



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:11 PM UTC

PDB ID : 3GJF / pdb_00003gjf
Title : Rational development of high-affinity T-cell receptor-like antibodies
Authors : Stewart-Jones, G.; Wadle, A.; Hombach, A.; Shenderov, E.; Held, G.; Fischer, E.; Kleber, S.; Stenner-Liewen, F.; Bauer, S.; McMichael, A.; Knuth, A.; Abken, H.; Hombach, A.A.; Cerundolo, V.; Jones, E.Y.; Renner, C.
Deposited on : 2009-03-08
Resolution : 1.90 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

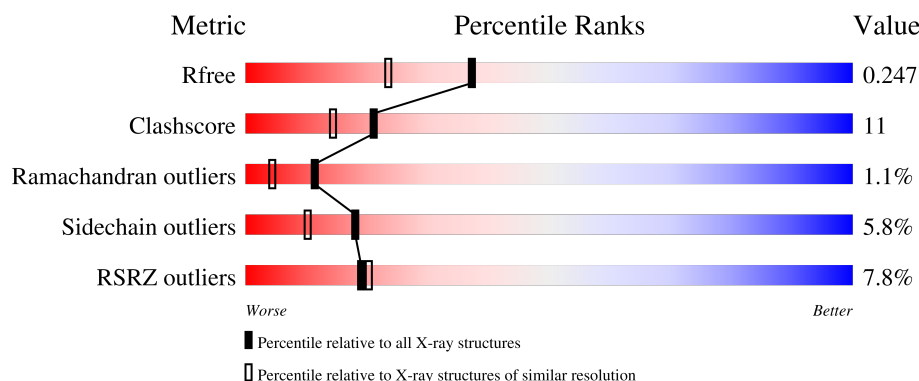
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	276	2% 84% 14% .
1	D	276	% 83% 16% .
2	B	100	6% 81% 14% .
2	E	100	% 78% 19% .
3	C	9	11% 56% 33% 11%

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Mol	Chain	Length	Quality of chain
3	F	9	89% 11%
4	K	212	5% 84% 13%
4	L	212	17% 76% 13%
5	H	220	25% 78% 18%
5	M	220	4% 89% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14331 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	D	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
E	0	MET	-	expression tag	UNP P61769

- Molecule 3 is a protein called NYESO-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			

- Molecule 4 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	206	Total	C	N	O	S	0	0	0
			1559	976	262	317	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	212	Total	C	N	O	S	0	0	0
			1600	1001	269	326	4			

- Molecule 5 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	220	Total	C	N	O	S	0	0	0
			1621	1020	269	325	7			
5	M	220	Total	C	N	O	S	0	0	0
			1620	1020	269	324	7			

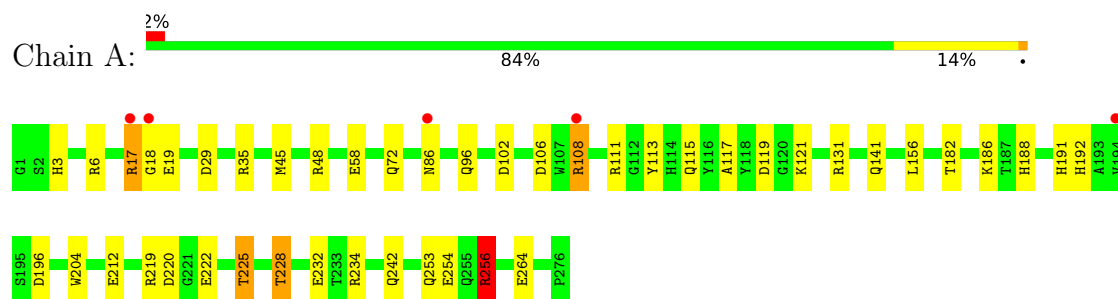
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	289	Total	O	0	0
			289	289		
6	B	144	Total	O	0	0
			144	144		
6	C	9	Total	O	0	0
			9	9		
6	D	291	Total	O	0	0
			291	291		
6	E	104	Total	O	0	0
			104	104		
6	F	7	Total	O	0	0
			7	7		
6	L	172	Total	O	0	0
			172	172		
6	K	178	Total	O	0	0
			178	178		
6	H	189	Total	O	0	0
			189	189		
6	M	220	Total	O	0	0
			220	220		

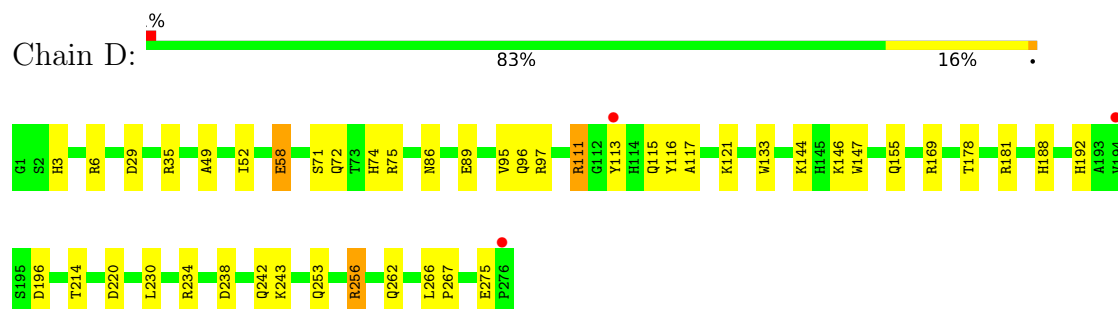
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

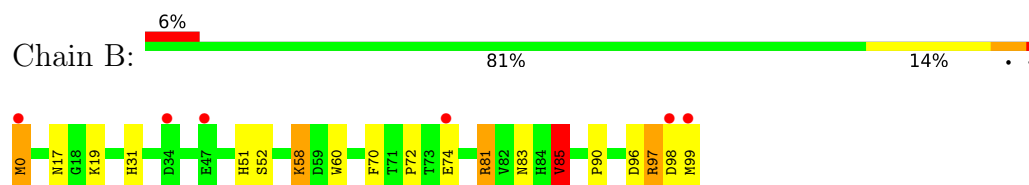
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



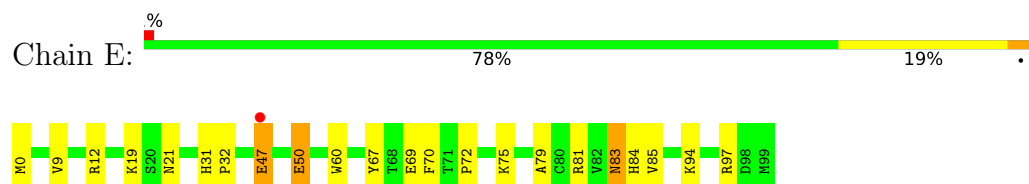
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



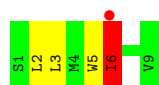
- Molecule 2: Beta-2-microglobulin



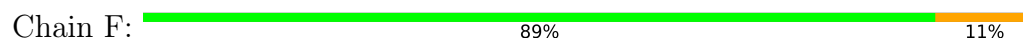
- Molecule 2: Beta-2-microglobulin



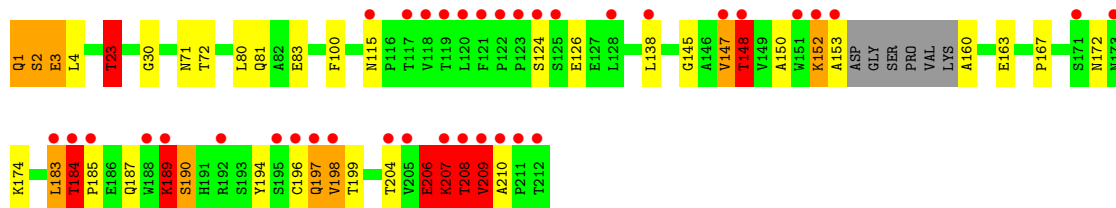
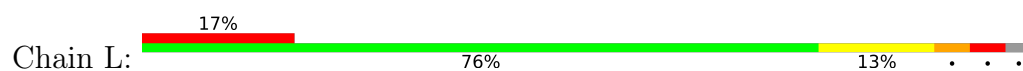
- Molecule 3: NYESO-1 peptide



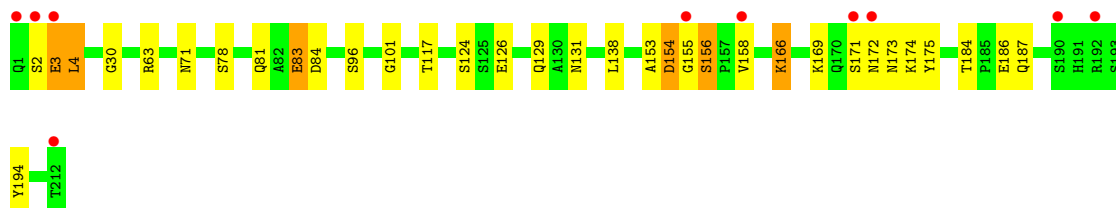
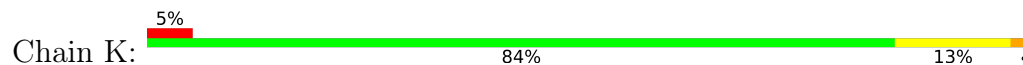
- Molecule 3: NYESO-1 peptide



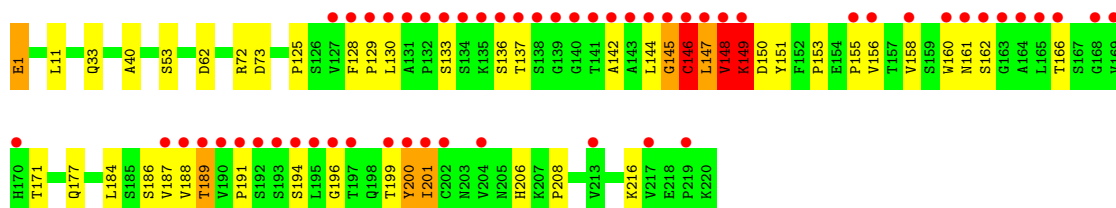
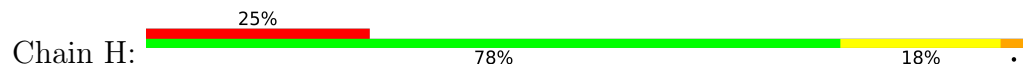
- Molecule 4: Antibody light chain



- Molecule 4: Antibody light chain

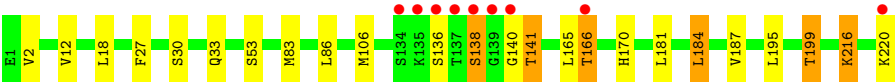


- Molecule 5: Antibody heavy chain



- Molecule 5: Antibody heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 111.84Å 124.72Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 25.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-1.90) 99.7 (25.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.251 0.199 , 0.247	Depositor DCC
R_{free} test set	7718 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14331	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.80	0/2319	0.90	1/3149 (0.0%)
1	D	0.77	0/2319	0.87	0/3149
2	B	0.85	0/859	0.91	1/1162 (0.1%)
2	E	0.70	0/859	0.88	0/1162
3	C	0.82	0/76	1.29	1/103 (1.0%)
3	F	0.73	0/76	0.95	0/103
4	K	0.78	0/1641	0.93	0/2240
4	L	0.80	1/1598 (0.1%)	1.05	7/2180 (0.3%)
5	H	0.81	0/1658	1.10	18/2257 (0.8%)
5	M	0.78	1/1657 (0.1%)	0.90	0/2255
All	All	0.79	2/13062 (0.0%)	0.95	28/17760 (0.2%)

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	B	0	1
4	L	0	2
5	H	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	23	THR	CA-CB	5.31	1.61	1.53
5	M	181	LEU	CA-C	5.23	1.58	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3	GLU	N-CA-C	10.74	125.65	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	146	CYS	CA-C-N	7.84	135.82	121.70
5	H	146	CYS	C-N-CA	7.84	135.82	121.70
5	H	147	LEU	CA-C-N	6.83	134.00	121.70
5	H	147	LEU	C-N-CA	6.83	134.00	121.70
2	B	85	VAL	CB-CA-C	-6.51	102.06	112.16
3	C	6	ILE	CB-CA-C	-6.45	101.35	110.12
5	H	155	PRO	CA-C-N	6.16	132.79	121.70
5	H	155	PRO	C-N-CA	6.16	132.79	121.70
4	L	147	VAL	N-CA-C	6.01	121.83	109.34
5	H	148	VAL	CA-C-N	5.93	132.38	121.70
5	H	148	VAL	C-N-CA	5.93	132.38	121.70
5	H	72	ARG	CA-C-N	-5.91	113.64	122.39
5	H	72	ARG	C-N-CA	-5.91	113.64	122.39
5	H	150	ASP	N-CA-C	-5.79	94.80	111.00
5	H	145	GLY	CA-C-N	5.74	132.03	121.70
5	H	145	GLY	C-N-CA	5.74	132.03	121.70
5	H	162	SER	N-CA-C	5.64	119.47	112.47
5	H	40	ALA	CA-C-N	-5.50	113.89	119.83
5	H	40	ALA	C-N-CA	-5.50	113.89	119.83
4	L	206	GLU	CA-C-N	5.42	131.45	121.70
4	L	206	GLU	C-N-CA	5.42	131.45	121.70
5	H	149	LYS	CA-C-N	5.37	131.36	121.70
5	H	149	LYS	C-N-CA	5.37	131.36	121.70
4	L	189	LYS	CA-C-N	5.29	131.22	121.70
4	L	189	LYS	C-N-CA	5.29	131.22	121.70
4	L	184	THR	N-CA-C	5.09	116.25	109.93
1	A	256	ARG	NE-CZ-NH1	-5.08	116.42	121.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	0	MET	Peptide
5	H	148	VAL	Peptide
4	L	2	SER	Peptide
4	L	206	GLU	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	2253	0	2103	61	0
1	D	2253	0	2103	45	0
2	B	836	0	803	27	0
2	E	836	0	803	19	0
3	C	75	0	83	3	0
3	F	75	0	83	2	0
4	K	1600	0	1534	31	0
4	L	1559	0	1492	45	0
5	H	1621	0	1592	35	0
5	M	1620	0	1592	19	0
6	A	289	0	0	21	0
6	B	144	0	0	9	0
6	C	9	0	0	0	0
6	D	291	0	0	12	0
6	E	104	0	0	6	0
6	F	7	0	0	0	0
6	H	189	0	0	11	0
6	K	178	0	0	6	0
6	L	172	0	0	6	0
6	M	220	0	0	9	0
All	All	14331	0	12188	274	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 11.

All (274) 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:A:106:ASP:OD1	1:A:108:ARG:HD2	1.40	1.21
1:A:35:ARG:NH1	1:A:48:ARG:HD3	1.56	1.20
1:A:256:ARG:HH11	1:A:256:ARG:CG	1.54	1.19
1:D:256:ARG:HG3	1:D:256:ARG:HH11	1.08	1.10
4:L:115:ASN:HB3	6:L:1463:HOH:O	1.51	1.10
1:A:256:ARG:HG3	1:A:256:ARG:NH1	1.48	1.10
4:L:207:LYS:HA	4:L:208:THR:CB	1.82	1.08
4:L:150:ALA:H	4:L:197:GLN:HB2	1.15	1.07
1:A:35:ARG:HH11	1:A:48:ARG:HD3	0.89	1.03
4:L:197:GLN:HB3	4:L:198:VAL:HA	1.37	1.02
1:A:72:GLN:HG3	6:A:1524:HOH:O	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:207:LYS:CA	4:L:208:THR:HB	1.88	1.02
4:K:83:GLU:HG3	6:K:1470:HOH:O	1.60	0.99
1:A:220:ASP:OD2	1:A:256:ARG:HD2	1.63	0.98
2:B:81:ARG:HG2	2:B:81:ARG:HH11	1.27	0.98
1:A:6:ARG:NH2	1:A:113:TYR:CD1	2.32	0.96
4:L:207:LYS:HA	4:L:208:THR:HB	0.97	0.96
1:A:108:ARG:O	1:A:108:ARG:HD3	1.69	0.93
1:D:256:ARG:HH11	1:D:256:ARG:CG	1.83	0.92
6:D:1563:HOH:O	3:F:6:ILE:HG21	1.70	0.92
1:A:35:ARG:CZ	6:A:1530:HOH:O	2.18	0.90
1:D:6:ARG:NH2	1:D:113:TYR:CD1	2.40	0.88
2:E:50:GLU:HG3	2:E:67:TYR:CE1	2.09	0.87
1:A:106:ASP:OD1	1:A:108:ARG:CD	2.23	0.86
1:D:188:HIS:HD2	6:D:291:HOH:O	1.59	0.86
1:D:256:ARG:HG3	1:D:256:ARG:NH1	1.87	0.85
4:L:189:LYS:HB3	4:L:190:SER:HB2	1.60	0.84
5:H:148:VAL:HA	5:H:149:LYS:O	1.76	0.83
2:B:99:MET:HE3	6:B:103:HOH:O	1.77	0.82
4:L:197:GLN:CB	4:L:198:VAL:HA	2.09	0.81
2:B:81:ARG:NH2	6:B:1526:HOH:O	1.98	0.81
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.43	0.81
1:D:111:ARG:HH11	1:D:111:ARG:CG	1.93	0.80
1:D:74:HIS:HE1	1:D:97:ARG:HE	1.29	0.80
2:B:81:ARG:NH1	6:B:1526:HOH:O	2.13	0.79
6:A:1541:HOH:O	2:B:99:MET:SD	2.39	0.79
5:H:73:ASP:CB	6:H:1525:HOH:O	2.32	0.78
1:D:220:ASP:OD2	1:D:256:ARG:HD2	1.83	0.78
5:H:73:ASP:HB2	6:H:1525:HOH:O	1.83	0.78
2:B:97:ARG:HG2	2:B:98:ASP:N	2.00	0.77
5:H:73:ASP:CG	6:H:1525:HOH:O	2.28	0.77
1:A:219:ARG:O	1:A:222:GLU:HG2	1.84	0.77
1:A:182:THR:HG22	1:A:264:GLU:OE2	1.83	0.77
5:M:199:THR:HG22	6:M:1365:HOH:O	1.84	0.77
4:L:189:LYS:CA	4:L:190:SER:HB2	2.15	0.76
1:A:220:ASP:OD2	1:A:256:ARG:CD	2.35	0.75
1:D:192:HIS:HD2	6:D:1418:HOH:O	1.70	0.75
2:E:47:GLU:HG2	6:E:1279:HOH:O	1.86	0.74
1:D:3:HIS:HD2	1:D:29:ASP:OD2	1.70	0.74
4:L:189:LYS:N	4:L:190:SER:HB2	2.02	0.74
4:L:184:THR:HG22	4:L:185:PRO:HD2	1.70	0.74
4:L:150:ALA:N	4:L:197:GLN:HB2	1.98	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.35	0.72
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.72	0.72
1:A:256:ARG:HH11	1:A:256:ARG:HG3	0.65	0.72
4:L:208:THR:HG23	4:L:209:VAL:N	2.05	0.71
4:L:189:LYS:CB	4:L:190:SER:HB2	2.19	0.71
5:H:128:PHE:O	5:H:146:CYS:HB3	1.90	0.71
5:H:145:GLY:O	5:H:160:TRP:CH2	2.45	0.70
4:L:147:VAL:O	4:L:199:THR:O	2.10	0.70
5:M:136:SER:HB3	6:M:1466:HOH:O	1.92	0.69
4:L:199:THR:HG22	4:L:204:THR:OG1	1.93	0.69
4:L:148:THR:HG22	6:L:432:HOH:O	1.93	0.68
1:D:253:GLN:HE21	1:D:256:ARG:HH12	1.42	0.68
1:A:131:ARG:HD2	6:A:362:HOH:O	1.95	0.66
1:D:6:ARG:HH22	1:D:113:TYR:HD1	1.36	0.66
2:B:19:LYS:HE3	6:B:944:HOH:O	1.96	0.65
5:H:191:PRO:HG2	5:H:194:SER:HB3	1.78	0.65
1:A:182:THR:CG2	1:A:264:GLU:OE2	2.44	0.65
1:A:253:GLN:HE21	1:A:256:ARG:HH12	1.43	0.65
1:D:111:ARG:HH11	1:D:111:ARG:HG3	1.61	0.65
2:B:81:ARG:HG2	2:B:81:ARG:NH1	2.04	0.65
5:H:145:GLY:O	5:H:160:TRP:HH2	1.79	0.64
5:M:138:SER:HA	6:M:720:HOH:O	1.97	0.64
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.44	0.64
5:H:146:CYS:O	5:H:186:SER:N	2.28	0.64
1:A:191:HIS:HE1	1:A:254:GLU:OE2	1.81	0.64
1:A:35:ARG:NH1	1:A:48:ARG:CD	2.49	0.63
1:A:188:HIS:HD2	6:A:391:HOH:O	1.81	0.63
4:L:208:THR:HG23	4:L:209:VAL:H	1.63	0.63
4:K:131:ASN:HB2	6:K:1375:HOH:O	1.97	0.63
1:A:204:TRP:HZ2	2:B:99:MET:HB2	1.63	0.63
1:A:121:LYS:HE3	6:A:305:HOH:O	1.99	0.63
1:D:3:HIS:HE1	6:D:324:HOH:O	1.82	0.62
1:A:182:THR:HG23	6:A:1379:HOH:O	1.98	0.62
2:E:85:VAL:HG13	6:E:211:HOH:O	1.98	0.62
1:A:256:ARG:CG	1:A:256:ARG:NH1	2.28	0.62
4:K:81:GLN:NE2	4:K:83:GLU:OE1	2.32	0.62
2:B:81:ARG:CZ	6:B:1526:HOH:O	2.37	0.62
4:K:154:ASP:N	4:K:155:GLY:CA	2.62	0.61
5:M:166:THR:HB	6:M:1550:HOH:O	2.00	0.61
4:K:63:ARG:HD2	4:K:78:SER:O	2.01	0.60
5:H:200:TYR:HD2	6:H:1370:HOH:O	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:HB3	6:A:1354:HOH:O	2.01	0.60
1:D:155:GLN:HE22	4:K:96:SER:HB2	1.67	0.60
5:H:144:LEU:O	5:H:187:VAL:HA	2.02	0.59
5:H:144:LEU:HD13	5:H:188:VAL:HG13	1.83	0.59
1:A:256:ARG:NH2	6:A:1527:HOH:O	2.21	0.59
4:L:124:SER:OG	5:H:129:PRO:O	2.21	0.59
5:H:73:ASP:OD2	6:H:1525:HOH:O	2.16	0.59
1:A:6:ARG:NH2	1:A:113:TYR:CG	2.71	0.59
1:D:111:ARG:HH11	1:D:111:ARG:HG2	1.66	0.59
2:B:74:GLU:HG2	6:B:1369:HOH:O	2.02	0.58
5:M:141:THR:HG23	6:M:683:HOH:O	2.02	0.58
1:A:253:GLN:NE2	1:A:256:ARG:HH12	2.01	0.58
4:L:208:THR:CG2	4:L:209:VAL:N	2.67	0.58
4:K:155:GLY:HA2	4:K:156:SER:CB	2.34	0.58
4:K:155:GLY:HA2	4:K:156:SER:HB2	1.85	0.58
4:K:30:GLY:HA3	4:K:71:ASN:HD22	1.69	0.57
5:H:145:GLY:CA	6:H:1548:HOH:O	2.53	0.57
5:M:199:THR:CG2	6:M:1365:HOH:O	2.48	0.57
4:L:145:GLY:O	4:L:167:PRO:HG3	2.05	0.57
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.86	0.56
4:L:160:ALA:N	6:L:1540:HOH:O	2.39	0.56
4:K:155:GLY:CA	4:K:156:SER:HB2	2.34	0.56
4:L:183:LEU:HB3	4:L:187:GLN:OE1	2.05	0.56
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.18	0.56
2:B:31:HIS:HD2	6:B:102:HOH:O	1.89	0.56
1:D:253:GLN:HE21	1:D:256:ARG:NH1	2.02	0.56
1:D:72:GLN:NE2	1:D:75:ARG:HE	2.05	0.55
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.89	0.55
1:A:225:THR:O	1:A:228:THR:HB	2.07	0.54
1:A:220:ASP:OD1	6:A:1527:HOH:O	2.18	0.54
1:D:58:GLU:CD	1:D:58:GLU:H	2.15	0.54
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.19	0.54
5:H:158:VAL:HG13	6:H:711:HOH:O	2.06	0.54
4:K:138:LEU:CD1	5:M:187:VAL:HG21	2.37	0.54
4:K:155:GLY:CA	4:K:156:SER:CB	2.86	0.53
5:H:148:VAL:O	5:H:184:LEU:N	2.30	0.53
5:H:1:GLU:HB2	6:H:766:HOH:O	2.07	0.53
4:L:1:GLN:H2	4:L:3:GLU:HB2	1.74	0.53
1:A:108:ARG:HD2	1:A:108:ARG:H	1.73	0.53
1:A:3:HIS:HE1	6:A:539:HOH:O	1.90	0.53
4:K:153:ALA:O	4:K:156:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:137:THR:HG22	5:H:142:ALA:HB2	1.92	0.52
5:M:33:GLN:NE2	5:M:53:SER:H	2.08	0.52
4:L:23:THR:HB	4:L:72:THR:OG1	2.09	0.52
1:A:256:ARG:NE	6:A:1527:HOH:O	2.34	0.52
2:B:58:LYS:NZ	2:B:58:LYS:HB3	2.24	0.52
4:L:194:TYR:O	4:L:208:THR:O	2.27	0.52
1:A:17:ARG:CG	1:A:18:GLY:HA3	2.39	0.52
1:A:6:ARG:HH22	1:A:113:TYR:HD1	1.42	0.52
5:H:171:THR:O	6:H:1534:HOH:O	2.19	0.52
1:A:121:LYS:HE2	6:A:297:HOH:O	2.09	0.51
2:E:50:GLU:HG2	2:E:67:TYR:O	2.10	0.51
5:M:170:HIS:HE1	6:M:622:HOH:O	1.94	0.51
2:E:50:GLU:HG3	2:E:67:TYR:CZ	2.44	0.51
4:L:152:LYS:O	4:L:153:ALA:HB3	2.11	0.51
1:A:17:ARG:CB	1:A:18:GLY:HA3	2.41	0.51
4:L:184:THR:CG2	4:L:185:PRO:HD2	2.39	0.51
5:M:140:GLY:N	6:M:1468:HOH:O	2.32	0.51
1:A:108:ARG:HH11	1:A:108:ARG:CG	2.17	0.50
1:D:111:ARG:CG	1:D:111:ARG:NH1	2.62	0.50
1:D:238:ASP:HB3	2:E:12:ARG:HD3	1.92	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.50
2:B:96:ASP:HB3	2:B:99:MET:HE2	1.92	0.50
5:M:33:GLN:HE22	5:M:53:SER:H	1.58	0.50
1:D:169:ARG:NH2	6:D:498:HOH:O	2.44	0.50
4:K:126:GLU:HB2	6:K:411:HOH:O	2.12	0.50
1:D:275:GLU:HG2	6:D:710:HOH:O	2.10	0.50
4:K:154:ASP:N	4:K:155:GLY:HA2	2.27	0.50
1:A:108:ARG:HD3	1:A:108:ARG:C	2.36	0.49
2:B:17:ASN:ND2	2:B:74:GLU:OE2	2.39	0.49
5:M:2:VAL:HG13	5:M:27:PHE:CD2	2.47	0.49
2:E:47:GLU:HG3	6:E:814:HOH:O	2.12	0.49
4:L:126:GLU:OE1	4:L:126:GLU:N	2.28	0.49
1:D:178:THR:HG23	6:D:922:HOH:O	2.11	0.49
1:A:186:LYS:NZ	6:A:414:HOH:O	2.46	0.49
6:A:1601:HOH:O	3:C:6:ILE:HG23	2.13	0.49
1:A:6:ARG:HG3	6:A:293:HOH:O	2.11	0.49
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.47	0.49
4:L:138:LEU:HD12	5:H:187:VAL:HG11	1.95	0.48
4:L:115:ASN:CB	6:L:1463:HOH:O	2.32	0.48
4:L:189:LYS:N	4:L:190:SER:CB	2.73	0.48
1:D:6:ARG:HD2	6:D:1212:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ARG:HG2	1:D:111:ARG:NH1	2.27	0.48
1:D:146:LYS:HG2	1:D:147:TRP:HD1	1.79	0.48
5:H:145:GLY:O	5:H:160:TRP:CZ2	2.66	0.48
5:M:12:VAL:HG11	5:M:86:LEU:HD13	1.95	0.48
5:H:171:THR:HA	5:H:186:SER:HA	1.94	0.48
4:K:175:TYR:OH	6:K:1595:HOH:O	2.20	0.48
2:E:19:LYS:O	2:E:72:PRO:HD2	2.14	0.48
4:L:81:GLN:NE2	4:L:83:GLU:OE1	2.47	0.48
4:K:30:GLY:HA3	4:K:71:ASN:ND2	2.29	0.48
1:A:119:ASP:O	2:B:0:MET:HB3	2.13	0.48
1:D:95:VAL:HG11	1:D:116:TYR:OH	2.13	0.48
1:D:178:THR:CG2	6:D:922:HOH:O	2.61	0.48
2:E:81:ARG:HD2	6:E:169:HOH:O	2.13	0.48
1:A:108:ARG:NH1	1:A:108:ARG:CG	2.77	0.48
4:K:153:ALA:HA	4:K:154:ASP:HA	1.70	0.47
1:D:178:THR:O	1:D:181:ARG:HD3	2.15	0.47
6:K:596:HOH:O	5:M:170:HIS:HD2	1.97	0.47
5:H:142:ALA:O	5:H:189:THR:HA	2.14	0.47
3:F:6:ILE:HD11	6:M:712:HOH:O	2.13	0.47
5:M:216:LYS:HE3	5:M:216:LYS:HB2	1.72	0.47
4:K:4:LEU:HB2	4:K:101:GLY:HA2	1.96	0.47
5:M:184:LEU:HD12	5:M:184:LEU:C	2.40	0.47
1:D:230:LEU:HD11	1:D:243:LYS:HE3	1.96	0.47
2:E:79:ALA:HB2	2:E:94:LYS:HD2	1.97	0.47
2:E:83:ASN:HD22	2:E:84:HIS:H	1.62	0.47
5:H:177:GLN:HG3	6:H:1419:HOH:O	2.15	0.46
1:A:106:ASP:HB2	6:A:1073:HOH:O	2.15	0.46
5:M:30:SER:O	5:M:53:SER:HB2	2.16	0.46
4:K:166:LYS:HD3	6:K:574:HOH:O	2.15	0.46
2:B:0:MET:HA	6:B:1480:HOH:O	2.16	0.46
2:E:50:GLU:HG3	2:E:67:TYR:CD1	2.49	0.46
1:A:121:LYS:HG2	6:A:297:HOH:O	2.16	0.46
4:L:206:GLU:C	4:L:207:LYS:HD2	2.41	0.46
4:K:172:ASN:OD1	4:K:174:LYS:HB2	2.16	0.46
5:H:206:HIS:CD2	5:H:208:PRO:HD2	2.51	0.46
5:H:133:SER:HB3	5:H:136:SER:H	1.81	0.45
4:K:138:LEU:HD12	5:M:187:VAL:HG21	1.97	0.45
5:H:158:VAL:HG11	5:H:186:SER:CB	2.46	0.45
4:L:197:GLN:HB3	4:L:198:VAL:CA	2.27	0.45
5:H:145:GLY:C	6:H:1548:HOH:O	2.59	0.45
2:B:81:ARG:HD2	2:B:90:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:OD2	1:A:256:ARG:NE	2.50	0.45
2:E:31:HIS:HD2	6:E:382:HOH:O	2.00	0.45
5:H:130:LEU:HD12	5:H:145:GLY:HA3	1.98	0.45
1:D:71:SER:OG	6:D:1372:HOH:O	2.21	0.44
2:B:51:HIS:HD2	2:B:52:SER:O	2.01	0.44
3:C:3:LEU:HG	3:C:5:TRP:O	2.16	0.44
1:A:17:ARG:HG2	1:A:18:GLY:HA3	1.99	0.44
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.53	0.44
1:D:192:HIS:HA	6:D:1168:HOH:O	2.18	0.44
4:L:189:LYS:HB3	4:L:190:SER:CB	2.38	0.44
4:L:83:GLU:H	4:L:83:GLU:CD	2.26	0.44
1:A:232:GLU:HG2	6:A:406:HOH:O	2.18	0.44
5:H:160:TRP:HA	5:H:201:ILE:O	2.18	0.44
2:E:31:HIS:CD2	2:E:32:PRO:HA	2.54	0.43
4:L:30:GLY:HA3	4:L:71:ASN:HD22	1.83	0.43
2:E:69:GLU:HG2	6:E:1076:HOH:O	2.18	0.43
4:K:81:GLN:O	4:K:84:ASP:HB2	2.19	0.43
2:B:81:ARG:NH1	2:B:81:ARG:CG	2.72	0.43
2:E:50:GLU:HG2	2:E:50:GLU:H	1.48	0.43
4:K:154:ASP:N	4:K:154:ASP:OD2	2.51	0.43
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.54	0.42
5:H:11:LEU:HB2	5:H:153:PRO:HG3	2.01	0.42
5:M:18:LEU:HB3	5:M:83:MET:HE3	2.00	0.42
5:H:33:GLN:NE2	5:H:53:SER:H	2.17	0.42
1:A:102:ASP:OD2	1:A:113:TYR:OH	2.33	0.42
4:L:172:ASN:ND2	4:L:174:LYS:HD2	2.34	0.42
2:B:19:LYS:O	2:B:72:PRO:HD2	2.20	0.42
1:D:6:ARG:NH2	1:D:113:TYR:CG	2.87	0.42
1:D:256:ARG:CG	1:D:256:ARG:NH1	2.54	0.42
2:B:96:ASP:O	2:B:99:MET:HG3	2.19	0.42
4:L:3:GLU:O	4:L:100:PHE:O	2.38	0.42
4:L:160:ALA:O	4:L:183:LEU:HD11	2.20	0.42
4:K:153:ALA:HB2	4:K:194:TYR:CD2	2.54	0.42
4:K:184:THR:OG1	4:K:187:GLN:HG3	2.19	0.42
6:A:1127:HOH:O	2:B:99:MET:HE2	2.20	0.41
4:L:189:LYS:CA	4:L:190:SER:CB	2.91	0.41
1:A:108:ARG:CD	1:A:108:ARG:H	2.34	0.41
1:D:253:GLN:NE2	1:D:256:ARG:NH1	2.69	0.41
1:D:266:LEU:HA	1:D:267:PRO:HD2	1.86	0.41
5:H:130:LEU:HD12	5:H:145:GLY:CA	2.51	0.41
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ASP:HB3	2:B:99:MET:CE	2.51	0.41
1:D:6:ARG:HG3	6:D:320:HOH:O	2.20	0.41
4:K:2:SER:O	4:K:3:GLU:HB2	2.21	0.41
4:K:81:GLN:NE2	4:K:83:GLU:CD	2.79	0.41
2:B:85:VAL:HG22	6:B:105:HOH:O	2.20	0.41
4:K:166:LYS:HD2	4:K:166:LYS:HA	1.80	0.40
5:H:125:PRO:HB3	5:H:151:TYR:HB3	2.03	0.40
1:D:133:TRP:HB2	1:D:144:LYS:HG3	2.03	0.40
4:L:1:GLN:HG3	6:L:770:HOH:O	2.21	0.40
4:K:169:LYS:HE3	4:K:173:ASN:HA	2.03	0.40
4:L:2:SER:HB2	6:L:583:HOH:O	2.21	0.40
4:L:196:CYS:O	4:L:197:GLN:O	2.40	0.40
1:A:35:ARG:NE	6:A:1530:HOH:O	2.44	0.40
1:D:49:ALA:O	1:D:52:ILE:HG22	2.21	0.40
1:D:214:THR:HB	1:D:262:GLN:HB2	2.04	0.40
1:A:45:MET:CE	3:C:2:LEU:HD11	2.52	0.40
4:K:81:GLN:HE21	4:K:83:GLU:CD	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	264 (96%)	9 (3%)	1 (0%)	30	22
1	D	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
4	K	210/212 (99%)	202 (96%)	6 (3%)	2 (1%)	12	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	202/212 (95%)	182 (90%)	11 (5%)	9 (4%)	2	0
5	H	218/220 (99%)	203 (93%)	10 (5%)	5 (2%)	5	1
5	M	218/220 (99%)	214 (98%)	4 (2%)	0	100	100
All	All	1606/1634 (98%)	1539 (96%)	50 (3%)	17 (1%)	11	4

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	190	SER
4	L	197	GLN
4	L	208	THR
5	H	149	LYS
5	H	156	VAL
4	L	148	THR
4	L	183	LEU
4	L	209	VAL
4	L	210	ALA
5	H	196	GLY
4	L	207	LYS
4	K	3	GLU
4	L	4	LEU
5	H	147	LEU
1	A	19	GLU
4	K	156	SER
5	H	148	VAL

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	232/232 (100%)	219 (94%)	13 (6%)	19	11
1	D	232/232 (100%)	223 (96%)	9 (4%)	28	21
2	B	95/95 (100%)	89 (94%)	6 (6%)	16	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	95/95 (100%)	88 (93%)	7 (7%)	13	6
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	2
3	F	9/9 (100%)	8 (89%)	1 (11%)	6	2
4	K	179/179 (100%)	169 (94%)	10 (6%)	19	11
4	L	174/179 (97%)	161 (92%)	13 (8%)	12	6
5	H	182/182 (100%)	171 (94%)	11 (6%)	17	9
5	M	182/182 (100%)	172 (94%)	10 (6%)	19	11
All	All	1389/1394 (100%)	1308 (94%)	81 (6%)	18	10

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	58	GLU
1	A	86	ASN
1	A	108	ARG
1	A	115	GLN
1	A	141	GLN
1	A	156	LEU
1	A	192	HIS
1	A	196	ASP
1	A	212	GLU
1	A	225	THR
1	A	228	THR
1	A	256	ARG
2	B	58	LYS
2	B	70	PHE
2	B	81	ARG
2	B	83	ASN
2	B	85	VAL
2	B	97	ARG
3	C	6	ILE
1	D	35	ARG
1	D	58	GLU
1	D	86	ASN
1	D	89	GLU
1	D	111	ARG
1	D	115	GLN
1	D	121	LYS
1	D	196	ASP

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Mol	Chain	Res	Type
1	D	256	ARG
2	E	0	MET
2	E	9	VAL
2	E	47	GLU
2	E	50	GLU
2	E	75	LYS
2	E	83	ASN
2	E	97	ARG
3	F	6	ILE
4	L	1	GLN
4	L	23	THR
4	L	80	LEU
4	L	148	THR
4	L	152	LYS
4	L	163	GLU
4	L	184	THR
4	L	189	LYS
4	L	198	VAL
4	L	206	GLU
4	L	207	LYS
4	L	208	THR
4	L	209	VAL
4	K	4	LEU
4	K	83	GLU
4	K	117	THR
4	K	124	SER
4	K	129	GLN
4	K	154	ASP
4	K	158	VAL
4	K	166	LYS
4	K	171	SER
4	K	186	GLU
5	H	1	GLU
5	H	62	ASP
5	H	146	CYS
5	H	148	VAL
5	H	161	ASN
5	H	166	THR
5	H	189	THR
5	H	199	THR
5	H	200	TYR
5	H	201	ILE

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Mol	Chain	Res	Type
5	H	216	LYS
5	M	106	MET
5	M	138	SER
5	M	141	THR
5	M	165	LEU
5	M	166	THR
5	M	184	LEU
5	M	195	LEU
5	M	199	THR
5	M	216	LYS
5	M	220	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	115	GLN
1	A	141	GLN
1	A	155	GLN
1	A	174	ASN
1	A	188	HIS
1	A	191	HIS
1	A	224	GLN
1	A	242	GLN
1	A	253	GLN
2	B	2	GLN
2	B	13	HIS
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
3	C	8	GLN
1	D	3	HIS
1	D	72	GLN
1	D	74	HIS
1	D	115	GLN
1	D	145	HIS
1	D	155	GLN
1	D	174	ASN
1	D	188	HIS
1	D	191	HIS
1	D	242	GLN
1	D	253	GLN

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Mol	Chain	Res	Type
1	D	255	GLN
2	E	2	GLN
2	E	13	HIS
2	E	31	HIS
2	E	51	HIS
2	E	83	ASN
2	E	89	GLN
3	F	8	GLN
4	L	1	GLN
4	L	71	ASN
4	L	115	ASN
4	L	131	ASN
4	L	197	GLN
4	K	1	GLN
4	K	39	GLN
4	K	71	ASN
4	K	81	GLN
4	K	170	GLN
4	K	173	ASN
4	K	197	GLN
5	H	33	GLN
5	H	77	ASN
5	H	111	GLN
5	H	177	GLN
5	H	205	ASN
5	M	3	GLN
5	M	33	GLN
5	M	77	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.04	5 (1%) 67 71	16, 28, 43, 57	0
1	D	276/276 (100%)	-0.06	3 (1%) 78 80	17, 28, 43, 55	0
2	B	100/100 (100%)	0.19	6 (6%) 27 29	19, 27, 45, 51	0
2	E	100/100 (100%)	0.26	1 (1%) 79 82	17, 34, 50, 57	0
3	C	9/9 (100%)	0.40	1 (11%) 10 11	23, 28, 33, 35	0
3	F	9/9 (100%)	0.09	0 100 100	20, 27, 31, 32	0
4	K	212/212 (100%)	0.31	10 (4%) 36 39	19, 31, 50, 55	0
4	L	206/212 (97%)	0.87	37 (17%) 3 3	16, 35, 69, 84	1 (0%)
5	H	220/220 (100%)	0.92	55 (25%) 2 1	17, 32, 82, 90	0
5	M	220/220 (100%)	0.18	9 (4%) 41 44	18, 29, 43, 66	0
All	All	1628/1634 (99%)	0.33	127 (7%) 19 20	16, 30, 58, 90	1 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	196	CYS	7.3
5	H	190	VAL	6.7
1	A	18	GLY	6.2
5	H	148	VAL	6.1
4	L	183	LEU	6.0
5	H	195	LEU	5.7
4	L	210	ALA	5.6
5	M	139	GLY	5.5
4	L	211	PRO	5.4
5	H	144	LEU	5.3
5	H	132	PRO	5.3
5	M	137	THR	5.1
5	H	147	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	0	MET	4.6
5	M	138	SER	4.6
5	M	135	LYS	4.3
5	H	200	TYR	4.1
5	H	143	ALA	4.0
5	H	191	PRO	4.0
5	M	136	SER	3.9
4	L	197	GLN	3.8
4	L	205	VAL	3.7
5	H	199	THR	3.7
5	H	130	LEU	3.7
5	H	164	ALA	3.6
5	H	217	VAL	3.6
5	H	141	THR	3.6
5	H	192	SER	3.6
5	H	146	CYS	3.6
4	L	184	THR	3.5
5	H	165	LEU	3.5
5	H	127	VAL	3.5
4	K	1	GLN	3.4
4	L	188	TRP	3.4
5	H	189	THR	3.4
5	H	201	ILE	3.4
4	L	148	THR	3.4
5	H	137	THR	3.4
5	H	188	VAL	3.3
5	H	139	GLY	3.3
4	K	158	VAL	3.3
4	L	212	THR	3.3
2	B	98	ASP	3.2
4	L	208	THR	3.2
5	H	131	ALA	3.2
1	A	194	VAL	3.2
5	H	196	GLY	3.2
5	H	202	CYS	3.1
5	H	169	VAL	3.1
5	H	135	LYS	3.1
5	H	162	SER	3.1
5	H	142	ALA	3.1
4	L	153	ALA	3.0
5	H	168	GLY	3.0
5	H	136	SER	2.9

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Mol	Chain	Res	Type	RSRZ
5	H	155	PRO	2.9
4	K	2	SER	2.9
5	H	194	SER	2.9
4	L	209	VAL	2.9
4	K	155	GLY	2.9
5	H	156	VAL	2.9
1	D	113	TYR	2.9
4	L	115	ASN	2.9
4	L	125	SER	2.9
5	H	219	PRO	2.8
5	H	133	SER	2.8
5	H	197	THR	2.8
4	L	121	PHE	2.8
4	L	123	PRO	2.8
4	L	118	VAL	2.8
4	L	147	VAL	2.8
5	M	134	SER	2.7
5	H	140	GLY	2.7
2	B	99	MET	2.7
5	H	161	ASN	2.7
1	D	194	VAL	2.7
5	H	193	SER	2.6
4	L	173	ASN	2.6
4	K	212	THR	2.6
1	A	108	ARG	2.5
4	L	152	LYS	2.5
4	L	195	SER	2.5
2	B	74	GLU	2.5
5	H	204	VAL	2.5
5	H	213	VAL	2.5
5	H	145	GLY	2.5
4	K	3	GLU	2.4
3	C	6	ILE	2.4
5	M	166	THR	2.4
4	L	151	TRP	2.4
1	D	276	PRO	2.4
4	L	185	PRO	2.4
5	H	160	TRP	2.4
1	A	86	ASN	2.4
2	B	34	ASP	2.3
5	H	129	PRO	2.3
4	L	128	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	L	120	LEU	2.3
5	H	166	THR	2.3
5	H	149	LYS	2.3
1	A	17	ARG	2.3
5	H	138	SER	2.3
4	L	204	THR	2.3
2	E	47	GLU	2.2
5	H	128	PHE	2.2
5	H	134	SER	2.2
4	L	171	SER	2.2
5	H	163	GLY	2.2
5	H	170	HIS	2.2
4	L	198	VAL	2.2
5	H	158	VAL	2.2
4	L	117	THR	2.2
4	K	171	SER	2.2
5	M	140	GLY	2.2
4	L	138	LEU	2.2
2	B	47	GLU	2.1
4	L	124	SER	2.1
4	L	119	THR	2.1
4	L	192	ARG	2.1
5	H	187	VAL	2.1
5	M	220	LYS	2.0
4	K	172	ASN	2.0
4	L	122	PRO	2.0
4	K	192	ARG	2.0
4	L	189	LYS	2.0
4	L	207	LYS	2.0
4	K	190	SER	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.