



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:10 AM EDT

PDB ID : 4PLK
Title : Hepatitis E Virus E2s domain (Genotype I) in complex with a neutralizing antibody 8G12
Authors : Tang, X.H.; Li, S.W.; Sivaraman, J.
Deposited on : 2014-05-18
Resolution : 4.00 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)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

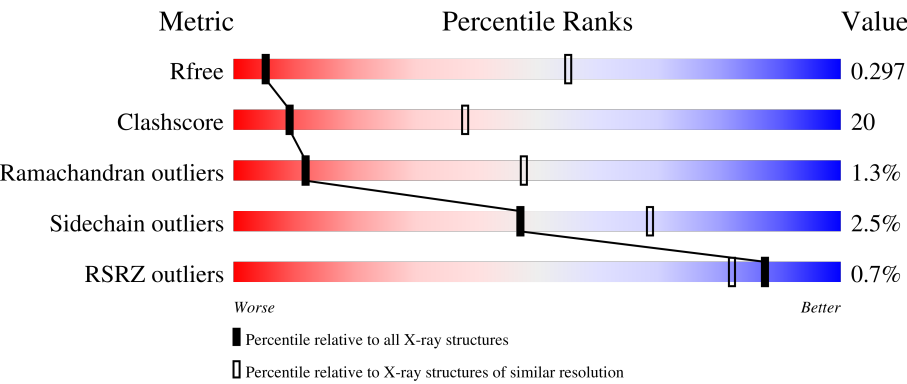
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	147	<div><div></div><div>57%42%</div><div></div></div>
1	B	147	<div><div></div><div>67%32%</div><div></div></div>
1	E	147	<div><div>%</div><div></div><div>64%35%</div><div></div></div>
1	F	147	<div><div></div><div>55%44%</div><div></div></div>
2	C	212	<div><div></div><div>46%42%</div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	212	<div><div></div><div>58%32%7%</div></div>
2	K	212	<div><div></div><div>62%33%</div></div>
2	L	212	<div><div>2%</div><div></div><div>61%34%</div></div>
3	D	229	<div><div>2%</div><div></div><div>65%29%5%</div></div>
3	H	229	<div><div></div><div>63%29%6%</div></div>
3	I	229	<div><div>%</div><div></div><div>64%26%5%</div></div>
3	J	229	<div><div></div><div>66%27%6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17362 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 Capsid protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	0	0	0
			1104	702	186	216			
1	B	147	Total	C	N	O	0	0	0
			1104	702	186	216			
1	E	147	Total	C	N	O	0	0	0
			1104	702	186	216			
1	F	147	Total	C	N	O	0	0	0
			1104	702	186	216			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	PRO	-	expression tag	UNP L0L7P5
A	605	PRO	-	expression tag	UNP L0L7P5
B	604	PRO	-	expression tag	UNP L0L7P5
B	605	PRO	-	expression tag	UNP L0L7P5
E	604	PRO	-	expression tag	UNP L0L7P5
E	605	PRO	-	expression tag	UNP L0L7P5
F	604	PRO	-	expression tag	UNP L0L7P5
F	605	PRO	-	expression tag	UNP L0L7P5

- Molecule 2 is a protein called 8G12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	208	Total	C	N	O	S	0	0	0
			1618	1010	271	331	6			
2	C	198	Total	C	N	O	S	0	0	0
			1533	959	257	312	5			
2	K	208	Total	C	N	O	S	0	0	0
			1618	1010	271	331	6			
2	G	198	Total	C	N	O	S	0	0	0
			1531	957	257	312	5			

- Molecule 3 is a protein called 8G12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1654	1056	271	320	7			
3	D	218	Total	C	N	O	S	0	0	0
			1669	1064	274	324	7			
3	J	216	Total	C	N	O	S	0	0	0
			1654	1056	271	320	7			
3	I	218	Total	C	N	O	S	0	0	0
			1669	1064	274	324	7			

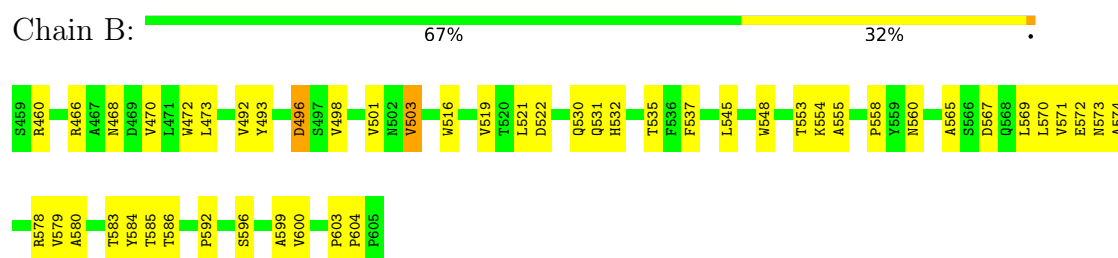
3 Residue-property plots

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.

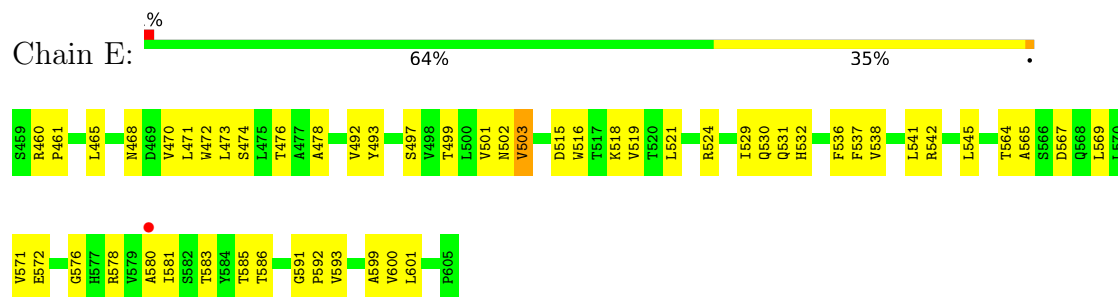
• Molecule 1: Capsid protein



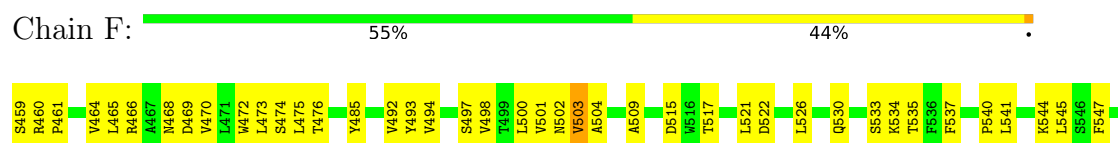
• Molecule 1: Capsid protein

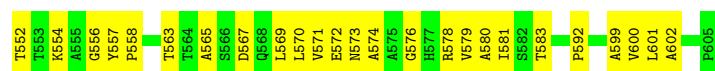


• Molecule 1: Capsid protein

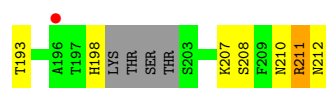
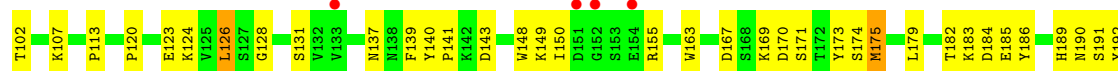


• Molecule 1: Capsid protein

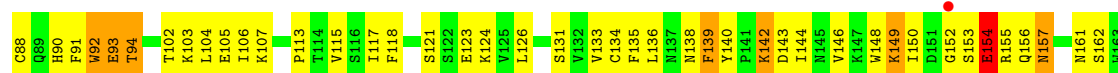
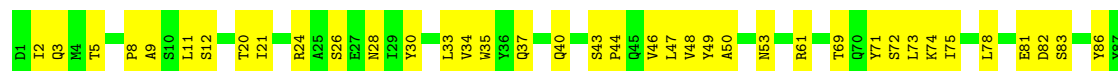




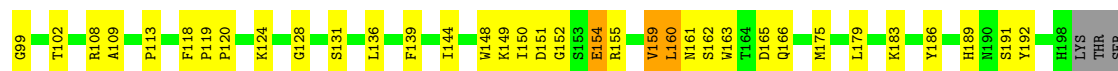
• Molecule 2: 8G12 light chain



• Molecule 2: 8G12 light chain

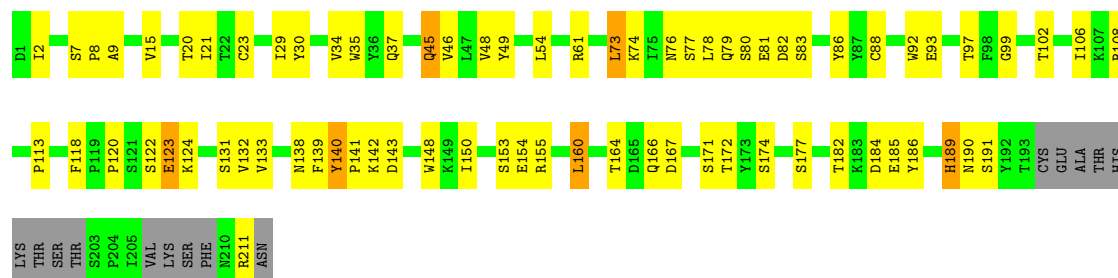


• Molecule 2: 8G12 light chain



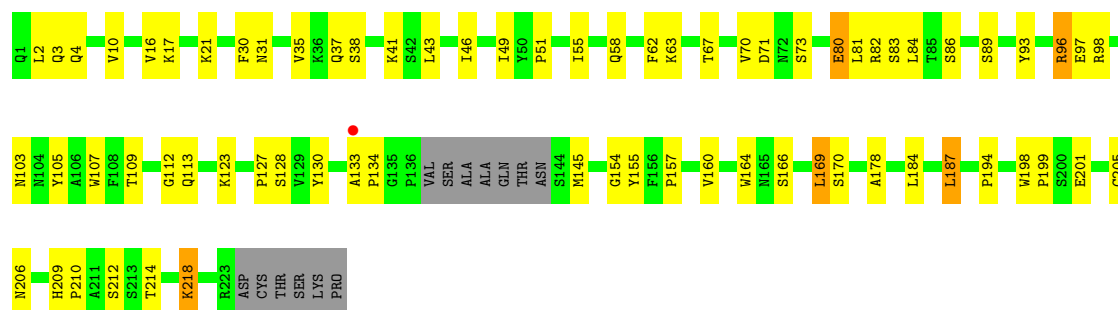
• Molecule 2: 8G12 light chain





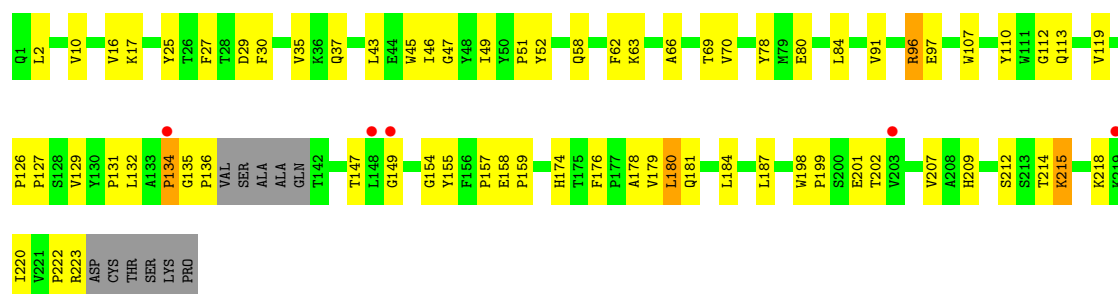
• Molecule 3: 8G12 heavy chain

Chain H: 63% 29% 6%



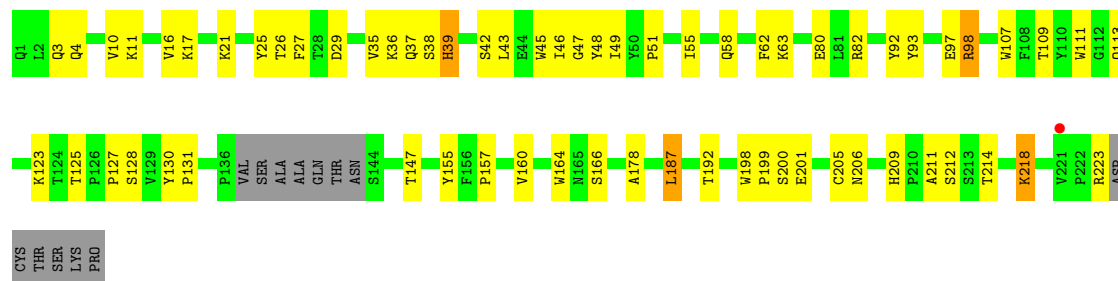
• Molecule 3: 8G12 heavy chain

Chain D: 2% 65% 29% 5%

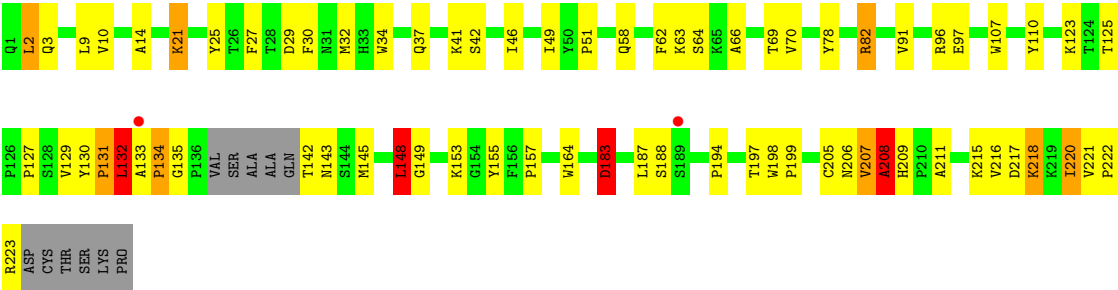


• Molecule 3: 8G12 heavy chain

Chain J: 66% 27% 6%



• Molecule 3: 8G12 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.20Å 191.99Å 192.58Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	33.99 – 4.00 33.99 – 3.90	Depositor EDS
% Data completeness (in resolution range)	91.2 (33.99-4.00) 79.8 (33.99-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.264 , 0.296 0.271 , 0.297	Depositor DCC
R_{free} test set	1971 reflections (6.20%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.378 for -h,l,k 0.379 for -h,-l,-k 0.399 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	17362	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.29	0/1131	0.62	0/1552
1	B	0.30	0/1131	0.61	0/1552
1	E	0.32	0/1131	0.66	1/1552 (0.1%)
1	F	0.31	0/1131	0.65	0/1552
2	C	0.36	0/1567	0.84	3/2126 (0.1%)
2	G	0.37	0/1565	0.87	2/2122 (0.1%)
2	K	0.34	0/1655	0.81	4/2246 (0.2%)
2	L	0.33	0/1655	0.76	3/2246 (0.1%)
3	D	0.34	0/1717	0.73	2/2346 (0.1%)
3	H	0.28	0/1702	0.63	2/2325 (0.1%)
3	I	0.33	0/1717	0.86	9/2346 (0.4%)
3	J	0.29	0/1702	0.67	1/2325 (0.0%)
All	All	0.32	0/17804	0.74	27/24290 (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
2	C	0	1
2	G	0	1
2	K	0	2
3	I	0	2
All	All	0	6

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	92	TRP	CB-CA-C	-9.47	91.46	110.40
3	I	132	LEU	N-CA-C	9.33	136.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	131	PRO	C-N-CA	8.04	141.80	121.70
3	I	131	PRO	CA-C-N	-7.84	99.96	117.20
3	I	131	PRO	N-CA-C	7.21	130.85	112.10
2	C	152	GLY	N-CA-C	6.79	130.08	113.10
2	K	160	LEU	CA-CB-CG	6.67	130.65	115.30
3	I	220	ILE	N-CA-C	6.60	128.82	111.00
3	I	148	LEU	CA-CB-CG	6.53	130.31	115.30
2	G	140	TYR	C-N-CD	-6.34	106.65	120.60
3	H	187	LEU	CA-CB-CG	6.30	129.80	115.30
3	D	52	TYR	CA-CB-CG	6.24	125.25	113.40
3	J	187	LEU	CA-CB-CG	6.20	129.56	115.30
3	I	132	LEU	N-CA-CB	-6.10	98.20	110.40
2	C	149	LYS	CA-CB-CG	-6.04	100.11	113.40
2	K	92	TRP	CA-CB-CG	5.89	124.88	113.70
2	G	73	LEU	CA-CB-CG	5.53	128.01	115.30
2	K	94	THR	N-CA-C	-5.42	96.35	111.00
3	H	169	LEU	CA-CB-CG	5.39	127.69	115.30
2	L	73	LEU	CA-CB-CG	5.33	127.57	115.30
3	I	131	PRO	CA-C-O	5.33	133.00	120.20
2	C	188	ARG	N-CA-C	-5.28	96.74	111.00
2	L	126	LEU	CA-CB-CG	5.21	127.28	115.30
3	I	183	ASP	CB-CG-OD1	5.20	122.97	118.30
3	D	180	LEU	CA-CB-CG	5.19	127.25	115.30
1	E	576	GLY	N-CA-C	-5.16	100.20	113.10
2	L	81	GLU	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	172	THR	Peptide
2	G	141	PRO	Peptide
3	I	207	VAL	Peptide
3	I	208	ALA	Peptide
2	K	159	VAL	Peptide
2	K	209	PHE	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	1104	0	1092	65	0
1	B	1104	0	1090	53	0
1	E	1104	0	1092	40	0
1	F	1104	0	1092	56	0
2	C	1533	0	1464	103	0
2	G	1531	0	1456	62	0
2	K	1618	0	1544	75	0
2	L	1618	0	1542	95	0
3	D	1669	0	1624	64	0
3	H	1654	0	1611	51	0
3	I	1669	0	1624	64	0
3	J	1654	0	1611	52	0
All	All	17362	0	16842	680	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 20.

All (680) 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:B:554:LYS:CD	2:C:92:TRP:CZ2	2.15	1.27
1:B:554:LYS:HD2	2:C:92:TRP:CE2	1.70	1.24
1:B:554:LYS:CD	2:C:92:TRP:CE2	2.19	1.23
1:B:554:LYS:HD2	2:C:92:TRP:CZ2	1.79	1.16
1:A:554:LYS:HE2	2:L:93:GLU:HG3	1.23	1.15
1:A:554:LYS:HG2	2:L:93:GLU:CG	1.76	1.15
1:A:554:LYS:HG2	2:L:93:GLU:HG2	1.24	1.15
1:B:554:LYS:HD3	2:C:92:TRP:CZ2	1.80	1.11
1:B:554:LYS:CE	2:C:92:TRP:CE2	2.33	1.07
1:B:554:LYS:HE3	2:C:92:TRP:CG	1.94	1.00
1:F:460:ARG:NH2	1:F:464:VAL:O	1.96	0.98
1:A:588:LEU:HA	2:L:93:GLU:OE1	1.63	0.97
1:B:554:LYS:HE3	2:C:93:GLU:HG3	1.44	0.97
1:A:554:LYS:CE	2:L:93:GLU:HG3	1.94	0.96
3:D:2:LEU:HD21	3:D:96:ARG:HH12	1.31	0.96
1:F:501:VAL:HG12	1:F:503:VAL:H	1.32	0.94
2:C:34:VAL:HG21	3:D:107:TRP:HB3	1.48	0.94
1:A:501:VAL:HG12	1:A:503:VAL:H	1.35	0.92
1:B:554:LYS:HD3	2:C:92:TRP:CH2	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:190:ASN:O	2:C:210:ASN:ND2	2.02	0.91
1:E:501:VAL:HG12	1:E:503:VAL:H	1.33	0.90
2:K:2:ILE:HB	2:K:92:TRP:CZ2	2.07	0.89
1:B:501:VAL:HG12	1:B:503:VAL:H	1.37	0.88
1:A:554:LYS:HE2	2:L:93:GLU:CG	2.04	0.87
2:G:20:THR:HG22	2:G:74:LYS:HD3	1.57	0.86
2:G:34:VAL:HG21	3:I:107:TRP:HB3	1.56	0.85
3:I:135:GLY:HA3	3:I:223:ARG:HD3	1.59	0.83
3:H:127:PRO:HB3	3:H:155:TYR:HB3	1.60	0.82
1:B:554:LYS:CE	2:C:93:GLU:HG3	2.08	0.82
1:F:460:ARG:NH1	1:F:461:PRO:O	2.12	0.82
1:E:537:PHE:HB2	1:E:571:VAL:HG23	1.61	0.81
1:B:554:LYS:HE3	2:C:92:TRP:CE2	2.11	0.80
1:A:588:LEU:CA	2:L:93:GLU:OE1	2.29	0.80
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.63	0.80
3:H:96:ARG:HD2	3:H:97:GLU:H	1.45	0.80
2:G:61:ARG:NH1	2:G:77:SER:O	2.16	0.79
2:K:92:TRP:HB3	2:K:93:GLU:OE1	1.82	0.79
2:L:46:VAL:HG21	3:H:107:TRP:HD1	1.48	0.79
3:D:154:GLY:HA2	3:D:184:LEU:HD13	1.64	0.78
1:A:554:LYS:CG	2:L:93:GLU:CG	2.61	0.78
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.17	0.77
2:L:189:HIS:HD2	2:L:190:ASN:H	1.30	0.77
2:C:75:ILE:HD13	2:C:78:LEU:HD13	1.65	0.77
1:B:554:LYS:HD2	2:C:92:TRP:NE1	2.00	0.76
3:H:96:ARG:HD2	3:H:97:GLU:N	2.00	0.76
1:B:554:LYS:HE3	2:C:92:TRP:CD1	2.20	0.75
1:E:585:THR:HG22	1:E:586:THR:H	1.50	0.75
1:B:473:LEU:HD11	1:B:569:LEU:HD21	1.67	0.75
1:A:554:LYS:HG2	2:L:93:GLU:HG3	1.65	0.74
1:F:592:PRO:HG2	3:I:58:GLN:HG3	1.68	0.74
2:K:6:GLN:HE21	2:K:102:THR:HG23	1.52	0.73
3:H:166:SER:H	3:H:206:ASN:HD21	1.36	0.73
3:I:216:VAL:HG12	3:I:218:LYS:HE3	1.70	0.73
3:J:200:SER:OG	3:J:201:GLU:OE1	2.06	0.73
2:C:93:GLU:O	2:C:94:THR:O	2.07	0.72
2:L:124:LYS:HE3	2:L:131:SER:H	1.54	0.72
2:C:148:TRP:HZ3	2:C:179:LEU:HB2	1.54	0.72
1:E:572:GLU:OE2	1:E:578:ARG:N	2.23	0.72
1:F:570:LEU:HB2	1:F:580:ALA:HB3	1.70	0.71
2:C:133:VAL:HG11	3:D:132:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TRP:HH2	1:B:468:ASN:HD22	1.38	0.71
3:D:131:PRO:HB3	3:D:220:ILE:HD12	1.72	0.71
2:K:148:TRP:HB2	2:K:155:ARG:HG3	1.72	0.71
1:A:534:LYS:HD2	1:A:535:THR:H	1.54	0.71
1:E:545:LEU:HB2	1:E:567:ASP:OD2	1.90	0.71
2:K:119:PRO:HB3	2:K:209:PHE:HE1	1.54	0.71
2:K:155:ARG:HH12	2:K:179:LEU:HD22	1.56	0.71
2:K:165:ASP:OD1	2:K:166:GLN:N	2.24	0.71
1:F:535:THR:HG23	1:F:573:ASN:HB3	1.72	0.71
1:E:592:PRO:HG2	3:J:58:GLN:HG3	1.72	0.70
2:C:174:SER:HB2	3:D:174:HIS:NE2	2.06	0.70
3:D:97:GLU:CD	3:D:97:GLU:H	1.94	0.70
1:E:564:THR:OG1	1:F:554:LYS:NZ	2.24	0.70
1:E:472:TRP:HH2	1:F:468:ASN:HD22	1.38	0.69
2:C:148:TRP:O	2:C:149:LYS:HD2	1.92	0.69
2:K:61:ARG:NH1	2:K:82:ASP:OD2	2.26	0.69
1:A:554:LYS:CG	2:L:93:GLU:HG2	2.14	0.68
2:L:61:ARG:HH22	2:L:82:ASP:CG	1.97	0.68
3:H:67:THR:HB	3:H:80:GLU:HG2	1.76	0.68
2:G:164:THR:HG22	2:G:174:SER:H	1.59	0.68
3:I:132:LEU:HD23	3:I:148:LEU:HD21	1.76	0.68
1:F:492:VAL:HG11	1:F:580:ALA:HB1	1.76	0.68
3:I:127:PRO:HB3	3:I:155:TYR:HB3	1.74	0.68
1:B:545:LEU:HD12	1:B:599:ALA:HB2	1.75	0.68
1:B:492:VAL:HG11	1:B:580:ALA:HB1	1.74	0.67
1:F:592:PRO:HG3	3:I:63:LYS:HD3	1.76	0.67
3:J:127:PRO:HB3	3:J:155:TYR:HB3	1.75	0.67
2:C:46:VAL:HG21	3:D:107:TRP:HD1	1.60	0.67
2:G:166:GLN:NE2	2:G:167:ASP:OD1	2.28	0.67
2:C:37:GLN:HG2	2:C:47:LEU:HG	1.75	0.67
1:A:554:LYS:CG	2:L:93:GLU:HG3	2.21	0.67
2:L:61:ARG:HH21	2:L:78:LEU:HA	1.56	0.67
3:I:206:ASN:ND2	3:I:217:ASP:OD1	2.14	0.67
1:A:492:VAL:HG11	1:A:580:ALA:HB1	1.77	0.66
2:L:189:HIS:CD2	2:L:190:ASN:H	2.13	0.66
2:L:21:ILE:HB	2:L:73:LEU:HG	1.76	0.66
2:C:61:ARG:NH1	2:C:82:ASP:OD2	2.28	0.66
1:F:472:TRP:HB3	1:F:501:VAL:HB	1.78	0.66
1:A:545:LEU:HB2	1:A:567:ASP:OD2	1.95	0.66
2:G:150:ILE:C	2:G:190:ASN:HD21	1.99	0.66
2:K:92:TRP:CB	2:K:93:GLU:OE1	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:PRO:HG2	3:H:58:GLN:HG3	1.77	0.66
3:D:129:VAL:HG21	3:D:207:VAL:HG11	1.76	0.66
1:E:591:GLY:HA2	1:E:593:VAL:HG13	1.78	0.66
2:K:186:TYR:O	2:K:192:TYR:OH	2.14	0.66
3:I:58:GLN:HE21	3:I:63:LYS:HA	1.61	0.65
1:F:537:PHE:HB2	1:F:571:VAL:HB	1.77	0.65
1:F:563:THR:HG23	1:F:565:ALA:H	1.61	0.65
1:E:572:GLU:N	1:E:572:GLU:OE1	2.28	0.65
2:G:61:ARG:NH1	2:G:79:GLN:HG2	2.12	0.65
1:A:468:ASN:HD22	1:B:472:TRP:HH2	1.43	0.65
1:A:591:GLY:HA2	1:A:593:VAL:HG13	1.79	0.65
3:I:207:VAL:HG12	3:I:208:ALA:HB2	1.79	0.65
1:B:554:LYS:HG2	2:C:93:GLU:HG2	1.80	0.64
2:C:146:VAL:O	2:C:155:ARG:NH1	2.30	0.64
1:F:473:LEU:HD11	1:F:569:LEU:HD21	1.79	0.64
2:K:119:PRO:HB3	2:K:209:PHE:CE1	2.32	0.64
2:L:61:ARG:HH21	2:L:78:LEU:HD12	1.62	0.64
3:I:142:THR:OG1	3:I:143:ASN:N	2.31	0.64
2:L:82:ASP:OD1	2:L:82:ASP:N	2.25	0.64
3:I:129:VAL:HG11	3:I:218:LYS:HE2	1.79	0.64
2:K:90:HIS:CE1	2:K:96:PHE:HA	2.32	0.63
2:G:154:GLU:O	2:G:155:ARG:NH1	2.31	0.63
1:A:470:VAL:HG11	1:B:470:VAL:HG11	1.79	0.63
1:E:492:VAL:HG11	1:E:580:ALA:HB1	1.79	0.63
1:F:485:TYR:HD2	1:F:494:VAL:HG11	1.63	0.63
2:C:164:THR:HG21	3:D:174:HIS:NE2	2.13	0.63
3:D:69:THR:HG23	3:D:78:TYR:HB2	1.79	0.63
2:K:46:VAL:HG21	3:J:107:TRP:HD1	1.64	0.63
3:I:132:LEU:HG	3:I:149:GLY:O	1.98	0.63
1:B:470:VAL:HG22	1:B:600:VAL:HG22	1.82	0.62
2:C:210:ASN:OD1	2:C:211:ARG:N	2.32	0.62
2:C:81:GLU:N	2:C:81:GLU:OE2	2.32	0.62
2:C:149:LYS:HE2	2:C:153:SER:O	2.00	0.62
1:F:475:LEU:HA	1:F:498:VAL:HG12	1.80	0.62
1:A:549:GLU:OE2	2:L:93:GLU:OE2	2.16	0.62
1:F:554:LYS:HD3	2:G:93:GLU:OE1	1.99	0.62
3:J:131:PRO:HB3	3:J:218:LYS:HE2	1.82	0.62
3:I:32:MET:SD	3:I:96:ARG:NH1	2.70	0.62
2:K:37:GLN:HG3	2:K:47:LEU:HG	1.82	0.62
2:L:193:THR:HG23	2:L:208:SER:HB3	1.81	0.61
1:A:588:LEU:C	2:L:93:GLU:OE1	2.38	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:ILE:HD13	2:L:191:SER:O	2.00	0.61
3:D:37:GLN:HG2	3:D:91:VAL:HB	1.81	0.61
2:K:149:LYS:HE2	2:K:152:GLY:HA2	1.81	0.61
2:K:6:GLN:NE2	2:K:102:THR:HG23	2.16	0.61
3:H:97:GLU:HA	3:H:107:TRP:O	2.00	0.61
1:E:521:LEU:HD12	1:E:601:LEU:HD13	1.83	0.61
3:D:174:HIS:HE1	3:D:176:PHE:CD1	2.19	0.60
1:B:460:ARG:HH22	1:B:466:ARG:HH12	1.50	0.60
2:L:150:ILE:HD11	2:L:189:HIS:CE1	2.36	0.60
2:C:5:THR:OG1	2:C:24:ARG:HB3	2.00	0.60
3:I:132:LEU:HB3	3:I:148:LEU:HG	1.84	0.60
3:J:166:SER:H	3:J:206:ASN:HD21	1.49	0.60
2:G:35:TRP:HB2	2:G:48:VAL:HG12	1.83	0.60
2:G:35:TRP:CD2	2:G:73:LEU:HD23	2.37	0.60
2:L:35:TRP:CE3	2:L:73:LEU:HD23	2.37	0.60
2:C:124:LYS:HD2	2:C:131:SER:H	1.66	0.60
3:J:147:THR:HG22	3:J:192:THR:HG23	1.83	0.60
1:E:542:ARG:NH1	1:F:552:THR:O	2.30	0.60
2:K:99:GLY:O	3:J:42:SER:OG	2.13	0.60
3:I:218:LYS:HD2	3:I:218:LYS:N	2.17	0.59
2:L:24:ARG:HD3	2:L:70:GLN:OE1	2.02	0.59
2:K:90:HIS:CE1	2:K:92:TRP:CD2	2.90	0.59
3:I:194:PRO:O	3:I:197:THR:OG1	2.14	0.59
1:E:501:VAL:HG12	1:E:503:VAL:N	2.13	0.59
1:A:459:SER:O	1:A:460:ARG:NH1	2.35	0.59
2:L:8:PRO:HG2	2:L:11:LEU:HD11	1.84	0.59
3:D:96:ARG:HB3	3:D:110:TYR:HB2	1.84	0.59
2:C:138:ASN:HA	2:C:172:THR:OG1	2.02	0.59
3:H:166:SER:H	3:H:206:ASN:ND2	1.99	0.59
3:J:98:ARG:HG2	3:J:109:THR:OG1	2.02	0.58
1:A:570:LEU:HB2	1:A:580:ALA:HB3	1.85	0.58
1:A:542:ARG:HG2	1:B:553:THR:HG22	1.85	0.58
2:G:140:TYR:OH	2:G:171:SER:O	2.11	0.58
3:H:4:GLN:O	3:H:113:GLN:NE2	2.31	0.58
3:J:11:LYS:HD2	3:J:11:LYS:H	1.67	0.58
1:A:565:ALA:HB2	2:C:30:TYR:CZ	2.38	0.58
3:D:127:PRO:HB3	3:D:155:TYR:HB3	1.86	0.58
2:K:113:PRO:HB3	2:K:139:PHE:HB3	1.86	0.58
2:L:21:ILE:HD12	2:L:73:LEU:HD11	1.86	0.58
2:L:37:GLN:NE2	2:L:45:GLN:HB2	2.19	0.58
3:D:17:LYS:HD3	3:D:80:GLU:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:124:LYS:HD2	2:G:131:SER:H	1.69	0.58
1:A:515:ASP:OD1	1:A:517:THR:HG22	2.04	0.58
2:K:42:LYS:HD2	2:K:43:SER:H	1.68	0.58
2:K:124:LYS:HE2	3:J:130:TYR:CD2	2.39	0.58
2:K:160:LEU:CG	2:K:161:ASN:H	2.16	0.58
2:G:123:GLU:N	2:G:123:GLU:OE1	2.36	0.58
2:L:61:ARG:NH2	2:L:78:LEU:HA	2.19	0.57
2:L:167:ASP:OD2	2:L:171:SER:N	2.34	0.57
3:I:64:SER:O	3:I:82:ARG:NH2	2.38	0.57
2:L:184:ASP:OD1	2:L:185:GLU:N	2.38	0.57
1:F:485:TYR:HE1	1:F:534:LYS:HZ3	1.53	0.57
1:A:554:LYS:CD	2:L:93:GLU:HG3	2.35	0.57
3:D:136:PRO:O	3:D:223:ARG:NH2	2.38	0.57
1:F:545:LEU:N	1:F:567:ASP:OD2	2.31	0.57
2:K:98:PHE:CD2	3:J:43:LEU:HB2	2.40	0.57
2:G:184:ASP:OD1	2:G:185:GLU:N	2.36	0.57
3:D:46:ILE:HG13	3:D:62:PHE:HD2	1.70	0.57
1:F:460:ARG:NH1	1:F:464:VAL:HB	2.20	0.57
2:G:78:LEU:HD21	2:G:106:ILE:HG23	1.87	0.57
2:K:108:ARG:HG3	2:K:109:ALA:H	1.69	0.57
1:A:543:GLY:HA2	1:B:555:ALA:HB2	1.87	0.57
3:J:10:VAL:HG11	3:J:16:VAL:HB	1.86	0.57
1:F:460:ARG:HH12	1:F:464:VAL:H	1.53	0.56
2:L:8:PRO:O	2:L:102:THR:HG22	2.06	0.56
1:F:554:LYS:HE2	1:F:554:LYS:HA	1.86	0.56
2:L:123:GLU:O	2:L:126:LEU:HG	2.05	0.56
2:C:175:MET:SD	2:C:176:SER:N	2.79	0.56
2:K:159:VAL:O	2:K:160:LEU:HB2	2.05	0.56
1:F:501:VAL:HG12	1:F:503:VAL:N	2.11	0.56
2:G:9:ALA:HA	2:G:102:THR:HA	1.88	0.56
1:F:466:ARG:O	1:F:601:LEU:HD11	2.06	0.56
2:G:118:PHE:HB2	2:G:133:VAL:HG13	1.87	0.56
1:B:554:LYS:CE	2:C:93:GLU:CG	2.82	0.56
3:I:132:LEU:HA	3:I:149:GLY:O	2.06	0.55
2:C:20:THR:HG22	2:C:74:LYS:HG3	1.88	0.55
2:C:143:ASP:OD1	2:C:144:ILE:N	2.39	0.55
3:D:2:LEU:HG	3:D:96:ARG:HH22	1.72	0.55
2:K:154:GLU:CG	2:K:155:ARG:H	2.20	0.55
1:A:501:VAL:HG12	1:A:503:VAL:N	2.13	0.55
1:B:603:PRO:HB2	3:H:103:ASN:OD1	2.06	0.55
3:I:143:ASN:HB2	3:I:145:MET:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:493:TYR:CD1	1:F:583:THR:HG21	2.42	0.55
2:G:34:VAL:HG21	3:I:107:TRP:CB	2.32	0.55
1:B:592:PRO:HG2	3:D:63:LYS:HD3	1.88	0.54
3:H:17:LYS:NZ	3:H:80:GLU:OE1	2.35	0.54
2:C:37:GLN:O	2:C:44:PRO:HA	2.07	0.54
2:C:135:PHE:HE1	3:D:132:LEU:HD11	1.71	0.54
3:D:35:VAL:HG11	3:D:43:LEU:HD13	1.89	0.54
2:C:140:TYR:OH	2:C:171:SER:O	2.17	0.54
3:D:181:GLN:O	3:D:184:LEU:HG	2.07	0.54
2:L:128:GLY:HA2	2:L:183:LYS:HD3	1.89	0.54
3:I:209:HIS:NE2	3:I:211:ALA:HB3	2.22	0.54
2:L:12:SER:HB3	2:L:107:LYS:HD3	1.89	0.54
3:J:36:LYS:HG3	3:J:92:TYR:CE1	2.42	0.54
3:D:209:HIS:HD2	3:D:212:SER:HB2	1.72	0.54
3:J:35:VAL:CG1	3:J:93:TYR:HB2	2.37	0.54
2:C:166:GLN:HA	2:C:172:THR:O	2.08	0.54
2:C:164:THR:HG21	3:D:174:HIS:CE1	2.42	0.54
1:E:493:TYR:CD1	1:E:583:THR:HG21	2.43	0.54
1:A:566:SER:OG	1:B:553:THR:O	2.10	0.54
3:H:31:ASN:O	3:H:96:ARG:HD3	2.08	0.54
2:K:8:PRO:HG2	2:K:11:LEU:HD11	1.90	0.54
3:J:4:GLN:O	3:J:113:GLN:NE2	2.39	0.54
2:L:82:ASP:HB2	2:L:86:TYR:OH	2.08	0.54
1:E:460:ARG:HD3	1:E:461:PRO:HD2	1.88	0.54
2:G:124:LYS:HE2	3:I:130:TYR:CD2	2.42	0.54
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.43	0.53
2:C:135:PHE:CE1	3:D:132:LEU:HD11	2.43	0.53
1:E:565:ALA:HB2	2:G:30:TYR:OH	2.07	0.53
1:F:515:ASP:OD1	1:F:517:THR:HG22	2.08	0.53
1:B:516:TRP:HA	1:B:519:VAL:HG23	1.91	0.53
2:C:28:ASN:HA	2:C:69:THR:HG22	1.89	0.53
2:C:167:ASP:OD1	2:C:168:SER:N	2.41	0.53
3:D:174:HIS:CE1	3:D:176:PHE:CE1	2.97	0.53
2:C:3:GLN:HB2	2:C:26:SER:HB3	1.90	0.53
2:G:190:ASN:ND2	2:G:191:SER:H	2.07	0.53
3:I:46:ILE:HD11	3:I:66:ALA:CB	2.39	0.53
2:L:38:GLN:HE22	3:H:37:GLN:HE22	1.56	0.53
3:I:58:GLN:NE2	3:I:63:LYS:HA	2.24	0.53
2:L:167:ASP:OD2	2:L:170:ASP:N	2.40	0.53
2:L:120:PRO:HG2	2:L:186:TYR:CE1	2.43	0.52
2:C:118:PHE:HB2	2:C:133:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:TYR:CD1	1:A:583:THR:HG21	2.44	0.52
1:F:493:TYR:HD1	1:F:583:THR:HG21	1.75	0.52
1:F:545:LEU:HD12	1:F:599:ALA:HB2	1.91	0.52
2:K:8:PRO:O	2:K:102:THR:HG22	2.09	0.52
2:K:160:LEU:HD12	2:K:161:ASN:H	1.73	0.52
3:J:166:SER:H	3:J:206:ASN:ND2	2.06	0.52
2:G:46:VAL:HG21	3:I:107:TRP:HD1	1.75	0.52
3:I:164:TRP:CZ3	3:I:205:CYS:HB3	2.45	0.52
1:B:472:TRP:HB3	1:B:501:VAL:HB	1.90	0.52
1:A:476:THR:HG21	3:H:55:ILE:HD12	1.91	0.52
2:C:115:VAL:HG13	2:C:136:LEU:HD13	1.92	0.52
3:D:46:ILE:HD11	3:D:66:ALA:CB	2.40	0.52
1:F:498:VAL:HG21	1:F:579:VAL:HG21	1.92	0.52
2:L:82:ASP:O	2:L:86:TYR:OH	2.19	0.52
2:K:34:VAL:HG21	3:J:107:TRP:HB2	1.91	0.52
2:L:35:TRP:CD2	2:L:73:LEU:HD23	2.45	0.52
2:C:9:ALA:O	2:C:102:THR:HA	2.10	0.52
3:D:69:THR:CG2	3:D:78:TYR:HB2	2.40	0.52
1:F:563:THR:HG1	2:K:30:TYR:HH	1.57	0.52
1:B:501:VAL:HG12	1:B:503:VAL:N	2.16	0.52
2:L:11:LEU:HD22	2:L:19:VAL:HG23	1.92	0.52
3:D:131:PRO:HD3	3:D:218:LYS:HD2	1.92	0.52
3:I:132:LEU:HD23	3:I:148:LEU:CD2	2.38	0.52
1:B:554:LYS:HE3	2:C:92:TRP:NE1	2.25	0.52
2:C:92:TRP:CD1	2:C:93:GLU:OE2	2.63	0.52
2:K:120:PRO:HG2	2:K:186:TYR:CE1	2.46	0.51
1:A:466:ARG:N	1:A:469:ASP:OD2	2.37	0.51
3:H:10:VAL:HG11	3:H:16:VAL:HB	1.92	0.51
3:D:84:LEU:HB3	3:D:119:VAL:HG21	1.91	0.51
3:D:126:PRO:HB3	3:D:214:THR:HG21	1.92	0.51
2:G:124:LYS:HZ3	2:G:131:SER:HB3	1.75	0.51
2:G:120:PRO:HD3	2:G:132:VAL:HG22	1.91	0.51
2:G:139:PHE:CG	2:G:140:TYR:N	2.79	0.51
2:K:108:ARG:HG3	2:K:109:ALA:N	2.26	0.51
3:I:97:GLU:HA	3:I:107:TRP:O	2.10	0.51
2:L:190:ASN:O	2:L:211:ARG:HG3	2.09	0.51
2:C:35:TRP:CE2	2:C:73:LEU:HB2	2.45	0.51
2:C:106:ILE:HG22	2:C:166:GLN:NE2	2.26	0.51
2:C:34:VAL:HG21	3:D:107:TRP:CB	2.30	0.51
2:K:35:TRP:CZ3	2:K:88:CYS:HB3	2.45	0.51
2:C:188:ARG:O	2:C:188:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:PHE:HB2	1:B:571:VAL:HB	1.93	0.51
2:L:62:PHE:CD2	2:L:75:ILE:HD12	2.46	0.51
3:H:198:TRP:CD2	3:H:199:PRO:HA	2.45	0.51
2:G:150:ILE:HG13	2:G:153:SER:OG	2.11	0.50
3:D:49:ILE:O	3:D:51:PRO:HD3	2.11	0.50
3:J:178:ALA:HB2	3:J:187:LEU:HD23	1.92	0.50
3:I:96:ARG:HG3	3:I:110:TYR:HB2	1.93	0.50
1:A:462:PHE:CG	1:A:509:ALA:HB2	2.46	0.50
1:A:475:LEU:HD23	1:A:495:SER:HB3	1.92	0.50
1:A:534:LYS:HD2	1:A:535:THR:N	2.24	0.50
2:L:210:ASN:O	2:L:212:ASN:N	2.39	0.50
2:K:11:LEU:HD22	2:K:19:VAL:HG23	1.92	0.50
3:I:218:LYS:HD2	3:I:218:LYS:H	1.76	0.50
2:C:43:SER:OG	3:D:112:GLY:O	2.23	0.50
1:E:592:PRO:HG3	3:J:63:LYS:HD3	1.93	0.50
1:E:470:VAL:HG11	1:F:470:VAL:HG11	1.93	0.50
3:J:29:ASP:OD1	3:J:29:ASP:N	2.45	0.50
3:J:160:VAL:CG2	3:J:187:LEU:HD21	2.41	0.50
1:A:496:ASP:OD1	1:A:578:ARG:NE	2.44	0.50
1:A:516:TRP:CD2	1:A:571:VAL:HG11	2.47	0.50
3:D:157:PRO:O	3:D:209:HIS:HE1	1.95	0.50
3:J:131:PRO:HG3	3:J:218:LYS:NZ	2.27	0.50
2:C:34:VAL:HG22	2:C:49:TYR:HA	1.93	0.49
1:F:476:THR:HB	1:F:497:SER:HB3	1.94	0.49
2:K:52:THR:HG22	2:K:65:SER:HA	1.94	0.49
2:L:182:THR:OG1	2:L:184:ASP:OD1	2.26	0.49
2:K:62:PHE:CD2	2:K:75:ILE:HD12	2.47	0.49
2:G:35:TRP:CE3	2:G:73:LEU:HD23	2.48	0.49
2:L:79:GLN:HE21	2:L:81:GLU:HG3	1.78	0.49
2:K:90:HIS:ND1	2:K:92:TRP:CD1	2.81	0.49
2:G:124:LYS:NZ	2:G:131:SER:HB3	2.27	0.49
1:A:576:GLY:O	1:A:578:ARG:N	2.45	0.49
2:G:34:VAL:HG22	2:G:49:TYR:HA	1.94	0.49
2:G:80:SER:HA	2:G:106:ILE:HD12	1.95	0.49
1:A:516:TRP:HA	1:A:519:VAL:HG23	1.95	0.49
3:D:10:VAL:HG21	3:D:16:VAL:HB	1.95	0.49
2:K:20:THR:HG22	2:K:74:LYS:HG2	1.95	0.49
3:I:198:TRP:CD2	3:I:199:PRO:HA	2.48	0.49
2:L:149:LYS:O	2:L:193:THR:HB	2.12	0.49
1:E:515:ASP:CG	1:E:518:LYS:HG3	2.33	0.49
1:B:460:ARG:HH22	1:B:466:ARG:NH1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:GLU:O	2:C:93:GLU:OE1	2.30	0.49
2:C:93:GLU:O	2:C:94:THR:C	2.50	0.49
2:C:156:GLN:NE2	2:C:157:ASN:HB2	2.28	0.49
3:D:25:TYR:CE1	3:D:27:PHE:HA	2.48	0.49
2:L:137:ASN:HA	2:L:174:SER:HB2	1.93	0.48
1:E:493:TYR:HD1	1:E:583:THR:HG21	1.78	0.48
2:K:90:HIS:NE2	2:K:96:PHE:HA	2.28	0.48
2:K:128:GLY:HA2	2:K:183:LYS:HD3	1.94	0.48
2:L:131:SER:HA	2:L:179:LEU:O	2.13	0.48
2:K:42:LYS:CD	2:K:43:SER:H	2.26	0.48
2:L:141:PRO:HG2	2:L:143:ASP:OD1	2.12	0.48
2:L:50:ALA:HB3	2:L:53:ASN:ND2	2.29	0.48
3:J:198:TRP:CD2	3:J:199:PRO:HA	2.49	0.48
1:B:530:GLN:HG2	1:B:535:THR:HG22	1.96	0.48
2:C:105:GLU:HG2	2:C:166:GLN:OE1	2.13	0.48
3:I:132:LEU:HD13	3:I:220:ILE:HD11	1.94	0.48
1:A:459:SER:OG	1:A:460:ARG:N	2.44	0.48
2:L:46:VAL:HG21	3:H:107:TRP:CD1	2.37	0.48
2:C:2:ILE:HD11	2:C:93:GLU:OE2	2.13	0.48
3:I:32:MET:CE	3:I:96:ARG:HH12	2.25	0.48
3:H:82:ARG:HG3	3:H:83:SER:N	2.29	0.48
3:D:29:ASP:C	3:D:30:PHE:HD1	2.17	0.48
2:K:136:LEU:HD13	2:K:175:MET:HE2	1.96	0.48
3:I:37:GLN:HG2	3:I:91:VAL:HB	1.95	0.48
3:I:132:LEU:HB2	3:I:220:ILE:CD1	2.44	0.48
1:A:537:PHE:HB2	1:A:571:VAL:HB	1.96	0.48
2:L:34:VAL:HG21	3:H:107:TRP:HB2	1.95	0.48
2:L:163:TRP:CD1	2:L:175:MET:HB2	2.49	0.48
3:H:38:SER:HB3	3:H:41:LYS:HE2	1.96	0.48
1:F:530:GLN:HE22	1:F:533:SER:HA	1.78	0.48
3:H:63:LYS:HD2	3:H:63:LYS:O	2.13	0.48
3:D:158:GLU:HG3	3:D:159:PRO:HA	1.96	0.48
3:D:180:LEU:HD12	3:D:184:LEU:C	2.34	0.48
2:G:81:GLU:OE2	2:G:81:GLU:N	2.35	0.48
1:B:531:GLN:OE1	1:B:532:HIS:CE1	2.67	0.47
1:B:565:ALA:HB2	2:L:30:TYR:CZ	2.49	0.47
2:C:172:THR:OG1	2:C:173:TYR:O	2.31	0.47
2:K:150:ILE:HG12	2:K:155:ARG:NH2	2.28	0.47
1:A:554:LYS:HE2	2:L:93:GLU:CB	2.43	0.47
2:L:6:GLN:NE2	2:L:102:THR:HG23	2.29	0.47
3:H:164:TRP:CH2	3:H:205:CYS:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:209:HIS:HD2	3:H:212:SER:OG	1.97	0.47
2:C:139:PHE:CZ	2:C:144:ILE:HB	2.49	0.47
2:K:154:GLU:O	2:K:155:ARG:HD3	2.14	0.47
1:A:476:THR:HB	1:A:497:SER:OG	2.13	0.47
2:L:139:PHE:N	2:L:173:TYR:O	2.35	0.47
1:A:493:TYR:HD1	1:A:583:THR:HG21	1.79	0.47
2:K:37:GLN:HG2	2:K:86:TYR:CE2	2.49	0.47
1:A:460:ARG:HA	1:A:460:ARG:HD3	1.74	0.47
3:D:25:TYR:CE2	3:D:96:ARG:NH1	2.83	0.47
2:K:154:GLU:HG3	2:K:155:ARG:H	1.79	0.47
2:K:160:LEU:CD1	2:K:161:ASN:H	2.27	0.47
3:D:209:HIS:HB3	3:D:214:THR:OG1	2.15	0.47
3:J:46:ILE:HG12	3:J:62:PHE:CD2	2.49	0.47
3:I:135:GLY:CA	3:I:223:ARG:HD3	2.38	0.47
3:H:157:PRO:O	3:H:209:HIS:HE1	1.97	0.47
3:H:160:VAL:CG2	3:H:187:LEU:HD21	2.45	0.47
2:K:148:TRP:O	2:K:155:ARG:HG2	2.15	0.47
2:C:46:VAL:HG21	3:D:107:TRP:CD1	2.45	0.47
1:F:540:PRO:O	1:F:602:ALA:N	2.42	0.47
2:K:90:HIS:CE1	2:K:92:TRP:CE2	3.02	0.47
3:I:130:TYR:HA	3:I:131:PRO:HD3	1.63	0.47
3:H:164:TRP:CZ3	3:H:205:CYS:HB3	2.50	0.47
2:C:2:ILE:HD12	2:C:90:HIS:CE1	2.50	0.47
2:C:78:LEU:HG	2:C:106:ILE:HD11	1.97	0.47
3:D:178:ALA:HB2	3:D:187:LEU:HD23	1.97	0.47
1:E:468:ASN:HD22	1:F:472:TRP:HH2	1.62	0.47
3:I:29:ASP:C	3:I:30:PHE:HD1	2.19	0.47
1:A:530:GLN:HG3	1:A:535:THR:HA	1.97	0.47
1:F:526:LEU:HD22	1:F:537:PHE:HB3	1.97	0.47
3:I:183:ASP:OD1	3:I:183:ASP:O	2.32	0.47
2:L:6:GLN:HE21	2:L:102:THR:HG23	1.80	0.46
2:L:20:THR:HG22	2:L:74:LYS:HD2	1.97	0.46
2:C:142:LYS:H	2:C:142:LYS:HG2	1.37	0.46
2:G:35:TRP:HB2	2:G:48:VAL:CG1	2.44	0.46
2:C:12:SER:HB2	2:C:107:LYS:NZ	2.30	0.46
3:D:96:ARG:NH1	3:D:96:ARG:HB2	2.30	0.46
2:G:160:LEU:O	2:G:177:SER:HA	2.15	0.46
3:D:201:GLU:CD	3:D:202:THR:H	2.18	0.46
3:D:209:HIS:HD2	3:D:212:SER:CB	2.28	0.46
1:F:572:GLU:HB3	1:F:578:ARG:H	1.80	0.46
3:J:63:LYS:HD2	3:J:63:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:138:ASN:HA	2:G:172:THR:HB	1.96	0.46
3:I:130:TYR:HE2	3:I:153:LYS:HD3	1.81	0.46
2:C:117:ILE:HG23	2:C:134:CYS:SG	2.55	0.46
1:F:557:TYR:HA	1:F:558:PRO:HD3	1.72	0.46
2:K:98:PHE:CG	3:J:43:LEU:HB2	2.49	0.46
3:J:209:HIS:HB3	3:J:214:THR:HB	1.98	0.46
2:G:118:PHE:HB2	2:G:133:VAL:CG1	2.45	0.46
1:A:588:LEU:HA	2:L:93:GLU:CD	2.33	0.46
2:L:61:ARG:NH2	2:L:78:LEU:HD12	2.28	0.46
3:H:178:ALA:HB2	3:H:187:LEU:HD23	1.98	0.46
1:F:502:ASN:O	1:F:504:ALA:N	2.42	0.46
2:L:189:HIS:CD2	2:L:190:ASN:N	2.81	0.46
2:C:115:VAL:HG21	2:C:205:ILE:HD13	1.98	0.46
3:H:71:ASP:OD1	3:H:73:SER:OG	2.27	0.46
3:D:63:LYS:HD2	3:D:63:LYS:O	2.15	0.46
3:D:113:GLN:OE1	3:D:113:GLN:N	2.44	0.46
1:F:558:PRO:HA	1:F:583:THR:HA	1.98	0.46
2:G:15:VAL:HG21	2:G:108:ARG:CZ	2.45	0.46
2:G:61:ARG:HG3	2:G:76:ASN:OD1	2.16	0.46
3:I:132:LEU:H	3:I:132:LEU:HD12	1.81	0.46
1:B:548:TRP:NE1	1:B:596:SER:HB2	2.30	0.46
2:L:189:HIS:O	2:L:211:ARG:HD3	2.16	0.46
1:E:492:VAL:HG13	1:E:581:ILE:O	2.16	0.46
1:F:530:GLN:HE22	1:F:533:SER:CA	2.29	0.46
3:J:35:VAL:HG11	3:J:111:TRP:HZ3	1.80	0.46
2:L:124:LYS:CE	2:L:131:SER:H	2.24	0.46
2:C:121:SER:HB2	3:D:131:PRO:O	2.15	0.46
1:E:473:LEU:HD21	1:E:569:LEU:HD21	1.98	0.46
3:I:34:TRP:O	3:I:46:ILE:HG22	2.16	0.46
3:I:123:LYS:O	3:I:125:THR:HG23	2.16	0.46
3:H:30:PHE:HB3	3:H:96:ARG:HE	1.81	0.46
2:K:150:ILE:HG12	2:K:155:ARG:HH21	1.79	0.46
2:K:189:HIS:HD1	2:K:191:SER:N	2.13	0.46
3:J:209:HIS:HD2	3:J:212:SER:OG	1.99	0.46
2:L:61:ARG:HG3	2:L:77:SER:H	1.81	0.45
2:C:33:LEU:HD13	2:C:71:TYR:CD2	2.51	0.45
2:K:191:SER:HA	2:K:209:PHE:O	2.16	0.45
3:I:25:TYR:OH	3:I:96:ARG:NE	2.49	0.45
2:L:123:GLU:OE1	3:H:218:LYS:HE2	2.16	0.45
1:F:547:PHE:CE2	1:F:556:GLY:HA3	2.52	0.45
2:G:21:ILE:HD12	2:G:102:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:198:TRP:CD2	3:D:199:PRO:HA	2.51	0.45
3:J:46:ILE:HG12	3:J:62:PHE:CE2	2.50	0.45
1:B:545:LEU:N	1:B:567:ASP:OD2	2.41	0.45
2:C:149:LYS:NZ	2:C:155:ARG:HA	2.32	0.45
2:K:39:LYS:NZ	2:K:40:GLN:O	2.45	0.45
3:I:220:ILE:HD13	3:I:220:ILE:HA	1.72	0.45
2:L:107:LYS:HZ1	2:L:140:TYR:HE1	1.64	0.45
1:F:469:ASP:O	1:F:600:VAL:HG13	2.17	0.45
2:G:37:GLN:O	2:G:45:GLN:N	2.36	0.45
2:G:123:GLU:OE2	3:I:131:PRO:HG2	2.17	0.45
2:L:62:PHE:HD2	2:L:75:ILE:HD12	1.81	0.45
2:L:189:HIS:HD2	2:L:190:ASN:N	2.06	0.45
1:E:476:THR:HG21	3:J:55:ILE:HD12	1.99	0.45
2:G:186:TYR:O	2:G:189:HIS:HD2	2.00	0.45
1:A:545:LEU:HD12	1:A:599:ALA:HB2	1.98	0.45
2:C:35:TRP:CD1	2:C:48:VAL:HG13	2.52	0.45
2:C:50:ALA:HB3	2:C:53:ASN:ND2	2.32	0.45
2:C:162:SER:H	2:C:175:MET:HE1	1.81	0.45
3:I:132:LEU:CA	3:I:149:GLY:O	2.65	0.45
1:B:554:LYS:CD	2:C:92:TRP:CH2	2.78	0.45
2:L:124:LYS:HB3	2:L:124:LYS:HE2	1.52	0.45
1:E:465:LEU:HD23	1:E:519:VAL:HG13	1.99	0.45
1:F:492:VAL:HG13	1:F:581:ILE:O	2.17	0.45
2:G:82:ASP:O	2:G:86:TYR:OH	2.26	0.45
2:K:59:PRO:HG2	2:K:62:PHE:CE1	2.52	0.45
2:K:73:LEU:HD21	2:K:75:ILE:HD11	1.99	0.44
2:K:155:ARG:HH12	2:K:179:LEU:CD2	2.28	0.44
1:A:465:LEU:HD23	1:A:519:VAL:HG13	1.98	0.44
3:H:35:VAL:CG1	3:H:93:TYR:HB2	2.47	0.44
3:J:3:GLN:O	3:J:21:LYS:HG2	2.17	0.44
2:G:29:ILE:HA	2:G:92:TRP:CD1	2.52	0.44
2:C:123:GLU:O	2:C:126:LEU:HB3	2.17	0.44
3:D:134:PRO:HB2	3:D:135:GLY:H	1.53	0.44
2:G:124:LYS:HB2	3:I:130:TYR:CG	2.52	0.44
2:L:186:TYR:O	2:L:192:TYR:OH	2.35	0.44
2:K:96:PHE:HB2	3:J:45:TRP:CG	2.52	0.44
3:J:131:PRO:HG3	3:J:218:LYS:HZ3	1.82	0.44
3:I:10:VAL:HG12	3:I:14:ALA:HB3	2.00	0.44
3:H:154:GLY:HA2	3:H:184:LEU:HB3	2.00	0.44
2:C:131:SER:HA	2:C:179:LEU:O	2.18	0.44
2:C:148:TRP:CZ3	2:C:179:LEU:HB2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:46:ILE:HD11	3:D:66:ALA:HB2	1.99	0.44
2:C:113:PRO:HB3	2:C:139:PHE:HB2	1.98	0.44
1:A:470:VAL:HG22	1:A:600:VAL:HG12	1.99	0.44
1:B:535:THR:OG1	1:B:573:ASN:HB3	2.18	0.44
3:H:2:LEU:O	3:H:112:GLY:HA2	2.18	0.44
2:K:94:THR:HG21	3:J:48:TYR:CE1	2.52	0.44
2:G:23:CYS:SG	2:G:35:TRP:CH2	3.11	0.44
3:I:129:VAL:CG1	3:I:218:LYS:HE2	2.46	0.44
1:B:585:THR:OG1	1:B:586:THR:N	2.50	0.44
3:H:145:MET:HB2	3:H:194:PRO:HA	2.00	0.44
2:G:9:ALA:HA	2:G:102:THR:HG23	2.00	0.44
1:A:554:LYS:CD	2:L:93:GLU:CG	2.93	0.43
1:B:522:ASP:OD1	1:B:604:PRO:HD3	2.18	0.43
2:L:12:SER:CB	2:L:107:LYS:HD3	2.48	0.43
3:H:16:VAL:O	3:H:80:GLU:HA	2.18	0.43
3:H:201:GLU:N	3:H:201:GLU:OE1	2.51	0.43
1:E:585:THR:HG22	1:E:586:THR:N	2.25	0.43
3:J:97:GLU:HA	3:J:107:TRP:O	2.18	0.43
2:L:140:TYR:CD1	2:L:141:PRO:HA	2.53	0.43
3:H:3:GLN:O	3:H:21:LYS:HG2	2.17	0.43
2:C:192:TYR:O	2:C:193:THR:HB	2.19	0.43
2:L:35:TRP:O	2:L:47:LEU:N	2.45	0.43
3:H:46:ILE:HG12	3:H:62:PHE:CD2	2.53	0.43
1:A:541:LEU:HD13	1:A:599:ALA:HB1	1.99	0.43
2:L:148:TRP:HB3	2:L:155:ARG:NH1	2.33	0.43
3:H:49:ILE:O	3:H:51:PRO:HD3	2.18	0.43
2:C:165:ASP:N	2:C:165:ASP:OD1	2.48	0.43
1:E:541:LEU:HD23	1:E:601:LEU:HA	1.99	0.43
1:F:500:LEU:HB2	1:F:509:ALA:HB3	1.99	0.43
3:J:26:THR:O	3:J:29:ASP:OD1	2.36	0.43
3:I:2:LEU:HA	3:I:21:LYS:O	2.18	0.43
2:C:37:GLN:NE2	2:C:86:TYR:CD2	2.86	0.43
3:D:45:TRP:CH2	3:D:47:GLY:HA2	2.53	0.43
3:D:215:LYS:HE2	3:D:215:LYS:HB3	1.77	0.43
2:K:124:LYS:NZ	2:K:131:SER:HB2	2.33	0.43
2:K:160:LEU:HG	2:K:161:ASN:H	1.82	0.43
3:J:45:TRP:CH2	3:J:47:GLY:HA2	2.54	0.43
1:A:585:THR:OG1	1:A:586:THR:N	2.51	0.43
1:B:572:GLU:OE2	1:B:574:ALA:HB3	2.18	0.43
3:H:169:LEU:HD12	3:H:169:LEU:O	2.19	0.43
2:K:192:TYR:HE2	2:K:211:ARG:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:210:ASN:O	2:K:212:ASN:N	2.51	0.43
3:H:209:HIS:HB3	3:H:214:THR:HB	1.99	0.43
2:C:153:SER:HB3	2:C:154:GLU:OE1	2.19	0.43
1:E:470:VAL:HG22	1:E:600:VAL:HG12	2.01	0.43
1:E:474:SER:HB2	1:E:499:THR:OG1	2.19	0.43
2:C:131:SER:OG	2:C:178:THR:HG22	2.19	0.43
1:F:534:LYS:HE2	1:F:578:ARG:HH21	1.84	0.43
3:J:164:TRP:CZ3	3:J:205:CYS:HB2	2.54	0.43
1:A:548:TRP:CE2	1:A:596:SER:HB2	2.54	0.43
2:L:61:ARG:NH2	2:L:79:GLN:H	2.16	0.43
1:F:498:VAL:HG21	1:F:579:VAL:CG2	2.48	0.43
3:I:133:ALA:HA	3:I:134:PRO:HD3	1.63	0.43
3:H:30:PHE:HB3	3:H:96:ARG:NE	2.33	0.43
2:C:86:TYR:HE1	2:C:104:LEU:HB3	1.84	0.43
1:E:516:TRP:HA	1:E:519:VAL:HG23	2.01	0.43
1:E:541:LEU:HD13	1:E:599:ALA:HB1	2.01	0.43
1:F:544:LYS:NZ	1:F:565:ALA:O	2.50	0.43
2:K:86:TYR:HB2	2:K:102:THR:OG1	2.19	0.43
3:J:123:LYS:O	3:J:125:THR:HG23	2.18	0.43
3:I:69:THR:OG1	3:I:70:VAL:N	2.50	0.43
1:A:474:SER:O	1:A:498:VAL:HA	2.19	0.42
1:E:531:GLN:HG3	1:E:532:HIS:CE1	2.54	0.42
1:F:565:ALA:HB2	2:K:30:TYR:CZ	2.54	0.42
2:G:2:ILE:O	2:G:97:THR:HG21	2.18	0.42
3:J:35:VAL:HG11	3:J:111:TRP:CZ3	2.55	0.42
2:G:122:SER:OG	2:G:123:GLU:OE1	2.28	0.42
3:I:49:ILE:O	3:I:51:PRO:HD3	2.19	0.42
1:F:474:SER:O	1:F:498:VAL:HA	2.19	0.42
3:H:128:SER:HB2	3:H:130:TYR:CZ	2.55	0.42
2:C:118:PHE:HZ	3:D:147:THR:HG1	1.66	0.42
3:J:49:ILE:O	3:J:51:PRO:HD3	2.19	0.42
2:C:92:TRP:CD1	2:C:93:GLU:HG3	2.55	0.42
2:K:24:ARG:HA	2:K:69:THR:O	2.20	0.42
2:K:150:ILE:O	2:K:151:ASP:OD1	2.38	0.42
2:G:99:GLY:O	3:I:42:SER:OG	2.29	0.42
1:B:493:TYR:CD1	1:B:583:THR:HG21	2.55	0.42
1:B:592:PRO:CG	3:D:63:LYS:HD3	2.50	0.42
3:H:81:LEU:HB3	3:H:84:LEU:HD21	2.02	0.42
1:F:465:LEU:O	1:F:521:LEU:HA	2.18	0.42
1:F:466:ARG:HG2	1:F:522:ASP:OD1	2.19	0.42
2:G:186:TYR:O	2:G:189:HIS:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LYS:CD	1:A:535:THR:H	2.28	0.42
2:L:107:LYS:HE3	2:L:107:LYS:HA	2.02	0.42
1:E:536:PHE:HA	1:E:572:GLU:HA	2.01	0.42
2:K:207:LYS:HD2	2:K:207:LYS:HA	1.77	0.42
1:A:478:ALA:O	1:A:592:PRO:HA	2.19	0.42
1:A:544:LYS:NZ	1:A:565:ALA:O	2.37	0.42
2:L:79:GLN:O	2:L:82:ASP:OD1	2.37	0.42
2:C:21:ILE:O	2:C:72:SER:HA	2.20	0.42
2:C:83:SER:HA	2:C:104:LEU:HD22	2.02	0.42
2:C:149:LYS:HG3	2:C:150:ILE:N	2.35	0.42
1:E:471:LEU:HD23	1:E:502:ASN:HA	2.02	0.42
3:J:17:LYS:HG2	3:J:80:GLU:HB2	2.00	0.42
3:J:25:TYR:CE2	3:J:27:PHE:HA	2.55	0.42
1:A:541:LEU:HD11	1:A:569:LEU:HD13	2.01	0.41
3:H:133:ALA:HA	3:H:134:PRO:HD3	1.91	0.41
2:C:139:PHE:CG	2:C:140:TYR:N	2.88	0.41
2:G:29:ILE:HG22	2:G:92:TRP:CD1	2.55	0.41
2:G:182:THR:HB	2:G:184:ASP:OD1	2.19	0.41
3:I:134:PRO:HB2	3:I:135:GLY:H	1.52	0.41
3:H:209:HIS:HA	3:H:210:PRO:HD2	1.82	0.41
2:G:148:TRP:O	2:G:148:TRP:CE3	2.73	0.41
2:L:59:PRO:HG2	2:L:62:PHE:CE1	2.55	0.41
3:D:178:ALA:HA	3:D:187:LEU:HB3	2.03	0.41
3:I:46:ILE:HG13	3:I:62:PHE:HD2	1.85	0.41
1:B:521:LEU:HG	1:B:522:ASP:OD1	2.19	0.41
1:B:558:PRO:O	1:B:584:TYR:HB2	2.20	0.41
2:L:207:LYS:HD2	2:L:207:LYS:HA	1.80	0.41
2:C:161:ASN:O	3:D:179:VAL:HG21	2.20	0.41
2:C:167:ASP:HB2	2:C:172:THR:HG22	2.02	0.41
2:G:7:SER:OG	2:G:8:PRO:HA	2.20	0.41
3:I:25:TYR:CE1	3:I:27:PHE:HA	2.56	0.41
1:B:545:LEU:CD1	1:B:599:ALA:HB2	2.47	0.41
2:L:37:GLN:OE1	2:L:47:LEU:HG	2.20	0.41
3:H:46:ILE:HG12	3:H:62:PHE:CE2	2.55	0.41
1:E:531:GLN:HA	1:E:531:GLN:OE1	2.21	0.41
2:K:118:PHE:HZ	3:J:147:THR:O	2.04	0.41
3:J:157:PRO:O	3:J:209:HIS:HE1	2.03	0.41
2:G:124:LYS:CD	2:G:131:SER:H	2.34	0.41
3:D:97:GLU:HA	3:D:107:TRP:O	2.21	0.41
1:E:478:ALA:O	1:E:592:PRO:HA	2.21	0.41
2:G:54:LEU:HD23	2:G:54:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:163:TRP:CD1	2:K:175:MET:HG3	2.56	0.41
2:G:150:ILE:HG13	2:G:150:ILE:O	2.20	0.41
3:I:164:TRP:CH2	3:I:205:CYS:HB3	2.55	0.41
1:A:547:PHE:CE2	1:A:556:GLY:HA3	2.56	0.41
1:A:554:LYS:HE2	2:L:93:GLU:HB2	2.02	0.41
1:A:601:LEU:HD23	1:A:601:LEU:HA	1.94	0.41
2:L:54:LEU:HD23	2:L:54:LEU:HA	1.88	0.41
3:H:86:SER:O	3:H:89:SER:OG	2.35	0.41
3:H:98:ARG:HB2	3:H:109:THR:OG1	2.21	0.41
2:C:20:THR:HA	2:C:73:LEU:O	2.21	0.41
2:C:210:ASN:O	2:C:211:ARG:HB3	2.21	0.41
3:D:46:ILE:HG13	3:D:62:PHE:CD2	2.54	0.41
3:D:51:PRO:HB3	3:D:70:VAL:HG21	2.03	0.41
1:E:564:THR:CB	1:F:554:LYS:HZ3	2.30	0.41
1:F:554:LYS:HE3	2:G:92:TRP:CZ2	2.56	0.41
2:K:108:ARG:CG	2:K:109:ALA:N	2.84	0.41
3:J:209:HIS:NE2	3:J:211:ALA:HB3	2.36	0.41
3:D:132:LEU:HG	3:D:149:GLY:C	2.41	0.41
2:G:35:TRP:CZ3	2:G:88:CYS:HB3	2.55	0.41
2:G:113:PRO:HB3	2:G:139:PHE:HB2	2.02	0.41
3:I:187:LEU:HG	3:I:188:SER:N	2.36	0.41
1:B:570:LEU:HB2	1:B:580:ALA:HB3	2.03	0.40
2:L:91:PHE:O	3:H:105:TYR:HB2	2.21	0.40
2:L:120:PRO:HG2	2:L:186:TYR:CZ	2.56	0.40
1:E:476:THR:HB	1:E:497:SER:OG	2.21	0.40
3:I:69:THR:HG23	3:I:78:TYR:HB2	2.01	0.40
1:B:496:ASP:OD1	1:B:578:ARG:HG2	2.21	0.40
2:C:8:PRO:HG2	2:C:11:LEU:HD11	2.03	0.40
2:C:34:VAL:HG23	2:C:91:PHE:CE2	2.57	0.40
2:K:47:LEU:HD23	2:K:47:LEU:HA	1.80	0.40
3:J:80:GLU:HG2	3:J:82:ARG:HE	1.85	0.40
3:I:9:LEU:HB2	3:I:157:PRO:HG3	2.03	0.40
1:B:498:VAL:HG21	1:B:579:VAL:HB	2.03	0.40
2:C:149:LYS:HZ3	2:C:155:ARG:HA	1.87	0.40
1:F:541:LEU:HD23	1:F:601:LEU:HA	2.03	0.40
3:I:132:LEU:CB	3:I:220:ILE:HG13	2.51	0.40
1:A:492:VAL:HG13	1:A:581:ILE:O	2.21	0.40
2:L:163:TRP:HE1	2:L:175:MET:HE3	1.86	0.40
2:C:35:TRP:CD2	2:C:73:LEU:HB2	2.57	0.40
2:K:136:LEU:HD23	2:K:144:ILE:HD13	2.03	0.40
3:J:16:VAL:O	3:J:80:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:128:SER:HB2	3:J:130:TYR:CZ	2.57	0.40
1:E:529:ILE:HG23	1:E:538:VAL:HG21	2.02	0.40
2:K:90:HIS:CD2	2:K:97:THR:HB	2.56	0.40
3:J:37:GLN:HG2	3:J:39:HIS:H	1.87	0.40
2:G:30:TYR:N	2:G:30:TYR:CD1	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	145/147 (99%)	139 (96%)	4 (3%)	2 (1%)	11	46
1	B	145/147 (99%)	140 (97%)	4 (3%)	1 (1%)	22	61
1	E	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	22	61
1	F	145/147 (99%)	136 (94%)	6 (4%)	3 (2%)	7	39
2	C	192/212 (91%)	176 (92%)	11 (6%)	5 (3%)	5	34
2	G	192/212 (91%)	176 (92%)	13 (7%)	3 (2%)	9	44
2	K	204/212 (96%)	193 (95%)	8 (4%)	3 (2%)	10	45
2	L	204/212 (96%)	192 (94%)	9 (4%)	3 (2%)	10	45
3	D	214/229 (93%)	202 (94%)	10 (5%)	2 (1%)	17	55
3	H	212/229 (93%)	208 (98%)	4 (2%)	0	100	100
3	I	214/229 (93%)	205 (96%)	5 (2%)	4 (2%)	8	40
3	J	212/229 (93%)	207 (98%)	3 (1%)	2 (1%)	17	55
All	All	2224/2352 (95%)	2112 (95%)	83 (4%)	29 (1%)	12	48

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	577	HIS
1	B	503	VAL
2	L	169	LYS
2	C	154	GLU
2	C	157	ASN
3	D	134	PRO
3	D	222	PRO
1	F	503	VAL
2	K	92	TRP
2	K	154	GLU
3	J	39	HIS
2	G	142	LYS
3	I	132	LEU
3	I	134	PRO
3	I	208	ALA
3	I	222	PRO
1	A	503	VAL
2	L	211	ARG
2	C	40	GLN
1	E	503	VAL
2	K	211	ARG
2	L	40	GLN
2	C	92	TRP
2	C	94	THR
1	F	574	ALA
2	G	143	ASP
1	F	576	GLY
3	J	38	SER
2	G	189	HIS

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	120/120 (100%)	119 (99%)	1 (1%)	81	89
1	B	120/120 (100%)	118 (98%)	2 (2%)	60	78
1	E	120/120 (100%)	118 (98%)	2 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	C	175/190 (92%)	167 (95%)	8 (5%)	27	54
2	G	175/190 (92%)	170 (97%)	5 (3%)	42	65
2	K	186/190 (98%)	184 (99%)	2 (1%)	73	85
2	L	186/190 (98%)	182 (98%)	4 (2%)	52	71
3	D	190/199 (96%)	187 (98%)	3 (2%)	62	79
3	H	188/199 (94%)	181 (96%)	7 (4%)	34	60
3	I	190/199 (96%)	180 (95%)	10 (5%)	22	51
3	J	188/199 (94%)	185 (98%)	3 (2%)	62	79
All	All	1958/2036 (96%)	1910 (98%)	48 (2%)	47	68

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	VAL
1	B	496	ASP
1	B	560	ASN
2	L	24	ARG
2	L	93	GLU
2	L	175	MET
2	L	198	HIS
3	H	43	LEU
3	H	70	VAL
3	H	80	GLU
3	H	96	ARG
3	H	123	LYS
3	H	170	SER
3	H	218	LYS
2	C	88	CYS
2	C	93	GLU
2	C	103	LYS
2	C	139	PHE
2	C	142	LYS
2	C	154	GLU
2	C	173	TYR
2	C	188	ARG
3	D	58	GLN
3	D	96	ARG
3	D	215	LYS

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Mol	Chain	Res	Type
1	E	524	ARG
1	E	530	GLN
1	F	459	SER
2	K	89	GLN
2	K	162	SER
3	J	98	ARG
3	J	218	LYS
3	J	223	ARG
2	G	45	GLN
2	G	83	SER
2	G	123	GLU
2	G	160	LEU
2	G	211	ARG
3	I	2	LEU
3	I	3	GLN
3	I	21	LYS
3	I	41	LYS
3	I	82	ARG
3	I	148	LEU
3	I	183	ASP
3	I	215	LYS
3	I	218	LYS
3	I	221	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	HIS
1	B	508	GLN
2	L	38	GLN
2	L	53	ASN
2	L	79	GLN
2	L	138	ASN
2	L	189	HIS
2	L	212	ASN
3	H	72	ASN
3	H	104	ASN
3	H	174	HIS
3	H	206	ASN
3	H	209	HIS
2	C	32	ASN
2	C	53	ASN

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Mol	Chain	Res	Type
2	C	79	GLN
2	C	138	ASN
3	D	37	GLN
3	D	174	HIS
3	D	209	HIS
1	E	577	HIS
1	F	508	GLN
1	F	531	GLN
1	F	532	HIS
2	K	137	ASN
2	K	138	ASN
3	J	31	ASN
3	J	174	HIS
3	J	206	ASN
3	J	209	HIS
2	G	37	GLN
2	G	166	GLN
2	G	190	ASN
3	I	3	GLN
3	I	37	GLN
3	I	58	GLN

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 monosaccharides 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	147/147 (100%)	-0.29	0 100 100	73, 103, 146, 165	0
1	B	147/147 (100%)	-0.23	0 100 100	79, 104, 153, 193	0
1	E	147/147 (100%)	-0.21	1 (0%) 87 82	81, 108, 159, 180	0
1	F	147/147 (100%)	-0.31	0 100 100	68, 107, 158, 175	0
2	C	198/212 (93%)	-0.26	1 (0%) 91 85	55, 169, 218, 283	0
2	G	198/212 (93%)	-0.22	0 100 100	51, 167, 208, 237	0
2	K	208/212 (98%)	-0.26	0 100 100	63, 167, 209, 234	0
2	L	208/212 (98%)	-0.13	5 (2%) 59 49	49, 163, 234, 272	0
3	D	218/229 (95%)	-0.19	5 (2%) 60 51	96, 135, 210, 233	0
3	H	216/229 (94%)	-0.28	1 (0%) 91 85	85, 128, 202, 253	0
3	I	218/229 (95%)	-0.28	2 (0%) 84 77	98, 135, 211, 235	0
3	J	216/229 (94%)	-0.32	1 (0%) 91 85	95, 134, 192, 219	0
All	All	2268/2352 (96%)	-0.25	16 (0%) 87 82	49, 135, 210, 283	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	152	GLY	4.6
2	L	154	GLU	4.1
2	L	152	GLY	3.8
3	H	133	ALA	3.4
3	D	149	GLY	3.4
3	J	221	VAL	3.0
2	L	151	ASP	3.0
2	L	133	VAL	3.0
3	I	189	SER	2.8
3	D	219	LYS	2.4
3	I	133	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	203	VAL	2.4
2	L	196	ALA	2.3
1	E	580	ALA	2.3
3	D	148	LEU	2.1
3	D	134	PRO	2.1

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.