



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:23 PM EDT

PDB ID : 4HKB / pdb_00004hkb
Title : CH67 Fab (unbound) from the CH65-67 Lineage
Authors : Schmidt, A.G.; Harrison, S.C.
Deposited on : 2012-10-15
Resolution : 3.60 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

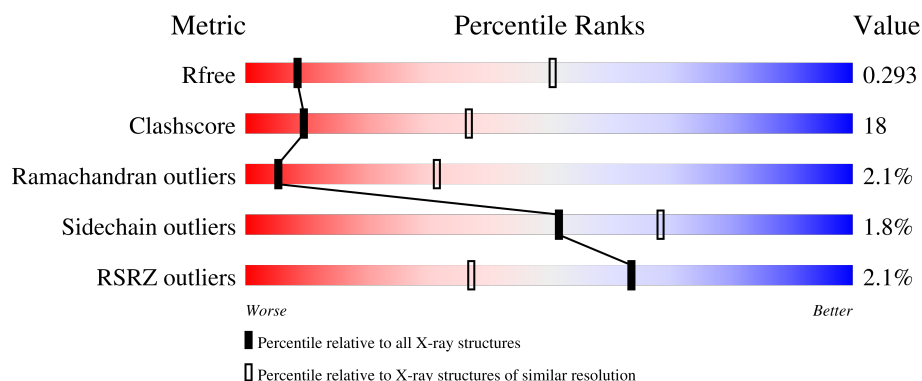
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	236	 2% 64% 25% 5% 7%
1	C	236	 2% 68% 22% • 8%
1	E	236	 2% 64% 27% • 7%
1	G	236	 67% 24% • 8%
1	I	236	 2% 67% 24% • 7%

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Mol	Chain	Length	Quality of chain
1	J	236	3% 62% 27% • 8%
2	B	213	% 46% 29% • 23%
2	D	213	4% 53% 27% • 16%
2	F	213	2% 50% 28% • 19%
2	H	213	2% 51% 27% • 18%
2	K	213	% 54% 28% • 15%
2	N	213	65% 24% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17971 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 CH67 heavy chain.

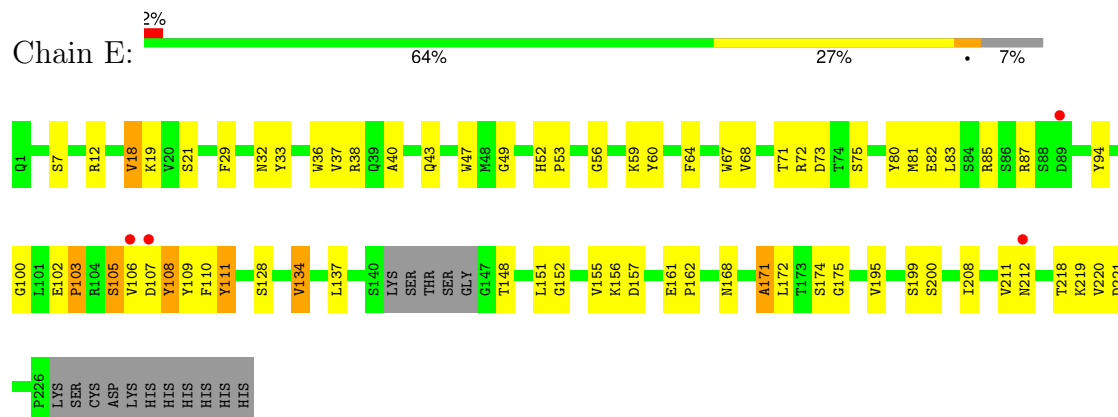
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	218	Total	C	N	O	S	0	0	0
			1665	1056	281	321	7			
1	A	220	Total	C	N	O	S	0	0	0
			1675	1061	283	324	7			
1	C	218	Total	C	N	O	S	0	0	0
			1662	1053	281	321	7			
1	E	220	Total	C	N	O	S	0	0	0
			1675	1061	283	324	7			
1	G	218	Total	C	N	O	S	0	0	0
			1664	1055	281	321	7			
1	I	220	Total	C	N	O	S	0	0	0
			1675	1061	283	324	7			

- Molecule 2 is a protein called CH67 light chain.

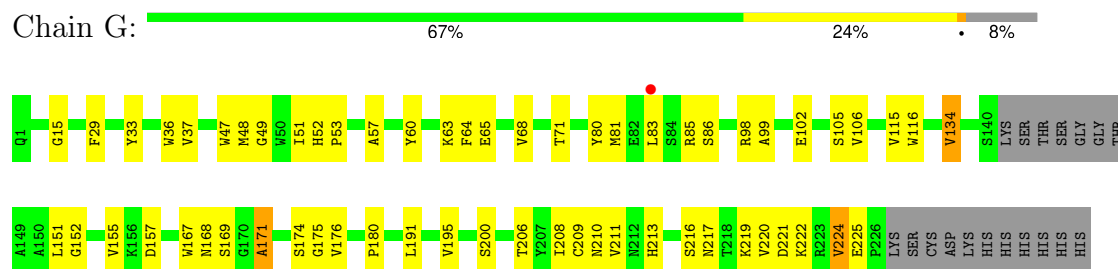
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	193	Total	C	N	O	S	0	0	0
			1433	894	241	294	4			
2	B	164	Total	C	N	O	S	0	0	0
			1216	755	205	252	4			
2	D	179	Total	C	N	O	S	0	0	0
			1341	834	228	275	4			
2	F	173	Total	C	N	O	S	0	0	0
			1303	809	222	268	4			
2	H	174	Total	C	N	O	S	0	0	0
			1306	813	221	268	4			
2	K	182	Total	C	N	O	S	0	0	0
			1356	845	229	278	4			

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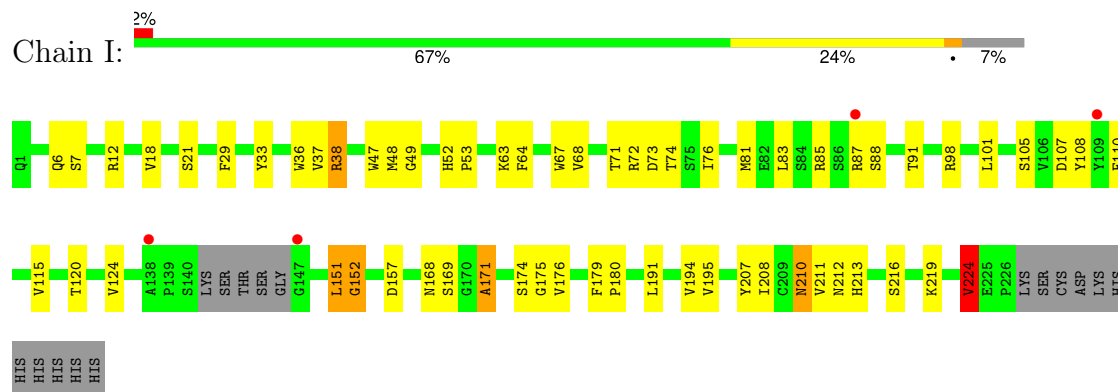
• Molecule 1: CH67 heavy chain



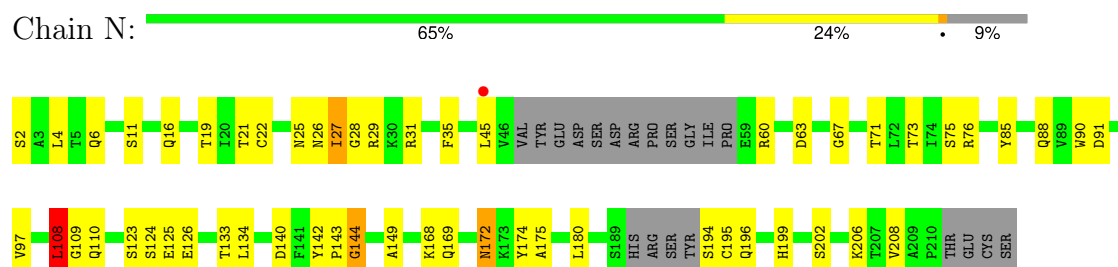
• Molecule 1: CH67 heavy chain



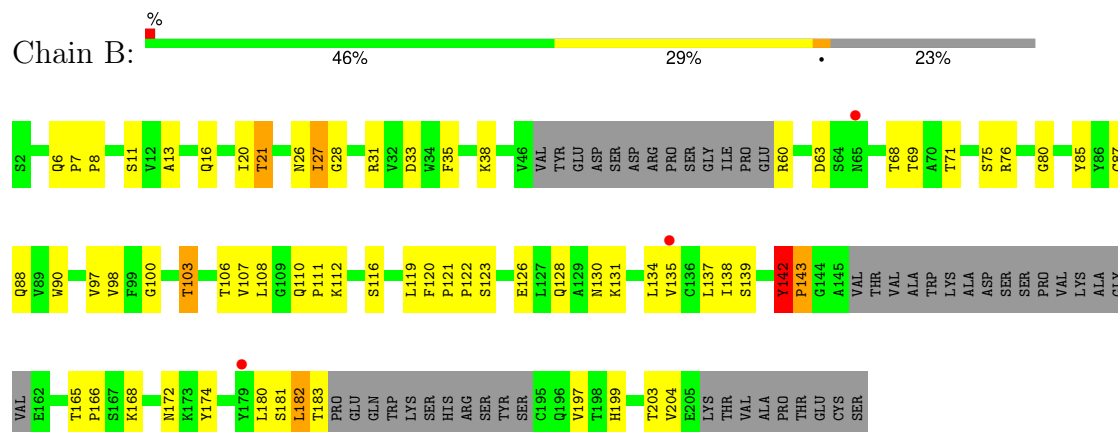
• Molecule 1: CH67 heavy chain



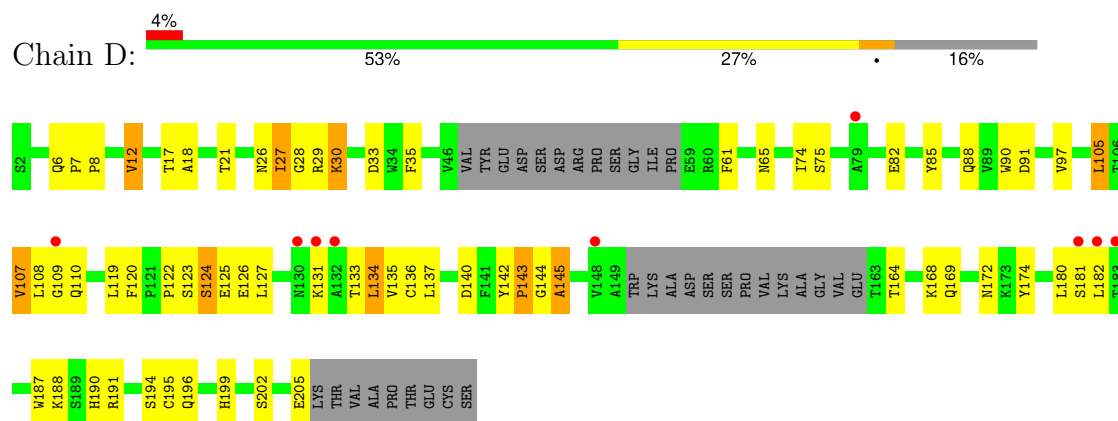
• Molecule 2: CH67 light chain



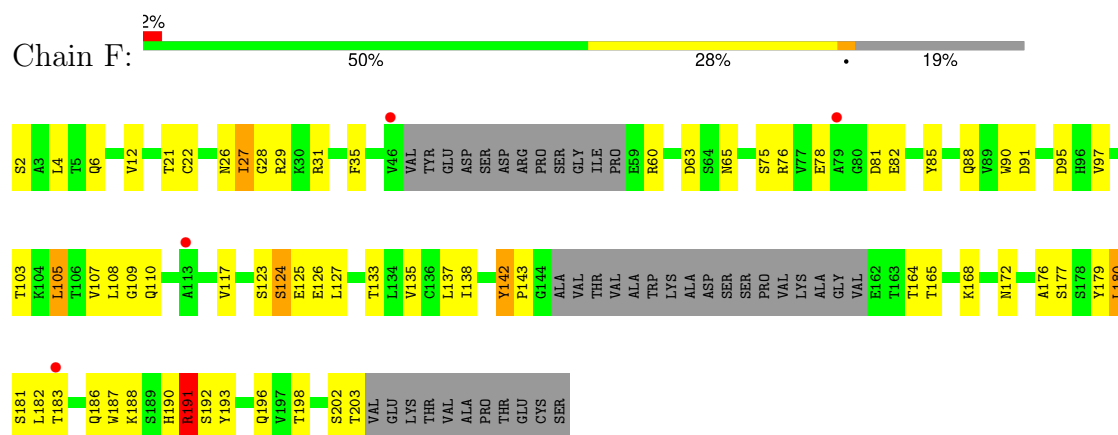
- Molecule 2: CH67 light chain



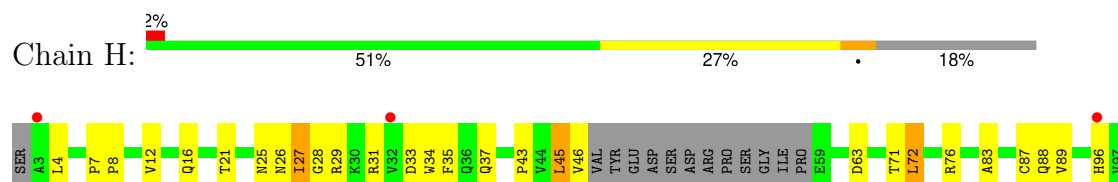
- Molecule 2: CH67 light chain

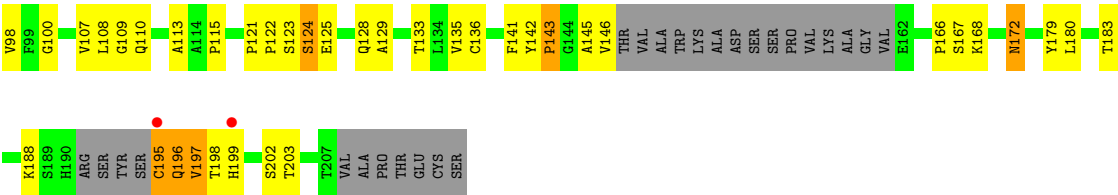


- Molecule 2: CH67 light chain

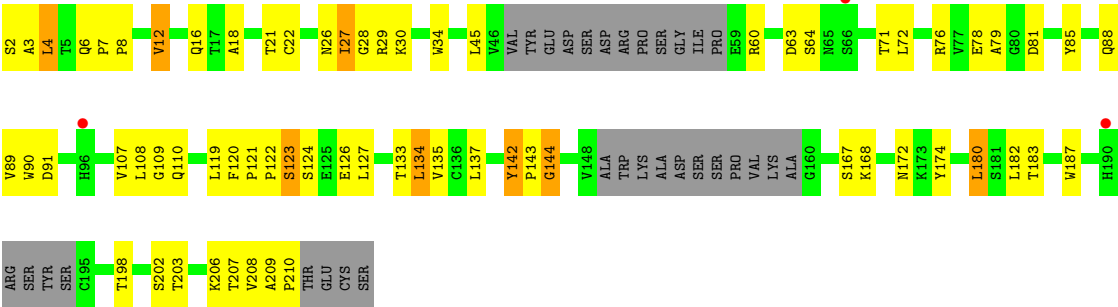


- Molecule 2: CH67 light chain





● Molecule 2: CH67 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.25Å 123.27Å 228.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 3.60 41.70 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (41.70-3.60) 93.6 (41.70-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.258 , 0.306 0.254 , 0.293	Depositor DCC
R_{free} test set	2005 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	89.7	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17971	wwPDB-VP
Average B, all atoms (Å ²)	122.0	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 33.56 % 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 7.8460e-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	0.46	2/1720 (0.1%)	1.09	14/2348 (0.6%)
1	C	0.42	0/1706	1.05	7/2328 (0.3%)
1	E	0.42	2/1720 (0.1%)	1.01	8/2348 (0.3%)
1	G	0.40	0/1709	0.97	6/2333 (0.3%)
1	I	0.39	0/1720	0.96	6/2348 (0.3%)
1	J	0.37	0/1710	0.92	3/2335 (0.1%)
2	B	0.43	1/1239 (0.1%)	1.11	10/1689 (0.6%)
2	D	0.41	1/1370 (0.1%)	1.03	6/1870 (0.3%)
2	F	0.41	0/1332	0.99	5/1816 (0.3%)
2	H	0.36	0/1333	0.97	6/1817 (0.3%)
2	K	0.39	0/1384	0.96	7/1889 (0.4%)
2	N	0.41	0/1464	0.93	2/2000 (0.1%)
All	All	0.41	6/18407 (0.0%)	1.00	80/25121 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GLU	C-N	5.92	1.41	1.33
1	E	102	GLU	C-N	5.77	1.41	1.33
1	A	103	PRO	N-CD	5.41	1.55	1.47
2	D	122	PRO	N-CD	5.30	1.55	1.47
2	B	143	PRO	N-CD	5.27	1.55	1.47
1	E	103	PRO	N-CD	5.26	1.55	1.47

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	GLY	N-CA-C	13.41	125.62	112.08
1	G	152	GLY	N-CA-C	12.49	124.69	112.08
1	E	152	GLY	N-CA-C	9.80	121.98	112.08
1	C	98	ARG	N-CA-C	8.89	124.84	112.04
1	C	107	ASP	N-CA-C	7.55	120.58	111.82
1	I	151	LEU	N-CA-C	6.73	114.30	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	VAL	N-CA-C	6.70	117.73	108.89
1	A	67	TRP	N-CA-C	-6.65	105.46	113.97
2	B	31	ARG	N-CA-C	6.62	119.49	108.96
1	G	102	GLU	CA-C-N	6.59	127.13	120.14
1	G	102	GLU	C-N-CA	6.59	127.13	120.14
2	B	103	THR	N-CA-C	6.58	119.26	109.59
1	E	102	GLU	CA-C-N	-6.54	113.02	119.76
1	E	102	GLU	C-N-CA	-6.54	113.02	119.76
1	G	222	LYS	N-CA-C	6.50	119.01	108.41
2	H	121	PRO	CA-C-N	6.50	126.46	119.76
2	H	121	PRO	C-N-CA	6.50	126.46	119.76
1	A	102	GLU	CA-C-N	-6.48	113.00	119.99
1	A	102	GLU	C-N-CA	-6.48	113.00	119.99
1	E	111	TYR	N-CA-C	6.39	118.32	111.36
1	J	82	GLU	N-CA-C	6.35	119.25	108.90
1	A	224	VAL	N-CA-C	6.28	116.67	107.37
1	I	152	GLY	N-CA-C	6.17	118.31	112.08
2	D	181	SER	N-CA-C	6.11	118.75	107.99
1	I	151	LEU	CA-C-O	6.10	121.48	117.94
1	A	66	GLY	N-CA-C	6.09	123.13	115.21
2	B	21	THR	N-CA-C	6.07	119.57	107.62
2	K	134	LEU	CA-C-N	-6.07	115.67	123.19
2	K	134	LEU	C-N-CA	-6.07	115.67	123.19
1	G	224	VAL	N-CA-C	6.00	117.87	112.17
1	E	134	VAL	N-CA-C	5.97	116.77	108.89
2	K	144	GLY	N-CA-C	5.95	127.27	113.18
1	A	150	ALA	CA-C-N	-5.92	111.69	123.99
1	A	150	ALA	C-N-CA	-5.92	111.69	123.99
2	H	183	THR	CA-C-N	5.89	125.76	119.28
2	H	183	THR	C-N-CA	5.89	125.76	119.28
2	K	142	TYR	C-N-CD	-5.69	108.08	120.60
1	C	170	GLY	N-CA-C	5.68	122.60	115.21
1	C	151	LEU	CA-C-O	5.59	121.18	117.94
2	B	130	ASN	N-CA-C	-5.58	104.44	111.92
1	A	138	ALA	CA-C-N	5.58	126.82	119.84
1	A	138	ALA	C-N-CA	5.58	126.82	119.84
1	E	137	LEU	N-CA-C	5.54	117.56	108.52
2	B	13	ALA	CA-C-N	5.54	125.48	119.78
2	B	13	ALA	C-N-CA	5.54	125.48	119.78
2	F	183	THR	CA-C-N	5.48	125.31	119.28
2	F	183	THR	C-N-CA	5.48	125.31	119.28
2	B	142	TYR	CA-C-N	-5.47	113.00	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	142	TYR	C-N-CA	-5.47	113.00	119.84
2	F	181	SER	N-CA-C	5.36	117.42	107.99
2	D	134	LEU	CA-C-N	-5.35	116.56	123.19
2	D	134	LEU	C-N-CA	-5.35	116.56	123.19
2	F	191	ARG	N-CA-C	5.33	122.16	110.80
1	I	108	TYR	N-CA-C	5.32	119.67	107.48
1	A	52	HIS	CA-C-N	5.32	125.13	119.28
1	A	52	HIS	C-N-CA	5.32	125.13	119.28
2	D	190	HIS	N-CA-C	5.31	118.24	109.85
1	G	134	VAL	N-CA-C	5.28	115.86	108.89
1	J	224	VAL	N-CA-C	5.27	115.17	107.37
1	A	173	THR	N-CA-C	-5.25	107.90	114.56
2	D	21	THR	N-CA-C	5.21	117.89	107.62
2	K	79	ALA	N-CA-C	-5.20	107.48	113.88
1	I	151	LEU	CB-CA-C	-5.20	109.58	117.07
2	N	67	GLY	N-CA-C	-5.20	108.90	115.08
1	I	224	VAL	N-CA-C	5.19	115.06	107.37
2	D	30	LYS	N-CA-C	-5.17	102.62	110.28
1	C	13	LYS	CA-C-N	5.17	125.10	119.78
1	C	13	LYS	C-N-CA	5.17	125.10	119.78
2	N	144	GLY	N-CA-C	5.14	125.37	113.18
2	B	139	SER	N-CA-C	5.12	116.97	109.24
2	F	21	THR	N-CA-C	5.11	117.68	107.62
2	H	129	ALA	CA-C-N	-5.09	114.18	123.34
2	H	129	ALA	C-N-CA	-5.09	114.18	123.34
2	K	183	THR	CA-C-N	5.08	124.87	119.28
2	K	183	THR	C-N-CA	5.08	124.87	119.28
1	A	204	THR	N-CA-C	-5.06	106.24	112.72
2	B	107	VAL	N-CA-C	5.06	114.57	106.88
1	A	104	ARG	CA-CB-CG	-5.06	103.99	114.10
1	J	152	GLY	N-CA-C	5.04	117.18	112.04
1	E	151	LEU	CA-C-O	5.04	120.86	117.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1675	0	1623	59	0
1	C	1662	0	1611	49	0
1	E	1675	0	1623	62	0
1	G	1664	0	1613	41	0
1	I	1675	0	1623	55	0
1	J	1665	0	1617	71	0
2	B	1216	0	1167	84	0
2	D	1341	0	1288	67	0
2	F	1303	0	1242	49	0
2	H	1306	0	1255	60	0
2	K	1356	0	1307	52	0
2	N	1433	0	1387	41	0
All	All	17971	0	17356	627	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 18.

All (627) 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)
2:B:182:LEU:CD1	2:B:183:THR:H	1.19	1.52
2:B:182:LEU:HD12	2:B:183:THR:N	1.12	1.43
1:J:160:PRO:C	1:J:162:PRO:HD2	1.47	1.38
2:D:142:TYR:CD2	2:D:143:PRO:HA	1.61	1.33
2:B:180:LEU:CD1	2:B:181:SER:O	1.82	1.28
2:D:142:TYR:HA	2:D:143:PRO:O	1.30	1.26
2:B:180:LEU:CA	2:B:181:SER:HB3	1.67	1.25
2:B:180:LEU:HA	2:B:181:SER:HB3	1.16	1.14
2:D:142:TYR:CD2	2:D:143:PRO:CA	2.31	1.14
1:J:160:PRO:C	1:J:162:PRO:CD	2.26	1.08
2:H:145:ALA:O	2:H:146:VAL:CG1	2.04	1.05
2:H:145:ALA:O	2:H:146:VAL:HG13	1.56	1.04
2:B:180:LEU:HD12	2:B:181:SER:O	0.87	1.04
2:B:180:LEU:HA	2:B:181:SER:CB	1.88	1.00
1:J:163:VAL:HG23	1:J:212:ASN:O	1.61	0.99
1:A:137:LEU:HB2	1:A:152:GLY:HA3	1.43	0.98
2:B:182:LEU:HD12	2:B:183:THR:CA	1.94	0.97
1:J:160:PRO:O	1:J:162:PRO:HD2	1.63	0.96
2:D:142:TYR:CG	2:D:143:PRO:HA	2.00	0.96
2:D:142:TYR:HA	2:D:143:PRO:C	1.90	0.95
2:D:142:TYR:CA	2:D:143:PRO:O	2.15	0.95
1:J:153:CYS:SG	1:J:209:CYS:CB	2.57	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HG11	1:A:98:ARG:HH21	1.35	0.91
1:J:153:CYS:SG	1:J:209:CYS:HB3	2.12	0.90
2:B:142:TYR:HB3	2:B:143:PRO:HD3	1.53	0.90
1:J:134:VAL:HG12	1:J:155:VAL:HG22	1.56	0.86
2:B:182:LEU:CG	2:B:183:THR:H	1.88	0.85
1:J:139:PRO:HB3	1:J:150:ALA:O	1.74	0.85
1:J:161:GLU:N	1:J:162:PRO:CD	2.39	0.85
1:C:137:LEU:HB3	2:D:120:PHE:CD1	2.12	0.84
1:A:137:LEU:HD21	1:A:154:LEU:HD23	1.58	0.84
2:H:145:ALA:C	2:H:146:VAL:HG13	2.03	0.84
1:J:163:VAL:HG22	1:J:164:THR:N	1.92	0.82
2:D:142:TYR:CD2	2:D:143:PRO:N	2.47	0.82
2:D:142:TYR:CE2	2:D:143:PRO:HA	2.16	0.81
1:I:73:ASP:OD2	1:I:76:ILE:HG12	1.79	0.81
2:F:60:ARG:HH12	2:F:78:GLU:HG3	1.45	0.81
1:E:12:ARG:HD3	1:E:18:VAL:HG12	1.63	0.80
1:E:106:VAL:HG11	2:F:29:ARG:HH21	1.45	0.80
2:H:110:GLN:HB2	2:H:142:TYR:CE1	2.16	0.80
2:B:180:LEU:N	2:B:181:SER:HB3	1.96	0.80
2:H:110:GLN:HB2	2:H:142:TYR:CZ	2.16	0.80
1:C:148:THR:HA	1:C:199:SER:HB3	1.63	0.79
2:D:144:GLY:HA3	2:D:174:TYR:CD2	2.18	0.79
2:H:35:PHE:HE2	2:H:88:GLN:HG2	1.48	0.79
2:B:112:LYS:HZ3	2:B:112:LYS:HB2	1.48	0.79
2:B:142:TYR:HB3	2:B:143:PRO:CD	2.12	0.79
1:C:99:ALA:HB2	1:C:113:LEU:HD23	1.65	0.79
2:H:115:PRO:HD2	2:H:199:HIS:NE2	1.97	0.79
2:B:35:PHE:HE2	2:B:88:GLN:HG2	1.47	0.78
2:K:206:LYS:HG3	2:K:207:THR:H	1.45	0.78
2:B:135:VAL:CG2	2:B:137:LEU:HD21	2.15	0.77
2:H:115:PRO:CD	2:H:199:HIS:CD2	2.67	0.77
1:E:103:PRO:HG3	1:E:111:TYR:HA	1.67	0.77
2:H:115:PRO:HD2	2:H:199:HIS:CD2	2.20	0.76
2:D:35:PHE:HE2	2:D:88:GLN:HG2	1.50	0.76
2:B:180:LEU:CA	2:B:181:SER:CB	2.49	0.76
2:H:145:ALA:O	2:H:146:VAL:HG12	1.86	0.76
1:I:179:PHE:CE1	2:K:137:LEU:HD13	2.20	0.75
2:D:17:THR:HG22	2:D:75:SER:HA	1.67	0.75
1:J:160:PRO:HB2	1:J:162:PRO:HD3	1.68	0.75
2:B:142:TYR:HD2	2:B:143:PRO:HD3	1.52	0.75
2:N:35:PHE:HE2	2:N:88:GLN:HG2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:PRO:HB2	2:B:199:HIS:HE2	1.52	0.74
2:B:142:TYR:CD2	2:B:143:PRO:HD3	2.23	0.74
2:B:120:PHE:HB2	2:B:135:VAL:CG1	2.18	0.73
2:F:35:PHE:HE2	2:F:88:GLN:HG2	1.52	0.72
1:C:213:HIS:HD1	1:C:216:SER:HG	1.31	0.72
1:I:169:SER:H	1:I:210:ASN:HD21	1.36	0.72
2:B:20:ILE:HG21	2:B:103:THR:HG21	1.71	0.72
1:J:101:LEU:HD22	2:N:45:LEU:HD21	1.72	0.72
2:N:123:SER:O	2:N:125:GLU:N	2.22	0.71
2:D:6:GLN:NE2	2:D:85:TYR:O	2.23	0.71
2:D:142:TYR:HD2	2:D:143:PRO:N	1.86	0.71
2:N:126:GLU:OE2	2:N:133:THR:N	2.23	0.71
1:J:163:VAL:HG22	1:J:164:THR:H	1.55	0.71
2:D:134:LEU:HD12	2:D:180:LEU:HD23	1.74	0.70
2:F:6:GLN:NE2	2:F:85:TYR:O	2.23	0.70
1:G:213:HIS:ND1	1:G:216:SER:OG	2.22	0.70
1:J:213:HIS:HD1	1:J:216:SER:HG	1.37	0.70
1:C:99:ALA:HA	1:C:112:GLY:O	1.92	0.69
2:N:169:GLN:HE21	2:N:175:ALA:HB2	1.57	0.69
1:E:148:THR:HA	1:E:199:SER:HB2	1.73	0.69
1:J:108:TYR:CD2	2:N:31:ARG:HG2	2.28	0.69
2:H:198:THR:HG22	2:H:203:THR:HG23	1.72	0.69
2:F:142:TYR:HB3	2:F:143:PRO:HD3	1.76	0.68
1:J:163:VAL:CG2	1:J:164:THR:N	2.55	0.67
2:D:144:GLY:CA	2:D:174:TYR:HD2	2.06	0.67
2:H:115:PRO:CD	2:H:199:HIS:CG	2.77	0.67
1:J:163:VAL:CG2	1:J:164:THR:H	2.06	0.67
1:A:98:ARG:HH11	1:A:100:GLY:HA3	1.58	0.67
2:F:60:ARG:NH1	2:F:76:ARG:O	2.27	0.67
2:B:143:PRO:O	2:B:199:HIS:NE2	2.27	0.67
2:H:145:ALA:C	2:H:146:VAL:CG1	2.66	0.66
1:A:68:VAL:HG22	1:A:83:LEU:HD23	1.76	0.66
2:D:120:PHE:HB2	2:D:135:VAL:CG2	2.26	0.66
2:B:142:TYR:HD2	2:B:143:PRO:CD	2.08	0.66
1:J:156:LYS:HG3	1:J:190:SER:OG	1.96	0.65
1:J:105:SER:OG	1:J:106:VAL:N	2.27	0.64
1:A:137:LEU:HB2	1:A:152:GLY:CA	2.23	0.64
1:A:137:LEU:HD21	1:A:154:LEU:CD2	2.27	0.64
1:G:134:VAL:HG12	1:G:155:VAL:HG22	1.80	0.64
2:H:115:PRO:HD3	2:H:199:HIS:CD2	2.32	0.64
2:B:6:GLN:HE21	2:B:7:PRO:HD2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:PRO:HD2	2:H:199:HIS:CE1	2.32	0.64
1:E:218:THR:O	1:E:219:LYS:HD3	1.99	0.63
2:F:123:SER:O	2:F:125:GLU:N	2.29	0.63
1:E:106:VAL:HG11	2:F:29:ARG:NH2	2.13	0.63
2:D:145:ALA:O	2:D:199:HIS:HD2	1.82	0.63
1:A:212:ASN:OD1	1:A:219:LYS:HG2	1.98	0.63
2:B:112:LYS:HB2	2:B:112:LYS:NZ	2.13	0.63
2:D:82:GLU:HA	2:D:105:LEU:HD22	1.81	0.62
2:H:115:PRO:HD3	2:H:199:HIS:CG	2.35	0.62
2:B:143:PRO:HB2	2:B:199:HIS:NE2	2.15	0.62
1:A:2:VAL:HG11	1:A:98:ARG:NH2	2.12	0.62
1:G:217:ASN:O	1:G:217:ASN:ND2	2.33	0.62
1:J:85:ARG:HG3	1:G:85:ARG:HG3	1.82	0.61
1:E:110:PHE:HE2	2:F:88:GLN:HE22	1.48	0.61
1:J:87:ARG:HG2	1:J:88:SER:N	2.16	0.61
1:E:109:TYR:CE2	1:I:219:LYS:HB3	2.35	0.61
2:B:182:LEU:CD1	2:B:183:THR:OG1	2.47	0.61
1:G:37:VAL:HG23	1:G:47:TRP:HA	1.82	0.61
2:D:123:SER:O	2:D:125:GLU:N	2.32	0.61
1:A:168:ASN:OD1	1:A:208:ILE:HG12	2.01	0.61
2:D:120:PHE:HB2	2:D:135:VAL:HG22	1.83	0.61
1:J:33:TYR:CE1	1:J:52:HIS:HD2	2.18	0.61
1:E:19:LYS:HD3	1:E:82:GLU:HB2	1.81	0.61
2:B:142:TYR:CB	2:B:143:PRO:HD3	2.30	0.61
2:K:144:GLY:HA3	2:K:174:TYR:HD2	1.66	0.61
2:N:2:SER:N	2:N:91:ASP:OD2	2.33	0.60
2:B:121:PRO:HA	2:B:134:LEU:HD12	1.82	0.60
2:B:182:LEU:CD1	2:B:183:THR:N	2.02	0.60
1:A:135:PHE:HE2	1:A:156:LYS:HE2	1.67	0.60
2:K:180:LEU:HD11	2:K:182:LEU:HD12	1.84	0.60
2:K:122:PRO:HB2	2:K:127:LEU:HD11	1.83	0.60
1:J:162:PRO:HG2	1:J:215:PRO:HG2	1.84	0.60
1:I:101:LEU:HD22	2:K:45:LEU:HD21	1.84	0.60
2:B:182:LEU:HD12	2:B:183:THR:CB	2.32	0.60
2:K:120:PHE:HB2	2:K:135:VAL:HG22	1.84	0.60
2:D:144:GLY:CA	2:D:174:TYR:CD2	2.82	0.60
2:K:144:GLY:HA3	2:K:174:TYR:CD2	2.37	0.60
1:A:33:TYR:CE1	1:A:52:HIS:HD2	2.20	0.59
1:A:152:GLY:O	1:A:153:CYS:HB2	2.02	0.59
1:J:161:GLU:N	1:J:162:PRO:HD3	2.17	0.59
2:B:20:ILE:CG2	2:B:103:THR:HG21	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:SER:N	2:K:91:ASP:OD2	2.36	0.59
2:K:119:LEU:HB3	2:K:206:LYS:HG2	1.85	0.59
2:F:126:GLU:OE2	2:F:133:THR:N	2.28	0.59
2:N:168:LYS:HA	2:N:174:TYR:HD1	1.68	0.59
1:A:64:PHE:HA	1:A:67:TRP:HE1	1.67	0.59
1:E:134:VAL:HG12	1:E:155:VAL:HG22	1.84	0.59
2:F:26:ASN:C	2:F:28:GLY:H	2.11	0.59
2:F:196:GLN:HG2	2:F:203:THR:HG21	1.84	0.59
2:B:134:LEU:H	2:B:181:SER:H	1.49	0.59
1:E:208:ILE:HD11	1:E:221:ASP:HB3	1.85	0.58
1:G:134:VAL:HG21	1:G:220:VAL:HG11	1.85	0.58
2:D:142:TYR:CA	2:D:143:PRO:C	2.72	0.58
2:B:6:GLN:NE2	2:B:7:PRO:HD2	2.19	0.58
2:D:136:CYS:HG	2:D:195:CYS:HG	0.64	0.58
1:J:129:THR:O	1:E:128:SER:HB2	2.03	0.58
2:B:63:ASP:OD1	2:B:63:ASP:N	2.37	0.58
1:J:160:PRO:CA	1:J:162:PRO:HD2	2.30	0.58
1:A:151:LEU:HD23	1:A:151:LEU:H	1.69	0.58
1:G:68:VAL:HG22	1:G:83:LEU:HD23	1.85	0.58
2:N:60:ARG:HD2	2:N:76:ARG:HB2	1.85	0.58
2:K:133:THR:HA	2:K:180:LEU:O	2.03	0.58
1:C:83:LEU:HD21	1:C:90:ASP:HB3	1.86	0.58
1:G:63:LYS:HG3	1:G:64:PHE:CD1	2.39	0.58
2:K:209:ALA:HB3	2:K:210:PRO:HD3	1.86	0.58
2:B:21:THR:HG22	2:B:71:THR:HG22	1.85	0.58
1:C:33:TYR:CE1	1:C:52:HIS:CD2	2.92	0.57
2:B:135:VAL:HG22	2:B:137:LEU:CD2	2.34	0.57
1:A:164:THR:HG23	1:A:212:ASN:HB2	1.85	0.57
2:B:119:LEU:HD11	2:B:134:LEU:HG	1.85	0.57
1:I:12:ARG:NH1	1:I:18:VAL:HA	2.19	0.57
1:J:160:PRO:HB2	1:J:162:PRO:CD	2.35	0.57
2:H:136:CYS:HG	2:H:195:CYS:HG	1.36	0.57
1:J:64:PHE:HB3	1:J:68:VAL:HG11	1.87	0.57
2:B:119:LEU:HD12	2:B:135:VAL:O	2.05	0.57
2:H:142:TYR:N	2:H:143:PRO:HD2	2.20	0.57
1:C:7:SER:OG	1:C:21:SER:OG	2.20	0.57
2:D:124:SER:HA	2:D:127:LEU:HD13	1.86	0.56
2:B:135:VAL:HG22	2:B:137:LEU:HD21	1.86	0.56
2:K:120:PHE:HB2	2:K:135:VAL:CG2	2.35	0.56
1:A:87:ARG:HH21	1:I:87:ARG:NH1	2.03	0.56
1:C:182:VAL:HG22	2:D:164:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:GLU:HB2	2:D:107:VAL:HG12	1.87	0.56
2:N:63:ASP:OD1	2:N:63:ASP:N	2.38	0.56
1:C:213:HIS:ND1	1:C:216:SER:OG	2.31	0.56
2:B:6:GLN:HG2	2:B:103:THR:H	1.70	0.56
2:H:63:ASP:N	2:H:63:ASP:OD1	2.38	0.56
2:B:181:SER:O	2:B:182:LEU:HB3	2.05	0.56
1:A:47:TRP:CG	2:B:97:VAL:HB	2.39	0.56
1:C:151:LEU:O	2:D:120:PHE:CZ	2.59	0.56
2:N:21:THR:HG22	2:N:71:THR:HG22	1.86	0.56
2:H:142:TYR:O	2:H:143:PRO:C	2.49	0.56
2:K:63:ASP:OD1	2:K:63:ASP:N	2.39	0.56
2:B:110:GLN:HB3	2:B:111:PRO:HD2	1.88	0.56
2:F:63:ASP:OD1	2:F:63:ASP:N	2.39	0.56
2:N:19:THR:HG22	2:N:73:THR:HG22	1.88	0.55
2:D:144:GLY:O	2:D:145:ALA:HB2	2.05	0.55
2:F:168:LYS:HE2	2:F:172:ASN:OD1	2.06	0.55
2:K:26:ASN:C	2:K:28:GLY:H	2.14	0.55
2:H:133:THR:HA	2:H:180:LEU:O	2.05	0.55
2:B:33:ASP:HB2	2:B:88:GLN:HG3	1.89	0.55
1:I:179:PHE:CZ	2:K:137:LEU:HB3	2.41	0.55
1:E:7:SER:OG	1:E:21:SER:OG	2.24	0.55
1:G:169:SER:H	1:G:210:ASN:ND2	2.04	0.55
2:B:142:TYR:CD2	2:B:143:PRO:CD	2.86	0.55
2:H:142:TYR:N	2:H:143:PRO:CD	2.70	0.55
1:E:134:VAL:HG11	1:E:211:VAL:HG21	1.88	0.55
2:H:31:ARG:NH2	2:H:33:ASP:OD1	2.39	0.55
2:H:195:CYS:O	2:H:196:GLN:HB2	2.06	0.55
1:I:37:VAL:HG23	1:I:47:TRP:HA	1.88	0.54
1:G:209:CYS:O	1:G:221:ASP:HA	2.08	0.54
1:C:33:TYR:CE1	1:C:52:HIS:HD2	2.26	0.54
1:C:197:VAL:HG22	1:C:198:PRO:HD2	1.90	0.54
1:E:134:VAL:HG21	1:E:220:VAL:HG11	1.90	0.54
2:N:194:SER:HA	2:N:208:VAL:HG23	1.90	0.54
1:A:208:ILE:HB	1:A:221:ASP:OD1	2.08	0.54
1:E:33:TYR:CE1	1:E:52:HIS:HD2	2.26	0.54
1:I:152:GLY:HA3	1:I:194:VAL:HG12	1.87	0.54
2:N:26:ASN:C	2:N:28:GLY:H	2.16	0.54
1:E:33:TYR:CE1	1:E:52:HIS:CD2	2.96	0.54
1:J:98:ARG:HB3	1:J:115:VAL:HG13	1.90	0.53
1:J:172:LEU:HD11	1:J:207:TYR:CE1	2.43	0.53
1:A:87:ARG:NH2	1:I:87:ARG:HD3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:PHE:CE2	2:B:88:GLN:HG2	2.37	0.53
2:K:144:GLY:CA	2:K:174:TYR:HD2	2.20	0.53
1:I:33:TYR:CE1	1:I:52:HIS:HD2	2.26	0.53
1:J:129:THR:HB	1:E:128:SER:HB3	1.90	0.53
1:C:87:ARG:HH12	1:E:87:ARG:NE	2.07	0.53
1:I:169:SER:N	1:I:210:ASN:HD21	2.06	0.53
1:J:73:ASP:O	1:J:74:THR:HB	2.08	0.53
1:G:169:SER:H	1:G:210:ASN:HD21	1.54	0.53
1:I:33:TYR:CE1	1:I:52:HIS:CD2	2.97	0.53
1:J:213:HIS:ND1	1:J:216:SER:OG	2.29	0.53
2:D:142:TYR:CD2	2:D:142:TYR:C	2.86	0.53
2:H:168:LYS:HE2	2:H:172:ASN:HA	1.91	0.53
1:J:151:LEU:HG	1:J:224:VAL:HG11	1.91	0.53
2:B:142:TYR:CB	2:B:143:PRO:CD	2.86	0.53
2:H:45:LEU:HD22	2:H:46:VAL:H	1.73	0.53
2:K:60:ARG:HH12	2:K:78:GLU:HG3	1.74	0.53
1:A:138:ALA:HB1	1:A:226:PRO:HA	1.90	0.52
1:C:38:ARG:HH21	1:C:90:ASP:HA	1.74	0.52
1:E:32:ASN:ND2	1:E:100:GLY:HA2	2.23	0.52
2:B:197:VAL:HG12	2:B:204:VAL:HB	1.91	0.52
1:C:36:TRP:CE2	1:C:81:MET:HB2	2.44	0.52
1:J:71:THR:OG1	1:J:80:TYR:HB2	2.10	0.52
1:G:211:VAL:O	1:G:219:LYS:HA	2.10	0.52
1:G:98:ARG:HG2	1:G:115:VAL:HB	1.90	0.52
1:E:103:PRO:HG3	1:E:110:PHE:O	2.09	0.52
1:G:176:VAL:HG12	1:G:195:VAL:HG22	1.92	0.52
2:F:82:GLU:HB2	2:F:107:VAL:HG22	1.91	0.52
2:B:134:LEU:HB3	2:B:180:LEU:O	2.09	0.52
1:C:87:ARG:HH12	1:E:87:ARG:CD	2.23	0.52
1:J:32:ASN:OD1	1:J:98:ARG:NH1	2.43	0.51
1:A:29:PHE:CE2	1:A:53:PRO:HB3	2.45	0.51
1:A:64:PHE:HA	1:A:67:TRP:NE1	2.24	0.51
1:C:156:LYS:NZ	2:D:131:LYS:HD3	2.25	0.51
1:E:37:VAL:HG23	1:E:47:TRP:HA	1.92	0.51
1:E:105:SER:HB3	2:F:31:ARG:NH1	2.26	0.51
2:N:109:GLY:O	2:N:110:GLN:HG2	2.11	0.51
1:E:106:VAL:CG1	2:F:29:ARG:HH21	2.21	0.51
2:H:146:VAL:HG23	2:H:146:VAL:O	2.09	0.51
2:N:195:CYS:HB3	2:N:206:LYS:HB2	1.92	0.51
1:J:87:ARG:HG2	1:J:88:SER:H	1.75	0.51
1:J:156:LYS:HG2	1:J:157:ASP:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4:LEU:HD23	2:K:22:CYS:SG	2.51	0.51
1:C:197:VAL:CG2	1:C:198:PRO:HD2	2.40	0.51
2:F:124:SER:HA	2:F:127:LEU:HD23	1.93	0.51
2:F:180:LEU:HD11	2:F:182:LEU:HD12	1.91	0.51
2:K:206:LYS:CG	2:K:207:THR:H	2.21	0.51
1:J:172:LEU:HD11	1:J:207:TYR:HE1	1.76	0.51
1:C:137:LEU:HD22	2:D:120:PHE:HB3	1.93	0.51
1:J:47:TRP:CZ2	1:J:49:GLY:HA2	2.45	0.50
1:A:167:TRP:HB2	1:A:172:LEU:HB2	1.93	0.50
1:I:211:VAL:O	1:I:219:LYS:HA	2.11	0.50
1:C:37:VAL:HG23	1:C:47:TRP:HA	1.94	0.50
1:C:137:LEU:HB3	2:D:120:PHE:CE1	2.47	0.50
1:C:169:SER:H	1:C:210:ASN:ND2	2.08	0.50
2:B:135:VAL:CG2	2:B:137:LEU:CD2	2.86	0.50
1:J:36:TRP:CE2	1:J:81:MET:HB2	2.47	0.50
1:I:64:PHE:O	1:I:68:VAL:HG22	2.11	0.50
2:F:2:SER:N	2:F:91:ASP:OD2	2.44	0.50
1:I:64:PHE:HA	1:I:67:TRP:NE1	2.25	0.50
2:F:186:GLN:HG2	2:F:190:HIS:CE1	2.46	0.50
2:H:122:PRO:C	2:H:124:SER:H	2.20	0.50
1:A:135:PHE:CE2	1:A:156:LYS:HE2	2.46	0.50
2:N:140:ASP:H	2:N:169:GLN:HE22	1.58	0.50
2:K:2:SER:OG	2:K:3:ALA:N	2.36	0.50
1:E:212:ASN:HA	1:E:219:LYS:HD2	1.94	0.50
1:G:206:THR:OG1	1:G:225:GLU:OE1	2.22	0.50
2:N:149:ALA:O	2:N:196:GLN:HG2	2.12	0.50
2:D:30:LYS:NZ	2:D:91:ASP:OD1	2.42	0.50
2:D:134:LEU:HB2	2:D:180:LEU:HB3	1.94	0.50
1:C:158:TYR:OH	1:C:161:GLU:OE1	2.20	0.50
1:G:33:TYR:HB2	1:G:99:ALA:HB3	1.93	0.50
2:N:6:GLN:NE2	2:N:85:TYR:O	2.39	0.50
1:A:168:ASN:HA	1:A:208:ILE:HD11	1.93	0.49
1:I:107:ASP:OD1	1:I:107:ASP:N	2.42	0.49
2:K:168:LYS:HA	2:K:174:TYR:HD1	1.76	0.49
1:E:107:ASP:OD2	2:F:29:ARG:HD3	2.12	0.49
1:C:27:TYR:CZ	1:C:98:ARG:HD3	2.48	0.49
2:H:26:ASN:C	2:H:28:GLY:H	2.20	0.49
1:A:87:ARG:HD2	1:I:67:TRP:CD2	2.47	0.49
2:K:126:GLU:OE2	2:K:133:THR:HG22	2.12	0.49
1:A:176:VAL:HG12	1:A:195:VAL:HG22	1.94	0.49
1:I:7:SER:HB3	1:I:21:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:MET:HG2	1:I:64:PHE:CE2	2.47	0.49
1:I:212:ASN:ND2	1:I:219:LYS:HE2	2.27	0.49
2:B:123:SER:OG	2:B:126:GLU:HG3	2.12	0.49
1:J:33:TYR:CE1	1:J:52:HIS:CD2	3.00	0.49
2:B:120:PHE:HB2	2:B:135:VAL:HG13	1.95	0.49
1:A:85:ARG:HG3	1:I:85:ARG:HG3	1.94	0.49
1:A:110:PHE:HE2	2:B:88:GLN:HE22	1.60	0.49
1:E:168:ASN:HB2	1:E:171:ALA:HB3	1.95	0.49
2:F:60:ARG:NH2	2:F:81:ASP:OD2	2.45	0.49
1:A:154:LEU:C	1:A:154:LEU:HD12	2.37	0.49
1:E:59:LYS:HE2	2:F:95:ASP:HB3	1.95	0.49
2:K:6:GLN:NE2	2:K:85:TYR:O	2.42	0.49
2:K:30:LYS:HD2	2:K:90:TRP:O	2.13	0.49
1:A:47:TRP:CD2	2:B:97:VAL:HB	2.48	0.49
2:D:123:SER:O	2:D:125:GLU:HG2	2.12	0.49
2:H:107:VAL:O	2:H:109:GLY:N	2.45	0.49
1:E:47:TRP:CZ2	1:E:49:GLY:HA2	2.49	0.48
2:N:144:GLY:HA3	2:N:174:TYR:CD2	2.48	0.48
2:D:110:GLN:HE22	2:D:172:ASN:HB3	1.77	0.48
1:E:53:PRO:O	1:E:72:ARG:NE	2.46	0.48
2:H:115:PRO:HA	2:H:141:PHE:HB3	1.95	0.48
1:E:106:VAL:O	1:E:109:TYR:CZ	2.67	0.48
2:H:115:PRO:HG3	2:H:199:HIS:ND1	2.29	0.48
1:A:136:PRO:HB3	1:A:224:VAL:HG22	1.96	0.48
1:I:98:ARG:HD3	1:I:115:VAL:HB	1.95	0.48
2:D:187:TRP:CD1	2:D:188:LYS:HG3	2.49	0.48
1:E:108:TYR:CE1	2:F:90:TRP:HB3	2.48	0.48
1:G:47:TRP:CZ2	1:G:49:GLY:HA2	2.49	0.48
2:H:135:VAL:HG12	2:H:179:TYR:CD2	2.49	0.48
1:J:108:TYR:CE2	2:N:31:ARG:HG2	2.48	0.48
1:A:56:GLY:CA	1:A:72:ARG:HE	2.27	0.48
1:A:168:ASN:HB2	1:A:171:ALA:HB3	1.96	0.48
2:B:60:ARG:HD2	2:B:75:SER:O	2.13	0.48
1:C:7:SER:HG	1:C:21:SER:HG	1.58	0.48
1:A:48:MET:HA	1:A:64:PHE:CD2	2.49	0.47
2:K:12:VAL:HG21	2:K:18:ALA:HB2	1.96	0.47
1:E:40:ALA:HB3	1:E:43:GLN:HB2	1.96	0.47
2:D:168:LYS:HA	2:D:174:TYR:HD1	1.78	0.47
2:F:27:ILE:HG22	2:F:65:ASN:HD21	1.78	0.47
1:J:133:SER:O	1:J:133:SER:OG	2.32	0.47
2:D:26:ASN:C	2:D:28:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:ILE:O	2:D:65:ASN:ND2	2.37	0.47
1:J:168:ASN:HB2	1:J:171:ALA:HB3	1.96	0.47
1:A:15:GLY:N	1:A:86:SER:O	2.40	0.47
1:I:179:PHE:CD1	2:K:137:LEU:HD13	2.49	0.47
2:N:144:GLY:CA	2:N:174:TYR:HD2	2.28	0.47
2:H:37:GLN:O	2:H:83:ALA:HB1	2.14	0.47
1:E:71:THR:OG1	1:E:80:TYR:HB2	2.13	0.47
2:B:27:ILE:HD11	2:B:68:THR:C	2.40	0.47
2:K:7:PRO:HA	2:K:8:PRO:HD3	1.82	0.47
1:E:107:ASP:OD2	2:F:29:ARG:NE	2.47	0.47
1:J:107:ASP:OD2	2:N:29:ARG:NH1	2.47	0.47
1:J:160:PRO:HG2	1:J:162:PRO:HG3	1.95	0.47
1:C:66:GLY:O	1:E:85:ARG:NH2	2.48	0.47
1:E:18:VAL:HG23	1:E:83:LEU:HD23	1.97	0.47
1:G:29:PHE:CE2	1:G:53:PRO:HB3	2.50	0.47
1:I:64:PHE:HA	1:I:67:TRP:HE1	1.80	0.47
2:N:169:GLN:NE2	2:N:175:ALA:HB2	2.26	0.47
1:J:210:ASN:ND2	1:J:221:ASP:OD1	2.48	0.47
1:E:212:ASN:OD1	1:E:219:LYS:NZ	2.34	0.46
1:I:213:HIS:ND1	1:I:216:SER:OG	2.47	0.46
2:N:60:ARG:HD2	2:N:75:SER:O	2.15	0.46
2:B:135:VAL:HG21	2:B:137:LEU:HD21	1.94	0.46
1:A:108:TYR:CE1	2:B:90:TRP:HB3	2.51	0.46
1:C:47:TRP:CD2	2:D:97:VAL:HB	2.51	0.46
1:A:150:ALA:HA	1:A:195:VAL:O	2.15	0.46
1:I:38:ARG:HD3	1:I:64:PHE:CE2	2.50	0.46
1:I:87:ARG:HG2	1:I:88:SER:N	2.31	0.46
2:D:142:TYR:HD2	2:D:142:TYR:C	2.23	0.46
1:J:47:TRP:CG	2:N:97:VAL:HB	2.51	0.46
1:C:81:MET:HE3	1:C:81:MET:HB3	1.83	0.46
2:N:16:GLN:O	2:N:76:ARG:N	2.49	0.46
2:N:35:PHE:CE2	2:N:88:GLN:HG2	2.42	0.46
2:B:116:SER:O	2:B:116:SER:OG	2.29	0.46
2:D:61:PHE:CD1	2:D:74:ILE:HG22	2.50	0.46
2:D:144:GLY:HA3	2:D:174:TYR:CE2	2.50	0.46
2:H:115:PRO:CG	2:H:199:HIS:ND1	2.78	0.46
2:K:123:SER:OG	2:K:124:SER:N	2.48	0.46
2:K:142:TYR:HA	2:K:143:PRO:C	2.41	0.46
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.50	0.46
1:E:38:ARG:HD3	1:E:94:TYR:CE2	2.51	0.46
2:H:115:PRO:CD	2:H:199:HIS:CE1	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:VAL:HG12	1:E:83:LEU:HD13	1.98	0.46
1:G:48:MET:HG2	1:G:64:PHE:CE2	2.50	0.46
2:D:142:TYR:CG	2:D:143:PRO:CA	2.79	0.46
1:I:176:VAL:HG12	1:I:195:VAL:HG12	1.98	0.46
1:C:10:GLU:HB2	1:C:122:VAL:HA	1.98	0.46
1:C:37:VAL:HG12	1:C:95:TYR:HB2	1.97	0.46
2:D:18:ALA:HB3	2:D:74:ILE:HD11	1.96	0.46
2:H:87:CYS:O	2:H:100:GLY:N	2.47	0.46
1:J:14:PRO:HB2	1:G:65:GLU:O	2.16	0.46
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.51	0.46
2:B:128:GLN:HG2	2:H:128:GLN:O	2.16	0.46
2:H:113:ALA:HB3	2:H:142:TYR:H	1.81	0.46
2:K:121:PRO:HB3	2:K:208:VAL:CG1	2.46	0.46
2:K:121:PRO:HB3	2:K:208:VAL:HG11	1.97	0.46
1:E:56:GLY:CA	1:E:72:ARG:HD3	2.46	0.45
2:B:182:LEU:CG	2:B:183:THR:N	2.60	0.45
2:H:34:TRP:CE2	2:H:72:LEU:HB2	2.51	0.45
2:H:123:SER:O	2:H:125:GLU:HG2	2.16	0.45
2:K:4:LEU:HD11	2:K:89:VAL:HG22	1.99	0.45
2:K:187:TRP:HH2	2:K:208:VAL:HG11	1.82	0.45
1:C:182:VAL:HG22	2:D:164:THR:CG2	2.46	0.45
1:E:68:VAL:HG12	1:E:83:LEU:CD1	2.46	0.45
2:H:145:ALA:HA	2:H:166:PRO:HG2	1.97	0.45
1:A:87:ARG:HH21	1:I:87:ARG:HH11	1.64	0.45
2:D:145:ALA:O	2:D:199:HIS:CD2	2.66	0.45
1:A:37:VAL:HG11	1:A:116:TRP:HZ3	1.81	0.45
1:G:15:GLY:N	1:G:86:SER:O	2.47	0.45
1:G:33:TYR:CE1	1:G:52:HIS:HD2	2.34	0.45
1:I:47:TRP:CZ2	1:I:49:GLY:HA2	2.52	0.45
2:F:138:ILE:HD11	2:F:176:ALA:HB3	1.98	0.45
1:A:103:PRO:HG3	1:A:110:PHE:N	2.32	0.45
2:D:180:LEU:HG	2:D:182:LEU:HD13	1.98	0.45
2:F:107:VAL:O	2:F:109:GLY:N	2.50	0.45
1:I:68:VAL:HG12	1:I:83:LEU:HD13	1.97	0.45
2:D:133:THR:HA	2:D:180:LEU:O	2.16	0.45
2:H:197:VAL:C	2:H:198:THR:CG2	2.89	0.45
1:E:18:VAL:CG2	1:E:83:LEU:HB2	2.47	0.45
1:I:73:ASP:O	1:I:74:THR:HB	2.17	0.45
1:E:108:TYR:HE1	2:F:90:TRP:HB3	1.82	0.45
1:E:110:PHE:HB2	2:F:90:TRP:CE3	2.52	0.45
1:I:6:GLN:NE2	1:I:120:THR:HG23	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:ASP:OD2	2:K:29:ARG:HB3	2.17	0.45
1:I:110:PHE:HB2	2:K:90:TRP:CE3	2.52	0.45
2:F:191:ARG:NH1	2:F:192:SER:HB3	2.32	0.45
1:J:160:PRO:CB	1:J:162:PRO:CD	2.95	0.44
1:C:174:SER:OG	1:C:175:GLY:N	2.49	0.44
1:G:51:ILE:HD12	1:G:57:ALA:O	2.16	0.44
1:I:152:GLY:HA2	1:I:194:VAL:HA	1.98	0.44
2:B:20:ILE:O	2:B:71:THR:HA	2.17	0.44
1:J:161:GLU:HG3	1:J:189:TYR:CD1	2.52	0.44
1:C:87:ARG:HG2	1:E:67:TRP:CD1	2.52	0.44
1:I:180:PRO:HG2	2:K:167:SER:HB2	1.99	0.44
2:B:103:THR:HG23	2:B:103:THR:O	2.16	0.44
2:F:82:GLU:HA	2:F:105:LEU:HD22	1.98	0.44
2:K:134:LEU:HB2	2:K:180:LEU:HB3	1.99	0.44
1:I:219:LYS:HB2	1:I:219:LYS:HE3	1.69	0.44
2:N:142:TYR:HA	2:N:143:PRO:C	2.42	0.44
2:K:64:SER:OG	2:K:71:THR:OG1	2.35	0.44
1:G:151:LEU:HG	1:G:224:VAL:HG21	2.00	0.44
2:D:27:ILE:O	2:D:27:ILE:HG22	2.18	0.44
1:A:72:ARG:HH11	1:A:74:THR:HG23	1.82	0.44
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.52	0.44
1:G:29:PHE:CZ	1:G:53:PRO:HB3	2.51	0.44
2:B:16:GLN:O	2:B:76:ARG:N	2.51	0.44
1:J:174:SER:OG	1:J:175:GLY:N	2.50	0.44
1:A:33:TYR:CE1	1:A:52:HIS:CD2	3.04	0.44
1:C:13:LYS:HD3	1:C:125:SER:O	2.17	0.44
2:B:122:PRO:HD3	2:B:134:LEU:CD1	2.47	0.44
2:D:140:ASP:H	2:D:169:GLN:NE2	2.16	0.44
2:F:110:GLN:HB2	2:F:142:TYR:CZ	2.53	0.44
2:K:187:TRP:HH2	2:K:208:VAL:CG1	2.31	0.44
1:I:207:TYR:C	1:I:208:ILE:HG13	2.41	0.44
2:N:110:GLN:HE22	2:N:172:ASN:HB3	1.82	0.44
2:H:123:SER:O	2:H:125:GLU:N	2.47	0.44
2:K:21:THR:HG22	2:K:71:THR:HG22	2.00	0.44
1:A:156:LYS:NZ	2:B:131:LYS:HE2	2.33	0.44
1:C:87:ARG:HG3	1:C:87:ARG:HH11	1.83	0.44
1:I:36:TRP:CE2	1:I:81:MET:HB2	2.53	0.44
2:B:87:CYS:O	2:B:100:GLY:N	2.46	0.44
1:J:87:ARG:CG	1:J:88:SER:N	2.80	0.43
2:D:61:PHE:HD1	2:D:74:ILE:HG22	1.83	0.43
2:F:190:HIS:CB	2:F:193:TYR:HE2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:SER:OG	1:A:8:GLY:N	2.51	0.43
2:F:6:GLN:HG2	2:F:103:THR:OG1	2.17	0.43
2:H:124:SER:O	2:H:128:GLN:HG3	2.18	0.43
1:J:49:GLY:HA3	1:J:70:MET:HE1	2.00	0.43
1:E:56:GLY:HA2	1:E:72:ARG:HD3	2.00	0.43
1:E:107:ASP:O	1:E:109:TYR:CD2	2.71	0.43
1:I:88:SER:O	1:I:91:THR:HG22	2.18	0.43
2:N:134:LEU:HD12	2:N:180:LEU:HD23	2.01	0.43
2:B:11:SER:HA	2:B:106:THR:O	2.18	0.43
2:B:137:LEU:N	2:B:137:LEU:HD23	2.33	0.43
2:B:197:VAL:O	2:B:203:THR:HA	2.18	0.43
2:F:4:LEU:HD13	2:F:22:CYS:SG	2.58	0.43
2:F:164:THR:CG2	2:F:177:SER:H	2.31	0.43
1:C:167:TRP:O	1:C:168:ASN:ND2	2.51	0.43
1:G:180:PRO:HG2	2:H:167:SER:HB2	2.00	0.43
2:D:144:GLY:HA2	2:D:174:TYR:HD2	1.83	0.43
2:K:137:LEU:N	2:K:137:LEU:HD23	2.33	0.43
1:J:110:PHE:HB2	2:N:90:TRP:CE3	2.53	0.43
1:E:161:GLU:OE2	1:E:162:PRO:HA	2.18	0.43
2:N:143:PRO:O	2:N:199:HIS:HE1	2.02	0.43
2:F:198:THR:HA	2:F:203:THR:HA	1.99	0.43
2:K:27:ILE:O	2:K:27:ILE:HG22	2.19	0.43
1:E:200:SER:O	1:E:200:SER:OG	2.25	0.43
1:I:168:ASN:HB2	1:I:171:ALA:HB3	1.99	0.43
2:N:206:LYS:HD3	2:N:206:LYS:HA	1.75	0.43
2:K:16:GLN:O	2:K:76:ARG:N	2.52	0.43
2:K:22:CYS:HB2	2:K:34:TRP:CH2	2.53	0.43
2:K:81:ASP:O	2:K:85:TYR:OH	2.31	0.43
1:E:174:SER:OG	1:E:175:GLY:N	2.51	0.43
1:I:174:SER:OG	1:I:175:GLY:N	2.50	0.43
2:F:135:VAL:HG12	2:F:179:TYR:CD2	2.53	0.43
2:H:113:ALA:HB3	2:H:142:TYR:N	2.33	0.43
1:J:56:GLY:CA	1:J:72:ARG:HE	2.32	0.43
1:G:81:MET:HE3	1:G:81:MET:HB3	1.91	0.43
2:N:133:THR:HA	2:N:180:LEU:O	2.19	0.43
1:J:39:GLN:HB3	1:J:93:VAL:HG13	2.00	0.43
1:J:85:ARG:CG	1:G:85:ARG:HG3	2.49	0.43
1:J:159:PHE:HA	1:J:160:PRO:HA	1.71	0.43
1:J:172:LEU:HD21	1:J:207:TYR:CE1	2.53	0.43
1:A:159:PHE:HA	1:A:160:PRO:HA	1.84	0.43
1:A:211:VAL:CG2	1:A:220:VAL:HB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:ARG:HG2	1:I:115:VAL:HB	2.00	0.43
2:B:38:LYS:HE3	2:B:80:GLY:O	2.19	0.43
2:F:164:THR:OG1	2:F:165:THR:N	2.52	0.43
1:E:36:TRP:CE2	1:E:81:MET:HB2	2.53	0.43
1:G:33:TYR:CE1	1:G:52:HIS:CD2	3.07	0.43
2:B:126:GLU:HB3	2:B:131:LYS:O	2.18	0.43
2:K:122:PRO:HD3	2:K:134:LEU:HD13	2.00	0.43
2:K:198:THR:OG1	2:K:203:THR:HG22	2.18	0.43
1:C:24:ALA:HB1	1:C:27:TYR:CE1	2.54	0.42
1:G:200:SER:O	1:G:200:SER:OG	2.23	0.42
2:N:149:ALA:HB3	2:N:196:GLN:HE21	1.84	0.42
2:H:96:HIS:HD2	2:H:98:VAL:HG22	1.84	0.42
1:J:48:MET:HG2	1:J:64:PHE:CE2	2.53	0.42
1:A:110:PHE:HB2	2:B:90:TRP:CE3	2.55	0.42
1:C:73:ASP:O	1:C:75:SER:N	2.43	0.42
1:I:12:ARG:O	1:I:124:VAL:HA	2.19	0.42
1:I:151:LEU:HG	1:I:224:VAL:HG21	2.01	0.42
2:B:168:LYS:HA	2:B:174:TYR:HD1	1.83	0.42
1:C:71:THR:HG22	1:C:72:ARG:N	2.33	0.42
1:G:224:VAL:O	1:G:224:VAL:HG22	2.19	0.42
2:D:30:LYS:HE3	2:D:90:TRP:O	2.19	0.42
1:J:23:LYS:HA	1:J:78:THR:HG22	2.00	0.42
1:A:14:PRO:HG3	1:A:124:VAL:HG12	2.00	0.42
1:G:71:THR:OG1	1:G:80:TYR:HB2	2.19	0.42
1:G:174:SER:OG	1:G:175:GLY:N	2.52	0.42
1:I:81:MET:HE3	1:I:81:MET:HB3	1.87	0.42
2:K:107:VAL:O	2:K:109:GLY:N	2.53	0.42
1:G:168:ASN:HB2	1:G:171:ALA:HB3	2.01	0.42
2:N:27:ILE:HG22	2:N:27:ILE:O	2.19	0.42
2:D:196:GLN:HG2	2:D:205:GLU:HG2	1.99	0.42
2:F:26:ASN:C	2:F:28:GLY:N	2.77	0.42
2:K:168:LYS:HE3	2:K:172:ASN:OD1	2.20	0.42
1:C:156:LYS:HZ2	2:D:131:LYS:HD3	1.84	0.42
2:B:137:LEU:O	2:B:138:ILE:HD13	2.19	0.42
1:J:37:VAL:HG23	1:J:47:TRP:HA	2.00	0.42
1:I:71:THR:HG22	1:I:72:ARG:N	2.34	0.42
2:B:26:ASN:C	2:B:28:GLY:H	2.28	0.42
1:A:152:GLY:O	1:A:224:VAL:HG21	2.20	0.42
1:I:38:ARG:HD3	1:I:64:PHE:CZ	2.55	0.42
2:H:4:LEU:HD11	2:H:89:VAL:HG22	2.02	0.42
2:H:27:ILE:HG22	2:H:27:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:TRP:CD2	2:H:72:LEU:HB2	2.55	0.42
1:A:81:MET:HE3	1:A:81:MET:HB3	1.93	0.42
1:E:47:TRP:CD2	2:F:97:VAL:HB	2.54	0.42
1:G:63:LYS:HG3	1:G:64:PHE:HD1	1.84	0.42
2:N:134:LEU:HB2	2:N:180:LEU:HB3	2.02	0.42
2:F:187:TRP:CD1	2:F:188:LYS:HG3	2.55	0.42
1:A:179:PHE:CE1	2:B:137:LEU:HD13	2.55	0.42
1:E:73:ASP:O	1:E:75:SER:N	2.43	0.42
1:E:172:LEU:HD23	1:E:195:VAL:HG11	2.01	0.42
1:G:36:TRP:O	1:G:48:MET:HB2	2.20	0.42
2:H:21:THR:HG22	2:H:71:THR:HG22	2.02	0.42
1:J:158:TYR:OH	1:J:191:LEU:HD22	2.20	0.41
1:C:33:TYR:O	1:C:98:ARG:O	2.38	0.41
2:B:7:PRO:HA	2:B:8:PRO:HD3	1.89	0.41
2:B:35:PHE:O	2:B:85:TYR:HA	2.20	0.41
2:H:110:GLN:HB2	2:H:142:TYR:OH	2.20	0.41
1:E:29:PHE:CE2	1:E:53:PRO:HB3	2.55	0.41
2:D:35:PHE:CE2	2:D:88:GLN:HG2	2.40	0.41
2:H:142:TYR:HB3	2:H:143:PRO:HD3	2.01	0.41
1:C:83:LEU:HD21	1:C:90:ASP:CB	2.49	0.41
1:E:60:TYR:HB3	1:E:64:PHE:O	2.20	0.41
1:J:156:LYS:HZ1	2:N:133:THR:HB	1.84	0.41
1:C:151:LEU:HB3	1:C:152:GLY:H	1.62	0.41
1:E:156:LYS:HE3	1:E:156:LYS:HB3	1.93	0.41
1:C:37:VAL:CG1	1:C:95:TYR:HB2	2.51	0.41
1:I:105:SER:HB2	1:I:107:ASP:OD1	2.21	0.41
2:F:164:THR:HG22	2:F:177:SER:O	2.21	0.41
2:H:7:PRO:HA	2:H:8:PRO:HD3	1.80	0.41
2:H:110:GLN:CB	2:H:142:TYR:CE1	2.98	0.41
2:B:88:GLN:HA	2:B:98:VAL:O	2.21	0.41
2:B:165:THR:HA	2:B:166:PRO:HD3	1.97	0.41
2:B:182:LEU:CD1	2:B:183:THR:CB	2.98	0.41
1:J:49:GLY:CA	1:J:70:MET:HE1	2.50	0.41
1:J:158:TYR:CE2	1:J:161:GLU:HA	2.56	0.41
1:A:34:ILE:HG21	1:A:79:VAL:HG11	2.02	0.41
1:C:107:ASP:CG	2:D:29:ARG:HD3	2.46	0.41
2:N:4:LEU:HD13	2:N:22:CYS:SG	2.61	0.41
2:F:35:PHE:CE2	2:F:88:GLN:HG2	2.43	0.41
1:A:37:VAL:HG11	1:A:116:TRP:CZ3	2.55	0.41
1:J:87:ARG:CG	1:J:88:SER:H	2.34	0.41
1:C:179:PHE:CZ	2:D:137:LEU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:73:ASP:OD2	1:I:76:ILE:CG1	2.61	0.41
1:I:212:ASN:HD21	1:I:219:LYS:HE2	1.85	0.41
2:D:7:PRO:HA	2:D:8:PRO:HD3	1.82	0.41
2:F:133:THR:HA	2:F:180:LEU:O	2.21	0.41
1:A:204:THR:OG1	1:A:205:GLN:N	2.53	0.41
1:E:81:MET:HE3	1:E:81:MET:HB3	1.81	0.41
2:D:12:VAL:HG21	2:D:18:ALA:HB2	2.03	0.41
2:D:107:VAL:O	2:D:109:GLY:N	2.52	0.41
2:F:60:ARG:HD2	2:F:75:SER:O	2.21	0.41
2:K:110:GLN:HE22	2:K:172:ASN:HB3	1.86	0.41
1:E:103:PRO:HG3	1:E:110:PHE:C	2.46	0.40
1:G:105:SER:OG	1:G:106:VAL:N	2.54	0.40
1:I:29:PHE:CE2	1:I:53:PRO:HB3	2.56	0.40
2:N:11:SER:HB3	2:N:108:LEU:HD21	2.03	0.40
2:D:33:ASP:HB2	2:D:88:GLN:HG3	2.03	0.40
2:F:117:VAL:HA	2:F:137:LEU:O	2.21	0.40
2:H:195:CYS:HB3	2:H:196:GLN:H	1.70	0.40
1:J:85:ARG:HG3	1:G:85:ARG:CG	2.50	0.40
1:A:98:ARG:NH1	1:A:100:GLY:HA3	2.31	0.40
1:C:64:PHE:HA	1:C:67:TRP:CZ2	2.55	0.40
1:G:167:TRP:CZ2	1:G:195:VAL:HG23	2.57	0.40
2:D:126:GLU:OE2	2:D:133:THR:N	2.52	0.40
1:E:168:ASN:ND2	1:E:208:ILE:HG22	2.36	0.40
1:J:60:TYR:CD1	1:J:70:MET:HE3	2.56	0.40
1:G:60:TYR:HB3	1:G:64:PHE:O	2.21	0.40
1:G:116:TRP:CE3	2:H:43:PRO:HG2	2.56	0.40
2:B:27:ILE:HD11	2:B:69:THR:N	2.36	0.40
2:H:188:LYS:HE3	2:H:188:LYS:HB2	1.93	0.40
2:K:30:LYS:HE2	2:K:30:LYS:HB2	1.87	0.40
2:D:119:LEU:HD12	2:D:135:VAL:O	2.22	0.40
2:H:16:GLN:O	2:H:76:ARG:N	2.55	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	216/236 (92%)	199 (92%)	14 (6%)	3 (1%)	9	38
1	C	214/236 (91%)	195 (91%)	16 (8%)	3 (1%)	9	38
1	E	216/236 (92%)	194 (90%)	19 (9%)	3 (1%)	9	38
1	G	214/236 (91%)	196 (92%)	16 (8%)	2 (1%)	14	46
1	I	216/236 (92%)	199 (92%)	15 (7%)	2 (1%)	14	46
1	J	214/236 (91%)	193 (90%)	17 (8%)	4 (2%)	6	33
2	B	156/213 (73%)	139 (89%)	13 (8%)	4 (3%)	4	27
2	D	173/213 (81%)	149 (86%)	17 (10%)	7 (4%)	2	20
2	F	167/213 (78%)	143 (86%)	18 (11%)	6 (4%)	2	22
2	H	166/213 (78%)	145 (87%)	14 (8%)	7 (4%)	2	19
2	K	174/213 (82%)	154 (88%)	16 (9%)	4 (2%)	5	30
2	N	187/213 (88%)	163 (87%)	20 (11%)	4 (2%)	5	31
All	All	2313/2694 (86%)	2069 (90%)	195 (8%)	49 (2%)	5	31

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	161	GLU
1	A	153	CYS
2	B	142	TYR
2	B	182	LEU
2	D	191	ARG
2	F	191	ARG
2	H	197	VAL
1	C	105	SER
1	E	108	TYR
2	N	124	SER
2	N	202	SER
2	B	108	LEU
2	D	124	SER
2	D	202	SER
2	F	124	SER
2	F	202	SER
2	H	124	SER
2	H	202	SER
2	K	123	SER

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Mol	Chain	Res	Type
1	C	157	ASP
1	E	157	ASP
1	G	157	ASP
1	I	157	ASP
2	N	108	LEU
2	D	145	ALA
2	F	142	TYR
2	H	143	PRO
2	H	196	GLN
2	K	202	SER
1	J	157	ASP
1	A	157	ASP
2	N	27	ILE
2	B	27	ILE
2	D	108	LEU
2	F	108	LEU
2	H	108	LEU
2	K	108	LEU
1	J	171	ALA
1	A	171	ALA
1	C	171	ALA
1	E	171	ALA
1	G	171	ALA
1	I	171	ALA
2	D	27	ILE
2	F	27	ILE
2	H	27	ILE
2	K	27	ILE
1	J	162	PRO
2	D	143	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	185/200 (92%)	183 (99%)	2 (1%)	65 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	183/200 (92%)	182 (100%)	1 (0%)	81	80
1	E	185/200 (92%)	184 (100%)	1 (0%)	81	80
1	G	184/200 (92%)	182 (99%)	2 (1%)	65	74
1	I	185/200 (92%)	180 (97%)	5 (3%)	39	61
1	J	184/200 (92%)	181 (98%)	3 (2%)	55	69
2	B	137/180 (76%)	136 (99%)	1 (1%)	76	78
2	D	151/180 (84%)	147 (97%)	4 (3%)	40	62
2	F	147/180 (82%)	144 (98%)	3 (2%)	48	66
2	H	147/180 (82%)	140 (95%)	7 (5%)	23	50
2	K	153/180 (85%)	148 (97%)	5 (3%)	33	58
2	N	161/180 (89%)	158 (98%)	3 (2%)	50	67
All	All	2002/2280 (88%)	1965 (98%)	37 (2%)	51	68

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	68	VAL
1	J	115	VAL
1	J	161	GLU
1	A	79	VAL
1	A	208	ILE
1	C	191	LEU
1	E	105	SER
1	G	191	LEU
1	G	208	ILE
1	I	38	ARG
1	I	63	LYS
1	I	191	LEU
1	I	210	ASN
1	I	224	VAL
2	N	25	ASN
2	N	108	LEU
2	N	172	ASN
2	B	172	ASN
2	D	12	VAL
2	D	105	LEU
2	D	107	VAL
2	D	194	SER

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Mol	Chain	Res	Type
2	F	12	VAL
2	F	105	LEU
2	F	180	LEU
2	H	12	VAL
2	H	25	ASN
2	H	29	ARG
2	H	45	LEU
2	H	72	LEU
2	H	172	ASN
2	H	195	CYS
2	K	4	LEU
2	K	12	VAL
2	K	72	LEU
2	K	88	GLN
2	K	180	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	C	205	GLN
1	G	118	GLN
1	G	177	HIS
1	G	212	ASN
1	I	210	ASN
1	I	212	ASN
1	I	217	ASN
2	N	16	GLN
2	N	26	ASN
2	N	36	GLN
2	N	169	GLN
2	N	171	ASN
2	N	196	GLN
2	N	199	HIS
2	B	6	GLN
2	B	128	GLN
2	D	110	GLN
2	D	199	HIS
2	F	16	GLN
2	F	26	ASN
2	F	36	GLN
2	F	88	GLN

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Mol	Chain	Res	Type
2	F	110	GLN
2	H	25	ASN
2	H	96	HIS
2	K	110	GLN
2	K	171	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	220/236 (93%)	0.09	5 (2%) 61 35	48, 92, 208, 272	0
1	C	218/236 (92%)	0.13	5 (2%) 61 35	42, 102, 217, 358	0
1	E	220/236 (93%)	0.21	4 (1%) 67 40	25, 110, 239, 350	0
1	G	218/236 (92%)	-0.02	1 (0%) 87 66	43, 101, 217, 323	0
1	I	220/236 (93%)	0.06	4 (1%) 67 40	46, 87, 165, 256	0
1	J	218/236 (92%)	0.17	7 (3%) 50 29	46, 93, 178, 261	0
2	B	164/213 (76%)	0.16	3 (1%) 67 40	61, 130, 216, 258	0
2	D	179/213 (84%)	0.18	9 (5%) 34 19	53, 136, 219, 309	0
2	F	173/213 (81%)	0.14	4 (2%) 61 35	48, 129, 241, 351	0
2	H	174/213 (81%)	0.19	5 (2%) 53 30	66, 145, 263, 365	0
2	K	182/213 (85%)	0.09	3 (1%) 70 43	62, 119, 183, 266	0
2	N	193/213 (90%)	0.04	1 (0%) 87 66	60, 126, 187, 296	0
All	All	2379/2694 (88%)	0.12	51 (2%) 63 37	25, 113, 220, 365	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	ASP	5.4
2	D	130	ASN	4.1
1	J	204	THR	3.7
2	H	32	VAL	3.6
1	I	87	ARG	3.6
2	D	132	ALA	3.4
1	I	138	ALA	3.3
1	A	153	CYS	3.3
1	C	106	VAL	3.3
2	H	3	ALA	3.1
1	A	221	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	183	THR	3.1
2	H	96	HIS	3.0
2	K	96	HIS	3.0
2	K	66	SER	2.9
1	J	157	ASP	2.8
1	E	89	ASP	2.8
1	E	106	VAL	2.8
2	H	199	HIS	2.6
1	A	148	THR	2.6
1	J	87	ARG	2.6
2	D	182	LEU	2.6
2	D	131	LYS	2.5
1	C	201	SER	2.5
2	H	195	CYS	2.5
2	B	65	ASN	2.4
2	K	190	HIS	2.3
2	F	79	ALA	2.3
2	D	181	SER	2.3
2	F	46	VAL	2.3
1	A	147	GLY	2.3
1	J	192	SER	2.2
1	J	105	SER	2.2
1	A	169	SER	2.2
2	B	179	TYR	2.2
2	B	135	VAL	2.2
2	F	183	THR	2.2
2	D	79	ALA	2.2
2	D	109	GLY	2.2
2	N	45	LEU	2.1
1	C	104	ARG	2.1
1	G	83	LEU	2.1
1	I	147	GLY	2.1
2	F	113	ALA	2.1
1	C	200	SER	2.1
1	E	212	ASN	2.1
2	D	148	VAL	2.1
1	I	109	TYR	2.0
1	J	97	ALA	2.0
1	C	184	GLN	2.0
1	J	163	VAL	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 oligosaccharides 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.