



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:41 AM UTC

PDB ID : 5ZFP / pdb_00005zfp
Title : Structure of the ExbB/ExbD hexameric complex
Authors : Maki-Yonekura, S.; Matsuoka, R.; Yonekura, K.
Deposited on : 2018-03-06
Resolution : 2.84 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:

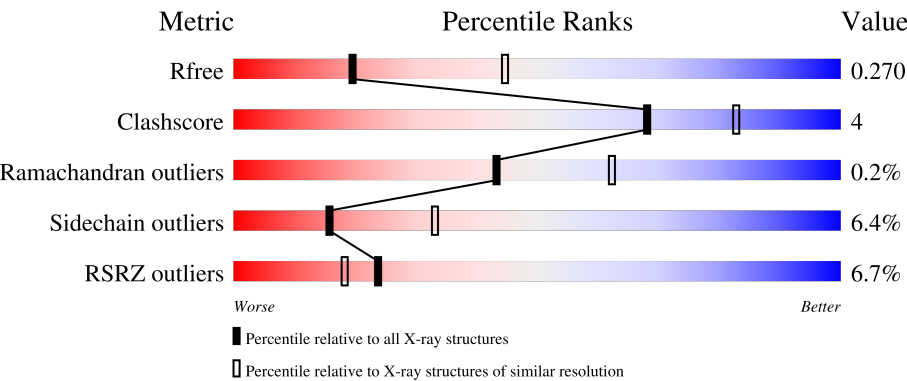
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	244	7% 77%13%•8%
1	B	244	8% 77%9%•12%
1	C	244	2% 77%12%•9%
1	D	244	8% 74%11%•12%
1	E	244	3% 82%8%•9%

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Mol	Chain	Length	Quality of chain
1	F	244	7% 79% 9% • 11%
1	G	244	7% 76% 14% • 8%
1	H	244	6% 76% 11% • 11%
1	I	244	6% 77% 11% • 9%
1	J	244	7% 72% 14% • 12%
1	K	244	8% 82% 9% • 8%
1	L	244	3% 74% 13% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20653 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 Biopolymer transport protein ExbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1704	1086	299	313	6			
1	B	215	Total	C	N	O	S	0	0	0
			1621	1031	285	300	5			
1	C	223	Total	C	N	O	S	0	0	0
			1687	1075	295	311	6			
1	D	215	Total	C	N	O	S	0	0	0
			1619	1029	285	300	5			
1	E	222	Total	C	N	O	S	0	0	0
			1679	1069	294	310	6			
1	F	216	Total	C	N	O	S	0	0	0
			1626	1034	286	301	5			
1	G	225	Total	C	N	O	S	0	0	0
			1704	1086	299	313	6			
1	H	216	Total	C	N	O	S	0	0	0
			1626	1034	286	301	5			
1	I	223	Total	C	N	O	S	0	0	0
			1687	1075	295	311	6			
1	J	214	Total	C	N	O	S	0	0	0
			1614	1026	284	299	5			
1	K	224	Total	C	N	O	S	0	0	0
			1696	1080	298	312	6			
1	L	215	Total	C	N	O	S	0	0	0
			1621	1031	285	300	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	53	Total	O	0	0
			53	53		
2	B	79	Total	O	0	0
			79	79		

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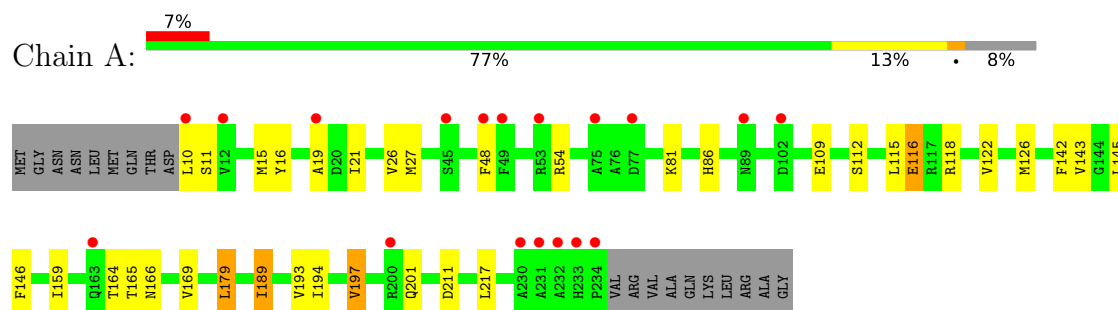
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	62	Total 62	O 62	0	0
2	D	53	Total 53	O 53	0	0
2	E	74	Total 74	O 74	0	0
2	F	75	Total 75	O 75	0	0
2	G	69	Total 69	O 69	0	0
2	H	57	Total 57	O 57	0	0
2	I	67	Total 67	O 67	0	0
2	J	60	Total 60	O 60	0	0
2	K	53	Total 53	O 53	0	0
2	L	67	Total 67	O 67	0	0

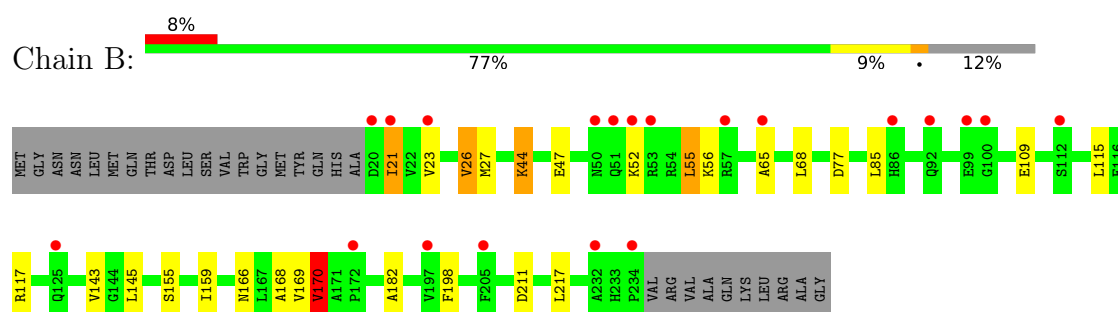
3 Residue-property plots [i](#)

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.

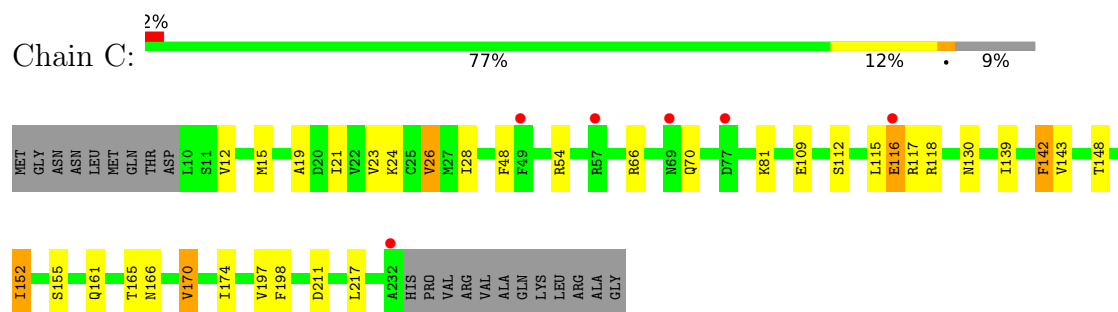
• Molecule 1: Biopolymer transport protein ExbB



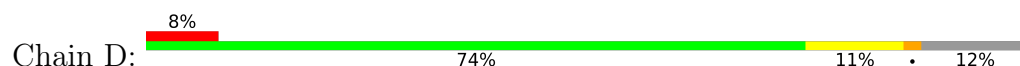
• Molecule 1: Biopolymer transport protein ExbB

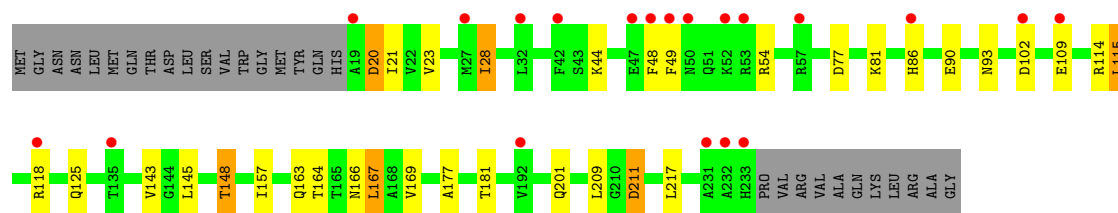


• Molecule 1: Biopolymer transport protein ExbB

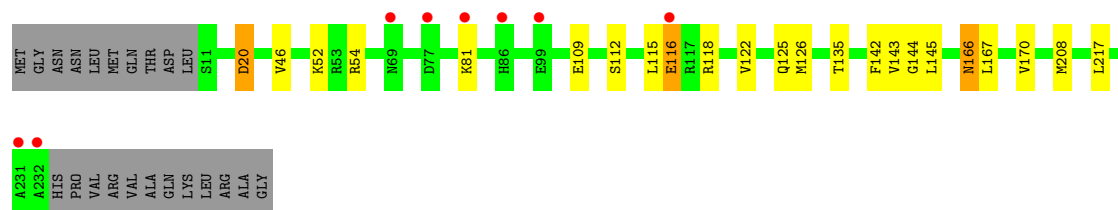
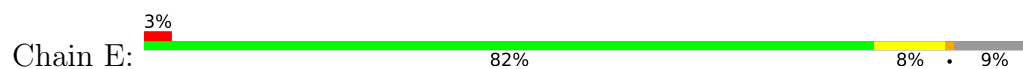


• Molecule 1: Biopolymer transport protein ExbB

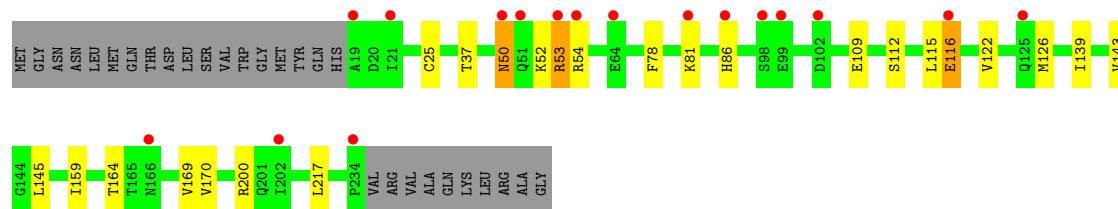
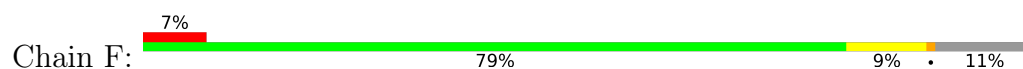




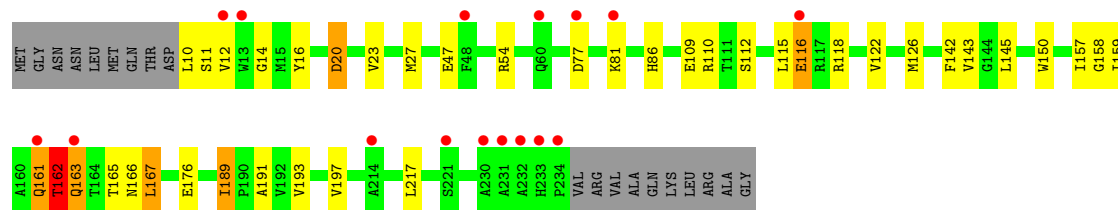
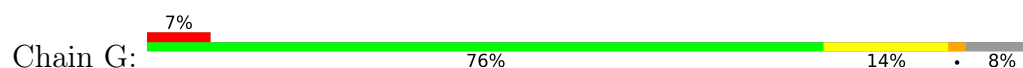
• Molecule 1: Biopolymer transport protein ExbB



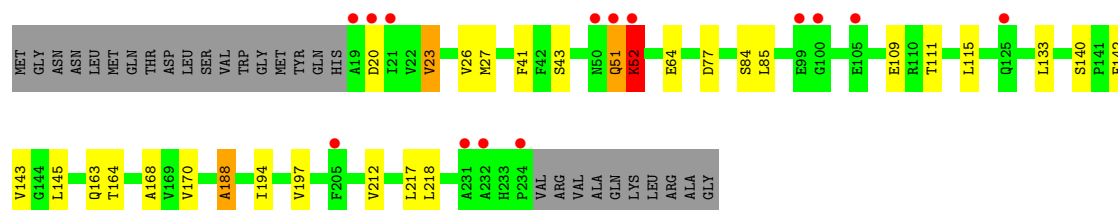
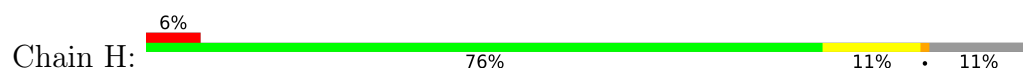
• Molecule 1: Biopolymer transport protein ExbB



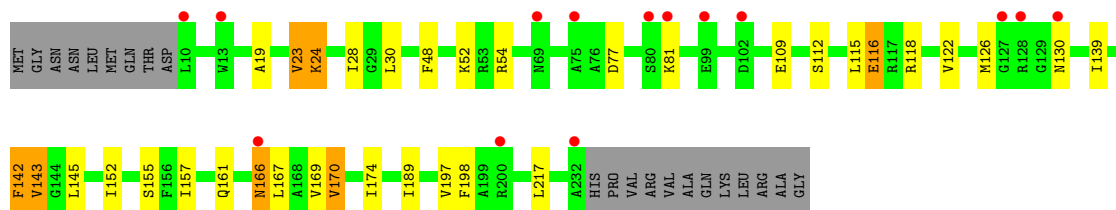
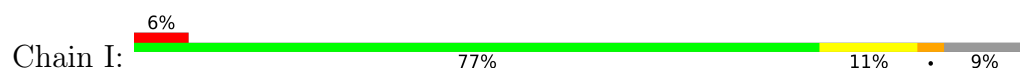
• Molecule 1: Biopolymer transport protein ExbB



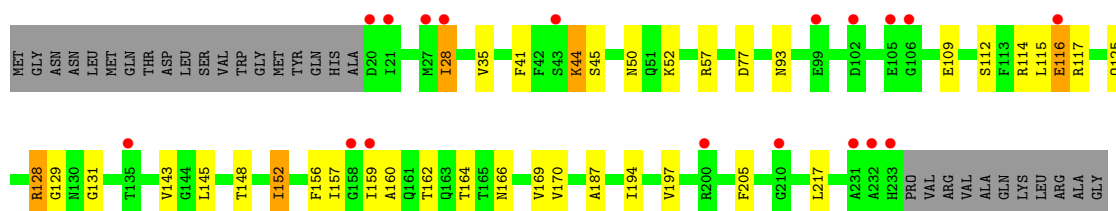
• Molecule 1: Biopolymer transport protein ExbB



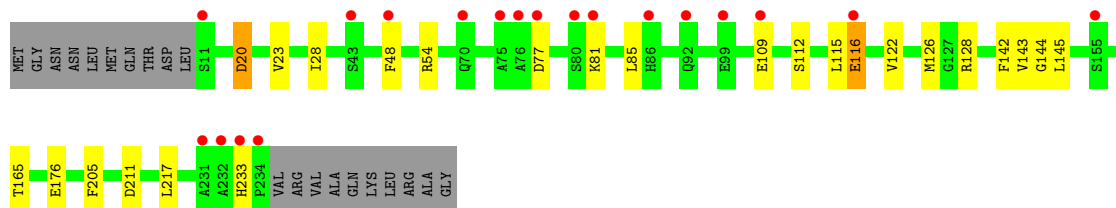
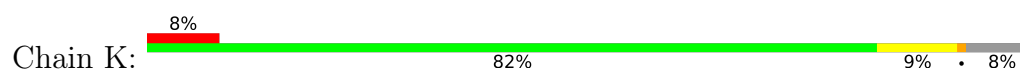
- Molecule 1: Biopolymer transport protein ExbB



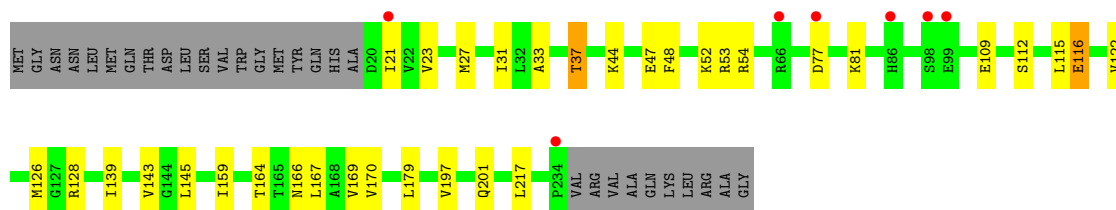
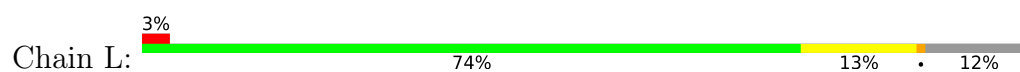
- Molecule 1: Biopolymer transport protein ExbB



- Molecule 1: Biopolymer transport protein ExbB



- Molecule 1: Biopolymer transport protein ExbB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.47Å 106.34Å 163.36Å 90.00° 111.75° 90.00°	Depositor
Resolution (Å)	50.18 – 2.84 50.18 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.18-2.84) 99.1 (50.18-2.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.245 , 0.288 (Not available) , 0.270	Depositor DCC
R_{free} test set	4546 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20653	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4364e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.85	0/1730	1.56	10/2342 (0.4%)
1	B	0.92	0/1643	1.57	5/2223 (0.2%)
1	C	0.90	0/1711	1.54	5/2315 (0.2%)
1	D	0.89	0/1640	1.56	12/2218 (0.5%)
1	E	0.85	0/1703	1.56	11/2304 (0.5%)
1	F	0.90	0/1648	1.55	7/2230 (0.3%)
1	G	0.88	0/1730	1.56	10/2342 (0.4%)
1	H	0.94	0/1648	1.56	13/2230 (0.6%)
1	I	0.89	0/1711	1.57	8/2315 (0.3%)
1	J	1.00	0/1635	1.59	13/2211 (0.6%)
1	K	0.85	0/1722	1.54	5/2331 (0.2%)
1	L	0.85	0/1643	1.55	4/2223 (0.2%)
All	All	0.90	0/20164	1.56	103/27284 (0.4%)

There are no bond length outliers.

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ALA	N-CA-C	14.38	126.45	111.07
1	J	128	ARG	N-CA-C	10.49	122.30	111.07
1	G	142	PHE	CA-CB-CG	10.27	124.07	113.80
1	C	142	PHE	CA-CB-CG	10.22	124.03	113.80
1	H	51	GLN	N-CA-C	9.51	124.89	112.72
1	G	162	THR	N-CA-C	-8.74	93.25	108.20
1	A	142	PHE	CA-CB-CG	8.61	122.41	113.80
1	E	20	ASP	CA-CB-CG	8.09	120.69	112.60
1	I	24	LYS	N-CA-C	-7.99	103.36	113.43
1	E	166	ASN	CA-CB-CG	7.26	119.86	112.60
1	H	52	LYS	N-CA-C	6.86	118.76	111.28
1	C	26	VAL	N-CA-CB	6.41	119.25	110.54
1	H	64	GLU	CB-CG-CD	6.39	123.46	112.60
1	I	142	PHE	CA-CB-CG	6.38	120.18	113.80
1	E	52	LYS	CA-C-N	6.20	128.50	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	52	LYS	C-N-CA	6.20	128.50	120.44
1	H	41	PHE	CA-CB-CG	6.15	119.95	113.80
1	L	197	VAL	N-CA-CB	6.15	117.74	110.55
1	K	20	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	166	ASN	CA-CB-CG	6.01	118.61	112.60
1	I	116	GLU	CB-CG-CD	5.93	122.68	112.60
1	J	160	ALA	N-CA-C	-5.92	105.72	113.12
1	D	157	ILE	N-CA-C	-5.90	104.77	110.72
1	A	19	ALA	CA-C-N	5.89	130.83	120.87
1	A	19	ALA	C-N-CA	5.89	130.83	120.87
1	J	41	PHE	CA-CB-CG	5.89	119.69	113.80
1	E	116	GLU	CB-CG-CD	5.87	122.59	112.60
1	G	20	ASP	CA-CB-CG	5.84	118.44	112.60
1	G	116	GLU	CB-CG-CD	5.84	122.52	112.60
1	I	197	VAL	N-CA-CB	5.82	117.36	110.55
1	K	116	GLU	CB-CG-CD	5.79	122.44	112.60
1	J	162	THR	N-CA-C	-5.77	99.33	108.73
1	D	211	ASP	CA-CB-CG	5.75	118.35	112.60
1	F	78	PHE	CA-CB-CG	5.70	119.50	113.80
1	C	48	PHE	CA-CB-CG	5.68	119.48	113.80
1	I	52	LYS	CA-C-N	5.67	127.82	120.44
1	I	52	LYS	C-N-CA	5.67	127.82	120.44
1	E	20	ASP	CB-CA-C	-5.64	99.20	110.42
1	A	116	GLU	CB-CG-CD	5.63	122.17	112.60
1	C	197	VAL	N-CA-CB	5.62	117.12	110.55
1	C	116	GLU	CB-CG-CD	5.56	122.05	112.60
1	J	131	GLY	CA-C-N	5.55	127.72	120.28
1	J	131	GLY	C-N-CA	5.55	127.72	120.28
1	A	197	VAL	N-CA-CB	5.53	117.65	110.57
1	F	116	GLU	CB-CG-CD	5.52	121.99	112.60
1	H	170	VAL	CA-C-N	5.50	126.96	120.09
1	H	170	VAL	C-N-CA	5.50	126.96	120.09
1	H	20	ASP	CA-CB-CG	5.49	118.09	112.60
1	J	116	GLU	CB-CG-CD	5.49	121.93	112.60
1	F	50	ASN	CA-CB-CG	5.47	118.07	112.60
1	D	209	LEU	CA-C-N	5.46	126.01	120.00
1	D	209	LEU	C-N-CA	5.46	126.01	120.00
1	L	116	GLU	CB-CG-CD	5.46	121.88	112.60
1	G	197	VAL	N-CA-CB	5.45	116.93	110.55
1	D	163	GLN	CA-C-N	5.41	128.39	120.71
1	D	163	GLN	C-N-CA	5.41	128.39	120.71
1	I	167	LEU	N-CA-C	-5.36	105.51	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	VAL	CA-C-N	5.33	126.75	120.09
1	B	170	VAL	C-N-CA	5.33	126.75	120.09
1	D	20	ASP	CA-CB-CG	5.33	117.93	112.60
1	J	157	ILE	CA-C-N	5.33	125.89	119.98
1	J	157	ILE	C-N-CA	5.33	125.89	119.98
1	I	48	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	179	LEU	CD1-CG-CD2	5.29	122.45	110.80
1	H	163	GLN	CA-C-N	5.28	128.20	120.71
1	H	163	GLN	C-N-CA	5.28	128.20	120.71
1	G	189	ILE	CA-C-O	-5.27	115.16	118.69
1	L	52	LYS	CA-C-N	5.27	127.34	120.28
1	L	52	LYS	C-N-CA	5.27	127.34	120.28
1	G	191	ALA	CA-C-N	5.26	127.29	120.56
1	G	191	ALA	C-N-CA	5.26	127.29	120.56
1	H	188	ALA	CA-C-N	5.24	125.46	120.43
1	H	188	ALA	C-N-CA	5.24	125.46	120.43
1	B	211	ASP	CA-CB-CG	5.23	117.83	112.60
1	G	150	TRP	CA-C-N	5.22	125.78	119.98
1	G	150	TRP	C-N-CA	5.22	125.78	119.98
1	D	157	ILE	CA-C-N	5.21	125.73	119.94
1	D	157	ILE	C-N-CA	5.21	125.73	119.94
1	B	26	VAL	N-CA-CB	5.21	118.40	110.58
1	A	26	VAL	CA-C-N	5.19	127.19	120.44
1	A	26	VAL	C-N-CA	5.19	127.19	120.44
1	A	189	ILE	CA-C-O	-5.16	115.23	118.69
1	F	53	ARG	CA-C-N	5.12	127.10	120.44
1	F	53	ARG	C-N-CA	5.12	127.10	120.44
1	J	166	ASN	CA-C-N	5.08	127.60	120.28
1	J	166	ASN	C-N-CA	5.08	127.60	120.28
1	F	52	LYS	CA-C-N	5.08	127.04	120.44
1	F	52	LYS	C-N-CA	5.08	127.04	120.44
1	K	142	PHE	CA-CB-CG	-5.07	108.73	113.80
1	E	46	VAL	CA-C-N	5.07	127.03	120.44
1	E	46	VAL	C-N-CA	5.07	127.03	120.44
1	D	115	LEU	CA-C-N	5.07	127.83	120.79
1	D	115	LEU	C-N-CA	5.07	127.83	120.79
1	A	211	ASP	CA-CB-CG	5.06	117.66	112.60
1	H	111	THR	CA-C-N	5.05	127.56	120.28
1	H	111	THR	C-N-CA	5.05	127.56	120.28
1	E	144	GLY	CA-C-N	5.04	127.04	120.28
1	E	144	GLY	C-N-CA	5.04	127.04	120.28
1	J	187	ALA	CA-C-N	5.04	127.00	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	187	ALA	C-N-CA	5.04	127.00	120.44
1	K	144	GLY	CA-C-N	5.04	127.03	120.28
1	K	144	GLY	C-N-CA	5.04	127.03	120.28
1	E	142	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

There are no planarity outliers.

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	1704	0	1737	14	0
1	B	1621	0	1661	13	0
1	C	1687	0	1723	20	0
1	D	1619	0	1659	17	0
1	E	1679	0	1712	7	0
1	F	1626	0	1666	9	0
1	G	1704	0	1737	18	0
1	H	1626	0	1666	10	0
1	I	1687	0	1723	17	0
1	J	1614	0	1654	20	0
1	K	1696	0	1726	7	0
1	L	1621	0	1661	12	0
2	A	53	0	0	0	0
2	B	79	0	0	1	0
2	C	62	0	0	0	0
2	D	53	0	0	1	0
2	E	74	0	0	1	0
2	F	75	0	0	1	0
2	G	69	0	0	0	0
2	H	57	0	0	1	0
2	I	67	0	0	0	0
2	J	60	0	0	2	0
2	K	53	0	0	0	0
2	L	67	0	0	0	0
All	All	20653	0	20325	143	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 4.

All (143) 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:H:52:LYS:NZ	2:H:301:HOH:O	1.98	0.95
1:D:148:THR:HG21	1:D:181:THR:OG1	1.71	0.89
1:K:23:VAL:HG21	1:K:176:GLU:HG2	1.59	0.85
1:G:23:VAL:HG21	1:G:176:GLU:HG2	1.60	0.81
1:G:158:GLY:O	1:G:162:THR:HG23	1.80	0.80
1:C:12:VAL:HA	1:C:15:MET:HE2	1.63	0.79
1:L:23:VAL:HG12	1:L:27:MET:HE2	1.65	0.77
1:I:19:ALA:HB1	1:I:23:VAL:HG13	1.68	0.76
1:A:16:TYR:HA	1:A:27:MET:HE1	1.69	0.75
1:C:19:ALA:HB1	1:C:23:VAL:HG13	1.70	0.73
1:C:161:GLN:OE1	1:J:50:ASN:HB3	1.89	0.72
1:G:161:GLN:HE21	1:G:162:THR:HG22	1.55	0.71
1:J:93:ASN:HD22	1:J:114:ARG:HH22	1.40	0.69
1:B:44:LYS:HA	1:B:47:GLU:HG2	1.75	0.69
1:D:93:ASN:HD22	1:D:114:ARG:HH22	1.40	0.69
1:I:170:VAL:HG13	1:I:174:ILE:HD12	1.75	0.68
1:A:193:VAL:HG21	1:F:139:ILE:HG21	1.75	0.67
1:B:21:ILE:HG22	2:B:310:HOH:O	1.96	0.64
1:D:148:THR:CG2	1:D:181:THR:OG1	2.43	0.63
1:C:170:VAL:HG13	1:C:174:ILE:HD12	1.81	0.61
1:J:93:ASN:ND2	1:J:114:ARG:HH22	1.99	0.60
1:C:66:ARG:HG2	1:C:70:GLN:OE1	2.02	0.60
1:A:86:HIS:HB3	1:A:118:ARG:HH11	1.68	0.59
1:G:110:ARG:HG2	1:H:218:LEU:HD23	1.83	0.59
1:J:115:LEU:HD12	1:J:217:LEU:HG	1.85	0.59
1:D:93:ASN:ND2	1:D:114:ARG:HH22	2.00	0.58
1:D:115:LEU:HD12	1:D:217:LEU:HG	1.85	0.58
1:C:155:SER:HB3	1:C:170:VAL:HG22	1.85	0.58
1:G:16:TYR:HA	1:G:27:MET:HE1	1.84	0.58
1:C:19:ALA:HB1	1:C:23:VAL:CG1	2.34	0.57
1:F:159:ILE:HD11	1:F:170:VAL:HG21	1.85	0.57
1:G:193:VAL:HG21	1:L:139:ILE:HG21	1.84	0.57
1:H:115:LEU:HD12	1:H:217:LEU:HG	1.87	0.57
1:L:159:ILE:HD11	1:L:170:VAL:HG21	1.86	0.57
1:A:54:ARG:HH12	1:A:81:LYS:HG3	1.69	0.56
1:F:115:LEU:HD12	1:F:217:LEU:HG	1.87	0.56
1:G:167:LEU:HD23	1:L:159:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD12	1:B:217:LEU:HG	1.88	0.55
1:K:115:LEU:HD12	1:K:217:LEU:HG	1.89	0.55
1:J:93:ASN:HD22	1:J:114:ARG:HH12	1.55	0.55
1:G:115:LEU:HD12	1:G:217:LEU:HG	1.89	0.55
1:I:155:SER:HB3	1:I:170:VAL:HG22	1.88	0.54
1:C:115:LEU:HD12	1:C:217:LEU:HG	1.88	0.54
1:D:49:PHE:HE2	1:I:157:ILE:HG21	1.72	0.54
1:C:170:VAL:HG13	1:C:174:ILE:CD1	2.37	0.54
1:G:23:VAL:HG21	1:G:176:GLU:CG	2.35	0.54
1:I:115:LEU:HD12	1:I:217:LEU:HG	1.88	0.54
1:L:115:LEU:HD12	1:L:217:LEU:HG	1.90	0.53
1:A:115:LEU:HD12	1:A:217:LEU:HG	1.89	0.53
1:G:159:ILE:HG22	1:H:168:ALA:HA	1.90	0.53
1:D:93:ASN:HD22	1:D:114:ARG:HH12	1.56	0.53
1:C:21:ILE:HG22	1:J:45:SER:HB2	1.90	0.53
1:E:115:LEU:HD12	1:E:217:LEU:HG	1.91	0.53
1:F:86:HIS:HB3	2:F:344:HOH:O	2.08	0.53
1:I:24:LYS:O	1:I:28:ILE:HG12	2.09	0.52
1:L:54:ARG:HH12	1:L:81:LYS:HG3	1.75	0.52
1:H:142:PHE:HB3	1:I:189:ILE:HD11	1.92	0.51
1:A:164:THR:HG23	1:A:169:VAL:HG21	1.93	0.51
1:D:86:HIS:HB3	1:D:118:ARG:NH2	2.26	0.51
1:D:93:ASN:HD22	1:D:114:ARG:NH2	2.08	0.51
1:G:86:HIS:HB3	1:G:118:ARG:HH11	1.76	0.50
1:J:52:LYS:HG2	1:J:205:PHE:CD1	2.45	0.50
1:H:140:SER:HB2	1:H:188:ALA:HB2	1.93	0.50
1:B:44:LYS:HB2	1:B:198:PHE:CE2	2.47	0.49
1:B:166:ASN:O	1:B:169:VAL:HG22	2.13	0.49
1:L:159:ILE:HA	1:L:164:THR:HG22	1.94	0.49
1:L:33:ALA:O	1:L:37:THR:HG23	2.12	0.49
1:J:93:ASN:HD22	1:J:114:ARG:NH2	2.06	0.49
1:C:54:ARG:HH12	1:C:81:LYS:HG3	1.78	0.49
1:I:54:ARG:HH12	1:I:81:LYS:HG3	1.78	0.48
1:C:117:ARG:HD3	1:D:211:ASP:OD1	2.14	0.48
1:I:139:ILE:O	1:I:142:PHE:HB2	2.12	0.48
1:E:54:ARG:HH12	1:E:81:LYS:HG3	1.79	0.48
1:B:155:SER:HB3	1:B:170:VAL:HG22	1.96	0.48
1:D:54:ARG:HH12	1:D:81:LYS:HG3	1.79	0.47
1:J:28:ILE:HD11	2:J:348:HOH:O	2.14	0.47
1:C:21:ILE:HD13	1:J:197:VAL:HG11	1.96	0.47
1:F:54:ARG:HH12	1:F:81:LYS:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:LYS:HE3	1:J:205:PHE:HB2	1.97	0.47
1:J:44:LYS:HE2	1:J:129:GLY:H	1.80	0.47
1:H:133:LEU:HD13	1:H:194:ILE:HG22	1.96	0.47
1:J:148:THR:O	1:J:152:ILE:HG23	2.14	0.46
1:G:112:SER:O	1:G:116:GLU:HG2	2.15	0.46
1:K:54:ARG:HH12	1:K:81:LYS:HG3	1.80	0.46
1:D:44:LYS:HE3	1:D:48:PHE:CE2	2.51	0.46
1:A:193:VAL:HG21	1:F:139:ILE:CG2	2.46	0.45
1:C:130:ASN:HD21	1:C:198:PHE:HB2	1.80	0.45
1:I:130:ASN:HD21	1:I:198:PHE:HB2	1.81	0.45
1:B:23:VAL:O	1:B:27:MET:HG2	2.17	0.45
1:E:112:SER:O	1:E:116:GLU:HG2	2.16	0.45
1:I:112:SER:O	1:I:116:GLU:HG2	2.17	0.45
1:A:112:SER:O	1:A:116:GLU:HG2	2.17	0.44
1:C:21:ILE:CG2	1:J:45:SER:HB2	2.45	0.44
1:K:112:SER:O	1:K:116:GLU:HG2	2.18	0.44
1:H:23:VAL:O	1:H:27:MET:HG2	2.17	0.44
1:D:148:THR:HB	1:D:177:ALA:O	2.17	0.44
1:E:135:THR:HG23	1:F:200:ARG:HH22	1.83	0.44
1:B:159:ILE:HD11	1:B:170:VAL:HG11	2.00	0.44
1:H:84:SER:OG	1:H:212:VAL:HG11	2.18	0.44
1:J:57:ARG:HD3	2:J:323:HOH:O	2.18	0.44
1:A:11:SER:O	1:A:15:MET:HG2	2.18	0.43
1:G:54:ARG:HH12	1:G:81:LYS:HG3	1.82	0.43
1:F:122:VAL:O	1:F:126:MET:HG2	2.18	0.43
1:G:193:VAL:HG21	1:L:139:ILE:CG2	2.48	0.43
1:A:146:PHE:CE1	1:B:182:ALA:HB1	2.53	0.43
1:C:112:SER:O	1:C:116:GLU:HG2	2.19	0.43
1:J:52:LYS:HA	1:J:205:PHE:HE1	1.84	0.43
1:I:122:VAL:O	1:I:126:MET:HG2	2.19	0.43
1:E:166:ASN:O	1:E:170:VAL:HG22	2.19	0.42
1:A:159:ILE:HG22	1:B:168:ALA:HA	2.00	0.42
1:L:112:SER:O	1:L:116:GLU:HG2	2.19	0.42
1:G:122:VAL:O	1:G:126:MET:HG2	2.19	0.42
1:K:122:VAL:O	1:K:126:MET:HG2	2.19	0.42
1:I:166:ASN:HB3	1:I:169:VAL:H	1.84	0.42
1:J:93:ASN:HD22	1:J:114:ARG:NH1	2.17	0.42
1:J:156:PHE:HA	1:J:159:ILE:HG12	2.01	0.42
1:B:117:ARG:HD3	1:C:211:ASP:OD1	2.20	0.42
1:G:10:LEU:HD22	1:G:14:GLY:HA3	2.01	0.42
1:C:24:LYS:O	1:C:28:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:O	1:A:126:MET:HG2	2.19	0.41
1:G:157:ILE:O	1:G:161:GLN:HG2	2.20	0.41
1:I:170:VAL:HG13	1:I:174:ILE:CD1	2.48	0.41
1:L:122:VAL:O	1:L:126:MET:HG2	2.20	0.41
1:B:44:LYS:HB2	1:B:198:PHE:CZ	2.54	0.41
1:D:28:ILE:HD11	2:D:334:HOH:O	2.21	0.41
1:I:30:LEU:HD21	1:I:143:VAL:HG22	2.02	0.41
1:C:139:ILE:O	1:C:142:PHE:HB2	2.20	0.41
1:J:117:ARG:HD3	1:K:211:ASP:OD1	2.20	0.41
1:A:48:PHE:CZ	1:A:201:GLN:HB3	2.55	0.41
1:D:167:LEU:HG	1:E:167:LEU:HD11	2.02	0.41
1:E:122:VAL:O	1:E:126:MET:HG2	2.21	0.41
1:F:112:SER:O	1:F:116:GLU:HG2	2.20	0.41
1:D:20:ASP:HB3	1:D:23:VAL:HB	2.03	0.41
1:H:142:PHE:HB3	1:I:189:ILE:CD1	2.51	0.41
1:B:55:LEU:HD23	1:B:55:LEU:HA	1.92	0.40
1:G:163:GLN:H	1:G:163:GLN:HG2	1.58	0.40
1:I:23:VAL:HG22	1:I:23:VAL:O	2.21	0.40
1:L:48:PHE:CZ	1:L:201:GLN:HB3	2.57	0.40
1:K:48:PHE:HE1	1:K:205:PHE:HB2	1.87	0.40
1:C:148:THR:O	1:C:152:ILE:HG23	2.21	0.40
1:D:102:ASP:HB2	2:E:333:HOH:O	2.21	0.40
1:A:194:ILE:HA	1:A:197:VAL:HG22	2.03	0.40
1:J:112:SER:O	1:J:116:GLU:HG2	2.21	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	223/244 (91%)	222 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/244 (87%)	209 (98%)	4 (2%)	0	100	100
1	C	221/244 (91%)	220 (100%)	1 (0%)	0	100	100
1	D	213/244 (87%)	212 (100%)	1 (0%)	0	100	100
1	E	220/244 (90%)	218 (99%)	1 (0%)	1 (0%)	24	43
1	F	214/244 (88%)	213 (100%)	1 (0%)	0	100	100
1	G	223/244 (91%)	222 (100%)	1 (0%)	0	100	100
1	H	214/244 (88%)	213 (100%)	1 (0%)	0	100	100
1	I	221/244 (91%)	219 (99%)	1 (0%)	1 (0%)	24	43
1	J	212/244 (87%)	211 (100%)	1 (0%)	0	100	100
1	K	222/244 (91%)	220 (99%)	0	2 (1%)	14	27
1	L	213/244 (87%)	213 (100%)	0	0	100	100
All	All	2609/2928 (89%)	2592 (99%)	13 (0%)	4 (0%)	43	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	20	ASP
1	K	233	HIS
1	K	20	ASP
1	I	23	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	175/190 (92%)	166 (95%)	9 (5%)	21	44
1	B	167/190 (88%)	154 (92%)	13 (8%)	11	25
1	C	173/190 (91%)	165 (95%)	8 (5%)	24	48
1	D	166/190 (87%)	153 (92%)	13 (8%)	11	25
1	E	172/190 (90%)	166 (96%)	6 (4%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	167/190 (88%)	158 (95%)	9 (5%)	20	42
1	G	175/190 (92%)	160 (91%)	15 (9%)	10	21
1	H	167/190 (88%)	155 (93%)	12 (7%)	13	28
1	I	173/190 (91%)	164 (95%)	9 (5%)	21	43
1	J	166/190 (87%)	152 (92%)	14 (8%)	10	22
1	K	174/190 (92%)	166 (95%)	8 (5%)	24	48
1	L	167/190 (88%)	152 (91%)	15 (9%)	9	20
All	All	2042/2280 (90%)	1911 (94%)	131 (6%)	16	33

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	21	ILE
1	A	109	GLU
1	A	143	VAL
1	A	145	LEU
1	A	165	THR
1	A	166	ASN
1	A	179	LEU
1	A	189	ILE
1	B	21	ILE
1	B	26	VAL
1	B	44	LYS
1	B	52	LYS
1	B	55	LEU
1	B	56	LYS
1	B	68	LEU
1	B	77	ASP
1	B	85	LEU
1	B	109	GLU
1	B	143	VAL
1	B	145	LEU
1	B	170	VAL
1	C	26	VAL
1	C	109	GLU
1	C	118	ARG
1	C	143	VAL
1	C	152	ILE
1	C	165	THR

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Mol	Chain	Res	Type
1	C	166	ASN
1	C	170	VAL
1	D	21	ILE
1	D	28	ILE
1	D	77	ASP
1	D	90	GLU
1	D	109	GLU
1	D	125	GLN
1	D	143	VAL
1	D	145	LEU
1	D	148	THR
1	D	164	THR
1	D	167	LEU
1	D	169	VAL
1	D	201	GLN
1	E	109	GLU
1	E	118	ARG
1	E	125	GLN
1	E	143	VAL
1	E	145	LEU
1	E	208	MET
1	F	25	CYS
1	F	37	THR
1	F	50	ASN
1	F	53	ARG
1	F	109	GLU
1	F	143	VAL
1	F	145	LEU
1	F	164	THR
1	F	169	VAL
1	G	11	SER
1	G	12	VAL
1	G	20	ASP
1	G	47	GLU
1	G	77	ASP
1	G	109	GLU
1	G	143	VAL
1	G	145	LEU
1	G	161	GLN
1	G	162	THR
1	G	163	GLN
1	G	165	THR

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Mol	Chain	Res	Type
1	G	166	ASN
1	G	167	LEU
1	G	189	ILE
1	H	23	VAL
1	H	26	VAL
1	H	43	SER
1	H	51	GLN
1	H	52	LYS
1	H	77	ASP
1	H	85	LEU
1	H	109	GLU
1	H	143	VAL
1	H	145	LEU
1	H	164	THR
1	H	197	VAL
1	I	77	ASP
1	I	109	GLU
1	I	118	ARG
1	I	143	VAL
1	I	145	LEU
1	I	152	ILE
1	I	161	GLN
1	I	166	ASN
1	I	170	VAL
1	J	28	ILE
1	J	35	VAL
1	J	44	LYS
1	J	77	ASP
1	J	109	GLU
1	J	125	GLN
1	J	128	ARG
1	J	143	VAL
1	J	145	LEU
1	J	152	ILE
1	J	164	THR
1	J	169	VAL
1	J	170	VAL
1	J	194	ILE
1	K	28	ILE
1	K	77	ASP
1	K	85	LEU
1	K	109	GLU

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Mol	Chain	Res	Type
1	K	128	ARG
1	K	143	VAL
1	K	145	LEU
1	K	165	THR
1	L	21	ILE
1	L	31	ILE
1	L	37	THR
1	L	44	LYS
1	L	47	GLU
1	L	53	ARG
1	L	77	ASP
1	L	109	GLU
1	L	128	ARG
1	L	143	VAL
1	L	145	LEU
1	L	166	ASN
1	L	167	LEU
1	L	169	VAL
1	L	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	50	ASN
1	A	72	ASN
1	A	86	HIS
1	A	92	GLN
1	A	166	ASN
1	A	196	ASN
1	B	51	GLN
1	B	70	GLN
1	B	86	HIS
1	B	92	GLN
1	B	163	GLN
1	B	166	ASN
1	B	196	ASN
1	C	18	HIS
1	C	72	ASN
1	C	92	GLN
1	C	130	ASN
1	C	196	ASN

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Mol	Chain	Res	Type
1	D	72	ASN
1	D	86	HIS
1	D	92	GLN
1	D	93	ASN
1	D	125	GLN
1	D	196	ASN
1	E	18	HIS
1	E	69	ASN
1	E	70	GLN
1	E	72	ASN
1	E	92	GLN
1	E	166	ASN
1	E	196	ASN
1	E	201	GLN
1	F	72	ASN
1	F	92	GLN
1	F	166	ASN
1	F	196	ASN
1	G	17	GLN
1	G	18	HIS
1	G	50	ASN
1	G	72	ASN
1	G	86	HIS
1	G	92	GLN
1	G	161	GLN
1	G	196	ASN
1	H	51	GLN
1	H	70	GLN
1	H	86	HIS
1	H	92	GLN
1	H	196	ASN
1	H	201	GLN
1	I	18	HIS
1	I	51	GLN
1	I	72	ASN
1	I	86	HIS
1	I	92	GLN
1	I	130	ASN
1	I	161	GLN
1	I	196	ASN
1	I	201	GLN
1	J	72	ASN

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Mol	Chain	Res	Type
1	J	86	HIS
1	J	92	GLN
1	J	93	ASN
1	J	161	GLN
1	J	196	ASN
1	J	233	HIS
1	K	18	HIS
1	K	72	ASN
1	K	89	ASN
1	K	92	GLN
1	K	196	ASN
1	K	220	GLN
1	L	72	ASN
1	L	92	GLN
1	L	196	ASN
1	L	201	GLN
1	L	233	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	225/244 (92%)	0.73	18 (8%) 18 14	27, 42, 71, 107	0
1	B	215/244 (88%)	0.67	20 (9%) 14 11	20, 38, 65, 103	0
1	C	223/244 (91%)	0.64	6 (2%) 56 47	24, 40, 60, 103	0
1	D	215/244 (88%)	0.69	20 (9%) 14 11	22, 40, 69, 112	0
1	E	222/244 (90%)	0.45	8 (3%) 46 37	20, 38, 61, 102	0
1	F	216/244 (88%)	0.64	17 (7%) 18 14	22, 41, 66, 86	0
1	G	225/244 (92%)	0.79	16 (7%) 22 16	27, 43, 73, 106	0
1	H	216/244 (88%)	0.56	14 (6%) 25 19	22, 38, 66, 108	0
1	I	223/244 (91%)	0.70	14 (6%) 26 20	24, 41, 66, 103	0
1	J	214/244 (87%)	0.71	18 (8%) 17 12	20, 40, 67, 113	0
1	K	224/244 (91%)	0.64	19 (8%) 16 12	22, 40, 67, 125	0
1	L	215/244 (88%)	0.60	7 (3%) 49 39	22, 41, 65, 90	0
All	All	2633/2928 (89%)	0.65	177 (6%) 24 18	20, 40, 67, 125	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	234	PRO	6.5
1	D	49	PHE	6.5
1	K	48	PHE	5.9
1	I	232	ALA	5.9
1	B	100	GLY	5.8
1	A	10	LEU	5.5
1	A	234	PRO	5.2
1	E	77	ASP	5.1
1	E	232	ALA	5.1
1	C	232	ALA	4.8
1	F	234	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	K	77	ASP	4.6
1	G	232	ALA	4.6
1	D	50	ASN	4.5
1	B	50	ASN	4.5
1	D	232	ALA	4.4
1	B	65	ALA	4.4
1	H	100	GLY	4.4
1	L	234	PRO	4.3
1	A	48	PHE	4.2
1	A	230	ALA	4.1
1	E	231	ALA	4.1
1	E	116	GLU	4.1
1	I	128	ARG	3.9
1	B	51	GLN	3.8
1	B	205	PHE	3.8
1	H	99	GLU	3.7
1	J	233	HIS	3.7
1	D	231	ALA	3.7
1	H	51	GLN	3.6
1	B	20	ASP	3.6
1	J	231	ALA	3.6
1	J	232	ALA	3.6
1	B	21	ILE	3.6
1	K	116	GLU	3.6
1	B	99	GLU	3.4
1	K	234	PRO	3.4
1	D	233	HIS	3.3
1	I	10	LEU	3.3
1	A	12	VAL	3.3
1	A	77	ASP	3.2
1	B	234	PRO	3.2
1	A	233	HIS	3.2
1	G	230	ALA	3.2
1	K	233	HIS	3.1
1	G	12	VAL	3.1
1	A	163	GLN	3.1
1	A	49	PHE	3.0
1	I	81	LYS	3.0
1	L	21	ILE	2.9
1	A	19	ALA	2.9
1	G	233	HIS	2.9
1	D	118	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	105	GLU	2.9
1	H	234	PRO	2.9
1	J	159	ILE	2.9
1	G	214	ALA	2.8
1	G	48	PHE	2.8
1	B	125	GLN	2.8
1	H	205	PHE	2.8
1	J	106	GLY	2.8
1	K	231	ALA	2.8
1	F	86	HIS	2.8
1	K	155	SER	2.8
1	H	232	ALA	2.8
1	D	47	GLU	2.7
1	J	105	GLU	2.7
1	G	77	ASP	2.7
1	G	116	GLU	2.7
1	F	99	GLU	2.7
1	J	21	ILE	2.7
1	E	69	ASN	2.7
1	F	125	GLN	2.7
1	G	161	GLN	2.7
1	K	81	LYS	2.6
1	D	86	HIS	2.6
1	F	98	SER	2.6
1	H	19	ALA	2.6
1	A	200	ARG	2.6
1	K	92	GLN	2.6
1	D	102	ASP	2.6
1	L	66	ARG	2.6
1	D	19	ALA	2.6
1	G	13	TRP	2.5
1	C	77	ASP	2.5
1	J	20	ASP	2.5
1	L	98	SER	2.5
1	E	99	GLU	2.5
1	C	69	ASN	2.5
1	B	197	VAL	2.5
1	G	60	GLN	2.5
1	A	89	ASN	2.5
1	K	80	SER	2.4
1	I	13	TRP	2.4
1	J	102	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	231	ALA	2.4
1	I	69	ASN	2.4
1	I	166	ASN	2.4
1	K	99	GLU	2.4
1	K	75	ALA	2.4
1	K	76	ALA	2.4
1	I	80	SER	2.4
1	K	43	SER	2.4
1	H	50	ASN	2.3
1	I	200	ARG	2.3
1	F	116	GLU	2.3
1	B	86	HIS	2.3
1	B	172	PRO	2.3
1	C	57	ARG	2.3
1	J	200	ARG	2.3
1	I	127	GLY	2.3
1	J	116	GLU	2.3
1	D	27	MET	2.3
1	J	27	MET	2.3
1	J	210	GLY	2.3
1	F	50	ASN	2.3
1	F	64	GLU	2.3
1	K	86	HIS	2.3
1	J	43	SER	2.3
1	A	45	SER	2.3
1	B	53	ARG	2.3
1	D	57	ARG	2.3
1	B	52	LYS	2.2
1	H	52	LYS	2.2
1	A	102	ASP	2.2
1	F	202	ILE	2.2
1	L	86	HIS	2.2
1	B	112	SER	2.2
1	F	19	ALA	2.2
1	F	166	ASN	2.2
1	G	163	GLN	2.2
1	H	20	ASP	2.2
1	A	75	ALA	2.2
1	I	99	GLU	2.2
1	L	99	GLU	2.2
1	I	130	ASN	2.2
1	F	51	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	86	HIS	2.2
1	D	109	GLU	2.2
1	H	231	ALA	2.2
1	K	232	ALA	2.2
1	F	54	ARG	2.2
1	F	102	ASP	2.2
1	D	52	LYS	2.2
1	D	48	PHE	2.2
1	A	231	ALA	2.2
1	K	109	GLU	2.2
1	B	57	ARG	2.1
1	K	70	GLN	2.1
1	L	77	ASP	2.1
1	J	135	THR	2.1
1	D	32	LEU	2.1
1	A	232	ALA	2.1
1	C	116	GLU	2.1
1	B	92	GLN	2.1
1	I	102	ASP	2.1
1	F	53	ARG	2.1
1	G	221	SER	2.1
1	D	53	ARG	2.1
1	B	232	ALA	2.1
1	J	28	ILE	2.1
1	K	11	SER	2.1
1	F	81	LYS	2.1
1	G	81	LYS	2.1
1	A	53	ARG	2.1
1	D	135	THR	2.1
1	I	75	ALA	2.1
1	E	81	LYS	2.0
1	D	42	PHE	2.0
1	H	21	ILE	2.0
1	J	99	GLU	2.0
1	D	192	VAL	2.0
1	H	125	GLN	2.0
1	C	49	PHE	2.0
1	J	158	GLY	2.0
1	F	21	ILE	2.0
1	B	23	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.