



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:24 PM UTC

PDB ID : 4PLK / pdb_00004plk
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	:	4-5-2 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

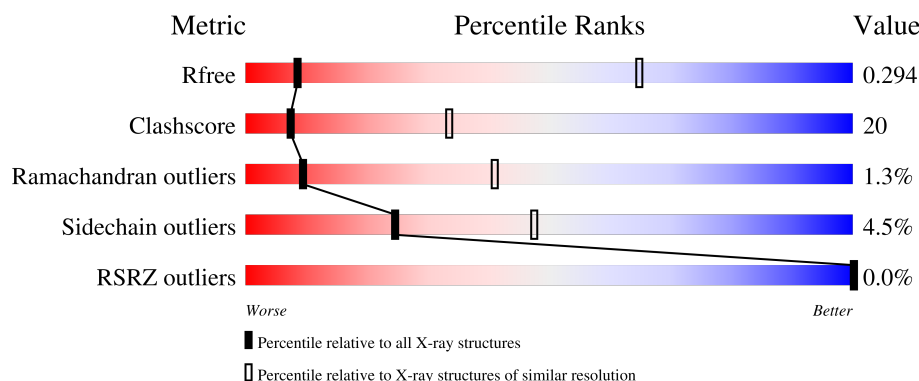
1 Overall quality at a glance i

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	55% 42% .
1	B	147	65% 33% .
1	E	147	59% 39% .
1	F	147	55% 40% 5%
2	C	212	44% 38% 9% . 7%

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Mol	Chain	Length	Quality of chain
2	G	212	53%32%8%7%
2	K	212	59%35%. .
2	L	212	56%38%. .
3	D	229	62%27%6%5%
3	H	229	62%30%. 6%
3	I	229	62%25%7%. 5%
3	J	229	64%28%. 6%

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			

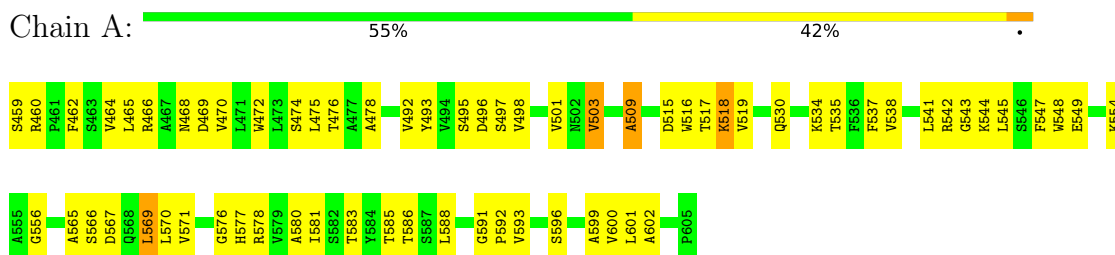
- Molecule 3 is a protein called 8G12 heavy chain.

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			

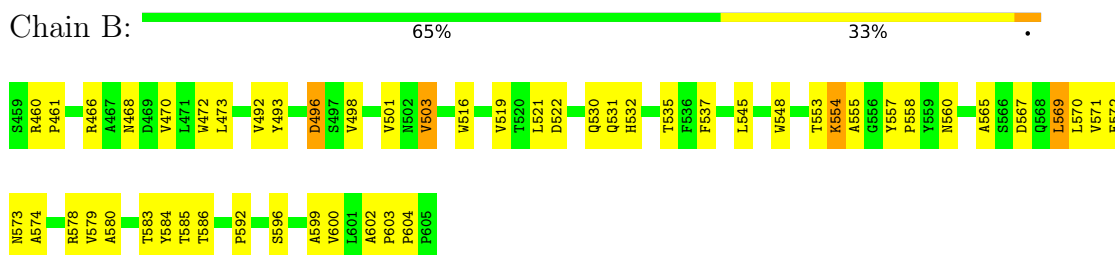
3 Residue-property plots

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.

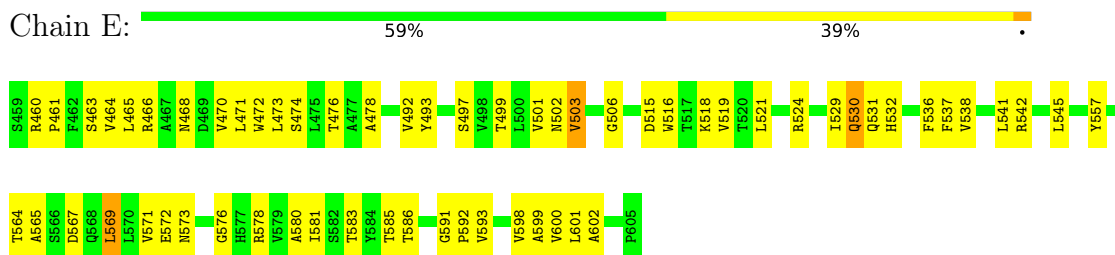
• Molecule 1: Capsid protein



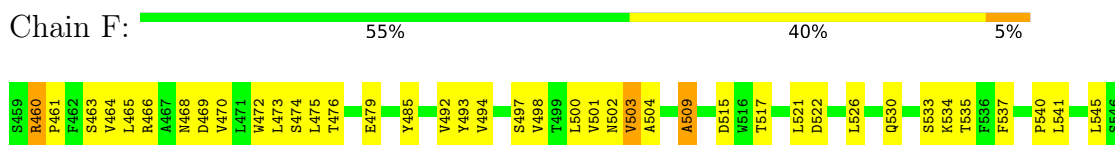
• Molecule 1: Capsid protein

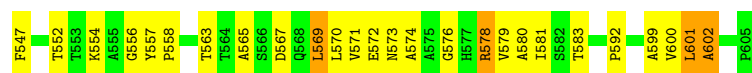


• Molecule 1: Capsid protein

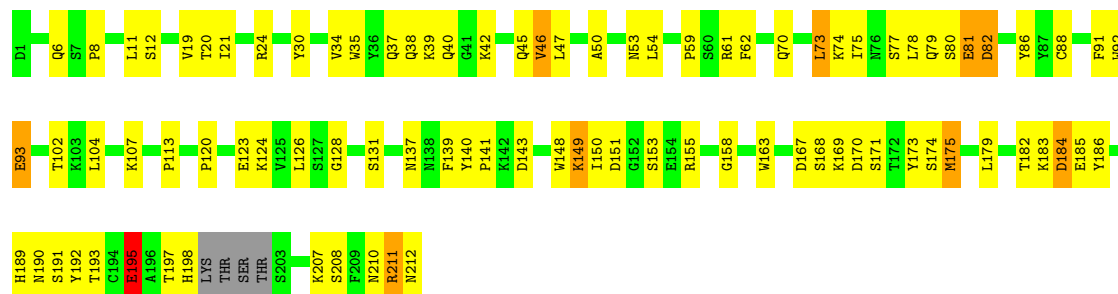


• Molecule 1: Capsid protein

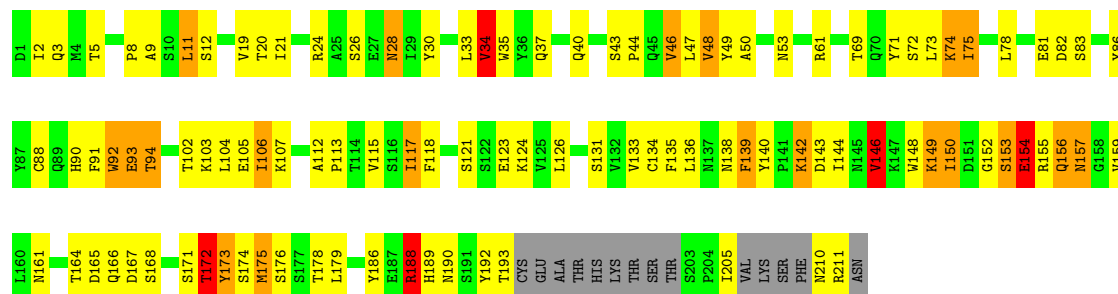




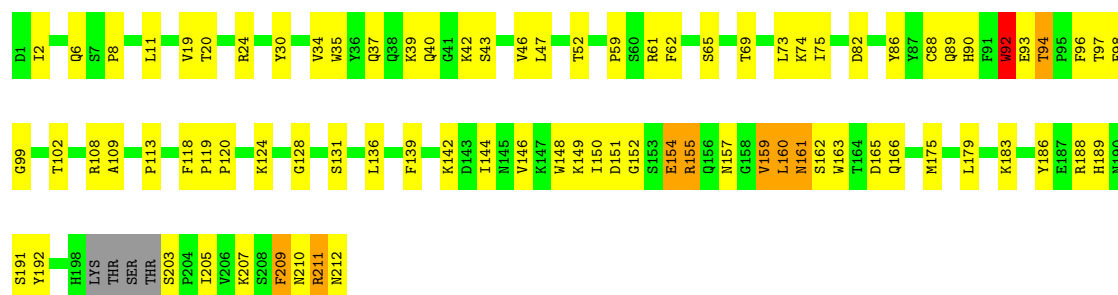
• Molecule 2: 8G12 light chain



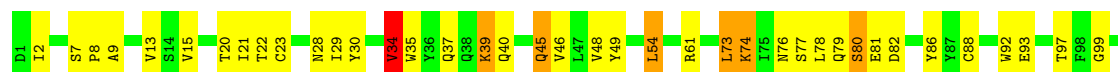
• Molecule 2: 8G12 light chain

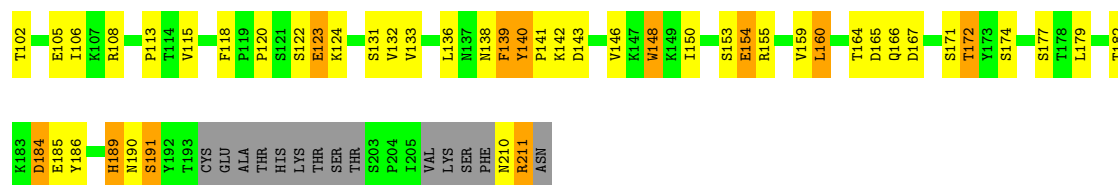


• Molecule 2: 8G12 light chain



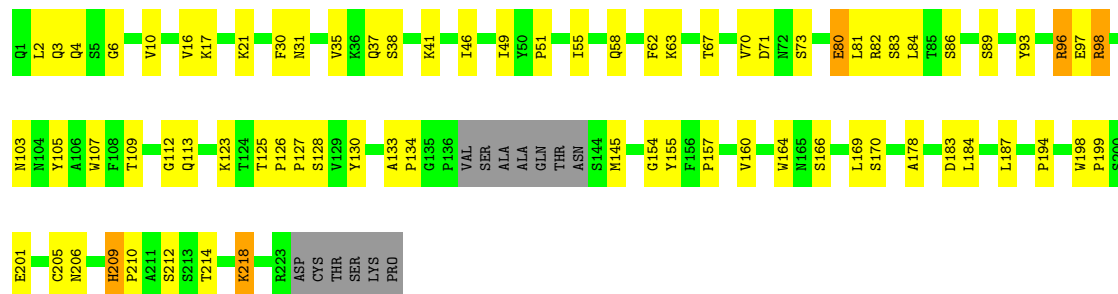
• Molecule 2: 8G12 light chain





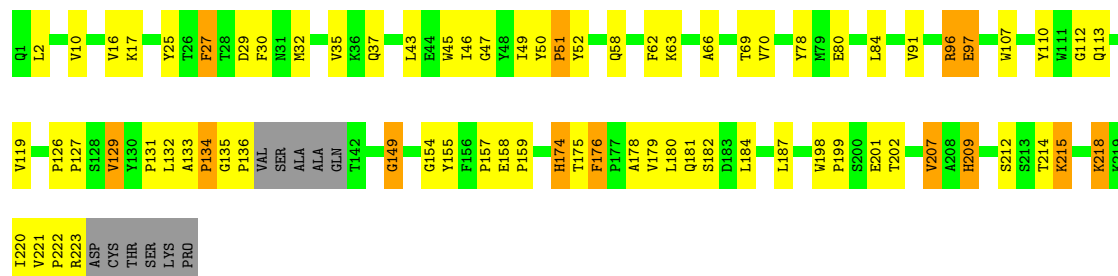
• Molecule 3: 8G12 heavy chain

Chain H: 62% 30% 6%



• Molecule 3: 8G12 heavy chain

Chain D: 62% 27% 6% 5%



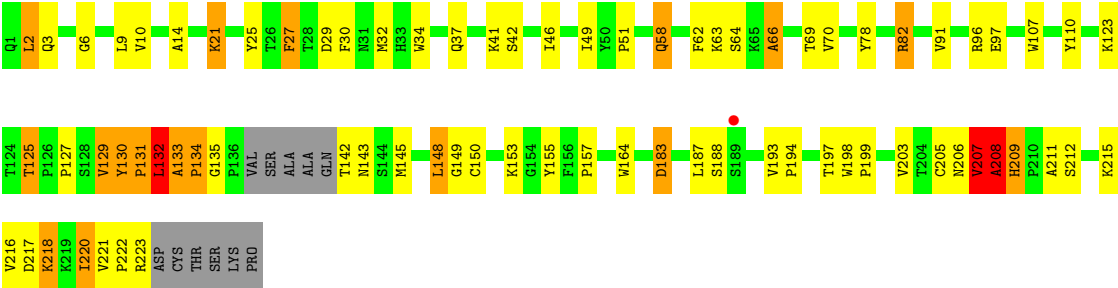
• Molecule 3: 8G12 heavy chain

Chain J: 64% 28% 6%



• Molecule 3: 8G12 heavy chain

Chain I: 62% 25% 7% 5%



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 – 4.00	Depositor EDS
% Data completeness (in resolution range)	91.2 (33.99-4.00) 82.2 (33.99-4.00)	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 0.273 , 0.294	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)	0.26 , 71.9	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	0.90	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	0.41	0/1131	1.01	3/1552 (0.2%)
1	B	0.44	0/1131	1.00	5/1552 (0.3%)
1	E	0.45	0/1131	1.08	9/1552 (0.6%)
1	F	0.43	0/1131	1.11	6/1552 (0.4%)
2	C	0.48	0/1567	1.29	20/2126 (0.9%)
2	G	0.48	0/1565	1.28	18/2122 (0.8%)
2	K	0.47	0/1655	1.23	13/2246 (0.6%)
2	L	0.43	0/1655	1.15	14/2246 (0.6%)
3	D	0.45	0/1717	1.14	15/2346 (0.6%)
3	H	0.37	0/1702	1.06	8/2325 (0.3%)
3	I	0.47	0/1717	1.40	27/2346 (1.2%)
3	J	0.39	0/1702	1.07	12/2325 (0.5%)
All	All	0.44	0/17804	1.17	150/24290 (0.6%)

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 (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	130	TYR	CA-C-N	14.97	134.97	119.85
3	I	130	TYR	C-N-CA	14.97	134.97	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	220	ILE	N-CA-C	13.46	128.82	108.23
2	C	152	GLY	N-CA-C	12.61	130.08	115.08
3	I	131	PRO	N-CA-C	12.25	130.85	111.38
3	I	132	LEU	N-CA-C	11.92	136.19	110.80
3	H	125	THR	CA-C-N	11.17	127.81	119.66
3	H	125	THR	C-N-CA	11.17	127.81	119.66
2	G	184	ASP	N-CA-C	10.92	122.75	111.07
2	K	94	THR	N-CA-C	-10.80	96.35	110.39
3	I	131	PRO	CA-C-N	10.61	141.80	121.54
3	I	131	PRO	C-N-CA	10.61	141.80	121.54
3	I	133	ALA	CA-C-N	10.30	132.71	119.84
3	I	133	ALA	C-N-CA	10.30	132.71	119.84
2	L	81	GLU	N-CA-C	9.61	124.54	113.01
2	K	92	TRP	CB-CA-C	-9.53	91.46	110.42
1	F	460	ARG	CA-C-N	9.38	129.44	119.78
1	F	460	ARG	C-N-CA	9.38	129.44	119.78
3	I	131	PRO	CA-C-O	9.29	133.00	121.67
3	I	133	ALA	N-CA-C	9.10	123.89	110.14
2	C	189	HIS	N-CA-C	9.05	122.62	109.14
3	D	51	PRO	N-CA-C	8.54	124.76	113.57
3	D	50	TYR	CA-C-N	8.08	127.76	119.19
3	D	50	TYR	C-N-CA	8.08	127.76	119.19
3	I	207	VAL	N-CA-C	7.89	119.16	108.11
3	D	209	HIS	CA-C-N	7.34	127.98	119.47
3	D	209	HIS	C-N-CA	7.34	127.98	119.47
3	I	132	LEU	N-CA-CB	-7.27	98.20	110.49
2	L	153	SER	CA-C-N	7.15	130.86	120.71
2	L	153	SER	C-N-CA	7.15	130.86	120.71
2	G	154	GLU	N-CA-C	7.15	120.59	110.23
2	L	168	SER	N-CA-C	-7.12	104.47	113.01
2	C	188	ARG	N-CA-C	-7.12	96.74	108.49
3	J	27	PHE	N-CA-C	7.10	119.63	111.11
2	G	139	PHE	N-CA-C	7.10	120.58	110.14
3	I	27	PHE	N-CA-C	7.02	119.53	111.11
2	C	149	LYS	CA-CB-CG	-7.00	100.11	114.10
2	L	153	SER	N-CA-C	6.93	120.96	109.46
2	C	46	VAL	N-CA-C	6.92	117.95	109.30
3	J	28	THR	N-CA-C	6.86	120.91	112.54
3	J	125	THR	CA-C-N	6.81	124.63	119.66
3	J	125	THR	C-N-CA	6.81	124.63	119.66
2	C	153	SER	N-CA-C	6.78	120.45	109.40
2	C	149	LYS	N-CA-C	6.64	119.20	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	602	ALA	CA-C-N	6.57	124.45	119.66
1	B	602	ALA	C-N-CA	6.57	124.45	119.66
2	K	92	TRP	CA-C-N	6.54	134.02	121.54
2	K	92	TRP	C-N-CA	6.54	134.02	121.54
2	K	160	LEU	N-CA-C	6.53	116.48	107.73
3	J	6	GLY	CA-C-N	6.45	126.47	119.89
3	J	6	GLY	C-N-CA	6.45	126.47	119.89
1	F	463	SER	N-CA-C	6.43	120.23	112.38
2	K	155	ARG	N-CA-C	6.42	119.61	108.76
2	K	157	ASN	N-CA-C	6.37	120.26	110.20
2	G	148	TRP	CA-C-N	-6.35	112.99	122.39
2	G	148	TRP	C-N-CA	-6.35	112.99	122.39
2	G	140	TYR	C-N-CD	-6.34	106.65	120.60
2	G	140	TYR	CA-C-N	6.31	142.14	127.00
2	G	140	TYR	C-N-CA	6.31	142.14	127.00
3	D	52	TYR	CA-CB-CG	6.30	125.25	113.90
1	E	602	ALA	CA-C-N	6.25	126.82	120.38
1	E	602	ALA	C-N-CA	6.25	126.82	120.38
3	H	98	ARG	N-CA-C	6.24	118.08	111.28
2	G	39	LYS	N-CA-C	-6.23	99.24	109.40
2	L	149	LYS	N-CA-C	6.13	119.12	108.76
3	I	125	THR	CA-C-N	6.12	124.13	119.66
3	I	125	THR	C-N-CA	6.12	124.13	119.66
3	D	176	PHE	CA-C-N	6.11	126.13	119.90
3	D	176	PHE	C-N-CA	6.11	126.13	119.90
2	C	146	VAL	CA-C-N	-6.11	113.91	123.13
2	C	146	VAL	C-N-CA	-6.11	113.91	123.13
3	H	6	GLY	CA-C-N	6.05	126.06	119.89
3	H	6	GLY	C-N-CA	6.05	126.06	119.89
1	E	530	GLN	N-CA-C	6.01	118.70	108.90
2	C	186	TYR	N-CA-C	5.95	117.44	111.07
2	L	42	LYS	N-CA-C	5.94	118.25	109.69
2	K	92	TRP	CA-CB-CG	5.94	124.88	113.60
2	G	22	THR	N-CA-C	5.92	119.32	110.14
3	I	209	HIS	CA-C-N	5.88	126.29	119.47
3	I	209	HIS	C-N-CA	5.88	126.29	119.47
3	H	209	HIS	CA-C-N	5.88	126.28	119.47
3	H	209	HIS	C-N-CA	5.88	126.28	119.47
3	I	193	VAL	CA-C-N	5.87	125.81	119.76
3	I	193	VAL	C-N-CA	5.87	125.81	119.76
3	I	212	SER	N-CA-C	-5.84	105.74	112.92
2	C	11	LEU	N-CA-C	5.82	117.86	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	509	ALA	N-CA-C	5.81	117.85	107.80
3	J	98	ARG	N-CA-C	5.80	117.60	111.28
2	G	172	THR	N-CA-C	5.80	118.92	110.17
1	B	461	PRO	N-CA-C	5.73	120.32	111.21
2	G	80	SER	N-CA-C	5.72	118.28	111.71
2	L	184	ASP	N-CA-C	5.71	117.18	111.07
3	I	150	CYS	N-CA-C	5.71	118.08	109.23
2	K	94	THR	N-CA-CB	5.70	119.57	110.10
2	G	28	ASN	N-CA-C	5.67	118.81	110.30
2	L	80	SER	N-CA-C	5.64	117.43	111.28
3	I	129	VAL	N-CA-C	5.64	116.25	107.28
2	C	154	GLU	N-CA-C	5.59	122.72	110.80
2	C	112	ALA	CA-C-N	5.59	126.03	119.99
2	C	112	ALA	C-N-CA	5.59	126.03	119.99
3	J	222	PRO	CA-C-N	5.57	131.73	121.70
3	J	222	PRO	C-N-CA	5.57	131.73	121.70
2	L	46	VAL	N-CA-C	5.56	116.18	108.84
2	L	151	ASP	CA-C-N	-5.54	114.77	122.86
2	L	151	ASP	C-N-CA	-5.54	114.77	122.86
2	K	142	LYS	N-CA-C	5.52	118.06	111.71
3	D	174	HIS	N-CA-C	5.48	117.33	108.34
1	E	576	GLY	N-CA-C	-5.47	100.20	113.18
3	H	126	PRO	N-CA-C	5.42	115.67	110.47
3	D	175	THR	N-CA-C	5.40	117.77	109.07
1	E	463	SER	N-CA-C	5.39	118.95	112.38
2	C	150	ILE	CA-C-N	5.38	130.00	122.08
2	C	150	ILE	C-N-CA	5.38	130.00	122.08
2	G	34	VAL	N-CA-C	5.37	116.46	108.46
2	C	34	VAL	N-CA-C	5.36	116.39	108.45
3	D	149	GLY	N-CA-C	5.34	121.03	110.83
2	L	195	GLU	N-CA-C	5.33	117.77	108.76
3	D	27	PHE	N-CA-C	5.33	117.78	111.33
2	G	105	GLU	CA-C-N	-5.32	115.72	122.43
2	G	105	GLU	C-N-CA	-5.32	115.72	122.43
3	D	129	VAL	N-CA-C	5.32	115.24	107.37
1	A	602	ALA	CA-C-N	5.30	125.84	120.38
1	A	602	ALA	C-N-CA	5.30	125.84	120.38
1	B	557	TYR	CA-C-N	5.24	125.24	120.21
1	B	557	TYR	C-N-CA	5.24	125.24	120.21
3	I	203	VAL	N-CA-C	5.17	115.41	108.17
2	L	158	GLY	N-CA-C	5.17	122.71	115.43
2	G	191	SER	N-CA-C	5.16	117.65	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	48	VAL	N-CA-C	5.15	115.45	107.78
3	J	209	HIS	CA-C-N	5.15	125.44	119.47
3	J	209	HIS	C-N-CA	5.15	125.44	119.47
2	C	28	ASN	N-CA-C	5.14	118.02	110.30
1	E	557	TYR	CA-C-N	5.12	125.13	120.21
1	E	557	TYR	C-N-CA	5.12	125.13	120.21
2	G	74	LYS	CA-CB-CG	5.12	124.34	114.10
2	K	161	ASN	N-CA-C	5.11	118.07	109.95
2	K	203	SER	CA-C-N	-5.09	114.99	120.03
2	K	203	SER	C-N-CA	-5.09	114.99	120.03
1	E	506	GLY	N-CA-C	-5.08	108.60	115.21
3	I	6	GLY	CA-C-N	5.07	125.06	119.89
3	I	6	GLY	C-N-CA	5.07	125.06	119.89
3	J	149	GLY	N-CA-C	5.07	120.30	110.66
1	A	509	ALA	N-CA-C	5.05	116.54	107.80
3	I	66	ALA	N-CA-C	5.04	117.27	108.76
1	E	573	ASN	N-CA-C	5.02	117.38	109.39
1	F	602	ALA	CA-C-N	5.02	125.55	120.38
1	F	602	ALA	C-N-CA	5.02	125.55	120.38
3	D	133	ALA	CA-C-N	5.01	126.10	119.84
3	D	133	ALA	C-N-CA	5.01	126.10	119.84
2	C	172	THR	N-CA-C	5.01	116.99	110.53

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	67	0
1	B	1104	0	1090	53	0
1	E	1104	0	1092	38	0
1	F	1104	0	1092	54	0
2	C	1533	0	1464	104	0
2	G	1531	0	1456	67	0
2	K	1618	0	1544	77	0
2	L	1618	0	1542	97	0
3	D	1669	0	1624	67	0
3	H	1654	0	1611	53	0
3	I	1669	0	1624	66	0
3	J	1654	0	1611	53	0
All	All	17362	0	16842	696	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 (696) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:97:GLU:CD	3:D:97:GLU:H	1.94	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:J:200:SER:OG	3:J:201:GLU:OE1	2.06	0.73
3:I:216:VAL:HG12	3:I:218:LYS:HE3	1.70	0.73
2:L:61:ARG:HH22	2:L:82:ASP:CG	1.97	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
1:A:472:TRP:HH2	1:B:468:ASN:HD22	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:150:ILE:C	2:G:190:ASN:HD21	1.99	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
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
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
1:A:588:LEU:C	2:L:93:GLU:OE1	2.38	0.66
2:K:92:TRP:CB	2:K:93:GLU:OE1	2.43	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:161:ASN:HB3	2:C:175:MET:HE1	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:82:ASP:O	2:K:86:TYR:OH	2.21	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
1:A:554:LYS:HZ3	2:L:92:TRP:CD1	2.25	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
2:L:182:THR:OG1	2:L:184:ASP:OD1	2.26	0.54
2:C:93:GLU:O	2:C:94:THR:C	2.50	0.54
1:E:460:ARG:HD3	1:E:461:PRO:HD2	1.88	0.54
1:E:515:ASP:CG	1:E:518:LYS:HG3	2.33	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
3:D:29:ASP:C	3:D:30:PHE:HD1	2.17	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
2:G:124:LYS:HZ3	2:G:131:SER:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:180:LEU:HD12	3:D:184:LEU:C	2.34	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
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
3:I:29:ASP:C	3:I:30:PHE:HD1	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:201:GLU:CD	3:D:202:THR:H	2.18	0.51
1:A:588:LEU:HA	2:L:93:GLU:CD	2.33	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
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:32:MET:HE2	3:I:96:ARG:HH22	1.76	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:K:146:VAL:HG21	2:K:175:MET:HE1	1.93	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
3:D:27:PHE:HE1	3:D:32:MET:HE2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:460:ARG:HH22	1:B:466:ARG:NH1	2.11	0.49
2:C:93:GLU:O	2:C:93:GLU:OE1	2.30	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
3:H:71:ASP:OD1	3:H:73:SER:OG	2.27	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:L:210:ASN:C	2:L:212:ASN:H	2.23	0.46
2:C:115:VAL:HG21	2:C:205:ILE:HD13	1.98	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
2:G:148:TRP:CD1	2:G:148:TRP:H	2.30	0.45
3:I:25:TYR:OH	3:I:96:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:123:GLU:OE1	3:H:218:LYS:HE2	2.16	0.45
2:L:195:GLU:OE2	2:L:197:THR:OG1	2.33	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
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
3:H:166:SER:O	3:H:166:SER:OG	2.34	0.45
3:D:132:LEU:HG	3:D:149:GLY:C	2.41	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
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
3:D:174:HIS:ND1	3:D:174:HIS:C	2.75	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
1:A:544:LYS:NZ	1:A:565:ALA:O	2.37	0.44
3:H:35:VAL:CG1	3:H:93:TYR:HB2	2.47	0.44
3:D:181:GLN:O	3:D:182:SER:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:J:37:GLN:C	3:J:39:HIS:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:82:ASP:O	2:G:86:TYR:OH	2.26	0.43
2:C:131:SER:OG	2:C:178:THR:HG22	2.19	0.43
1:F:460:ARG:HD2	1:F:460:ARG:C	2.43	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
2:C:104:LEU:C	2:C:104:LEU:HD23	2.44	0.43
1:F:498:VAL:HG21	1:F:579:VAL:CG2	2.48	0.43
2:G:40:GLN:CD	2:G:165:ASP:HB3	2.44	0.43
2:G:160:LEU:HD23	2:G:160:LEU:C	2.44	0.43
3:I:133:ALA:HA	3:I:134:PRO:HD3	1.63	0.43
1:A:515:ASP:CG	1:A:518:LYS:HG3	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:J:131:PRO:HG3	3:J:218:LYS:HZ1	1.84	0.42
1:A:478:ALA:O	1:A:592:PRO:HA	2.19	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
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:K:154:GLU:CD	2:K:155:ARG:H	2.28	0.41
2:G:148:TRP:O	2:G:148:TRP:CE3	2.73	0.41
3:I:27:PHE:HE1	3:I:32:MET:HE2	1.84	0.41
2:L:59:PRO:HG2	2:L:62:PHE:CE1	2.55	0.41
2:C:149:LYS:HG3	2:C:150:ILE:N	2.35	0.41
3:D:178:ALA:HA	3:D:187:LEU:HB3	2.03	0.41
2:G:210:ASN:C	2:G:211:ARG:HG2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:61:ARG:HH12	2:C:82:ASP:CG	2.28	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
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: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:H:183:ASP:C	3:H:184:LEU:HD12	2.45	0.41
2:C:164:THR:HG21	3:D:174:HIS:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:J:128:SER:HB2	3:J:130:TYR:CZ	2.57	0.40
2:G:123:GLU:CD	2:G:123:GLU:H	2.25	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%)	9	39
1	B	145/147 (99%)	140 (97%)	4 (3%)	1 (1%)	18	54
1	E	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	18	54
1	F	145/147 (99%)	136 (94%)	6 (4%)	3 (2%)	5	32
2	C	192/212 (91%)	176 (92%)	11 (6%)	5 (3%)	4	29
2	G	192/212 (91%)	176 (92%)	13 (7%)	3 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	204/212 (96%)	193 (95%)	8 (4%)	3 (2%)	8	38
2	L	204/212 (96%)	192 (94%)	9 (4%)	3 (2%)	8	38
3	D	214/229 (93%)	202 (94%)	10 (5%)	2 (1%)	14	48
3	H	212/229 (93%)	208 (98%)	4 (2%)	0	100	100
3	I	214/229 (93%)	205 (96%)	5 (2%)	4 (2%)	6	34
3	J	212/229 (93%)	207 (98%)	3 (1%)	2 (1%)	14	48
All	All	2224/2352 (95%)	2112 (95%)	83 (4%)	29 (1%)	9	41

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%)	116 (97%)	4 (3%)	33	56
1	B	120/120 (100%)	116 (97%)	4 (3%)	33	56
1	E	120/120 (100%)	114 (95%)	6 (5%)	22	45
1	F	120/120 (100%)	116 (97%)	4 (3%)	33	56
2	C	175/190 (92%)	158 (90%)	17 (10%)	8	27
2	G	175/190 (92%)	161 (92%)	14 (8%)	11	35
2	K	186/190 (98%)	182 (98%)	4 (2%)	45	65
2	L	186/190 (98%)	178 (96%)	8 (4%)	26	48
3	D	190/199 (96%)	183 (96%)	7 (4%)	30	52
3	H	188/199 (94%)	182 (97%)	6 (3%)	34	56
3	I	190/199 (96%)	179 (94%)	11 (6%)	18	42
3	J	188/199 (94%)	184 (98%)	4 (2%)	47	65
All	All	1958/2036 (96%)	1869 (96%)	89 (4%)	24	47

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	VAL
1	A	518	LYS
1	A	538	VAL
1	A	569	LEU
1	B	496	ASP
1	B	554	LYS
1	B	560	ASN
1	B	569	LEU
2	L	39	LYS
2	L	73	LEU
2	L	82	ASP
2	L	93	GLU
2	L	104	LEU
2	L	175	MET

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Mol	Chain	Res	Type
2	L	195	GLU
2	L	198	HIS
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	19	VAL
2	C	34	VAL
2	C	74	LYS
2	C	75	ILE
2	C	88	CYS
2	C	93	GLU
2	C	103	LYS
2	C	106	ILE
2	C	117	ILE
2	C	139	PHE
2	C	142	LYS
2	C	146	VAL
2	C	156	GLN
2	C	159	VAL
2	C	173	TYR
2	C	175	MET
2	C	188	ARG
3	D	58	GLN
3	D	96	ARG
3	D	97	GLU
3	D	207	VAL
3	D	215	LYS
3	D	218	LYS
3	D	221	VAL
1	E	464	VAL
1	E	466	ARG
1	E	524	ARG
1	E	530	GLN
1	E	569	LEU
1	E	598	VAL
1	F	479	GLU
1	F	569	LEU
1	F	578	ARG
1	F	601	LEU

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Mol	Chain	Res	Type
2	K	89	GLN
2	K	162	SER
2	K	188	ARG
2	K	205	ILE
3	J	98	ARG
3	J	145	MET
3	J	218	LYS
3	J	223	ARG
2	G	13	VAL
2	G	34	VAL
2	G	39	LYS
2	G	45	GLN
2	G	54	LEU
2	G	73	LEU
2	G	115	VAL
2	G	123	GLU
2	G	136	LEU
2	G	146	VAL
2	G	159	VAL
2	G	160	LEU
2	G	179	LEU
2	G	211	ARG
3	I	2	LEU
3	I	3	GLN
3	I	21	LYS
3	I	41	LYS
3	I	58	GLN
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 (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	GLN
1	A	532	HIS
1	B	508	GLN
2	L	38	GLN
2	L	79	GLN

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Mol	Chain	Res	Type
2	L	161	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	38	GLN
2	C	53	ASN
2	C	79	GLN
2	C	138	ASN
3	D	60	GLN
3	D	174	HIS
3	D	209	HIS
1	E	532	HIS
1	E	577	HIS
1	F	508	GLN
1	F	531	GLN
1	F	532	HIS
2	K	157	ASN
2	K	161	ASN
3	J	3	GLN
3	J	31	ASN
3	J	174	HIS
3	J	206	ASN
3	J	209	HIS
2	G	37	GLN
2	G	190	ASN
3	I	3	GLN
3	I	31	ASN
3	I	37	GLN
3	I	58	GLN
3	I	72	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	147/147 (100%)	-0.92	0	100	100	73, 103, 146, 165	0
1	B	147/147 (100%)	-0.95	0	100	100	79, 104, 153, 193	0
1	E	147/147 (100%)	-0.87	0	100	100	81, 108, 159, 180	0
1	F	147/147 (100%)	-0.91	0	100	100	68, 107, 158, 175	0
2	C	198/212 (93%)	-0.83	0	100	100	55, 169, 218, 283	0
2	G	198/212 (93%)	-0.82	0	100	100	51, 167, 208, 237	0
2	K	208/212 (98%)	-0.84	0	100	100	63, 167, 209, 234	0
2	L	208/212 (98%)	-0.83	0	100	100	49, 163, 234, 272	0
3	D	218/229 (95%)	-0.87	0	100	100	96, 135, 210, 233	0
3	H	216/229 (94%)	-0.92	0	100	100	85, 128, 202, 253	0
3	I	218/229 (95%)	-0.86	1 (0%)	87	73	98, 135, 211, 235	0
3	J	216/229 (94%)	-0.86	0	100	100	95, 134, 192, 219	0
All	All	2268/2352 (96%)	-0.87	1 (0%)	100	100	49, 135, 210, 283	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	189	SER	2.6

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.