



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:45 PM UTC

PDB ID : 3NH7 / pdb_00003nh7
Title : Crystal structure of the neutralizing Fab fragment AbD1556 bound to the BMP type I receptor IA
Authors : Mueller, T.D.; Harth, S.; Sebald, W.
Deposited on : 2010-06-14
Resolution : 2.70 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

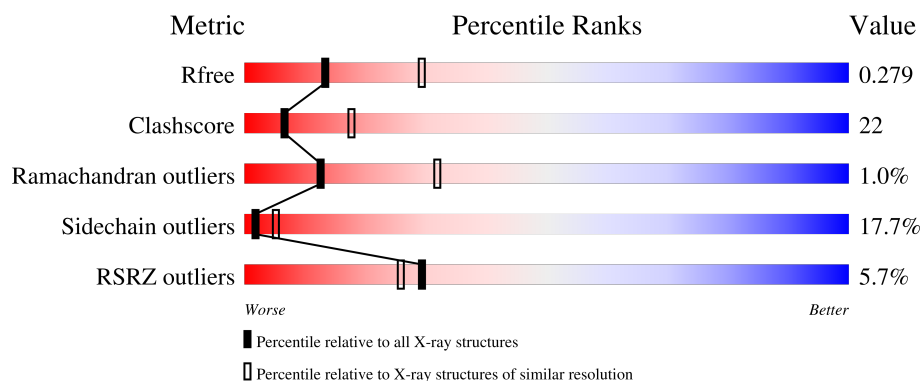
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	H	234	3% 44% 34% 9% 12%
1	I	234	% 56% 27% 8% 8%
1	J	234	4% 57% 29% 7% 6%
1	K	234	3% 57% 26% 8% 8%
2	L	213	8% 60% 31% 8%

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Mol	Chain	Length	Quality of chain
2	M	213	
2	N	213	
2	O	213	
3	A	129	
3	B	129	
3	C	129	
3	D	129	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15350 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 Antibody fragment Fab AbD1556, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	207	Total	C	N	O	S	0	0	0
			1569	992	269	303	5			
1	I	215	Total	C	N	O	S	0	0	0
			1620	1021	278	316	5			
1	J	221	Total	C	N	O	S	0	0	0
			1661	1045	286	325	5			
1	K	215	Total	C	N	O	S	0	0	0
			1625	1025	279	316	5			

- Molecule 2 is a protein called Antibody fragment Fab AbD1556, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			
2	M	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			
2	N	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			
2	O	210	Total	C	N	O	S	0	0	0
			1558	973	258	322	5			

- Molecule 3 is a protein called Bone morphogenetic protein receptor type-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			
3	B	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			
3	C	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			
3	D	85	Total	C	N	O	S	0	0	0
			654	400	112	131	11			

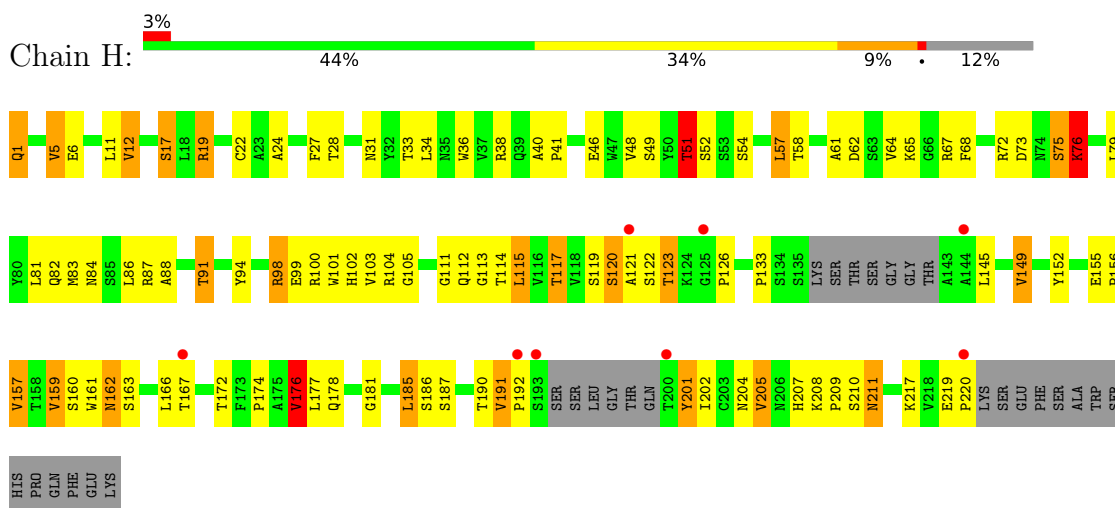
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	2	Total O 2 2	0	0
4	L	3	Total O 3 3	0	0
4	A	2	Total O 2 2	0	0
4	I	5	Total O 5 5	0	0
4	M	4	Total O 4 4	0	0
4	B	1	Total O 1 1	0	0
4	J	2	Total O 2 2	0	0
4	N	1	Total O 1 1	0	0
4	K	2	Total O 2 2	0	0
4	O	4	Total O 4 4	0	0
4	D	1	Total O 1 1	0	0

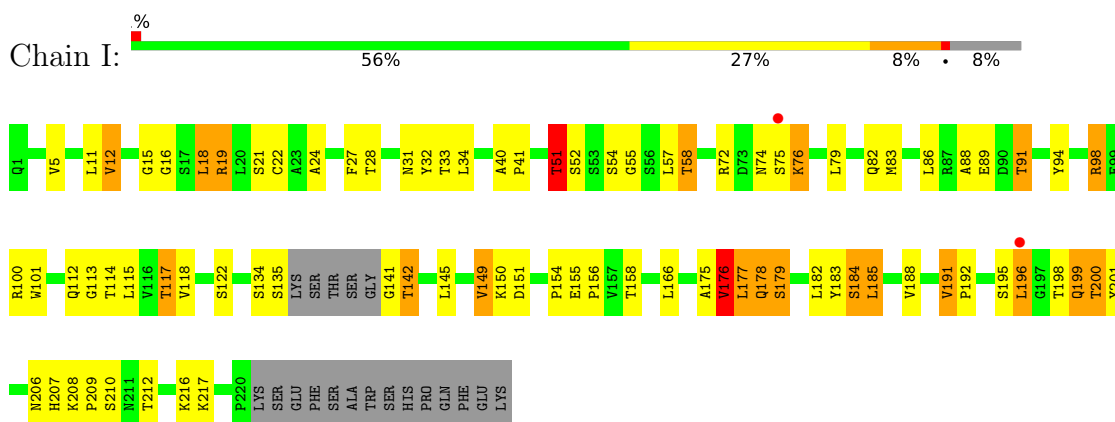
3 Residue-property plots

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.

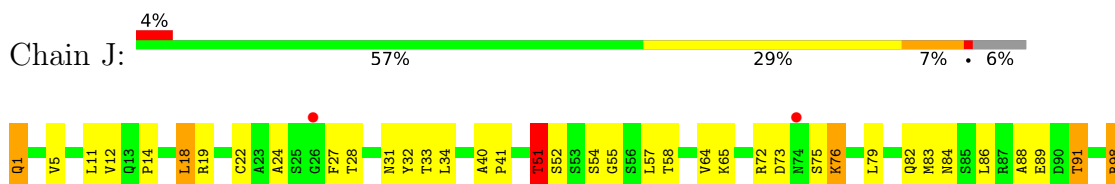
- Molecule 1: Antibody fragment Fab AbD1556, heavy chain

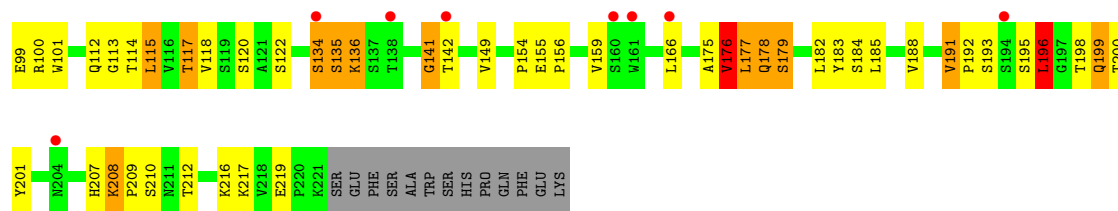


- Molecule 1: Antibody fragment Fab AbD1556, heavy chain

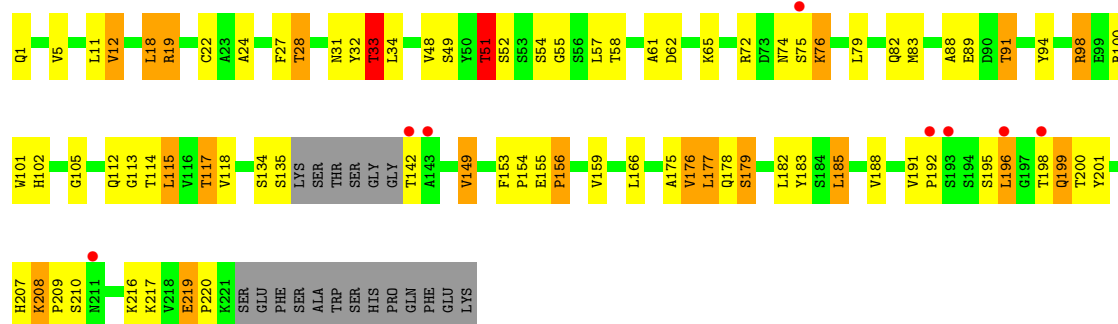


- Molecule 1: Antibody fragment Fab AbD1556, heavy chain

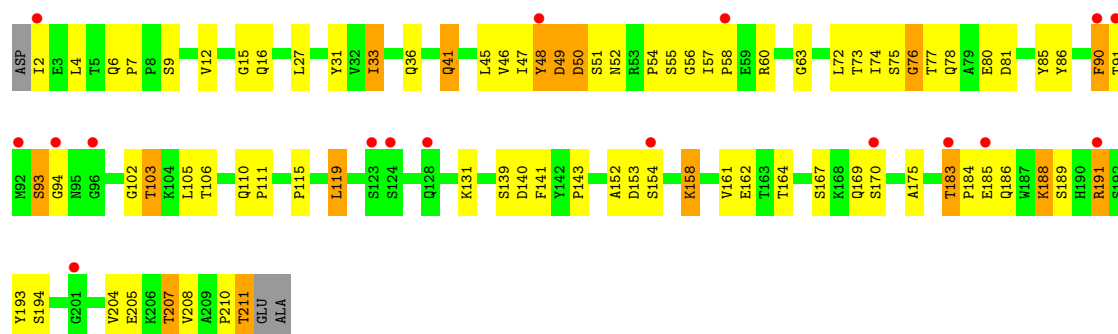




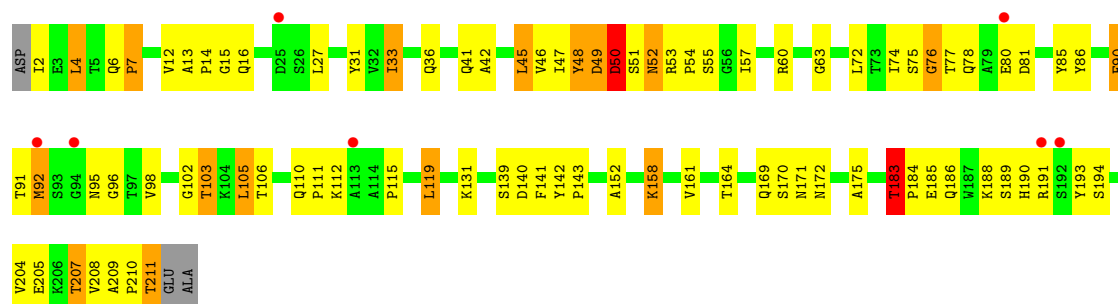
- Molecule 1: Antibody fragment Fab AbD1556, heavy chain



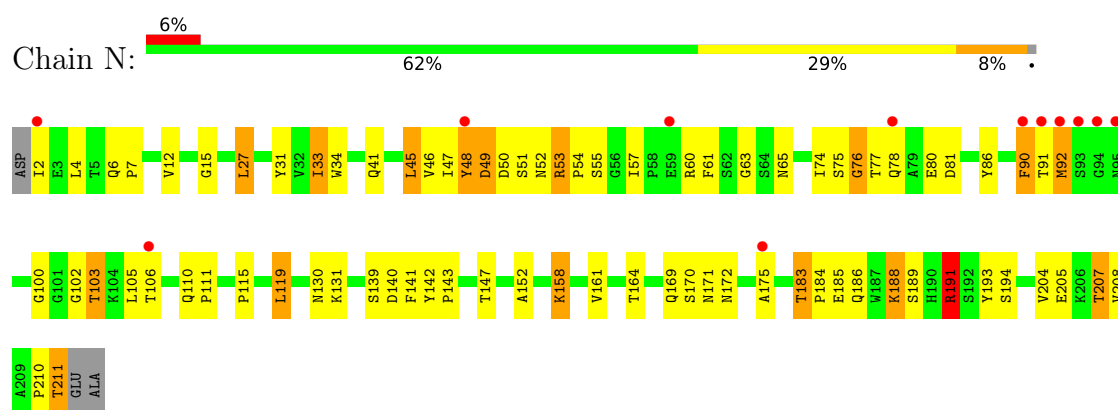
- Molecule 2: Antibody fragment Fab AbD1556, light chain



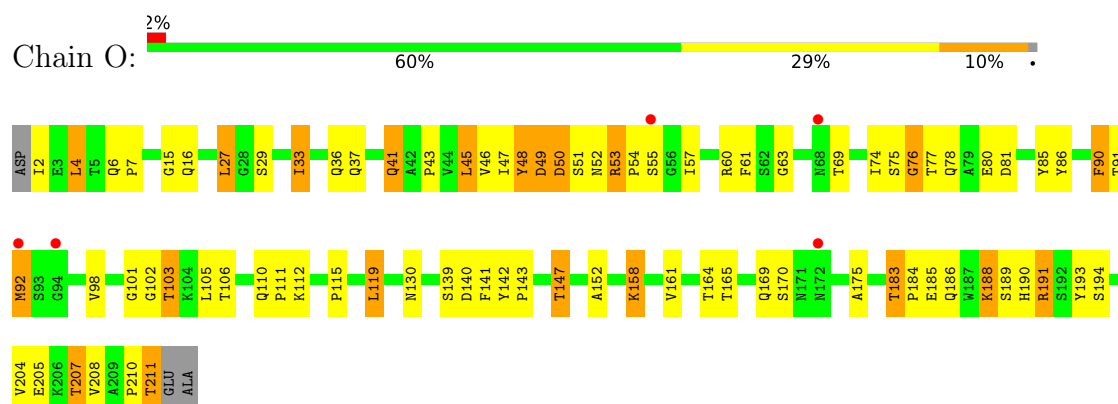
- Molecule 2: Antibody fragment Fab AbD1556, light chain



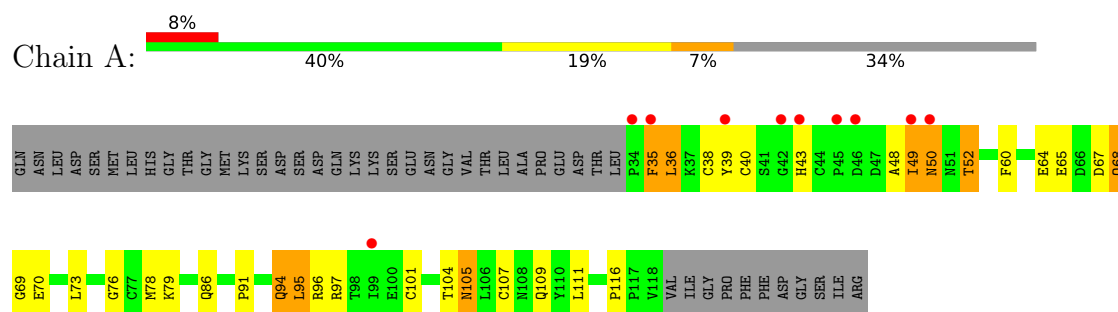
- Molecule 2: Antibody fragment Fab AbD1556, light chain



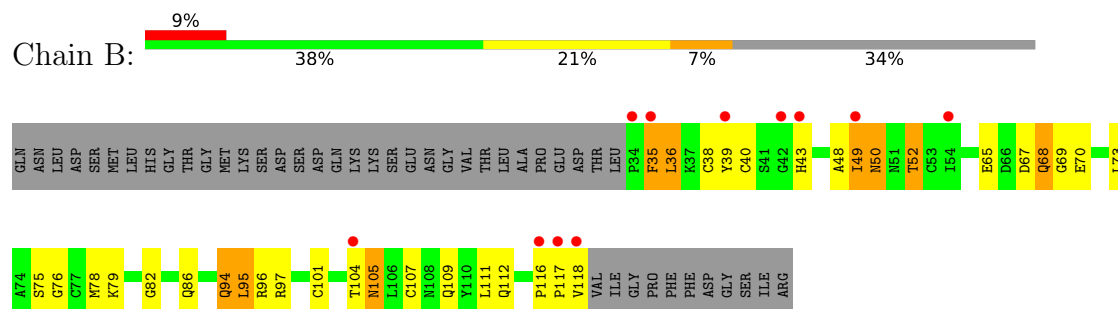
- Molecule 2: Antibody fragment Fab AbD1556, light chain



- Molecule 3: Bone morphogenetic protein receptor type-1A

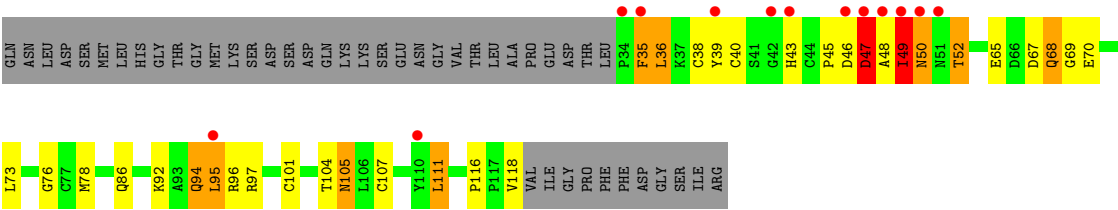


- Molecule 3: Bone morphogenetic protein receptor type-1A

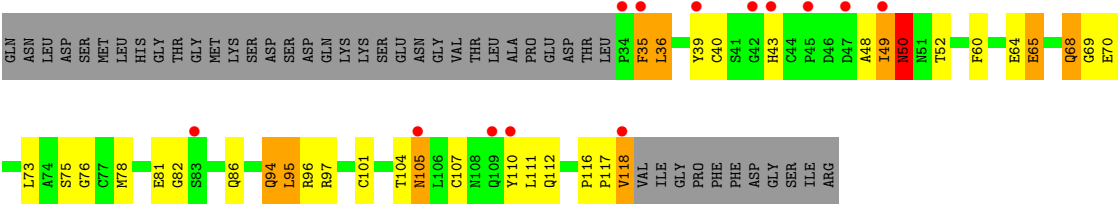


- Molecule 3: Bone morphogenetic protein receptor type-1A





● Molecule 3: Bone morphogenetic protein receptor type-1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.32Å 129.25Å 100.24Å 90.00° 92.27° 90.00°	Depositor
Resolution (Å)	30.40 – 2.70 30.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.40-2.70) 95.3 (30.40-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.280 0.235 , 0.279	Depositor DCC
R_{free} test set	3020 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15350	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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	H	0.82	0/1608	1.14	10/2190 (0.5%)
1	I	0.78	0/1660	1.08	5/2262 (0.2%)
1	J	0.73	0/1702	1.11	8/2318 (0.3%)
1	K	0.87	1/1665 (0.1%)	1.15	9/2268 (0.4%)
2	L	0.84	1/1595 (0.1%)	1.20	11/2180 (0.5%)
2	M	0.79	0/1595	1.18	20/2180 (0.9%)
2	N	0.84	0/1595	1.23	8/2180 (0.4%)
2	O	0.83	0/1595	1.16	14/2180 (0.6%)
3	A	0.68	0/667	0.97	1/903 (0.1%)
3	B	0.61	0/667	0.94	1/903 (0.1%)
3	C	0.69	0/667	1.06	4/903 (0.4%)
3	D	0.63	0/667	0.98	2/903 (0.2%)
All	All	0.79	2/15683 (0.0%)	1.13	93/21370 (0.4%)

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	L	0	1
3	A	0	1
3	B	0	1
3	C	0	1
3	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	191	ARG	CZ-NH2	5.88	1.41	1.33
1	K	33	THR	CB-CG2	-5.34	1.34	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	191	ARG	NE-CZ-NH1	-15.42	106.08	121.50
2	L	191	ARG	NE-CZ-NH2	14.29	132.06	119.20
2	O	49	ASP	N-CA-C	-12.41	90.45	109.94
2	N	49	ASP	N-CA-C	-11.72	91.53	109.94
2	N	191	ARG	NE-CZ-NH2	11.50	129.55	119.20
2	L	49	ASP	N-CA-C	-10.19	94.78	110.17
1	J	219	GLU	CA-C-N	10.12	130.22	119.90
1	J	219	GLU	C-N-CA	10.12	130.22	119.90
2	M	49	ASP	N-CA-C	-9.31	95.92	110.36
2	L	191	ARG	NE-CZ-NH1	-9.19	112.31	121.50
2	N	48	TYR	N-CA-C	8.92	124.14	112.72
2	O	48	TYR	N-CA-C	8.64	123.78	112.72
3	B	49	ILE	N-CA-C	-8.49	97.68	108.89
3	A	49	ILE	N-CA-C	-8.27	97.97	108.89
1	K	76	LYS	N-CA-C	-7.90	97.52	109.60
1	J	76	LYS	N-CA-C	-7.79	100.53	110.19
3	D	49	ILE	N-CA-C	-7.74	98.68	108.89
3	C	47	ASP	CB-CA-C	-7.66	97.61	110.56
1	H	120	SER	N-CA-C	-7.45	104.08	113.02
2	M	41	GLN	N-CA-C	7.34	120.08	109.14
3	C	49	ILE	N-CA-C	-7.29	99.27	108.89
2	N	53	ARG	CA-C-N	-7.19	112.37	119.78
2	N	53	ARG	C-N-CA	-7.19	112.37	119.78
1	K	219	GLU	CA-C-N	6.95	127.36	119.93
1	K	219	GLU	C-N-CA	6.95	127.36	119.93
2	M	191	ARG	NE-CZ-NH1	-6.85	114.65	121.50
2	M	48	TYR	N-CA-C	6.85	121.48	112.72
2	L	48	TYR	N-CA-C	6.80	121.42	112.72
1	J	51	THR	CB-CA-C	-6.77	97.45	109.70
1	K	51	THR	CB-CA-C	-6.50	97.93	109.70
3	C	47	ASP	N-CA-CB	-6.42	101.18	110.56
2	L	41	GLN	N-CA-C	6.40	118.68	109.14
1	I	176	VAL	CB-CA-C	-6.35	102.51	111.21
1	I	51	THR	CB-CA-C	-6.33	98.24	109.70
1	H	12	VAL	CB-CA-C	-6.29	103.05	111.80
1	H	5	VAL	N-CA-C	6.27	117.77	107.24
2	N	41	GLN	N-CA-C	6.22	118.23	108.96
2	O	49	ASP	CA-C-O	-6.11	113.86	121.55
1	J	141	GLY	N-CA-C	-6.06	106.88	115.30
1	H	76	LYS	N-CA-C	-6.05	100.34	109.60
2	M	49	ASP	CA-C-O	-5.92	114.65	121.82
1	J	196	LEU	N-CA-C	5.82	117.70	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	41	GLN	N-CA-C	5.77	117.56	108.96
2	O	101	GLY	N-CA-C	-5.70	108.40	114.67
2	M	53	ARG	CA-C-N	-5.68	113.93	119.78
2	M	53	ARG	C-N-CA	-5.68	113.93	119.78
1	K	48	VAL	CB-CA-C	-5.65	106.02	111.05
1	I	113	GLY	N-CA-C	5.64	119.98	112.65
2	L	139	SER	N-CA-C	5.56	117.52	109.07
2	M	139	SER	N-CA-C	5.52	117.47	109.07
2	M	42	ALA	CA-C-N	-5.49	114.04	119.92
2	M	42	ALA	C-N-CA	-5.49	114.04	119.92
2	L	93	SER	N-CA-C	5.44	117.27	108.41
2	N	139	SER	N-CA-C	5.44	117.06	108.96
1	H	51	THR	CB-CA-C	-5.43	98.59	109.35
1	H	176	VAL	CB-CA-C	-5.43	103.58	111.68
2	O	53	ARG	CA-C-N	-5.42	114.18	119.76
2	O	53	ARG	C-N-CA	-5.42	114.18	119.76
1	H	105	GLY	N-CA-C	5.40	117.68	111.36
1	J	176	VAL	CB-CA-C	-5.40	103.81	111.21
2	L	49	ASP	CA-C-N	-5.38	111.97	120.63
2	L	49	ASP	C-N-CA	-5.38	111.97	120.63
2	O	139	SER	N-CA-C	5.38	116.97	108.96
2	M	183	THR	CA-C-N	-5.36	113.66	119.24
2	M	183	THR	C-N-CA	-5.36	113.66	119.24
1	K	113	GLY	N-CA-C	5.34	119.59	112.65
2	O	50	ASP	N-CA-CB	5.33	119.39	110.32
1	H	181	GLY	N-CA-C	-5.32	107.34	115.00
2	L	48	TYR	CA-C-N	-5.31	113.24	122.64
2	L	48	TYR	C-N-CA	-5.31	113.24	122.64
2	M	50	ASP	N-CA-CB	5.31	119.74	110.18
2	M	209	ALA	CA-C-N	5.29	125.23	119.78
2	M	209	ALA	C-N-CA	5.29	125.23	119.78
2	O	69	THR	N-CA-C	5.26	117.65	108.76
2	M	48	TYR	CA-C-N	-5.25	112.10	122.02
2	M	48	TYR	C-N-CA	-5.25	112.10	122.02
2	M	7	PRO	N-CA-C	-5.24	104.98	110.58
1	I	151	ASP	N-CA-C	5.21	118.31	111.28
1	J	113	GLY	N-CA-C	5.18	119.39	112.65
2	M	49	ASP	CA-C-N	-5.18	112.29	120.63
2	M	49	ASP	C-N-CA	-5.18	112.29	120.63
2	O	191	ARG	CG-CD-NE	5.17	123.36	112.00
1	K	98	ARG	NE-CZ-NH1	-5.16	116.34	121.50
2	O	147	THR	N-CA-C	-5.11	101.06	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	50	ASN	N-CA-C	5.11	117.72	110.10
1	K	19	ARG	N-CA-C	5.11	117.11	108.02
3	C	47	ASP	N-CA-C	-5.10	106.65	112.92
1	K	49	SER	N-CA-C	5.06	116.21	108.42
2	O	191	ARG	CB-CA-C	5.05	118.49	109.29
1	I	19	ARG	N-CA-C	5.05	116.62	108.34
2	O	165	THR	N-CA-C	-5.03	102.85	110.39
1	H	49	SER	N-CA-C	5.01	116.14	108.52
1	H	201	TYR	N-CA-C	5.01	117.65	109.59

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	48	ALA	Peptide
3	B	48	ALA	Peptide
3	C	48	ALA	Peptide
3	D	48	ALA	Peptide
2	L	93	SER	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	H	1569	0	1526	95	0
1	I	1620	0	1576	68	0
1	J	1661	0	1623	63	0
1	K	1625	0	1586	57	0
2	L	1558	0	1507	70	0
2	M	1558	0	1507	78	0
2	N	1558	0	1507	75	0
2	O	1558	0	1507	69	0
3	A	654	0	608	41	0
3	B	654	0	608	40	0
3	C	654	0	608	40	0
3	D	654	0	608	41	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	1	0
4	D	1	0	0	0	0
4	H	2	0	0	1	0
4	I	5	0	0	1	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	3	0	0	0	0
4	M	4	0	0	2	0
4	N	1	0	0	0	0
4	O	4	0	0	0	0
All	All	15350	0	14771	651	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 22.

All (651) 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:O:52:ASN:ND2	3:D:43:HIS:CD2	1.99	1.31
2:L:52:ASN:ND2	3:A:43:HIS:CD2	2.07	1.22
1:I:33:THR:CG2	1:I:52:SER:HA	1.70	1.20
2:O:52:ASN:ND2	3:D:43:HIS:HD2	1.37	1.18
2:M:52:ASN:ND2	3:B:43:HIS:CD2	2.12	1.17
2:L:52:ASN:ND2	3:A:43:HIS:HD2	1.42	1.16
1:I:33:THR:HG22	1:I:52:SER:CA	1.78	1.12
1:J:1:GLN:OE1	1:J:1:GLN:HA	1.46	1.12
1:J:33:THR:CG2	1:J:52:SER:HA	1.86	1.06
1:K:33:THR:HG23	1:K:52:SER:HA	1.34	1.05
2:M:60:ARG:NH1	2:M:81:ASP:OD2	1.88	1.05
1:H:207:HIS:HD2	1:H:210:SER:OG	1.35	1.05
1:H:207:HIS:CD2	1:H:210:SER:OG	2.10	1.04
2:M:52:ASN:ND2	3:B:43:HIS:HD2	1.49	1.04
2:L:52:ASN:CG	3:A:43:HIS:CD2	2.38	1.02
1:J:33:THR:HG22	1:J:52:SER:CA	1.91	1.01
1:J:134:SER:HB2	1:J:136:LYS:HD2	1.43	0.99
2:N:52:ASN:ND2	3:C:43:HIS:CD2	2.32	0.98
1:J:33:THR:HG22	1:J:52:SER:HA	1.00	0.97
3:A:94:GLN:NE2	3:A:97:ARG:HB2	1.79	0.95
2:O:52:ASN:HD21	3:D:43:HIS:HD2	0.99	0.94
2:M:169:GLN:HE21	2:M:175:ALA:HB2	1.31	0.94
2:M:183:THR:HG22	2:M:186:GLN:H	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:90:PHE:C	2:N:90:PHE:CD1	2.47	0.94
3:C:94:GLN:NE2	3:C:97:ARG:HB2	1.83	0.94
2:M:90:PHE:CD1	2:M:90:PHE:C	2.45	0.93
2:N:191:ARG:CG	2:N:191:ARG:HH11	1.70	0.93
2:M:90:PHE:C	2:M:90:PHE:HD1	1.77	0.93
1:H:17:SER:HB3	1:H:84:ASN:HD22	1.34	0.92
1:I:33:THR:HG22	1:I:52:SER:HA	0.92	0.92
1:K:207:HIS:HD2	1:K:210:SER:OG	1.52	0.91
2:N:169:GLN:HE21	2:N:175:ALA:HB2	1.36	0.91
2:N:183:THR:HG21	2:N:185:GLU:HG2	1.53	0.91
2:O:183:THR:HG22	2:O:186:GLN:H	1.33	0.91
2:O:60:ARG:NH1	2:O:81:ASP:OD2	2.02	0.90
2:L:60:ARG:NH1	2:L:81:ASP:OD2	2.04	0.90
2:N:183:THR:HG22	2:N:186:GLN:H	1.35	0.90
1:H:185:LEU:C	1:H:185:LEU:HD12	1.96	0.90
3:A:94:GLN:HE22	3:A:97:ARG:HB2	1.32	0.90
2:M:52:ASN:HD21	3:B:43:HIS:HD2	1.13	0.90
2:L:183:THR:HG21	2:L:185:GLU:HG2	1.51	0.90
2:O:169:GLN:HE21	2:O:175:ALA:HB2	1.34	0.89
1:I:195:SER:O	1:I:199:GLN:HB2	1.71	0.89
2:N:90:PHE:C	2:N:90:PHE:HD1	1.78	0.89
2:N:52:ASN:ND2	3:C:43:HIS:HD2	1.70	0.88
2:N:60:ARG:NH1	2:N:81:ASP:OD2	2.05	0.88
1:H:1:GLN:OE1	1:H:1:GLN:O	1.91	0.88
2:L:6:GLN:HE21	2:L:103:THR:HG23	1.37	0.88
2:L:52:ASN:HD21	3:A:43:HIS:HD2	1.19	0.88
2:L:6:GLN:HE21	2:L:103:THR:CG2	1.86	0.87
1:I:88:ALA:O	1:I:91:THR:HG23	1.75	0.87
3:C:94:GLN:HE22	3:C:97:ARG:HB2	1.37	0.87
2:L:90:PHE:CD1	2:L:90:PHE:C	2.53	0.86
1:J:134:SER:CB	1:J:136:LYS:HD2	2.05	0.86
2:O:90:PHE:CD1	2:O:90:PHE:C	2.52	0.86
3:D:94:GLN:HE22	3:D:97:ARG:HB2	1.39	0.85
2:L:90:PHE:C	2:L:90:PHE:HD1	1.85	0.85
1:K:88:ALA:O	1:K:91:THR:HG23	1.76	0.85
2:M:6:GLN:HB3	2:M:103:THR:HG22	1.59	0.85
2:M:183:THR:HG21	2:M:185:GLU:HG2	1.57	0.84
2:O:90:PHE:C	2:O:90:PHE:HD1	1.85	0.84
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.60	0.83
3:B:94:GLN:NE2	3:B:97:ARG:HB2	1.93	0.83
2:L:41:GLN:OE1	1:I:122:SER:HB2	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:169:GLN:HE21	2:L:175:ALA:HB2	1.45	0.82
2:N:52:ASN:CG	3:C:43:HIS:CD2	2.58	0.81
1:J:88:ALA:O	1:J:91:THR:CG2	2.29	0.81
3:B:94:GLN:HE22	3:B:97:ARG:HB2	1.46	0.81
3:D:94:GLN:NE2	3:D:97:ARG:CB	2.43	0.81
2:L:7:PRO:O	2:L:103:THR:HB	1.82	0.80
3:D:94:GLN:NE2	3:D:97:ARG:HB2	1.94	0.80
2:L:6:GLN:HB3	2:L:103:THR:HG22	1.64	0.80
2:L:183:THR:CG2	2:L:185:GLU:HG2	2.11	0.79
2:L:183:THR:HG22	2:L:186:GLN:H	1.46	0.79
1:I:88:ALA:O	1:I:91:THR:CG2	2.30	0.79
1:K:88:ALA:O	1:K:91:THR:CG2	2.30	0.79
2:O:183:THR:HG21	2:O:185:GLU:HG2	1.62	0.79
1:H:101:TRP:CZ3	3:A:86:GLN:NE2	2.50	0.79
3:A:94:GLN:NE2	3:A:97:ARG:CB	2.44	0.79
1:I:207:HIS:HD2	1:I:210:SER:OG	1.65	0.79
2:M:52:ASN:CG	3:B:43:HIS:CD2	2.60	0.78
1:J:1:GLN:OE1	1:J:1:GLN:CA	2.31	0.78
2:O:74:ILE:HG22	2:O:77:THR:HG22	1.64	0.78
1:H:174:PRO:HG2	2:L:167:SER:OG	1.83	0.77
3:C:65:GLU:OE2	3:C:96:ARG:HD3	1.84	0.77
1:I:101:TRP:HH2	3:B:86:GLN:HE22	1.33	0.77
2:L:6:GLN:NE2	2:L:103:THR:HG23	2.00	0.77
2:O:7:PRO:O	2:O:103:THR:HB	1.85	0.77
2:N:6:GLN:HB3	2:N:103:THR:HG22	1.66	0.76
2:L:52:ASN:HA	3:A:43:HIS:NE2	2.01	0.76
3:C:94:GLN:NE2	3:C:97:ARG:CB	2.48	0.76
1:K:100:ARG:HG3	3:D:94:GLN:OE1	1.85	0.76
2:O:52:ASN:CG	3:D:43:HIS:CD2	2.63	0.76
2:L:194:SER:OG	2:L:207:THR:HB	1.86	0.75
1:J:207:HIS:HD2	1:J:210:SER:OG	1.68	0.75
2:N:191:ARG:CG	2:N:191:ARG:NH1	2.42	0.75
2:N:183:THR:CG2	2:N:185:GLU:HG2	2.15	0.75
1:J:88:ALA:O	1:J:91:THR:HG23	1.87	0.74
1:H:17:SER:HB3	1:H:84:ASN:ND2	2.02	0.74
2:M:6:GLN:HE21	2:M:103:THR:HG23	1.50	0.74
2:N:7:PRO:O	2:N:103:THR:HB	1.88	0.74
1:H:31:ASN:HA	3:A:95:LEU:HD22	1.70	0.74
1:H:176:VAL:HG13	2:L:164:THR:CG2	2.18	0.74
1:I:31:ASN:HB3	4:B:130:HOH:O	1.87	0.74
2:O:183:THR:CG2	2:O:185:GLU:HG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:50:ASP:OD1	2:N:65:ASN:HB3	1.87	0.73
2:O:119:LEU:HD13	2:O:208:VAL:HG13	1.69	0.73
1:H:33:THR:C	1:H:34:LEU:HD22	2.13	0.73
1:H:178:GLN:HG2	2:L:162:GLU:HG2	1.71	0.73
1:H:17:SER:CB	1:H:84:ASN:HD22	2.02	0.73
2:M:51:SER:HB3	2:M:63:GLY:O	1.89	0.73
2:M:60:ARG:NH1	2:M:81:ASP:CG	2.47	0.72
1:H:101:TRP:HZ3	3:A:86:GLN:NE2	1.88	0.71
3:D:94:GLN:HE21	3:D:97:ARG:HB3	1.54	0.71
2:N:106:THR:HG21	2:N:143:PRO:HB3	1.71	0.71
2:M:106:THR:HG21	2:M:143:PRO:HB3	1.73	0.71
3:B:65:GLU:OE2	3:B:96:ARG:HD3	1.91	0.71
1:K:33:THR:CG2	1:K:52:SER:HA	2.18	0.71
1:H:185:LEU:HD12	1:H:186:SER:N	2.05	0.71
2:M:183:THR:CG2	2:M:185:GLU:HG2	2.20	0.71
2:M:60:ARG:HH12	2:M:81:ASP:CG	1.99	0.70
2:N:191:ARG:NH1	2:N:191:ARG:HG3	2.06	0.70
2:O:6:GLN:HB3	2:O:103:THR:HG22	1.72	0.70
2:N:74:ILE:HG22	2:N:77:THR:HG22	1.74	0.70
1:H:88:ALA:O	1:H:91:THR:HG23	1.91	0.70
2:M:6:GLN:HE21	2:M:103:THR:CG2	2.05	0.70
1:J:134:SER:C	1:J:136:LYS:N	2.49	0.70
1:H:73:ASP:OD1	1:H:75:SER:HB2	1.91	0.70
3:B:94:GLN:NE2	3:B:97:ARG:CB	2.56	0.69
3:A:96:ARG:NH2	3:A:116:PRO:O	2.25	0.69
2:N:60:ARG:HH12	2:N:81:ASP:CG	2.01	0.69
1:H:52:SER:HB3	1:H:57:LEU:HB2	1.75	0.69
2:M:119:LEU:HD13	2:M:208:VAL:HG13	1.74	0.69
3:C:116:PRO:HB2	3:C:118:VAL:HG22	1.75	0.69
1:J:155:GLU:HG3	1:J:156:PRO:HA	1.75	0.69
2:N:110:GLN:HB2	2:N:111:PRO:HD2	1.74	0.69
2:L:49:ASP:O	2:L:51:SER:N	2.26	0.68
2:N:52:ASN:HD21	3:C:43:HIS:HD2	1.40	0.68
1:H:34:LEU:HD23	1:H:72:ARG:NH2	2.09	0.68
1:H:176:VAL:HG13	2:L:164:THR:HG23	1.73	0.68
2:M:6:GLN:NE2	2:M:103:THR:HG23	2.08	0.68
2:O:45:LEU:HD13	2:O:54:PRO:HG3	1.75	0.67
1:J:134:SER:HB2	1:J:136:LYS:CD	2.23	0.67
1:H:17:SER:CB	1:H:84:ASN:ND2	2.58	0.67
3:C:45:PRO:C	3:C:47:ASP:H	2.03	0.67
1:H:17:SER:HB3	1:H:84:ASN:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:GLN:NE2	2:L:103:THR:CG2	2.57	0.67
2:L:119:LEU:HD13	2:L:208:VAL:HG13	1.76	0.66
2:M:74:ILE:HG22	2:M:77:THR:HG22	1.76	0.66
2:L:41:GLN:CD	1:I:122:SER:HB2	2.19	0.66
2:L:106:THR:HG21	2:L:143:PRO:HB3	1.76	0.66
1:I:58:THR:HG21	4:I:239:HOH:O	1.95	0.66
1:I:101:TRP:CZ3	3:B:86:GLN:NE2	2.64	0.66
2:N:194:SER:OG	2:N:207:THR:HB	1.95	0.66
3:D:78:MET:HE1	3:D:101:CYS:SG	2.35	0.66
2:N:6:GLN:HE21	2:N:103:THR:CG2	2.09	0.66
2:N:191:ARG:HH11	2:N:191:ARG:HG3	1.59	0.65
2:O:46:VAL:O	2:O:47:ILE:HG13	1.96	0.65
2:M:7:PRO:O	2:M:103:THR:HB	1.97	0.65
2:N:52:ASN:CG	3:C:43:HIS:HD2	2.03	0.65
1:I:185:LEU:HD12	1:I:185:LEU:C	2.21	0.64
2:O:110:GLN:HB2	2:O:111:PRO:HD2	1.78	0.64
2:O:184:PRO:O	2:O:188:LYS:HG2	1.97	0.64
2:M:90:PHE:HD1	2:M:90:PHE:O	1.78	0.64
2:M:194:SER:OG	2:M:207:THR:HB	1.97	0.64
2:O:15:GLY:O	2:O:76:GLY:HA2	1.98	0.64
1:I:98:ARG:NH2	3:B:67:ASP:OD2	2.30	0.64
1:K:101:TRP:CZ3	3:D:86:GLN:NE2	2.66	0.64
3:A:65:GLU:OE2	3:A:96:ARG:HD3	1.98	0.64
2:L:49:ASP:O	2:L:50:ASP:C	2.35	0.64
3:D:65:GLU:OE2	3:D:96:ARG:HD3	1.98	0.63
2:L:31:TYR:CZ	3:A:79:LYS:HG2	2.33	0.63
2:L:60:ARG:NH1	2:L:81:ASP:CG	2.56	0.63
1:J:88:ALA:O	1:J:91:THR:HG22	1.97	0.63
3:C:96:ARG:NH2	3:C:116:PRO:O	2.31	0.63
1:J:89:GLU:N	1:J:89:GLU:OE1	2.29	0.63
2:N:6:GLN:HE21	2:N:103:THR:HG23	1.63	0.63
1:K:176:VAL:HG13	2:O:164:THR:CG2	2.28	0.63
2:M:152:ALA:HB2	2:M:193:TYR:CE1	2.33	0.63
2:O:60:ARG:NH1	2:O:81:ASP:CG	2.55	0.63
1:I:101:TRP:CH2	3:B:86:GLN:NE2	2.66	0.63
2:O:90:PHE:HD1	2:O:90:PHE:O	1.82	0.63
1:J:83:MET:C	1:J:84:ASN:HD22	2.06	0.62
1:K:102:HIS:ND1	3:D:64:GLU:OE1	2.31	0.62
2:O:194:SER:OG	2:O:207:THR:HB	1.99	0.62
2:N:90:PHE:HD1	2:N:90:PHE:O	1.82	0.62
1:K:195:SER:O	1:K:199:GLN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:78:MET:HE1	3:B:101:CYS:SG	2.40	0.62
1:K:33:THR:HG22	1:K:51:THR:O	1.99	0.62
2:O:106:THR:HG21	2:O:143:PRO:HB3	1.82	0.62
2:M:183:THR:HG22	2:M:186:GLN:N	2.11	0.62
1:J:122:SER:HB2	2:O:41:GLN:OE1	2.00	0.62
2:O:6:GLN:HE21	2:O:103:THR:CG2	2.13	0.62
1:I:100:ARG:HG3	3:B:94:GLN:OE1	2.00	0.62
1:J:177:LEU:HG	1:J:183:TYR:CE2	2.35	0.62
1:H:155:GLU:HG3	1:H:156:PRO:HA	1.81	0.61
1:K:51:THR:HG22	1:K:55:GLY:HA2	1.81	0.61
3:A:94:GLN:HE21	3:A:97:ARG:CB	2.13	0.61
2:M:183:THR:HB	2:M:186:GLN:OE1	1.99	0.61
2:L:52:ASN:CG	3:A:43:HIS:HD2	1.94	0.61
3:C:78:MET:HE1	3:C:101:CYS:SG	2.39	0.61
1:K:176:VAL:HG13	2:O:164:THR:HG23	1.82	0.61
2:O:33:ILE:HD13	2:O:48:TYR:O	2.00	0.61
2:M:90:PHE:CE1	2:M:91:THR:O	2.53	0.61
2:O:60:ARG:HH12	2:O:81:ASP:CG	2.08	0.61
2:O:183:THR:HG22	2:O:186:GLN:N	2.09	0.61
2:M:210:PRO:O	2:M:211:THR:C	2.44	0.61
2:L:183:THR:HB	2:L:186:GLN:OE1	2.00	0.61
2:L:110:GLN:HB2	2:L:111:PRO:CD	2.31	0.61
1:K:207:HIS:CD2	1:K:210:SER:OG	2.44	0.61
2:L:46:VAL:O	2:L:47:ILE:HG13	2.00	0.60
2:L:110:GLN:HB2	2:L:111:PRO:HD2	1.83	0.60
1:J:134:SER:C	1:J:136:LYS:H	2.09	0.60
3:C:104:THR:HB	3:C:107:CYS:HB3	1.83	0.60
1:H:219:GLU:HB3	1:H:220:PRO:CD	2.32	0.60
1:J:178:GLN:HG3	1:J:182:LEU:O	2.01	0.60
1:K:89:GLU:N	1:K:89:GLU:OE1	2.34	0.60
1:H:91:THR:HB	1:H:117:THR:HA	1.82	0.60
1:K:31:ASN:HA	3:D:95:LEU:HD22	1.83	0.60
1:H:185:LEU:C	1:H:185:LEU:CD1	2.68	0.60
1:I:19:ARG:HD3	1:I:82:GLN:NE2	2.16	0.60
1:H:159:VAL:HG21	1:H:187:SER:HB2	1.84	0.60
2:L:60:ARG:HH12	2:L:81:ASP:CG	2.10	0.60
3:C:94:GLN:HE21	3:C:97:ARG:CB	2.13	0.60
2:L:210:PRO:O	2:L:211:THR:C	2.44	0.60
1:H:100:ARG:HG3	3:A:94:GLN:OE1	2.02	0.60
3:B:65:GLU:HG2	3:B:96:ARG:HB3	1.84	0.60
1:H:208:LYS:HB2	1:H:209:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:184:PRO:O	2:L:188:LYS:HG2	2.01	0.59
1:I:178:GLN:HG3	1:I:182:LEU:O	2.01	0.59
2:N:140:ASP:H	2:N:169:GLN:HE22	1.50	0.59
3:D:35:PHE:N	3:D:35:PHE:CD2	2.69	0.59
1:I:51:THR:HG22	1:I:55:GLY:HA2	1.84	0.59
1:I:176:VAL:HG13	2:M:164:THR:HG23	1.85	0.59
1:H:34:LEU:HB3	1:H:79:LEU:HD22	1.85	0.59
2:N:60:ARG:NH1	2:N:81:ASP:CG	2.58	0.59
2:M:52:ASN:HA	3:B:43:HIS:NE2	2.17	0.58
2:M:110:GLN:HB2	2:M:111:PRO:HD2	1.84	0.58
1:J:185:LEU:C	1:J:185:LEU:HD12	2.27	0.58
1:H:19:ARG:HD3	1:H:82:GLN:NE2	2.19	0.58
1:H:217:LYS:NZ	1:H:219:GLU:OE2	2.34	0.58
1:H:219:GLU:HB3	1:H:220:PRO:HD2	1.84	0.58
2:N:210:PRO:O	2:N:211:THR:C	2.44	0.58
1:H:94:TYR:O	1:H:113:GLY:HA2	2.03	0.58
1:J:101:TRP:CZ3	3:C:86:GLN:NE2	2.71	0.58
2:L:90:PHE:HD1	2:L:90:PHE:O	1.85	0.58
2:M:110:GLN:HB2	2:M:111:PRO:CD	2.33	0.58
1:I:91:THR:HB	1:I:117:THR:HA	1.85	0.58
2:N:52:ASN:HD21	3:C:43:HIS:CD2	2.17	0.58
2:N:90:PHE:CE1	2:N:91:THR:O	2.57	0.58
2:N:110:GLN:HB2	2:N:111:PRO:CD	2.33	0.58
1:K:185:LEU:C	1:K:185:LEU:HD12	2.28	0.58
3:A:35:PHE:N	3:A:35:PHE:CD2	2.70	0.58
2:O:183:THR:HB	2:O:186:GLN:OE1	2.04	0.57
1:H:102:HIS:ND1	3:A:64:GLU:OE1	2.38	0.57
2:N:54:PRO:HG2	2:N:57:ILE:HG12	1.85	0.57
2:O:74:ILE:CG2	2:O:77:THR:HG22	2.33	0.57
1:H:101:TRP:HH2	3:A:86:GLN:HE22	1.48	0.57
3:A:65:GLU:HG2	3:A:96:ARG:HB3	1.87	0.57
2:N:51:SER:HB3	2:N:63:GLY:O	2.03	0.57
2:N:53:ARG:HD3	2:N:61:PHE:O	2.05	0.57
3:C:68:GLN:O	3:C:70:GLU:N	2.36	0.57
2:M:6:GLN:HB3	2:M:103:THR:CG2	2.31	0.57
2:L:6:GLN:HB3	2:L:103:THR:CG2	2.34	0.56
2:L:36:GLN:HB2	2:L:85:TYR:CE2	2.40	0.56
2:L:56:GLY:HA2	1:I:12:VAL:HG13	1.86	0.56
2:L:140:ASP:H	2:L:169:GLN:HE22	1.52	0.56
1:I:155:GLU:HG3	1:I:156:PRO:HA	1.86	0.56
3:A:94:GLN:HE21	3:A:97:ARG:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:ALA:HB2	1:I:185:LEU:HB3	1.86	0.56
3:C:35:PHE:H	3:C:35:PHE:HD2	1.54	0.56
1:K:75:SER:C	1:K:76:LYS:O	2.45	0.56
1:H:161:TRP:O	1:H:162:ASN:C	2.47	0.56
2:M:90:PHE:CZ	2:M:92:MET:SD	2.98	0.56
1:H:155:GLU:HG3	1:H:156:PRO:CA	2.36	0.56
2:M:6:GLN:NE2	2:M:103:THR:CG2	2.67	0.56
1:K:101:TRP:HZ3	3:D:86:GLN:NE2	2.02	0.56
2:M:90:PHE:CE1	2:M:92:MET:SD	2.99	0.56
2:N:15:GLY:O	2:N:76:GLY:HA2	2.06	0.56
1:J:101:TRP:HH2	3:C:86:GLN:HE22	1.54	0.56
3:D:96:ARG:NH2	3:D:116:PRO:O	2.39	0.56
1:H:145:LEU:C	1:H:145:LEU:HD12	2.32	0.55
1:I:149:VAL:O	1:I:149:VAL:CG2	2.54	0.55
3:C:94:GLN:HE21	3:C:97:ARG:HB3	1.71	0.55
3:A:35:PHE:H	3:A:35:PHE:HD2	1.54	0.55
3:D:35:PHE:N	3:D:35:PHE:HD2	2.02	0.55
1:H:34:LEU:HD22	1:H:34:LEU:N	2.21	0.55
2:L:115:PRO:HB3	2:L:141:PHE:HB3	1.88	0.55
2:M:31:TYR:CZ	3:B:79:LYS:HG2	2.41	0.55
1:H:122:SER:O	1:H:123:THR:O	2.24	0.55
1:H:75:SER:C	1:H:76:LYS:O	2.47	0.55
2:L:185:GLU:O	2:L:189:SER:HB3	2.06	0.55
2:N:6:GLN:NE2	2:N:103:THR:HG23	2.21	0.55
2:N:49:ASP:O	2:N:50:ASP:C	2.48	0.55
2:O:185:GLU:O	2:O:189:SER:HB3	2.06	0.55
1:H:34:LEU:HD23	1:H:72:ARG:HH22	1.69	0.55
1:K:178:GLN:HG3	1:K:182:LEU:O	2.07	0.55
3:C:35:PHE:CD2	3:C:35:PHE:N	2.71	0.55
1:H:24:ALA:HB1	1:H:27:PHE:CE1	2.42	0.54
1:H:87:ARG:HD3	4:H:235:HOH:O	2.06	0.54
2:L:75:SER:O	2:L:76:GLY:C	2.49	0.54
1:I:177:LEU:HG	1:I:183:TYR:CE2	2.42	0.54
3:C:50:ASN:C	3:C:50:ASN:HD22	2.15	0.54
3:C:65:GLU:HG2	3:C:96:ARG:HB3	1.89	0.54
1:H:19:ARG:HB2	1:H:82:GLN:HE22	1.72	0.54
2:L:52:ASN:ND2	3:A:43:HIS:NE2	2.55	0.54
1:J:19:ARG:HD3	1:J:82:GLN:NE2	2.22	0.54
3:C:35:PHE:HD2	3:C:35:PHE:N	2.05	0.54
1:H:98:ARG:NH2	3:A:67:ASP:OD2	2.39	0.54
2:L:74:ILE:HG22	2:L:77:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:119:LEU:HD13	2:N:208:VAL:HG13	1.90	0.54
3:B:104:THR:HB	3:B:107:CYS:HB3	1.90	0.54
3:B:35:PHE:CD2	3:B:35:PHE:N	2.73	0.54
2:M:75:SER:O	2:M:76:GLY:C	2.51	0.54
2:N:49:ASP:O	2:N:51:SER:N	2.41	0.54
1:H:101:TRP:HZ3	3:A:86:GLN:HE21	1.56	0.53
2:N:6:GLN:HB3	2:N:103:THR:CG2	2.37	0.53
1:I:154:PRO:O	1:I:207:HIS:HE1	1.89	0.53
2:M:95:ASN:HB2	4:M:217:HOH:O	2.08	0.53
2:O:140:ASP:H	2:O:169:GLN:HE22	1.56	0.53
2:M:86:TYR:CE2	2:M:102:GLY:HA3	2.43	0.53
1:H:119:SER:OG	1:H:121:ALA:HB3	2.09	0.53
2:O:210:PRO:O	2:O:211:THR:C	2.52	0.53
1:H:172:THR:HA	1:H:187:SER:HA	1.89	0.53
3:A:78:MET:HE1	3:A:101:CYS:SG	2.48	0.53
1:I:89:GLU:OE1	1:I:89:GLU:N	2.39	0.53
1:K:24:ALA:HB1	1:K:27:PHE:CE1	2.44	0.53
1:H:40:ALA:O	1:H:41:PRO:C	2.52	0.53
3:A:35:PHE:N	3:A:35:PHE:HD2	2.07	0.53
2:M:54:PRO:HG2	2:M:57:ILE:HG12	1.90	0.53
3:D:35:PHE:HD2	3:D:35:PHE:H	1.54	0.53
1:H:57:LEU:HD23	3:A:91:PRO:HB2	1.90	0.53
1:H:185:LEU:CD1	1:H:186:SER:N	2.71	0.53
3:C:68:GLN:C	3:C:70:GLU:H	2.17	0.53
3:B:40:CYS:HB3	3:B:76:GLY:HA2	1.90	0.53
2:L:58:PRO:HA	1:I:16:GLY:HA2	1.91	0.52
3:B:35:PHE:N	3:B:35:PHE:HD2	2.07	0.52
2:L:15:GLY:O	2:L:76:GLY:HA2	2.08	0.52
2:N:90:PHE:CZ	2:N:92:MET:SD	3.01	0.52
1:K:19:ARG:HD3	1:K:82:GLN:NE2	2.24	0.52
1:H:162:ASN:HD21	1:H:201:TYR:HA	1.74	0.52
2:N:183:THR:HG22	2:N:186:GLN:N	2.15	0.52
1:K:149:VAL:CG2	1:K:149:VAL:O	2.58	0.52
1:H:83:MET:HE2	1:H:86:LEU:HD21	1.91	0.52
1:H:176:VAL:HG13	2:L:164:THR:HG22	1.90	0.52
1:H:162:ASN:ND2	1:H:202:ILE:H	2.08	0.52
1:H:207:HIS:HD2	1:H:210:SER:HG	1.53	0.52
3:A:104:THR:HB	3:A:107:CYS:HB3	1.89	0.52
1:I:33:THR:HG22	1:I:52:SER:C	2.35	0.52
1:I:83:MET:CE	1:I:94:TYR:CZ	2.93	0.52
2:N:184:PRO:O	2:N:188:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:LEU:HD23	3:C:105:ASN:HD22	1.74	0.52
1:I:75:SER:C	1:I:76:LYS:O	2.52	0.52
2:N:6:GLN:NE2	2:N:103:THR:CG2	2.73	0.52
2:N:75:SER:O	2:N:76:GLY:C	2.52	0.52
1:H:176:VAL:CG1	2:L:164:THR:HG22	2.39	0.52
2:L:54:PRO:HG2	2:L:57:ILE:HG12	1.92	0.52
1:J:100:ARG:HG3	3:C:94:GLN:OE1	2.09	0.52
2:M:33:ILE:HD13	2:M:48:TYR:O	2.09	0.52
1:K:33:THR:C	1:K:34:LEU:HD22	2.35	0.52
2:L:183:THR:HG22	2:L:185:GLU:N	2.25	0.51
1:I:200:THR:O	1:I:200:THR:HG22	2.10	0.51
3:B:94:GLN:HE21	3:B:97:ARG:HB3	1.75	0.51
3:B:94:GLN:HE21	3:B:97:ARG:CB	2.23	0.51
2:N:152:ALA:HB2	2:N:193:TYR:CE1	2.45	0.51
2:O:90:PHE:CE1	2:O:92:MET:SD	3.03	0.51
1:H:88:ALA:O	1:H:91:THR:CG2	2.58	0.51
1:K:177:LEU:HG	1:K:183:TYR:CE2	2.46	0.51
1:I:40:ALA:O	1:I:41:PRO:C	2.51	0.51
2:O:51:SER:HB3	2:O:63:GLY:O	2.10	0.51
1:I:34:LEU:HB3	1:I:79:LEU:HD22	1.91	0.51
2:M:140:ASP:H	2:M:169:GLN:HE22	1.58	0.51
1:J:192:PRO:O	1:J:195:SER:OG	2.20	0.51
2:N:33:ILE:HD13	2:N:48:TYR:O	2.11	0.51
1:H:205:VAL:HG12	1:H:205:VAL:O	2.09	0.51
2:M:45:LEU:HD13	2:M:54:PRO:HG3	1.92	0.51
1:H:48:VAL:HG13	1:H:64:VAL:HG21	1.93	0.50
1:K:91:THR:HB	1:K:117:THR:HA	1.93	0.50
2:L:33:ILE:HD13	2:L:48:TYR:O	2.12	0.50
3:A:36:LEU:HD23	3:A:105:ASN:HD22	1.77	0.50
2:N:90:PHE:CE1	2:N:92:MET:SD	3.04	0.50
1:J:31:ASN:HA	3:C:95:LEU:HD22	1.94	0.50
2:M:115:PRO:HB3	2:M:141:PHE:HB3	1.93	0.50
3:B:50:ASN:C	3:B:50:ASN:HD22	2.07	0.50
1:K:101:TRP:HH2	3:D:86:GLN:HE22	1.54	0.50
3:B:35:PHE:HD2	3:B:35:PHE:H	1.59	0.50
1:J:51:THR:HG22	1:J:55:GLY:HA2	1.94	0.50
1:H:176:VAL:CG1	2:L:164:THR:CG2	2.88	0.50
2:N:183:THR:HB	2:N:186:GLN:OE1	2.11	0.50
2:M:190:HIS:HE1	3:D:82:GLY:O	1.95	0.50
3:D:40:CYS:HB3	3:D:76:GLY:HA2	1.94	0.50
3:D:50:ASN:O	3:D:50:ASN:ND2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:50:ASN:HD22	3:D:50:ASN:C	2.13	0.50
3:D:65:GLU:HG2	3:D:96:ARG:HB3	1.93	0.50
2:L:90:PHE:CE1	2:L:91:THR:O	2.65	0.49
1:J:91:THR:HB	1:J:117:THR:HA	1.93	0.49
1:J:175:ALA:HB2	1:J:185:LEU:HB3	1.94	0.49
2:M:90:PHE:CD1	2:M:91:THR:N	2.79	0.49
1:J:34:LEU:HB3	1:J:79:LEU:HD22	1.93	0.49
1:I:176:VAL:HG13	2:M:164:THR:CG2	2.41	0.49
1:J:154:PRO:O	1:J:207:HIS:HE1	1.95	0.49
2:N:46:VAL:O	2:N:47:ILE:HG13	2.12	0.49
2:O:6:GLN:NE2	2:O:103:THR:CG2	2.74	0.49
2:O:110:GLN:HB2	2:O:111:PRO:CD	2.42	0.49
1:I:33:THR:C	1:I:34:LEU:HD22	2.37	0.49
1:K:34:LEU:HB3	1:K:79:LEU:HD22	1.94	0.49
1:H:6:GLU:CD	1:H:113:GLY:H	2.21	0.49
1:J:73:ASP:OD1	1:J:73:ASP:C	2.55	0.49
2:O:6:GLN:HE21	2:O:103:THR:HG23	1.76	0.49
2:M:49:ASP:O	2:M:50:ASP:C	2.54	0.49
2:M:184:PRO:O	2:M:188:LYS:HG2	2.13	0.49
2:O:53:ARG:HD3	2:O:61:PHE:O	2.12	0.49
2:M:15:GLY:O	2:M:76:GLY:HA2	2.12	0.49
1:K:72:ARG:HD3	1:K:74:ASN:OD1	2.13	0.49
2:M:52:ASN:N	2:M:52:ASN:HD22	2.11	0.48
1:I:83:MET:HB3	1:I:86:LEU:HD21	1.93	0.48
1:I:185:LEU:HD12	1:I:185:LEU:O	2.14	0.48
1:J:24:ALA:HB1	1:J:27:PHE:CE1	2.47	0.48
2:O:115:PRO:HB3	2:O:141:PHE:HB3	1.95	0.48
3:D:104:THR:HB	3:D:107:CYS:HB3	1.96	0.48
2:M:90:PHE:CD1	2:M:90:PHE:O	2.61	0.48
2:O:54:PRO:HG2	2:O:57:ILE:HG12	1.96	0.48
1:J:98:ARG:NH2	3:C:67:ASP:OD2	2.40	0.48
1:J:191:VAL:HG21	1:J:201:TYR:CE1	2.49	0.48
1:K:154:PRO:O	1:K:207:HIS:HE1	1.97	0.48
1:H:36:TRP:NE1	1:H:81:LEU:HB2	2.29	0.48
2:M:52:ASN:ND2	3:B:43:HIS:NE2	2.59	0.48
3:B:36:LEU:HD23	3:B:105:ASN:HD22	1.79	0.48
1:H:191:VAL:HG11	1:H:201:TYR:CE2	2.48	0.48
3:D:117:PRO:O	3:D:118:VAL:C	2.56	0.48
1:H:160:SER:OG	1:H:204:ASN:HB2	2.14	0.47
1:H:208:LYS:HB2	1:H:209:PRO:CD	2.44	0.47
1:I:208:LYS:N	1:I:209:PRO:HD2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:45:LEU:HD13	2:N:54:PRO:HG3	1.96	0.47
1:H:208:LYS:N	1:H:209:PRO:HD2	2.29	0.47
1:I:24:ALA:HB1	1:I:27:PHE:CE1	2.50	0.47
1:J:101:TRP:HZ3	3:C:86:GLN:NE2	2.10	0.47
3:B:50:ASN:O	3:B:50:ASN:ND2	2.33	0.47
3:B:111:LEU:HD12	3:B:111:LEU:HA	1.70	0.47
2:N:34:TRP:O	2:N:46:VAL:HG22	2.14	0.47
2:N:185:GLU:O	2:N:189:SER:HB3	2.13	0.47
3:D:36:LEU:HD23	3:D:105:ASN:HD22	1.78	0.47
3:D:60:PHE:HB3	3:D:78:MET:HE3	1.96	0.47
3:C:111:LEU:HD12	3:C:111:LEU:HA	1.62	0.47
1:I:196:LEU:C	1:I:198:THR:H	2.22	0.47
2:N:74:ILE:CG2	2:N:77:THR:HG22	2.43	0.47
1:K:32:TYR:O	1:K:72:ARG:NH2	2.46	0.47
2:O:142:TYR:HA	2:O:143:PRO:C	2.40	0.47
1:H:67:ARG:C	1:H:68:PHE:HD1	2.23	0.47
2:N:90:PHE:CE1	2:N:91:THR:C	2.93	0.47
1:K:175:ALA:HB2	1:K:185:LEU:HB3	1.95	0.47
2:O:52:ASN:HA	3:D:43:HIS:NE2	2.30	0.47
2:O:152:ALA:HB2	2:O:193:TYR:CE1	2.50	0.47
1:K:149:VAL:O	1:K:149:VAL:HG23	2.15	0.47
2:O:75:SER:O	2:O:76:GLY:C	2.58	0.47
3:A:40:CYS:HB3	3:A:76:GLY:HA2	1.96	0.47
2:M:60:ARG:NH1	2:M:81:ASP:OD1	2.46	0.47
1:K:34:LEU:HD13	1:K:98:ARG:HA	1.97	0.47
2:O:6:GLN:NE2	2:O:103:THR:HG23	2.29	0.47
1:H:33:THR:HB	1:H:99:GLU:HB3	1.96	0.46
3:B:68:GLN:C	3:B:70:GLU:H	2.24	0.46
2:N:90:PHE:CD1	2:N:91:THR:N	2.81	0.46
2:N:140:ASP:H	2:N:169:GLN:NE2	2.13	0.46
2:N:115:PRO:HB3	2:N:141:PHE:HB3	1.96	0.46
1:I:88:ALA:O	1:I:91:THR:HG22	2.11	0.46
1:K:219:GLU:HA	1:K:220:PRO:HD2	1.69	0.46
2:L:56:GLY:CA	1:I:12:VAL:HG13	2.46	0.46
2:M:4:LEU:HD22	2:M:98:VAL:HG13	1.98	0.46
1:J:40:ALA:O	1:J:41:PRO:C	2.58	0.46
2:N:46:VAL:HA	2:N:57:ILE:HG13	1.98	0.46
1:K:83:MET:CE	1:K:94:TYR:CZ	2.98	0.46
2:L:51:SER:HB3	2:L:63:GLY:O	2.16	0.46
2:L:60:ARG:NH1	2:L:81:ASP:OD1	2.48	0.46
1:I:185:LEU:C	1:I:185:LEU:CD1	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:LEU:C	1:I:198:THR:N	2.72	0.46
2:O:48:TYR:C	2:O:49:ASP:O	2.51	0.46
1:I:149:VAL:O	1:I:149:VAL:HG23	2.16	0.46
3:B:82:GLY:O	2:O:190:HIS:HE1	1.99	0.46
1:K:195:SER:O	1:K:199:GLN:N	2.47	0.46
1:H:101:TRP:CH2	3:A:86:GLN:NE2	2.73	0.46
1:I:83:MET:HE1	1:I:94:TYR:CZ	2.51	0.46
1:J:33:THR:C	1:J:34:LEU:HD22	2.41	0.46
1:J:134:SER:O	1:J:136:LYS:N	2.48	0.46
1:K:155:GLU:HG3	1:K:156:PRO:HA	1.98	0.46
3:B:68:GLN:O	3:B:70:GLU:N	2.48	0.46
3:C:40:CYS:HB3	3:C:76:GLY:HA2	1.98	0.46
2:M:90:PHE:CE1	2:M:91:THR:C	2.94	0.46
2:O:37:GLN:HE21	2:O:43:PRO:HG3	1.81	0.46
2:M:52:ASN:HD21	3:B:43:HIS:CD2	2.00	0.45
1:J:208:LYS:N	1:J:209:PRO:HD2	2.31	0.45
2:M:95:ASN:CB	4:M:217:HOH:O	2.64	0.45
1:H:155:GLU:CG	1:H:156:PRO:HA	2.46	0.45
1:J:75:SER:C	1:J:76:LYS:O	2.58	0.45
2:N:52:ASN:ND2	3:C:43:HIS:NE2	2.64	0.45
1:K:88:ALA:O	1:K:91:THR:HG22	2.11	0.45
2:O:52:ASN:ND2	3:D:43:HIS:NE2	2.56	0.45
2:O:90:PHE:CE1	2:O:91:THR:O	2.69	0.45
1:H:6:GLU:OE2	1:H:111:GLY:HA3	2.16	0.45
2:M:46:VAL:HA	2:M:57:ILE:HG13	1.98	0.45
2:M:171:ASN:O	2:M:172:ASN:HB2	2.15	0.45
2:M:183:THR:HG22	2:M:185:GLU:N	2.30	0.45
1:I:141:GLY:C	1:I:142:THR:HG22	2.42	0.45
1:I:175:ALA:HB1	1:I:184:SER:O	2.17	0.45
1:J:34:LEU:HD13	1:J:98:ARG:HA	1.99	0.45
1:J:141:GLY:C	1:J:193:SER:OG	2.60	0.45
3:C:45:PRO:C	3:C:47:ASP:N	2.75	0.45
3:A:50:ASN:C	3:A:50:ASN:HD22	2.16	0.45
1:K:196:LEU:C	1:K:198:THR:H	2.24	0.45
3:A:68:GLN:C	3:A:70:GLU:H	2.25	0.45
1:I:91:THR:HB	1:I:118:VAL:H	1.82	0.45
2:M:48:TYR:C	2:M:49:ASP:O	2.57	0.45
1:H:162:ASN:HD21	1:H:202:ILE:H	1.65	0.45
1:H:185:LEU:HD12	1:H:186:SER:CA	2.47	0.45
2:L:86:TYR:CE2	2:L:102:GLY:HA3	2.52	0.45
3:D:68:GLN:OE1	3:D:68:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:38:CYS:O	3:A:52:THR:HA	2.17	0.44
1:J:18:LEU:HD23	1:J:18:LEU:HA	1.78	0.44
1:H:103:VAL:HG12	1:H:104:ARG:HG2	2.00	0.44
3:D:94:GLN:NE2	3:D:97:ARG:HB3	2.15	0.44
2:N:86:TYR:CE2	2:N:102:GLY:HA3	2.53	0.44
2:L:158:LYS:HD2	2:L:158:LYS:HA	1.77	0.44
1:K:91:THR:HB	1:K:118:VAL:H	1.82	0.44
1:I:145:LEU:C	1:I:145:LEU:HD12	2.42	0.44
2:M:74:ILE:CG2	2:M:77:THR:HG22	2.43	0.44
2:N:142:TYR:HA	2:N:143:PRO:C	2.43	0.44
1:K:12:VAL:HG21	1:K:18:LEU:HG	1.99	0.44
2:O:90:PHE:CZ	2:O:92:MET:SD	3.11	0.44
3:D:94:GLN:H	3:D:94:GLN:HG3	1.27	0.44
1:J:99:GLU:OE1	3:C:92:LYS:HE2	2.18	0.43
2:N:90:PHE:CD1	2:N:90:PHE:O	2.66	0.43
2:L:140:ASP:H	2:L:169:GLN:NE2	2.14	0.43
1:I:83:MET:HE3	1:I:94:TYR:CZ	2.54	0.43
2:O:37:GLN:NE2	2:O:43:PRO:HG3	2.32	0.43
2:O:60:ARG:NH1	2:O:81:ASP:OD1	2.50	0.43
1:I:191:VAL:HG21	1:I:201:TYR:CE1	2.53	0.43
2:M:6:GLN:CB	2:M:103:THR:HG22	2.41	0.43
3:C:38:CYS:O	3:C:52:THR:HA	2.18	0.43
1:H:38:ARG:HH21	1:H:46:GLU:CD	2.27	0.43
1:H:157:VAL:HG22	1:H:207:HIS:HB2	2.00	0.43
3:A:94:GLN:H	3:A:94:GLN:HG3	1.23	0.43
1:J:155:GLU:HG3	1:J:156:PRO:CA	2.46	0.43
1:H:210:SER:O	1:H:211:ASN:C	2.62	0.43
1:I:31:ASN:HA	3:B:95:LEU:HD22	1.99	0.43
3:B:38:CYS:O	3:B:52:THR:HA	2.18	0.43
1:K:192:PRO:O	1:K:195:SER:OG	2.31	0.43
1:K:196:LEU:C	1:K:198:THR:N	2.74	0.43
1:H:103:VAL:C	1:H:104:ARG:HG2	2.43	0.43
2:O:36:GLN:HB2	2:O:85:TYR:CE2	2.54	0.43
3:D:68:GLN:O	3:D:70:GLU:N	2.52	0.43
1:H:33:THR:HG23	1:H:51:THR:O	2.18	0.43
1:I:101:TRP:HZ3	3:B:86:GLN:NE2	2.12	0.43
1:I:150:LYS:HA	1:I:184:SER:OG	2.18	0.43
1:J:84:ASN:HD22	1:J:84:ASN:N	2.13	0.43
2:N:31:TYR:CD2	2:N:50:ASP:OD2	2.72	0.43
2:N:60:ARG:NH1	2:N:81:ASP:OD1	2.49	0.43
1:H:68:PHE:N	1:H:68:PHE:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:PHE:CD2	3:A:35:PHE:C	2.95	0.43
3:B:35:PHE:CD2	3:B:35:PHE:C	2.96	0.42
2:O:52:ASN:N	2:O:52:ASN:HD22	2.16	0.42
1:H:19:ARG:HD3	1:H:82:GLN:HE22	1.83	0.42
1:J:176:VAL:HG13	2:N:164:THR:HG23	2.01	0.42
1:K:28:THR:O	1:K:31:ASN:HB2	2.20	0.42
1:K:105:GLY:O	2:O:33:ILE:HD12	2.19	0.42
1:H:149:VAL:HG13	1:H:185:LEU:CD1	2.49	0.42
2:N:46:VAL:O	2:N:54:PRO:HD2	2.19	0.42
1:K:115:LEU:HD13	1:K:117:THR:HG22	2.01	0.42
1:H:34:LEU:N	1:H:34:LEU:CD2	2.83	0.42
2:L:152:ALA:HB2	2:L:193:TYR:CE1	2.55	0.42
1:H:61:ALA:O	1:H:62:ASP:C	2.62	0.42
1:I:207:HIS:HB3	1:I:212:THR:HB	2.01	0.42
1:J:84:ASN:N	1:J:84:ASN:ND2	2.67	0.42
2:N:183:THR:HG22	2:N:185:GLU:N	2.35	0.42
2:O:86:TYR:CE2	2:O:102:GLY:HA3	2.55	0.42
1:H:115:LEU:HD22	1:H:117:THR:HG22	2.02	0.42
1:I:72:ARG:HD3	1:I:74:ASN:OD1	2.19	0.42
1:J:32:TYR:O	1:J:72:ARG:NH2	2.48	0.42
2:M:13:ALA:O	2:M:14:PRO:C	2.63	0.42
2:M:105:LEU:HD23	2:M:105:LEU:HA	1.86	0.42
3:B:50:ASN:C	3:B:50:ASN:ND2	2.76	0.42
2:N:6:GLN:OE1	2:N:100:GLY:HA3	2.18	0.42
3:D:111:LEU:HD12	3:D:111:LEU:HA	1.65	0.42
2:M:142:TYR:HA	2:M:143:PRO:C	2.43	0.42
1:J:115:LEU:HD23	1:J:115:LEU:HA	1.84	0.42
1:K:83:MET:HE1	1:K:94:TYR:CZ	2.55	0.42
2:M:158:LYS:HD2	2:M:158:LYS:HA	1.80	0.42
1:K:176:VAL:CG1	2:O:164:THR:HG22	2.50	0.42
1:J:178:GLN:O	1:J:179:SER:C	2.62	0.42
3:D:68:GLN:C	3:D:70:GLU:H	2.27	0.42
1:H:133:PRO:HB3	1:H:145:LEU:HB3	2.01	0.41
1:J:195:SER:O	1:J:199:GLN:CB	2.69	0.41
1:H:115:LEU:HD13	1:H:117:THR:HG22	2.02	0.41
2:L:58:PRO:HB3	1:I:15:GLY:C	2.45	0.41
3:A:111:LEU:HD12	3:A:111:LEU:HA	1.74	0.41
1:I:191:VAL:HA	1:I:192:PRO:HD2	1.90	0.41
1:J:91:THR:HB	1:J:118:VAL:H	1.86	0.41
2:L:47:ILE:HD12	2:L:72:LEU:CD1	2.50	0.41
1:K:153:PHE:HA	1:K:154:PRO:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:158:LYS:HD2	2:O:158:LYS:HA	1.77	0.41
3:C:49:ILE:HG12	3:C:50:ASN:N	2.36	0.41
2:L:153:ASP:O	2:L:154:SER:OG	2.33	0.41
1:K:178:GLN:O	1:K:179:SER:C	2.64	0.41
3:A:60:PHE:CD1	3:A:60:PHE:C	2.99	0.41
3:A:68:GLN:O	3:A:70:GLU:N	2.53	0.41
2:M:36:GLN:HB2	2:M:85:TYR:CE2	2.56	0.41
2:M:86:TYR:CD2	2:M:102:GLY:HA3	2.56	0.41
2:M:140:ASP:H	2:M:169:GLN:NE2	2.18	0.41
1:J:176:VAL:HG13	2:N:164:THR:CG2	2.51	0.41
2:N:158:LYS:HD2	2:N:158:LYS:HA	1.86	0.41
1:I:199:GLN:HB3	1:I:201:TYR:CE2	2.55	0.41
2:M:49:ASP:O	2:M:51:SER:N	2.54	0.41
1:H:73:ASP:OD1	1:H:73:ASP:C	2.61	0.41
2:L:183:THR:HG22	2:L:186:GLN:N	2.23	0.41
1:I:12:VAL:HG21	1:I:18:LEU:HG	2.03	0.41
1:I:178:GLN:O	1:I:179:SER:C	2.64	0.41
1:I:195:SER:O	1:I:199:GLN:CB	2.57	0.41
2:M:185:GLU:O	2:M:189:SER:HB3	2.20	0.41
3:B:68:GLN:OE1	3:B:68:GLN:N	2.54	0.41
1:J:64:VAL:O	1:J:65:LYS:C	2.63	0.41
1:J:207:HIS:HB3	1:J:212:THR:HB	2.01	0.41
2:N:27:LEU:HA	2:N:27:LEU:HD23	1.79	0.41
1:K:208:LYS:N	1:K:209:PRO:HD2	2.36	0.41
2:O:29:SER:O	3:D:81:GLU:HG2	2.21	0.41
3:D:35:PHE:CD2	3:D:35:PHE:C	2.99	0.41
1:H:119:SER:OG	1:H:121:ALA:CB	2.69	0.41
2:M:47:ILE:HD12	2:M:72:LEU:CD1	2.51	0.41
1:J:83:MET:HB3	1:J:86:LEU:HD21	2.03	0.41
2:N:171:ASN:O	2:N:172:ASN:HB2	2.20	0.41
3:C:68:GLN:C	3:C:70:GLU:N	2.79	0.41
3:C:94:GLN:H	3:C:94:GLN:HG3	1.27	0.41
1:H:133:PRO:HD2	1:H:219:GLU:O	2.21	0.40
3:B:96:ARG:NH2	3:B:116:PRO:O	2.54	0.40
1:J:196:LEU:C	1:J:198:THR:H	2.28	0.40
1:K:61:ALA:O	1:K:62:ASP:C	2.62	0.40
1:K:199:GLN:HB3	1:K:201:TYR:CE2	2.57	0.40
1:H:159:VAL:HG23	1:H:159:VAL:O	2.21	0.40
1:I:32:TYR:O	1:I:72:ARG:NH2	2.48	0.40
1:K:176:VAL:CG1	2:O:164:THR:CG2	2.99	0.40
3:D:60:PHE:CD1	3:D:60:PHE:C	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:THR:OG1	1:I:206:ASN:HB3	2.22	0.40
1:J:185:LEU:C	1:J:185:LEU:CD1	2.95	0.40
2:O:27:LEU:HD23	2:O:27:LEU:HA	1.84	0.40
2:L:90:PHE:CE1	2:L:91:THR:C	3.00	0.40
2:M:91:THR:HG22	2:M:96:GLY:C	2.46	0.40
2:M:188:LYS:HE3	2:M:188:LYS:HB3	1.97	0.40
1:J:196:LEU:C	1:J:198:THR:N	2.80	0.40
1:K:185:LEU:C	1:K:185:LEU:CD1	2.94	0.40
2:O:4:LEU:HD22	2:O:98:VAL:HG13	2.04	0.40
2:O:90:PHE:CD1	2:O:91:THR:N	2.89	0.40
3:D:94:GLN:NE2	3:D:97:ARG:CD	2.84	0.40
1:J:14:PRO:HD2	1:J:120:SER:HB3	2.04	0.40
1:K:105:GLY:O	2:O:33:ILE:CD1	2.69	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	H	201/234 (86%)	171 (85%)	24 (12%)	6 (3%)	3	8
1	I	211/234 (90%)	202 (96%)	8 (4%)	1 (0%)	24	48
1	J	219/234 (94%)	205 (94%)	13 (6%)	1 (0%)	24	48
1	K	211/234 (90%)	201 (95%)	10 (5%)	0	100	100
2	L	208/213 (98%)	199 (96%)	7 (3%)	2 (1%)	12	32
2	M	208/213 (98%)	200 (96%)	7 (3%)	1 (0%)	24	48
2	N	208/213 (98%)	202 (97%)	5 (2%)	1 (0%)	24	48
2	O	208/213 (98%)	202 (97%)	5 (2%)	1 (0%)	24	48
3	A	83/129 (64%)	74 (89%)	8 (10%)	1 (1%)	10	27
3	B	83/129 (64%)	72 (87%)	9 (11%)	2 (2%)	4	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	83/129 (64%)	74 (89%)	7 (8%)	2 (2%)	4	12
3	D	83/129 (64%)	74 (89%)	7 (8%)	2 (2%)	4	12
All	All	2006/2304 (87%)	1876 (94%)	110 (6%)	20 (1%)	12	32

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	123	THR
1	H	192	PRO
2	L	76	GLY
2	L	94	GLY
2	M	76	GLY
2	N	76	GLY
3	C	69	GLY
2	O	76	GLY
1	H	163	SER
1	H	211	ASN
1	J	135	SER
1	H	76	LYS
1	H	162	ASN
3	B	117	PRO
3	C	46	ASP
3	D	110	TYR
3	A	69	GLY
1	I	76	LYS
3	B	69	GLY
3	D	69	GLY

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	H	175/198 (88%)	143 (82%)	32 (18%)	2	5
1	I	181/198 (91%)	146 (81%)	35 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	186/198 (94%)	149 (80%)	37 (20%)	1	4
1	K	182/198 (92%)	145 (80%)	37 (20%)	1	3
2	L	176/178 (99%)	148 (84%)	28 (16%)	2	7
2	M	176/178 (99%)	149 (85%)	27 (15%)	3	7
2	N	176/178 (99%)	149 (85%)	27 (15%)	3	7
2	O	176/178 (99%)	148 (84%)	28 (16%)	2	7
3	A	76/114 (67%)	64 (84%)	12 (16%)	2	7
3	B	76/114 (67%)	61 (80%)	15 (20%)	1	4
3	C	76/114 (67%)	63 (83%)	13 (17%)	2	6
3	D	76/114 (67%)	61 (80%)	15 (20%)	1	4
All	All	1732/1960 (88%)	1426 (82%)	306 (18%)	2	5

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	5	VAL
1	H	11	LEU
1	H	12	VAL
1	H	17	SER
1	H	19	ARG
1	H	22	CYS
1	H	28	THR
1	H	51	THR
1	H	54	SER
1	H	57	LEU
1	H	58	THR
1	H	65	LYS
1	H	75	SER
1	H	91	THR
1	H	98	ARG
1	H	112	GLN
1	H	114	THR
1	H	115	LEU
1	H	117	THR
1	H	120	SER
1	H	149	VAL
1	H	157	VAL

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Mol	Chain	Res	Type
1	H	159	VAL
1	H	166	LEU
1	H	167	THR
1	H	176	VAL
1	H	177	LEU
1	H	185	LEU
1	H	190	THR
1	H	191	VAL
1	H	205	VAL
2	L	2	ILE
2	L	4	LEU
2	L	9	SER
2	L	12	VAL
2	L	16	GLN
2	L	27	LEU
2	L	33	ILE
2	L	45	LEU
2	L	50	ASP
2	L	55	SER
2	L	73	THR
2	L	78	GLN
2	L	80	GLU
2	L	90	PHE
2	L	103	THR
2	L	105	LEU
2	L	119	LEU
2	L	131	LYS
2	L	158	LYS
2	L	161	VAL
2	L	170	SER
2	L	183	THR
2	L	188	LYS
2	L	191	ARG
2	L	204	VAL
2	L	205	GLU
2	L	207	THR
2	L	211	THR
3	A	35	PHE
3	A	36	LEU
3	A	39	TYR
3	A	49	ILE
3	A	50	ASN

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Mol	Chain	Res	Type
3	A	52	THR
3	A	68	GLN
3	A	73	LEU
3	A	94	GLN
3	A	95	LEU
3	A	105	ASN
3	A	109	GLN
1	I	5	VAL
1	I	11	LEU
1	I	12	VAL
1	I	18	LEU
1	I	21	SER
1	I	22	CYS
1	I	28	THR
1	I	51	THR
1	I	54	SER
1	I	57	LEU
1	I	58	THR
1	I	91	THR
1	I	98	ARG
1	I	112	GLN
1	I	114	THR
1	I	115	LEU
1	I	117	THR
1	I	134	SER
1	I	135	SER
1	I	142	THR
1	I	149	VAL
1	I	166	LEU
1	I	176	VAL
1	I	177	LEU
1	I	178	GLN
1	I	179	SER
1	I	184	SER
1	I	185	LEU
1	I	188	VAL
1	I	191	VAL
1	I	196	LEU
1	I	199	GLN
1	I	200	THR
1	I	216	LYS
1	I	217	LYS

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Mol	Chain	Res	Type
2	M	2	ILE
2	M	4	LEU
2	M	12	VAL
2	M	16	GLN
2	M	27	LEU
2	M	33	ILE
2	M	45	LEU
2	M	50	ASP
2	M	52	ASN
2	M	55	SER
2	M	78	GLN
2	M	80	GLU
2	M	90	PHE
2	M	92	MET
2	M	103	THR
2	M	105	LEU
2	M	112	LYS
2	M	119	LEU
2	M	131	LYS
2	M	158	LYS
2	M	161	VAL
2	M	170	SER
2	M	183	THR
2	M	204	VAL
2	M	205	GLU
2	M	207	THR
2	M	211	THR
3	B	35	PHE
3	B	36	LEU
3	B	39	TYR
3	B	49	ILE
3	B	50	ASN
3	B	52	THR
3	B	68	GLN
3	B	73	LEU
3	B	75	SER
3	B	94	GLN
3	B	95	LEU
3	B	105	ASN
3	B	109	GLN
3	B	112	GLN
3	B	118	VAL

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Mol	Chain	Res	Type
1	J	1	GLN
1	J	5	VAL
1	J	11	LEU
1	J	12	VAL
1	J	18	LEU
1	J	22	CYS
1	J	28	THR
1	J	51	THR
1	J	54	SER
1	J	57	LEU
1	J	58	THR
1	J	91	THR
1	J	98	ARG
1	J	112	GLN
1	J	114	THR
1	J	115	LEU
1	J	117	THR
1	J	134	SER
1	J	135	SER
1	J	136	LYS
1	J	142	THR
1	J	149	VAL
1	J	159	VAL
1	J	166	LEU
1	J	176	VAL
1	J	177	LEU
1	J	178	GLN
1	J	179	SER
1	J	184	SER
1	J	188	VAL
1	J	191	VAL
1	J	196	LEU
1	J	199	GLN
1	J	200	THR
1	J	208	LYS
1	J	216	LYS
1	J	217	LYS
2	N	2	ILE
2	N	4	LEU
2	N	12	VAL
2	N	27	LEU
2	N	33	ILE

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Mol	Chain	Res	Type
2	N	45	LEU
2	N	55	SER
2	N	78	GLN
2	N	80	GLU
2	N	90	PHE
2	N	92	MET
2	N	103	THR
2	N	105	LEU
2	N	119	LEU
2	N	130	ASN
2	N	131	LYS
2	N	147	THR
2	N	158	LYS
2	N	161	VAL
2	N	170	SER
2	N	183	THR
2	N	188	LYS
2	N	191	ARG
2	N	204	VAL
2	N	205	GLU
2	N	207	THR
2	N	211	THR
3	C	35	PHE
3	C	36	LEU
3	C	39	TYR
3	C	47	ASP
3	C	49	ILE
3	C	50	ASN
3	C	52	THR
3	C	68	GLN
3	C	73	LEU
3	C	94	GLN
3	C	95	LEU
3	C	105	ASN
3	C	111	LEU
1	K	1	GLN
1	K	5	VAL
1	K	11	LEU
1	K	12	VAL
1	K	18	LEU
1	K	22	CYS
1	K	28	THR

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Mol	Chain	Res	Type
1	K	33	THR
1	K	51	THR
1	K	54	SER
1	K	57	LEU
1	K	58	THR
1	K	65	LYS
1	K	91	THR
1	K	112	GLN
1	K	114	THR
1	K	115	LEU
1	K	117	THR
1	K	134	SER
1	K	135	SER
1	K	142	THR
1	K	149	VAL
1	K	156	PRO
1	K	159	VAL
1	K	166	LEU
1	K	176	VAL
1	K	177	LEU
1	K	179	SER
1	K	185	LEU
1	K	188	VAL
1	K	191	VAL
1	K	196	LEU
1	K	199	GLN
1	K	200	THR
1	K	208	LYS
1	K	216	LYS
1	K	217	LYS
2	O	2	ILE
2	O	4	LEU
2	O	16	GLN
2	O	27	LEU
2	O	33	ILE
2	O	45	LEU
2	O	50	ASP
2	O	55	SER
2	O	78	GLN
2	O	80	GLU
2	O	90	PHE
2	O	92	MET

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Mol	Chain	Res	Type
2	O	103	THR
2	O	105	LEU
2	O	112	LYS
2	O	119	LEU
2	O	130	ASN
2	O	147	THR
2	O	158	LYS
2	O	161	VAL
2	O	170	SER
2	O	183	THR
2	O	188	LYS
2	O	191	ARG
2	O	204	VAL
2	O	205	GLU
2	O	207	THR
2	O	211	THR
3	D	35	PHE
3	D	36	LEU
3	D	39	TYR
3	D	49	ILE
3	D	50	ASN
3	D	52	THR
3	D	65	GLU
3	D	68	GLN
3	D	73	LEU
3	D	75	SER
3	D	94	GLN
3	D	95	LEU
3	D	105	ASN
3	D	112	GLN
3	D	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	13	GLN
1	H	31	ASN
1	H	39	GLN
1	H	82	GLN
1	H	84	ASN
1	H	109	HIS

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Mol	Chain	Res	Type
1	H	112	GLN
1	H	162	ASN
1	H	171	HIS
1	H	178	GLN
1	H	207	HIS
2	L	16	GLN
2	L	36	GLN
2	L	52	ASN
2	L	65	ASN
2	L	95	ASN
2	L	169	GLN
2	L	190	HIS
3	A	43	HIS
3	A	86	GLN
3	A	105	ASN
3	A	109	GLN
1	I	13	GLN
1	I	39	GLN
1	I	82	GLN
1	I	84	ASN
1	I	109	HIS
1	I	162	ASN
1	I	171	HIS
1	I	178	GLN
1	I	207	HIS
2	M	52	ASN
2	M	65	ASN
2	M	95	ASN
2	M	169	GLN
2	M	190	HIS
3	B	43	HIS
3	B	51	ASN
3	B	86	GLN
3	B	105	ASN
3	B	109	GLN
1	J	13	GLN
1	J	39	GLN
1	J	82	GLN
1	J	84	ASN
1	J	162	ASN
1	J	178	GLN
1	J	207	HIS

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Mol	Chain	Res	Type
2	N	16	GLN
2	N	52	ASN
2	N	65	ASN
2	N	95	ASN
2	N	169	GLN
2	N	190	HIS
2	N	199	HIS
3	C	43	HIS
3	C	86	GLN
3	C	94	GLN
3	C	105	ASN
3	C	109	GLN
1	K	13	GLN
1	K	39	GLN
1	K	82	GLN
1	K	84	ASN
1	K	162	ASN
1	K	178	GLN
1	K	207	HIS
2	O	36	GLN
2	O	37	GLN
2	O	52	ASN
2	O	65	ASN
2	O	95	ASN
2	O	169	GLN
2	O	190	HIS
3	D	43	HIS
3	D	86	GLN
3	D	105	ASN
3	D	109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	H	207/234 (88%)	0.19	8 (3%) 43 39	37, 54, 91, 122	0
1	I	215/234 (91%)	0.22	2 (0%) 81 80	38, 56, 89, 114	0
1	J	221/234 (94%)	0.57	10 (4%) 38 34	44, 64, 102, 125	0
1	K	215/234 (91%)	0.35	8 (3%) 45 41	37, 54, 95, 123	0
2	L	210/213 (98%)	0.73	17 (8%) 18 15	44, 61, 86, 112	0
2	M	210/213 (98%)	0.42	7 (3%) 49 45	41, 59, 77, 92	0
2	N	210/213 (98%)	0.48	12 (5%) 29 26	48, 59, 78, 93	0
2	O	210/213 (98%)	0.38	5 (2%) 59 56	44, 57, 72, 86	0
3	A	85/129 (65%)	0.82	10 (11%) 9 7	51, 73, 107, 127	0
3	B	85/129 (65%)	0.96	11 (12%) 7 6	52, 79, 112, 135	0
3	C	85/129 (65%)	1.10	13 (15%) 5 4	58, 78, 108, 127	0
3	D	85/129 (65%)	1.10	13 (15%) 5 4	50, 80, 131, 157	0
All	All	2038/2304 (88%)	0.52	116 (5%) 29 26	37, 61, 99, 157	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	34	PRO	5.1
3	C	43	HIS	5.1
3	C	95	LEU	4.7
2	N	94	GLY	4.7
3	D	39	TYR	4.5
3	B	43	HIS	4.3
1	J	134	SER	3.9
2	O	55	SER	3.9
3	B	118	VAL	3.9
2	N	2	ILE	3.8
3	C	50	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
3	B	39	TYR	3.7
1	H	193	SER	3.7
3	C	39	TYR	3.6
3	D	34	PRO	3.5
3	D	42	GLY	3.5
3	B	42	GLY	3.4
2	L	90	PHE	3.4
2	N	90	PHE	3.4
3	A	43	HIS	3.4
3	A	34	PRO	3.3
3	D	110	TYR	3.3
3	C	48	ALA	3.3
1	H	200	THR	3.2
3	D	118	VAL	3.1
2	N	78	GLN	3.0
3	C	35	PHE	3.0
3	D	43	HIS	3.0
3	D	109	GLN	3.0
1	H	220	PRO	3.0
3	B	34	PRO	3.0
2	N	48	TYR	2.9
1	J	138	THR	2.9
3	D	83	SER	2.9
2	O	68	ASN	2.9
2	L	128	GLN	2.8
2	O	94	GLY	2.8
3	B	117	PRO	2.8
1	J	160	SER	2.8
3	B	49	ILE	2.8
2	M	191	ARG	2.7
1	H	192	PRO	2.7
1	I	75	SER	2.7
1	K	142	THR	2.7
2	M	25	ASP	2.7
1	K	75	SER	2.6
2	M	113	ALA	2.6
1	H	167	THR	2.5
3	A	46	ASP	2.5
3	B	35	PHE	2.5
1	J	142	THR	2.5
1	J	26	GLY	2.5
2	L	96	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	116	PRO	2.5
3	D	45	PRO	2.5
2	L	154	SER	2.5
3	D	49	ILE	2.4
3	A	49	ILE	2.4
2	L	123	SER	2.4
2	M	80	GLU	2.4
2	N	59	GLU	2.4
1	K	196	LEU	2.4
2	O	92	MET	2.4
2	L	124	SER	2.3
2	L	201	GLY	2.3
2	N	91	THR	2.3
1	J	194	SER	2.3
3	C	46	ASP	2.3
3	D	47	ASP	2.3
3	D	35	PHE	2.3
1	K	198	THR	2.3
1	K	193	SER	2.3
1	K	143	ALA	2.3
2	L	2	ILE	2.3
1	J	74	ASN	2.3
3	A	50	ASN	2.3
3	C	49	ILE	2.2
2	L	92	MET	2.2
2	N	106	THR	2.2
2	L	185	GLU	2.2
1	I	196	LEU	2.2
2	L	58	PRO	2.2
3	C	47	ASP	2.2
3	A	99	ILE	2.2
2	L	91	THR	2.2
1	K	211	ASN	2.2
3	C	42	GLY	2.2
2	L	191	ARG	2.1
1	H	144	ALA	2.1
2	M	92	MET	2.1
2	M	94	GLY	2.1
3	B	54	ILE	2.1
2	L	170	SER	2.1
2	N	93	SER	2.1
3	A	35	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	166	LEU	2.1
1	J	204	ASN	2.1
3	C	51	ASN	2.1
2	L	48	TYR	2.1
1	H	121	ALA	2.1
2	N	92	MET	2.1
2	O	172	ASN	2.1
3	A	39	TYR	2.1
3	C	110	TYR	2.1
2	M	192	SER	2.0
3	B	104	THR	2.0
1	K	192	PRO	2.0
3	A	45	PRO	2.0
2	N	95	ASN	2.0
2	L	94	GLY	2.0
2	N	175	ALA	2.0
1	J	161	TRP	2.0
2	L	183	THR	2.0
1	H	125	GLY	2.0
3	A	42	GLY	2.0
3	D	105	ASN	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.