	ASN
1	H	39	GLN
1	H	45	ASN
1	H	92	ASN
1	H	140	GLN
1	H	239	ASN

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Mol	Chain	Res	Type
1	H	246	GLN
1	H	363	GLN
1	H	466	HIS
1	H	513	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	517/524 (98%)	0.08	6 (1%) 76 75	8, 22, 36, 51	2 (0%)
1	B	517/524 (98%)	0.35	22 (4%) 40 38	9, 28, 47, 61	2 (0%)
1	C	517/524 (98%)	0.36	13 (2%) 58 57	12, 29, 42, 53	1 (0%)
1	D	517/524 (98%)	0.38	11 (2%) 63 62	13, 30, 42, 53	1 (0%)
1	E	517/524 (98%)	0.17	6 (1%) 76 75	10, 25, 36, 44	2 (0%)
1	F	517/524 (98%)	0.29	13 (2%) 58 57	9, 25, 41, 57	4 (0%)
1	G	517/524 (98%)	0.59	30 (5%) 30 28	11, 30, 51, 64	2 (0%)
1	H	517/524 (98%)	1.30	125 (24%) 2 2	22, 38, 67, 79	1 (0%)
2	I	0/3	-	-	-	-
2	J	0/3	-	-	-	-
2	K	0/3	-	-	-	-
2	L	0/3	-	-	-	-
2	M	0/3	-	-	-	-
2	N	0/3	-	-	-	-
2	O	0/3	-	-	-	-
2	P	0/3	-	-	-	-
All	All	4136/4216 (98%)	0.44	226 (5%) 32 30	8, 28, 48, 79	15 (0%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	126[A]	SER	6.2
1	H	97	VAL	6.0
1	H	193	VAL	5.5
1	H	209	GLY	4.5
1	D	330	ASN	4.4
1	H	482	VAL	4.4
1	H	86	VAL	4.2
1	H	484	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	347	TYR	4.0
1	H	162	VAL	4.0
1	H	223	VAL	3.9
1	B	284	LYS	3.8
1	E	484	ASP	3.8
1	H	147	ILE	3.8
1	H	145	ALA	3.7
1	H	93	LYS	3.7
1	H	169	THR	3.7
1	H	191	SER	3.7
1	H	96	LYS	3.7
1	H	196	ALA	3.7
1	H	120	VAL	3.6
1	H	218	THR	3.6
1	G	333	LYS	3.6
1	H	122	SER	3.5
1	C	482	VAL	3.5
1	F	347[A]	TYR	3.4
1	H	141	TYR	3.4
1	H	102	LEU	3.4
1	H	119	PHE	3.4
1	H	486	ALA	3.3
1	E	330	ASN	3.3
1	H	170	LEU	3.3
1	H	173	THR	3.3
1	H	479	THR	3.3
1	H	144	ILE	3.3
1	H	165	ILE	3.3
1	B	370	ALA	3.3
1	G	286	ILE	3.2
1	H	178	VAL	3.2
1	H	99	THR	3.2
1	H	192	PRO	3.2
1	H	230	LEU	3.2
1	H	354	THR	3.2
1	H	166	ASP	3.2
1	H	74	LEU	3.2
1	H	208	PRO	3.2
1	H	90	TRP	3.1
1	H	129	PRO	3.1
1	H	483	THR	3.1
1	B	278	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	457	LEU	3.1
1	H	216	ALA	3.1
1	H	98	TRP	3.1
1	H	168	HIS	3.1
1	H	116	ALA	3.1
1	H	157	ILE	3.1
1	G	110	ASP	3.1
1	H	95	ALA	3.0
1	H	150	ILE	3.0
1	D	117	GLN	3.0
1	H	491	LEU	3.0
1	H	100	PHE	3.0
1	G	284	LYS	3.0
1	H	180	TYR	2.9
1	H	215	GLY	2.9
1	G	212	VAL	2.9
1	H	103	ARG	2.9
1	H	108	TRP	2.9
1	H	194	PRO	2.9
1	B	334	ALA	2.9
1	H	201	PHE	2.9
1	H	177	PRO	2.8
1	G	543	HIS	2.8
1	D	406	SER	2.8
1	G	540	ILE	2.8
1	G	37	GLU	2.8
1	H	143	HIS	2.8
1	C	489	THR	2.8
1	C	330	ASN	2.7
1	H	197	ALA	2.7
1	C	540	ILE	2.7
1	H	112	THR	2.7
1	H	127	VAL	2.7
1	A	326	ASP	2.7
1	H	113	PRO	2.7
1	H	353	LEU	2.7
1	H	198	ILE	2.7
1	H	221	ASP	2.7
1	H	428	ASP	2.7
1	H	475	ILE	2.7
1	H	171	GLU	2.6
1	F	278	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	146	GLY	2.6
1	G	262	TYR	2.6
1	G	334	ALA	2.6
1	C	117	GLN	2.6
1	G	432	GLN	2.6
1	B	322	GLY	2.6
1	D	329	VAL	2.6
1	B	166	ASP	2.6
1	D	484	ASP	2.6
1	H	94	ASP	2.6
1	A	330	ASN	2.6
1	H	117	GLN	2.6
1	B	381	ALA	2.5
1	H	107	LYS	2.5
1	H	156	PRO	2.5
1	H	89	SER	2.5
1	H	210	ASN	2.5
1	H	27	ALA	2.5
1	A	37	GLU	2.5
1	D	526	GLY	2.5
1	H	375	ALA	2.5
1	F	126[A]	SER	2.4
1	E	428	ASP	2.4
1	G	428	ASP	2.4
1	H	487	GLN	2.4
1	B	375	ALA	2.4
1	F	375	ALA	2.4
1	H	240	ALA	2.4
1	B	354	THR	2.4
1	G	218	THR	2.4
1	H	235	THR	2.4
1	G	541	VAL	2.4
1	C	333	LYS	2.4
1	F	284	LYS	2.4
1	G	220	LYS	2.4
1	H	155	LYS	2.4
1	B	276	ILE	2.4
1	H	142	GLY	2.4
1	C	221	ASP	2.4
1	H	158	THR	2.4
1	B	409	LYS	2.4
1	H	200	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	188	PRO	2.4
1	H	70	PHE	2.4
1	B	364	GLU	2.4
1	B	484	ASP	2.4
1	D	487	GLN	2.4
1	H	146	GLY	2.4
1	G	33	VAL	2.3
1	H	172	VAL	2.3
1	F	373	LEU	2.3
1	G	409	LYS	2.3
1	H	481	LYS	2.3
1	C	483	THR	2.3
1	G	354	THR	2.3
1	H	363	GLN	2.3
1	B	542	LYS	2.3
1	F	282	LEU	2.3
1	G	282	LEU	2.3
1	F	380	THR	2.3
1	H	330	ASN	2.3
1	G	390	LEU	2.3
1	H	190	THR	2.3
1	H	477	ALA	2.3
1	H	493	THR	2.3
1	C	356	PRO	2.2
1	H	346	PRO	2.2
1	H	488	ARG	2.2
1	C	338	MET	2.2
1	H	151	LEU	2.2
1	H	160	LEU	2.2
1	B	34	THR	2.2
1	B	386	THR	2.2
1	C	493	THR	2.2
1	H	115	THR	2.2
1	G	31	ALA	2.2
1	F	409	LYS	2.2
1	H	365	LYS	2.2
1	B	257	THR	2.2
1	H	189	SER	2.2
1	H	163	LYS	2.2
1	G	202	GLY	2.2
1	H	85	GLY	2.2
1	H	187	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	2.2
1	B	347	TYR	2.2
1	H	164	ALA	2.2
1	C	526	GLY	2.2
1	H	130	ASN	2.2
1	D	280	GLN	2.2
1	E	37	GLU	2.1
1	G	244	ILE	2.1
1	G	516	LEU	2.1
1	H	244	ILE	2.1
1	H	222	TRP	2.1
1	H	460	SER	2.1
1	D	490	ALA	2.1
1	H	492	TYR	2.1
1	C	149	GLU	2.1
1	D	365	LYS	2.1
1	A	483	THR	2.1
1	G	34	THR	2.1
1	H	83	ALA	2.1
1	H	237	TRP	2.1
1	B	167	ASP	2.1
1	H	174	LEU	2.1
1	H	473	ASP	2.1
1	B	384	PRO	2.1
1	F	208	PRO	2.1
1	F	360	GLY	2.1
1	G	111	GLY	2.1
1	H	124	GLN	2.1
1	H	121	TYR	2.1
1	H	203	GLU	2.1
1	H	195	LYS	2.1
1	H	91	ASP	2.1
1	H	110	ASP	2.1
1	A	277	GLU	2.0
1	B	226	GLU	2.0
1	E	347	TYR	2.0
1	H	217	TYR	2.0
1	H	205	TRP	2.0
1	H	60	VAL	2.0
1	H	167	ASP	2.0
1	E	474	SER	2.0
1	G	126[A]	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	280	GLN	2.0
1	G	32	GLY	2.0
1	G	277	GLU	2.0
1	H	367	ASN	2.0
1	F	287	PRO	2.0
1	A	332	VAL	2.0
1	H	247	VAL	2.0
1	F	428	ASP	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.