



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:07 PM UTC

PDB ID : 2VXS / pdb_00002vxs
Title : Structure of IL-17A in complex with a potent, fully human neutralising antibody
Authors : Gerhardt, S.; Hargreaves, D.; Pauptit, R.A.; Davies, R.A.; Russell, C.; Welsh, F.; Tuske, S.J.; Coales, S.J.; Hamuro, Y.; Needham, M.R.C.; Langham, C.; Barker, W.; Bell, P.; Aziz, A.; Smith, M.J.; Dawson, S.; Abbott, W.M.
Deposited on : 2008-07-09
Resolution : 2.63 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

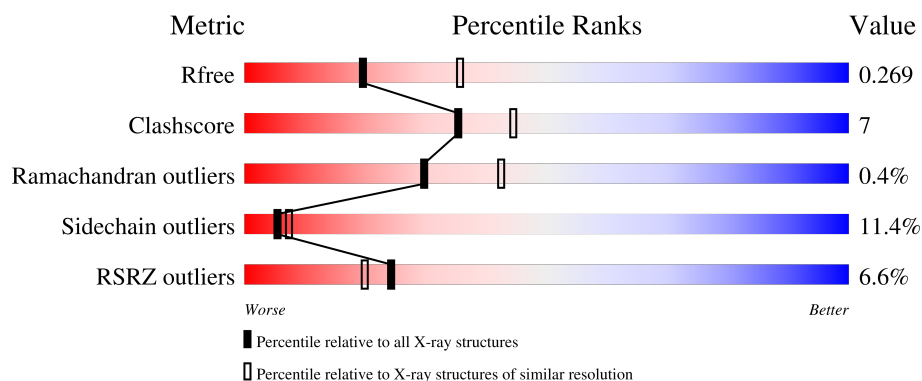
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	137	15% 39% 21% • 37%
1	B	137	7% 45% 11% • 42%
1	C	137	14% 46% 10% • 42%
1	D	137	10% 45% 12% • 44%

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Mol	Chain	Length	Quality of chain
2	H	225	
2	I	225	
2	J	225	
2	K	225	
3	L	216	
3	M	216	
3	N	216	
3	O	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1130	-	-	X	-
4	SO4	B	1129	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15669 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 INTERLEUKIN-17A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	0	0
			679	424	124	126	5			
1	B	80	Total	C	N	O	S	0	0	0
			635	398	115	117	5			
1	C	80	Total	C	N	O	S	0	0	0
			642	402	117	118	5			
1	D	77	Total	C	N	O	S	0	0	0
			612	382	111	114	5			

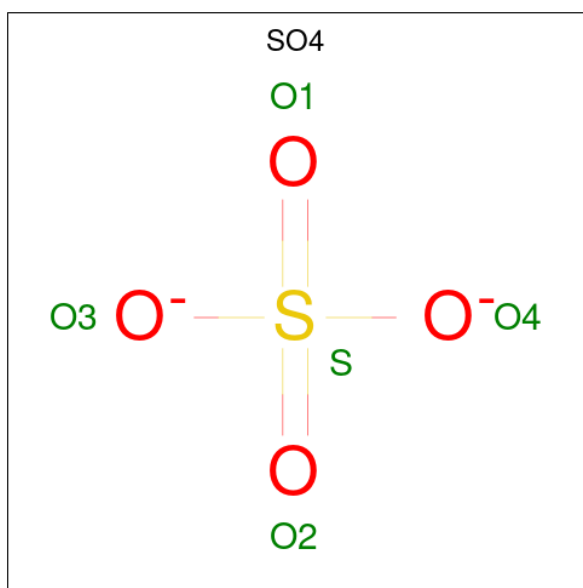
- Molecule 2 is a protein called FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1594	1001	273	313	7			
2	I	221	Total	C	N	O	S	0	0	0
			1620	1015	278	320	7			
2	J	211	Total	C	N	O	S	0	0	0
			1565	985	267	307	6			
2	K	217	Total	C	N	O	S	0	0	0
			1599	1005	275	313	6			

- Molecule 3 is a protein called FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1606	1006	266	329	5			
3	M	215	Total	C	N	O	S	0	0	0
			1621	1014	268	333	6			
3	N	213	Total	C	N	O	S	0	0	0
			1606	1006	266	329	5			
3	O	214	Total	C	N	O	S	0	0	0
			1616	1011	267	332	6			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		

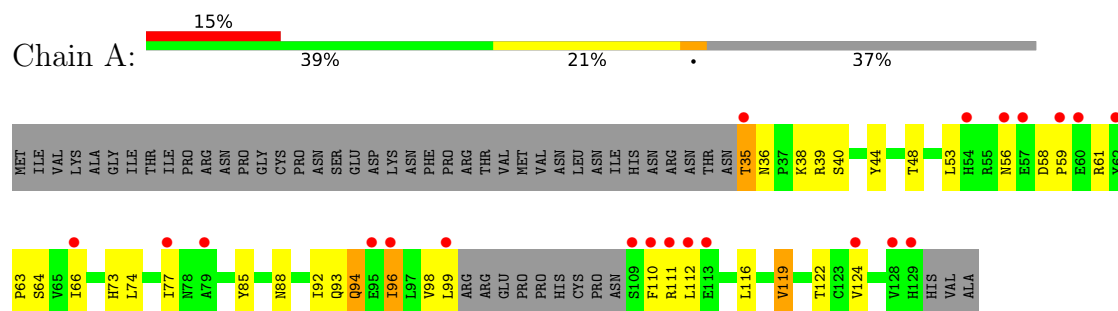
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total 9	O 9	0	0
5	B	15	Total 15	O 15	0	0
5	C	4	Total 4	O 4	0	0
5	D	2	Total 2	O 2	0	0
5	H	19	Total 19	O 19	0	0
5	I	52	Total 52	O 52	0	0
5	J	7	Total 7	O 7	0	0
5	K	28	Total 28	O 28	0	0
5	L	17	Total 17	O 17	0	0
5	M	31	Total 31	O 31	0	0
5	N	10	Total 10	O 10	0	0
5	O	20	Total 20	O 20	0	0

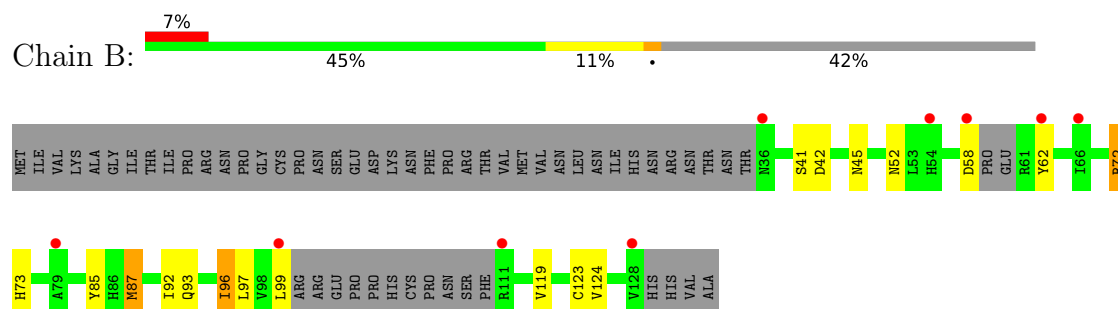
3 Residue-property plots [i](#)

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.

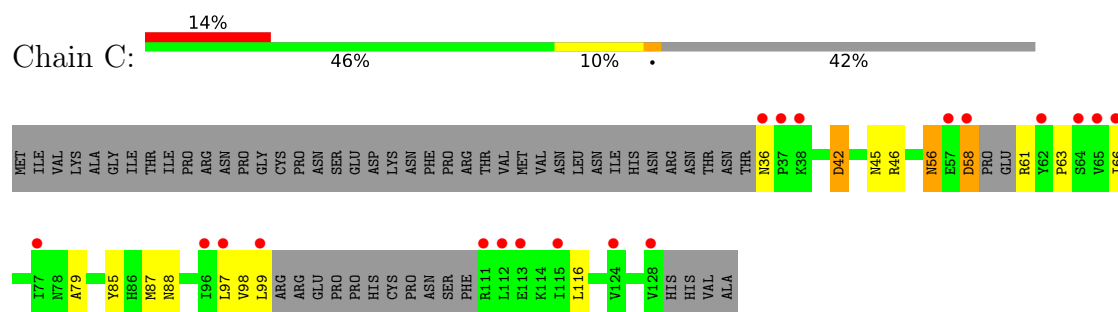
• Molecule 1: INTERLEUKIN-17A



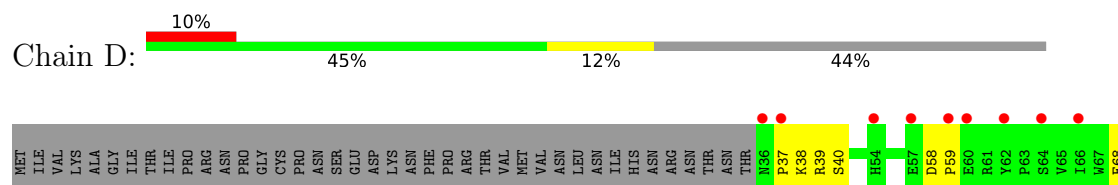
• Molecule 1: INTERLEUKIN-17A

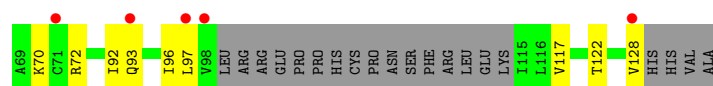


• Molecule 1: INTERLEUKIN-17A

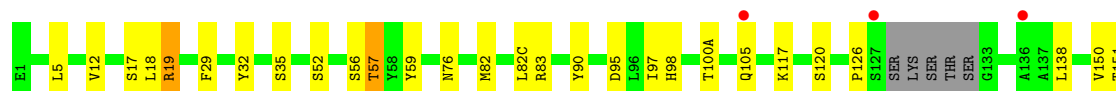
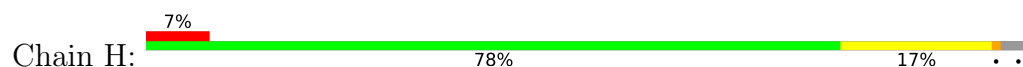


• Molecule 1: INTERLEUKIN-17A

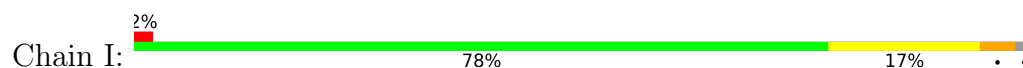




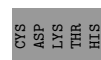
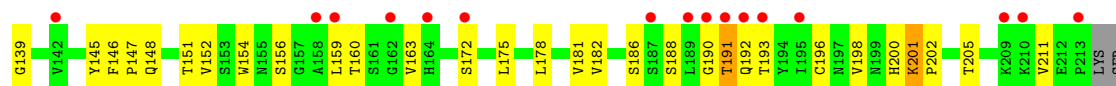
• Molecule 2: FAB FRAGMENT



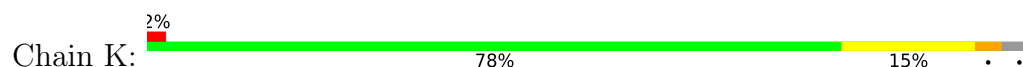
• Molecule 2: FAB FRAGMENT



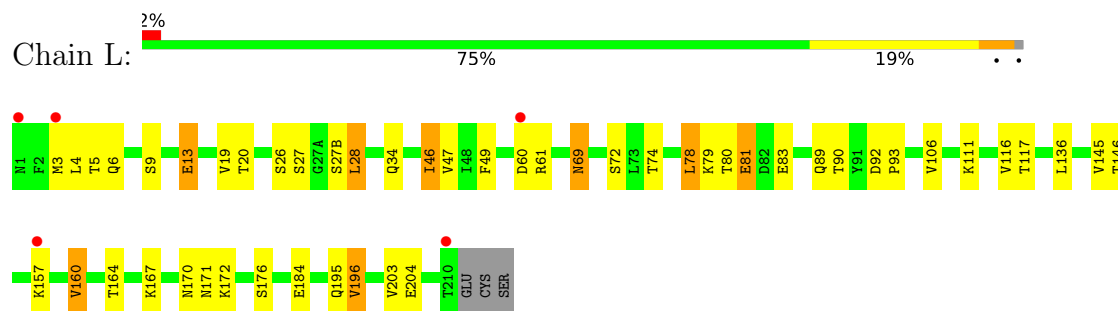
• Molecule 2: FAB FRAGMENT



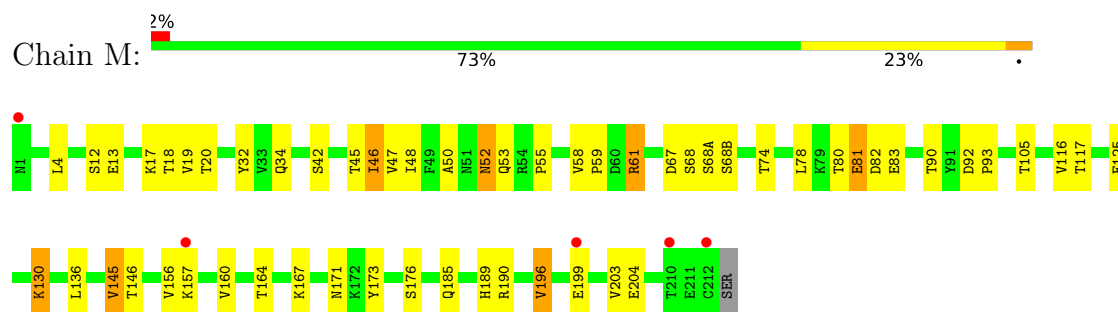
• Molecule 2: FAB FRAGMENT



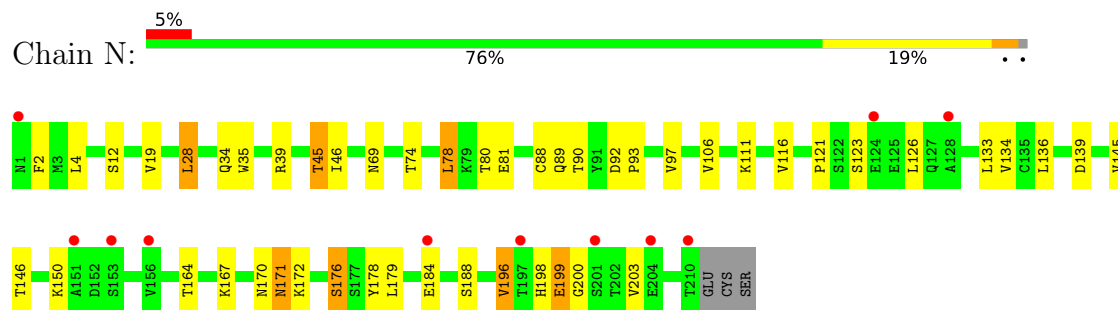
- Molecule 3: FAB FRAGMENT



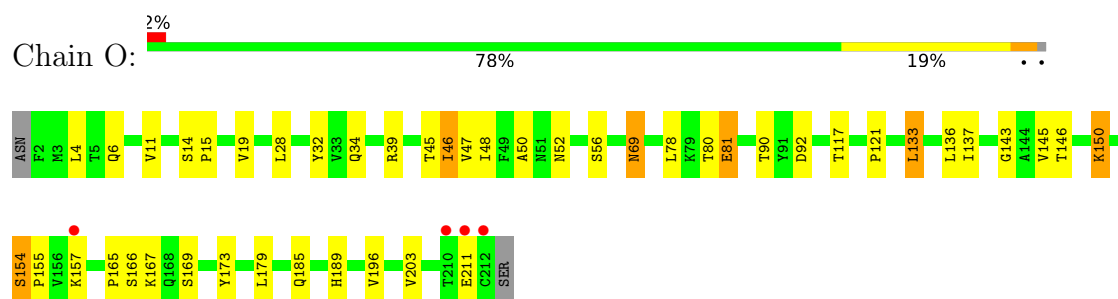
- Molecule 3: FAB FRAGMENT



- Molecule 3: FAB FRAGMENT



- Molecule 3: FAB FRAGMENT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.47Å 66.71Å 203.79Å 90.00° 91.65° 90.00°	Depositor
Resolution (Å)	204.12 – 2.63 203.71 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (204.12-2.63) 99.9 (203.71-2.63)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.5.0036	Depositor
R, R_{free}	0.213 , 0.264 0.217 , 0.269	Depositor DCC
R_{free} test set	3976 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15669	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.66	0/694	0.94	3/946 (0.3%)
1	B	0.59	0/648	0.79	0/881
1	C	0.58	0/655	0.95	2/889 (0.2%)
1	D	0.55	0/627	0.84	0/856
2	H	0.71	0/1629	0.90	0/2216
2	I	0.72	0/1656	0.94	3/2255 (0.1%)
2	J	0.61	0/1600	0.85	0/2179
2	K	0.71	1/1634 (0.1%)	0.93	3/2222 (0.1%)
3	L	0.68	1/1647 (0.1%)	0.88	1/2251 (0.0%)
3	M	0.71	0/1662	0.89	0/2271
3	N	0.60	0/1647	0.82	0/2251
3	O	0.63	0/1657	0.89	0/2264
All	All	0.66	2/15756 (0.0%)	0.89	12/21481 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	100	VAL	CA-CB	5.96	1.60	1.53
3	L	160	VAL	CA-CB	5.26	1.60	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	36	ASN	CA-C-N	7.48	129.19	119.84
1	C	36	ASN	C-N-CA	7.48	129.19	119.84
2	K	95	ASP	N-CA-C	6.44	121.17	113.12
1	A	40	SER	N-CA-C	-6.25	106.19	113.88
1	A	58	ASP	CA-C-N	5.47	126.68	119.84
1	A	58	ASP	C-N-CA	5.47	126.68	119.84
2	I	13	GLN	CA-C-N	-5.36	114.26	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	13	GLN	C-N-CA	-5.36	114.26	119.78
2	I	211	VAL	CB-CA-C	5.20	118.56	110.96
3	L	47	VAL	N-CA-C	-5.16	107.13	111.56
2	K	19	ARG	N-CA-C	5.14	116.79	108.41
2	K	29	PHE	N-CA-C	5.04	116.47	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	679	0	651	17	0
1	B	635	0	613	14	0
1	C	642	0	624	10	0
1	D	612	0	584	6	0
2	H	1594	0	1570	20	0
2	I	1620	0	1590	24	0
2	J	1565	0	1541	29	0
2	K	1599	0	1579	24	0
3	L	1606	0	1547	20	1
3	M	1621	0	1557	28	1
3	N	1606	0	1547	22	0
3	O	1616	0	1553	27	0
4	A	5	0	0	2	0
4	B	10	0	0	2	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	I	10	0	0	0	0
4	L	10	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	O	5	0	0	0	0
5	A	9	0	0	0	0
5	B	15	0	0	0	0
5	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	2	0	0	0	0
5	H	19	0	0	2	0
5	I	52	0	0	0	0
5	J	7	0	0	0	0
5	K	28	0	0	0	0
5	L	17	0	0	0	0
5	M	31	0	0	0	0
5	N	10	0	0	3	0
5	O	20	0	0	1	0
All	All	15669	0	14956	225	1

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 7.

All (225) 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:I:94:ARG:HH11	2:I:102:ASN:ND2	1.57	1.00
2:I:94:ARG:HH11	2:I:102:ASN:HD21	0.95	0.92
3:O:34:GLN:HE21	3:O:50:ALA:H	1.17	0.91
3:M:34:GLN:HE21	3:M:50:ALA:H	1.22	0.87
2:I:201:LYS:HD3	2:I:202:PRO:HD3	1.55	0.87
2:I:94:ARG:NH1	2:I:102:ASN:HD21	1.73	0.85
1:B:87:MET:HG3	1:B:123:CYS:SG	2.23	0.78
2:K:181:VAL:HG21	3:O:136:LEU:HD13	1.64	0.78
2:K:95:ASP:O	2:K:100:VAL:O	2.00	0.77
3:N:45:THR:HB	5:N:2004:HOH:O	1.83	0.77
2:K:95:ASP:O	2:K:96:LEU:HB2	1.90	0.70
3:O:34:GLN:NE2	3:O:50:ALA:H	1.90	0.70
3:O:39:ARG:NH2	3:O:81:GLU:O	2.25	0.70
2:H:19:ARG:HG2	2:H:19:ARG:HH11	1.57	0.70
3:O:28:LEU:H	3:O:69:ASN:HD21	1.40	0.70
1:A:63:PRO:HD2	1:A:98:VAL:HG12	1.74	0.69
1:A:92:ILE:HD12	1:B:92:ILE:HD12	1.74	0.69
1:A:94:GLN:HE21	1:A:94:GLN:HA	1.57	0.68
3:N:170:ASN:O	3:N:171:ASN:HB2	1.94	0.67
1:A:96:ILE:HD12	1:B:96:ILE:HG22	1.75	0.67
3:M:13:GLU:HG3	3:M:17:LYS:HB2	1.76	0.66
2:J:94:ARG:HH21	2:J:102:ASN:HD21	1.43	0.66
2:I:28:THR:HG22	2:I:28:THR:O	1.96	0.66
3:L:195:GLN:HG2	3:L:204:GLU:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TYR:OH	4:B:1129:SO4:O3	2.10	0.65
2:K:181:VAL:CG2	3:O:136:LEU:HD13	2.26	0.65
3:O:4:LEU:HD11	3:O:90:THR:HG22	1.78	0.64
2:H:126:PRO:HD3	2:H:138:LEU:HB3	1.79	0.63
3:L:92:ASP:HB2	3:L:93:PRO:CD	2.28	0.63
2:K:5:LEU:CD2	2:K:105:GLN:HE22	2.12	0.62
3:L:80:THR:HA	3:L:106:VAL:HG21	1.82	0.62
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.81	0.62
2:K:82:MET:HE2	2:K:82(C):LEU:HD21	1.83	0.61
1:B:41:SER:HA	2:I:28:THR:HG21	1.82	0.60
3:O:137:ILE:HG12	3:O:196:VAL:HG11	1.84	0.60
1:B:52:ASN:OD1	1:B:72:ARG:HD2	2.01	0.60
2:J:71:ARG:HE	2:J:73:ASN:HD21	1.50	0.59
3:O:121:PRO:HD3	3:O:133:LEU:CD1	2.32	0.59
3:L:13:GLU:HB2	3:L:19:VAL:CG1	2.32	0.59
2:J:152:VAL:HG22	2:J:198:VAL:HG22	1.84	0.59
3:M:46:ILE:C	3:M:46:ILE:HD13	2.27	0.59
3:L:3:MET:HG2	3:L:26:SER:HB3	1.86	0.58
3:M:167:LYS:HE3	3:M:173:TYR:CZ	2.39	0.57
2:H:19:ARG:HG2	2:H:19:ARG:NH1	2.16	0.56
2:J:135:THR:N	2:J:186:SER:HG	2.04	0.56
2:H:57:THR:HG23	2:H:59:TYR:CE2	2.40	0.56
3:N:133:LEU:HD12	3:N:179:LEU:HD23	1.88	0.55
3:M:167:LYS:HE2	3:M:171:ASN:O	2.05	0.55
2:J:94:ARG:HE	2:J:102:ASN:HD22	1.54	0.55
2:J:139:GLY:HA2	2:J:154:TRP:CZ2	2.42	0.55
3:O:28:LEU:H	3:O:69:ASN:ND2	2.05	0.54
2:H:152:VAL:HA	2:H:197:ASN:O	2.08	0.54
2:K:163:VAL:HG22	2:K:182:VAL:HG13	1.89	0.54
2:K:28:THR:HG22	2:K:28:THR:O	2.08	0.54
1:C:61:ARG:NH2	1:C:66:ILE:HG12	2.24	0.53
3:N:78:LEU:HD11	3:N:106:VAL:HG22	1.91	0.53
3:M:52:ASN:C	3:M:52:ASN:HD22	2.15	0.53
2:I:82:MET:HE2	2:I:82(C):LEU:HD21	1.91	0.53
1:A:56:ASN:HB3	1:A:66:ILE:HG13	1.91	0.53
2:J:188:SER:HB3	2:J:192:GLN:HB2	1.90	0.53
2:K:5:LEU:HD23	2:K:105:GLN:HE22	1.72	0.53
3:M:61:ARG:NH2	3:M:82:ASP:OD2	2.42	0.53
2:I:181:VAL:HG21	3:M:136:LEU:CD1	2.40	0.52
3:N:184:GLU:O	3:N:188:SER:HB2	2.09	0.52
1:C:85:TYR:OH	4:C:1129:SO4:O2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:94:ARG:HH21	2:J:102:ASN:ND2	2.08	0.52
3:N:116:VAL:HG21	3:N:196:VAL:CG1	2.40	0.52
3:O:167:LYS:HE3	3:O:173:TYR:CZ	2.45	0.52
2:I:94:ARG:HD3	2:I:102:ASN:HD22	1.75	0.51
2:J:66:ARG:HD3	2:J:83:ARG:NH2	2.26	0.51
3:L:28:LEU:H	3:L:69:ASN:HD21	1.58	0.51
1:B:62:TYR:HB3	1:B:99:LEU:HB2	1.92	0.51
2:K:181:VAL:HG21	3:O:136:LEU:CD1	2.36	0.51
3:O:32:TYR:HB3	3:O:50:ALA:HA	1.92	0.51
2:J:139:GLY:HA2	2:J:154:TRP:CH2	2.46	0.50
3:L:34:GLN:HB2	3:L:89:GLN:NE2	2.26	0.50
3:M:81:GLU:CD	3:M:81:GLU:H	2.17	0.50
2:H:57:THR:HG21	5:H:2007:HOH:O	2.10	0.50
3:M:4:LEU:HD11	3:M:90:THR:HG22	1.93	0.50
3:N:139:ASP:O	3:N:172:LYS:HD3	2.11	0.50
1:B:41:SER:HA	2:I:28:THR:CG2	2.41	0.50
2:K:29:PHE:CD1	2:K:76:ASN:HA	2.47	0.50
3:O:133:LEU:HD23	3:O:179:LEU:HD23	1.93	0.50
3:L:78:LEU:CD1	3:L:106:VAL:HG22	2.41	0.50
3:L:4:LEU:HD11	3:L:90:THR:HG22	1.94	0.50
3:M:185:GLN:O	3:M:189:HIS:HD2	1.94	0.50
3:M:32:TYR:HB3	3:M:34:GLN:HE22	1.76	0.49
1:C:58:ASP:HB3	1:C:61:ARG:HB3	1.94	0.49
1:A:61:ARG:HB3	1:A:64:SER:HA	1.93	0.49
3:N:4:LEU:HD11	3:N:90:THR:HG22	1.93	0.49
2:J:33:ALA:HB3	2:J:95:ASP:HB2	1.94	0.49
2:K:100:VAL:O	2:K:100:VAL:HG23	2.13	0.49
3:M:34:GLN:HE21	3:M:50:ALA:N	2.03	0.48
1:B:62:TYR:HB3	1:B:99:LEU:HD12	1.95	0.48
3:N:28:LEU:H	3:N:69:ASN:HD21	1.61	0.48
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	1.95	0.48
3:N:39:ARG:HG3	5:N:2005:HOH:O	2.13	0.48
3:O:150:LYS:HD3	3:O:155:PRO:HA	1.94	0.48
2:K:81:GLN:HE21	2:K:82(A):ASN:ND2	2.11	0.48
3:N:92:ASP:HB2	3:N:93:PRO:CD	2.43	0.48
3:N:111:LYS:HD2	3:N:199:GLU:HG3	1.94	0.48
1:A:85:TYR:OH	4:A:1130:SO4:O4	2.30	0.48
1:A:38:LYS:HB3	1:A:53:LEU:CD1	2.43	0.48
2:J:201:LYS:HB3	2:J:202:PRO:HD3	1.95	0.48
2:K:95:ASP:O	2:K:96:LEU:CB	2.59	0.48
3:L:13:GLU:HB2	3:L:19:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:HA	1:A:77:ILE:HG13	1.96	0.47
1:C:63:PRO:HD3	1:D:97:LEU:HD11	1.95	0.47
2:K:167:PRO:HG2	3:O:166:SER:OG	2.13	0.47
3:M:59:PRO:HB2	3:M:61:ARG:HG3	1.95	0.47
3:L:46:ILE:HD11	3:L:49:PHE:HD2	1.79	0.47
1:A:94:GLN:HA	1:A:94:GLN:NE2	2.28	0.47
3:L:83:GLU:HG2	3:L:167:LYS:HE3	1.96	0.47
1:A:119:VAL:HG21	1:B:119:VAL:HG11	1.97	0.47
1:A:36:ASN:O	1:A:39:ARG:HG3	2.15	0.47
3:M:92:ASP:HB2	3:M:93:PRO:CD	2.45	0.47
3:N:34:GLN:HE21	3:N:89:GLN:NE2	2.12	0.47
3:M:12:SER:HA	3:M:105:THR:O	2.14	0.47
2:J:163:VAL:HG22	2:J:182:VAL:HG22	1.97	0.47
1:B:87:MET:HB2	1:B:124:VAL:O	2.15	0.47
2:K:145:TYR:CE1	2:K:150:VAL:HG23	2.50	0.47
3:N:121:PRO:HB2	3:N:126:LEU:CD2	2.44	0.47
2:H:19:ARG:HH11	2:H:19:ARG:CG	2.24	0.47
2:H:95:ASP:OD1	2:H:100(A):THR:HG22	2.15	0.46
2:H:150:VAL:CG2	2:H:178:LEU:HD21	2.46	0.46
2:J:52:SER:HB3	2:J:56:SER:HB2	1.97	0.46
2:J:82:MET:HB3	2:J:82(C):LEU:HD21	1.97	0.46
1:A:35:THR:OG1	1:A:36:ASN:N	2.48	0.46
3:M:61:ARG:NH2	3:M:82:ASP:CG	2.74	0.46
2:I:101:ARG:HE	3:M:46:ILE:HG21	1.81	0.46
3:M:145:VAL:HG22	3:M:196:VAL:HG23	1.97	0.46
2:I:94:ARG:HD3	2:I:102:ASN:ND2	2.30	0.46
3:M:52:ASN:HD22	3:M:53:GLN:N	2.14	0.46
2:J:71:ARG:NE	2:J:73:ASN:HD21	2.13	0.46
3:O:14:SER:HB2	3:O:15:PRO:CD	2.45	0.46
3:O:81:GLU:CD	3:O:81:GLU:H	2.23	0.45
3:L:116:VAL:HG21	3:L:196:VAL:CG1	2.47	0.45
2:J:51:ILE:HD11	2:J:54:GLY:HA2	1.98	0.45
1:C:58:ASP:HB3	1:C:61:ARG:CB	2.46	0.45
2:J:188:SER:HA	2:J:191:THR:HG23	1.99	0.45
1:D:92:ILE:HD11	1:D:122:THR:HB	1.98	0.45
3:L:78:LEU:HD11	3:L:106:VAL:HG22	1.99	0.45
3:L:136:LEU:HD23	3:L:176:SER:HB3	1.99	0.45
2:H:82:MET:HE1	2:H:90:TYR:CZ	2.52	0.45
2:I:59:TYR:HB2	2:I:64:LYS:HE3	1.99	0.44
1:A:92:ILE:HD11	1:A:122:THR:HB	1.98	0.44
1:D:40:SER:O	2:K:28:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:94:ARG:HE	2:J:102:ASN:ND2	2.15	0.44
3:N:167:LYS:HE2	3:N:171:ASN:O	2.17	0.44
2:K:170:LEU:HD13	2:K:176:TYR:CZ	2.52	0.44
3:L:92:ASP:HB2	3:L:93:PRO:HD2	1.99	0.44
3:M:46:ILE:HD12	3:M:55:PRO:HG3	1.98	0.44
1:D:128:VAL:HG12	1:D:128:VAL:O	2.17	0.44
2:H:57:THR:HG23	2:H:59:TYR:HE2	1.81	0.44
3:O:121:PRO:HD3	3:O:133:LEU:HD12	1.98	0.44
2:H:97:ILE:O	2:H:98:HIS:C	2.60	0.44
2:K:100:VAL:O	2:K:100:VAL:CG2	2.66	0.43
3:O:46:ILE:HG22	5:O:2005:HOH:O	2.17	0.43
2:H:32:TYR:HA	5:H:2001:HOH:O	2.18	0.43
2:K:57:THR:HG23	2:K:59:TYR:CE2	2.53	0.43
2:J:97:ILE:O	2:J:98:HIS:C	2.60	0.43
2:K:81:GLN:HE21	2:K:82(A):ASN:HD21	1.64	0.43
2:J:66:ARG:HD3	2:J:83:ARG:HH21	1.84	0.43
1:B:42:ASP:N	2:I:28:THR:HG21	2.33	0.43
1:C:56:ASN:HB3	1:C:66:ILE:O	2.19	0.43
2:H:29:PHE:CD2	2:H:76:ASN:HA	2.54	0.43
3:L:170:ASN:O	3:L:171:ASN:HB2	2.18	0.43
3:M:58:VAL:HA	3:M:59:PRO:HD2	1.87	0.42
2:I:150:VAL:HG23	2:I:178:LEU:HD21	2.01	0.42
3:M:125:GLU:HG2	3:M:130:LYS:O	2.18	0.42
3:N:80:THR:HA	3:N:106:VAL:HG21	2.01	0.42
2:H:52:SER:HB3	2:H:56:SER:HB2	2.01	0.42
3:N:35:TRP:CZ3	3:N:88:CYS:HB3	2.54	0.42
1:A:73:HIS:HB3	4:A:1130:SO4:O1	2.19	0.42
1:B:41:SER:CA	2:I:28:THR:HG21	2.47	0.42
3:O:14:SER:HB2	3:O:15:PRO:HD2	2.01	0.42
1:C:87:MET:O	1:C:88:ASN:ND2	2.46	0.42
2:J:146:PHE:HB2	2:J:175:LEU:HD23	2.01	0.42
3:M:61:ARG:HH22	3:M:82:ASP:CG	2.27	0.42
3:O:154:SER:HA	3:O:155:PRO:HD3	1.84	0.42
2:I:6:GLU:CD	2:I:106:GLY:H	2.28	0.42
2:K:51:ILE:HG23	2:K:71:ARG:HH11	1.84	0.42
3:M:47:VAL:HG12	3:M:48:ILE:HG12	2.02	0.42
2:I:97:ILE:O	2:I:98:HIS:C	2.60	0.41
2:J:200:HIS:HB3	2:J:205:THR:HB	2.01	0.41
3:N:150:LYS:NZ	5:N:2008:HOH:O	2.53	0.41
2:I:95:ASP:OD1	2:I:100(A):THR:HB	2.19	0.41
2:K:119:PRO:HB3	2:K:145:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:185:GLN:O	3:O:189:HIS:HD2	2.02	0.41
1:D:37:PRO:O	1:D:39:ARG:N	2.53	0.41
2:H:199:ASN:ND2	2:H:206:LYS:HG3	2.34	0.41
3:O:143:GLY:O	3:O:165:PRO:HG2	2.20	0.41
1:A:74:LEU:O	1:A:88:ASN:HA	2.21	0.41
2:I:17:SER:HB2	2:I:82(A):ASN:HD22	1.86	0.41
2:H:201:LYS:N	2:H:202:PRO:CD	2.84	0.41
3:M:12:SER:HB3	3:M:105:THR:HB	2.02	0.41
3:O:92:ASP:C	3:O:92:ASP:OD1	2.63	0.41
2:J:12:VAL:HG11	2:J:82(C):LEU:HD12	2.03	0.41
2:H:12:VAL:CG2	2:H:18:LEU:HD22	2.50	0.41
2:I:34:MET:HB3	2:I:78:LEU:HD22	2.03	0.41
3:N:134:VAL:HG13	3:N:178:TYR:CE1	2.56	0.41
3:N:198:HIS:C	3:N:200:GLY:H	2.28	0.41
1:A:38:LYS:HB2	1:A:44:TYR:CE1	2.55	0.41
2:I:67:PHE:CZ	2:I:82:MET:HG2	2.56	0.41
2:I:193:THR:HB	2:I:210:LYS:HE3	2.02	0.41
2:J:82:MET:HE2	2:J:82(C):LEU:HD21	2.03	0.41
3:L:184:GLU:CD	3:L:184:GLU:H	2.28	0.41
3:M:136:LEU:HD23	3:M:176:SER:HB3	2.03	0.41
1:D:58:ASP:HA	1:D:59:PRO:HD2	1.83	0.40
2:H:17:SER:HA	2:H:82:MET:O	2.21	0.40
2:J:135:THR:HG22	2:J:136:ALA:N	2.36	0.40
2:K:181:VAL:CG2	3:O:136:LEU:CD1	2.97	0.40
3:M:116:VAL:HG21	3:M:196:VAL:HG13	2.02	0.40
3:N:2:PHE:CZ	3:N:97:VAL:HB	2.56	0.40
3:O:47:VAL:HG12	3:O:48:ILE:HG12	2.02	0.40
2:J:11:LEU:HB2	2:J:147:PRO:HG3	2.03	0.40
2:J:17:SER:HA	2:J:82:MET:O	2.21	0.40
3:N:136:LEU:HD23	3:N:176:SER:HB3	2.02	0.40
3:L:81:GLU:CD	3:L:81:GLU:H	2.29	0.40
1:C:87:MET:C	1:C:88:ASN:HD22	2.28	0.40
2:I:199:ASN:HD22	2:I:206:LYS:CG	2.34	0.40
3:L:46:ILE:HD13	3:L:49:PHE:HB3	2.04	0.40
1:B:73:HIS:HB3	4:B:1129:SO4:O2	2.21	0.40
1:C:42:ASP:HB3	1:C:46:ARG:HD3	2.02	0.40
1:C:63:PRO:HD2	1:C:98:VAL:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:9:SER:OG	3:M:67:ASP:OD1[2_745]	2.08	0.12

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	82/137 (60%)	77 (94%)	3 (4%)	2 (2%)	4	6
1	B	74/137 (54%)	74 (100%)	0	0	100	100
1	C	74/137 (54%)	71 (96%)	2 (3%)	1 (1%)	9	12
1	D	73/137 (53%)	69 (94%)	3 (4%)	1 (1%)	9	12
2	H	212/225 (94%)	204 (96%)	8 (4%)	0	100	100
2	I	219/225 (97%)	212 (97%)	7 (3%)	0	100	100
2	J	207/225 (92%)	195 (94%)	10 (5%)	2 (1%)	12	18
2	K	213/225 (95%)	208 (98%)	5 (2%)	0	100	100
3	L	211/216 (98%)	201 (95%)	9 (4%)	1 (0%)	24	36
3	M	213/216 (99%)	202 (95%)	11 (5%)	0	100	100
3	N	211/216 (98%)	200 (95%)	9 (4%)	2 (1%)	14	21
3	O	212/216 (98%)	202 (95%)	10 (5%)	0	100	100
All	All	2001/2312 (86%)	1915 (96%)	77 (4%)	9 (0%)	30	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	PHE
1	D	38	LYS
3	L	60	ASP
1	A	59	PRO
2	J	156	SER
3	N	199	GLU
1	C	79	ALA

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Mol	Chain	Res	Type
3	N	171	ASN
2	J	190	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	A	77/128 (60%)	67 (87%)	10 (13%)	4	5
1	B	73/128 (57%)	66 (90%)	7 (10%)	8	12
1	C	74/128 (58%)	67 (90%)	7 (10%)	8	12
1	D	71/128 (56%)	65 (92%)	6 (8%)	10	15
2	H	178/187 (95%)	162 (91%)	16 (9%)	9	13
2	I	181/187 (97%)	157 (87%)	24 (13%)	4	5
2	J	175/187 (94%)	155 (89%)	20 (11%)	5	7
2	K	178/187 (95%)	158 (89%)	20 (11%)	6	8
3	L	184/188 (98%)	159 (86%)	25 (14%)	3	4
3	M	186/188 (99%)	157 (84%)	29 (16%)	2	2
3	N	184/188 (98%)	169 (92%)	15 (8%)	10	17
3	O	186/188 (99%)	165 (89%)	21 (11%)	5	7
All	All	1747/2012 (87%)	1547 (89%)	200 (11%)	5	7

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	93	GLN
1	A	94	GLN
1	A	96	ILE
1	A	99	LEU
1	A	111	ARG
1	A	112	LEU
1	A	116	LEU

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Mol	Chain	Res	Type
1	A	119	VAL
1	A	124	VAL
1	B	45	ASN
1	B	58	ASP
1	B	72	ARG
1	B	87	MET
1	B	93	GLN
1	B	96	ILE
1	B	97	LEU
1	C	42	ASP
1	C	45	ASN
1	C	56	ASN
1	C	58	ASP
1	C	97	LEU
1	C	99	LEU
1	C	116	LEU
1	D	68	GLU
1	D	70	LYS
1	D	72	ARG
1	D	93	GLN
1	D	96	ILE
1	D	117	VAL
2	H	5	LEU
2	H	19	ARG
2	H	35	SER
2	H	57	THR
2	H	83	ARG
2	H	105	GLN
2	H	117	LYS
2	H	120	SER
2	H	151	THR
2	H	159	LEU
2	H	179	SER
2	H	181	VAL
2	H	193	THR
2	H	196	CYS
2	H	201	LYS
2	H	211	VAL
2	I	5	LEU
2	I	12	VAL
2	I	17	SER
2	I	28	THR

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Mol	Chain	Res	Type
2	I	35	SER
2	I	43	LYS
2	I	83	ARG
2	I	85	GLU
2	I	101	ARG
2	I	143	LYS
2	I	148	GLN
2	I	151	THR
2	I	159	LEU
2	I	178	LEU
2	I	182	VAL
2	I	191	THR
2	I	192	GLN
2	I	193	THR
2	I	196	CYS
2	I	201	LYS
2	I	206	LYS
2	I	211	VAL
2	I	214	LYS
2	I	215	SER
2	J	17	SER
2	J	43	LYS
2	J	57	THR
2	J	76	ASN
2	J	83	ARG
2	J	96	LEU
2	J	113	SER
2	J	138	LEU
2	J	148	GLN
2	J	151	THR
2	J	159	LEU
2	J	160	THR
2	J	172	SER
2	J	178	LEU
2	J	181	VAL
2	J	191	THR
2	J	193	THR
2	J	196	CYS
2	J	201	LYS
2	J	211	VAL
2	K	4	LEU
2	K	5	LEU

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Mol	Chain	Res	Type
2	K	12	VAL
2	K	57	THR
2	K	58	TYR
2	K	96	LEU
2	K	100	VAL
2	K	100(A)	THR
2	K	101	ARG
2	K	129	LYS
2	K	135	THR
2	K	151	THR
2	K	159	LEU
2	K	161	SER
2	K	182	VAL
2	K	192	GLN
2	K	193	THR
2	K	199	ASN
2	K	201	LYS
2	K	211	VAL
3	L	5	THR
3	L	6	GLN
3	L	13	GLU
3	L	20	THR
3	L	27	SER
3	L	27(B)	SER
3	L	28	LEU
3	L	46	ILE
3	L	61	ARG
3	L	69	ASN
3	L	72	SER
3	L	74	THR
3	L	78	LEU
3	L	79	LYS
3	L	81	GLU
3	L	111	LYS
3	L	117	THR
3	L	145	VAL
3	L	146	THR
3	L	157	LYS
3	L	160	VAL
3	L	164	THR
3	L	172	LYS
3	L	196	VAL

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Mol	Chain	Res	Type
3	L	203	VAL
3	M	18	THR
3	M	19	VAL
3	M	20	THR
3	M	42	SER
3	M	45	THR
3	M	46	ILE
3	M	52	ASN
3	M	61	ARG
3	M	68	SER
3	M	68(A)	SER
3	M	68(B)	SER
3	M	74	THR
3	M	78	LEU
3	M	80	THR
3	M	81	GLU
3	M	83	GLU
3	M	117	THR
3	M	130	LYS
3	M	145	VAL
3	M	146	THR
3	M	156	VAL
3	M	157	LYS
3	M	160	VAL
3	M	164	THR
3	M	190	ARG
3	M	196	VAL
3	M	199	GLU
3	M	203	VAL
3	M	204	GLU
3	N	12	SER
3	N	19	VAL
3	N	28	LEU
3	N	45	THR
3	N	46	ILE
3	N	74	THR
3	N	78	LEU
3	N	81	GLU
3	N	123	SER
3	N	145	VAL
3	N	146	THR
3	N	164	THR

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Mol	Chain	Res	Type
3	N	176	SER
3	N	196	VAL
3	N	203	VAL
3	O	6	GLN
3	O	11	VAL
3	O	19	VAL
3	O	45	THR
3	O	46	ILE
3	O	52	ASN
3	O	56	SER
3	O	69	ASN
3	O	78	LEU
3	O	80	THR
3	O	81	GLU
3	O	117	THR
3	O	133	LEU
3	O	145	VAL
3	O	146	THR
3	O	150	LYS
3	O	154	SER
3	O	157	LYS
3	O	169	SER
3	O	203	VAL
3	O	211	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	B	73	HIS
1	B	93	GLN
1	C	56	ASN
1	D	54	HIS
1	D	56	ASN
1	D	93	GLN
2	H	3	GLN
2	H	13	GLN
2	H	82(A)	ASN
2	H	148	GLN
2	H	199	ASN
2	I	81	GLN
2	I	82(A)	ASN

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Mol	Chain	Res	Type
2	I	102	ASN
2	I	192	GLN
2	I	199	ASN
2	J	73	ASN
2	J	81	GLN
2	J	82(A)	ASN
2	J	102	ASN
2	J	148	GLN
2	J	192	GLN
2	K	81	GLN
2	K	82(A)	ASN
2	K	98	HIS
2	K	148	GLN
3	L	53	GLN
3	L	69	ASN
3	L	89	GLN
3	L	109	GLN
3	L	168	GLN
3	L	171	ASN
3	M	34	GLN
3	M	52	ASN
3	M	89	GLN
3	M	171	ASN
3	M	189	HIS
3	N	69	ASN
3	N	89	GLN
3	N	109	GLN
3	N	129	ASN
3	N	171	ASN
3	N	189	HIS
3	O	34	GLN
3	O	69	ASN
3	O	89	GLN
3	O	109	GLN
3	O	127	GLN
3	O	129	ASN
3	O	189	HIS
3	O	195	GLN

5.3.3 RNA ⓘ

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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	C	1129	-	4,4,4	0.20	0	6,6,6	0.17	0
4	SO4	B	1130	-	4,4,4	0.24	0	6,6,6	0.17	0
4	SO4	I	1217	-	4,4,4	0.28	0	6,6,6	0.22	0
4	SO4	L	1212	-	4,4,4	0.20	0	6,6,6	0.08	0
4	SO4	D	1129	-	4,4,4	0.27	0	6,6,6	0.26	0
4	SO4	O	1213	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	A	1130	-	4,4,4	0.30	0	6,6,6	0.26	0
4	SO4	B	1129	-	4,4,4	0.33	0	6,6,6	0.52	0
4	SO4	I	1218	-	4,4,4	0.40	0	6,6,6	0.36	0
4	SO4	L	1211	-	4,4,4	0.27	0	6,6,6	0.39	0
4	SO4	M	1213	-	4,4,4	0.28	0	6,6,6	0.20	0
4	SO4	N	1211	-	4,4,4	0.26	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1129	SO4	1	0
4	A	1130	SO4	2	0
4	B	1129	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	86/137 (62%)	1.49	21 (24%) 2 1	33, 51, 62, 64	0
1	B	80/137 (58%)	0.87	9 (11%) 10 8	35, 50, 63, 65	0
1	C	80/137 (58%)	1.40	19 (23%) 2 1	34, 50, 63, 65	0
1	D	77/137 (56%)	1.12	14 (18%) 3 3	34, 48, 64, 65	0
2	H	216/225 (96%)	0.44	15 (6%) 23 19	29, 39, 47, 65	0
2	I	221/225 (98%)	0.17	5 (2%) 61 57	29, 39, 48, 79	0
2	J	211/225 (93%)	0.72	21 (9%) 12 10	31, 39, 46, 56	0
2	K	217/225 (96%)	0.14	5 (2%) 61 57	30, 39, 47, 66	0
3	L	213/216 (98%)	0.47	5 (2%) 61 57	32, 45, 55, 62	0
3	M	215/216 (99%)	0.33	5 (2%) 61 57	33, 45, 55, 80	0
3	N	213/216 (98%)	0.83	11 (5%) 33 27	33, 46, 55, 62	0
3	O	214/216 (99%)	0.56	4 (1%) 66 62	33, 45, 55, 74	0
All	All	2043/2312 (88%)	0.58	134 (6%) 24 20	29, 43, 58, 80	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	212	CYS	5.1
3	N	1	ASN	4.9
1	D	128	VAL	4.6
1	A	60	GLU	4.5
1	A	109	SER	4.5
2	J	187	SER	4.4
2	J	210	LYS	4.2
1	A	110	PHE	4.0
2	K	95	ASP	3.9
1	B	111	ARG	3.9
2	H	191	THR	3.8

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Mol	Chain	Res	Type	RSRZ
2	I	216	CYS	3.7
1	C	62	TYR	3.7
1	D	98	VAL	3.6
1	A	129	HIS	3.6
2	J	191	THR	3.6
3	O	212	CYS	3.6
1	D	60	GLU	3.5
1	C	36	ASN	3.5
1	C	99	LEU	3.5
1	D	59	PRO	3.4
1	A	99	LEU	3.4
2	H	189	LEU	3.4
2	J	189	LEU	3.4
3	O	157	LYS	3.4
1	B	36	ASN	3.3
1	D	37	PRO	3.3
1	D	36	ASN	3.3
1	A	113	GLU	3.2
2	H	127	SER	3.2
3	N	153	SER	3.2
1	C	64	SER	3.1
1	A	35	THR	3.1
2	H	214	LYS	3.1
1	C	37	PRO	3.1
1	C	112	LEU	3.0
1	A	59	PRO	3.0
2	J	158	ALA	3.0
2	H	216	CYS	3.0
2	J	125	ALA	3.0
2	H	164	HIS	2.9
2	J	213	PRO	2.9
1	B	99	LEU	2.9
2	J	195	ILE	2.9
2	J	193	THR	2.9
3	L	1	ASN	2.9
1	C	58	ASP	2.9
1	C	96	ILE	2.9
3	N	184	GLU	2.9
3	N	151	ALA	2.9
2	K	215	SER	2.8
1	D	66	ILE	2.8
1	B	58	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
3	N	156	VAL	2.8
2	I	1	GLU	2.8
2	I	214	LYS	2.8
1	A	112	LEU	2.8
3	L	210	THR	2.8
1	C	128	VAL	2.7
2	H	105	GLN	2.6
1	B	62	TYR	2.6
1	B	54	HIS	2.6
1	A	128	VAL	2.6
2	J	15	GLY	2.6
2	H	159	LEU	2.6
1	C	66	ILE	2.6
1	A	111	ARG	2.6
1	D	62	TYR	2.6
2	H	215	SER	2.5
2	J	209	LYS	2.5
2	J	164	HIS	2.5
1	A	57	GLU	2.5
3	M	199	GLU	2.5
3	O	211	GLU	2.5
3	L	60	ASP	2.5
1	A	66	ILE	2.5
3	L	157	LYS	2.5
1	A	56	ASN	2.5
3	N	210	THR	2.5
1	D	54	HIS	2.5
2	K	206	LYS	2.4
2	J	159	LEU	2.4
3	L	3	MET	2.4
1	A	54	HIS	2.4
1	D	64	SER	2.4
2	H	213	PRO	2.4
1	D	93	GLN	2.4
1	C	124	VAL	2.4
1	C	111	ARG	2.4
2	J	126	PRO	2.3
1	D	97	LEU	2.3
1	A	62	TYR	2.3
3	N	204	GLU	2.3
1	C	77	ILE	2.3
3	N	197	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	N	201	SER	2.3
2	K	133	GLY	2.3
1	A	124	VAL	2.3
1	B	66	ILE	2.2
3	M	157	LYS	2.2
1	C	113	GLU	2.2
1	D	57	GLU	2.2
1	A	77	ILE	2.2
2	J	136	ALA	2.2
3	M	210	THR	2.2
2	H	187	SER	2.2
2	H	136	ALA	2.2
3	N	128	ALA	2.2
3	M	1	ASN	2.2
2	H	188	SER	2.2
1	A	96	ILE	2.2
1	B	128	VAL	2.2
1	B	79	ALA	2.1
2	K	118	GLY	2.1
2	J	127	SER	2.1
2	J	172	SER	2.1
1	A	95	GLU	2.1
2	J	190	GLY	2.1
3	N	124	GLU	2.1
1	C	38	LYS	2.1
1	C	97	LEU	2.1
1	C	57	GLU	2.1
2	H	201	LYS	2.1
2	J	192	GLN	2.0
2	I	164	HIS	2.0
2	J	162	GLY	2.0
1	C	65	VAL	2.0
1	D	71	CYS	2.0
1	A	79	ALA	2.0
2	I	95	ASP	2.0
3	O	210	THR	2.0
1	C	115	ILE	2.0
2	H	190	GLY	2.0
2	J	142	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	N	1211	5/5	0.76	0.16	93,94,94,94	0
4	SO4	B	1130	5/5	0.83	0.20	82,82,83,84	0
4	SO4	A	1130	5/5	0.88	0.26	66,68,68,68	0
4	SO4	L	1212	5/5	0.89	0.22	85,85,85,85	0
4	SO4	I	1218	5/5	0.89	0.25	74,74,76,77	0
4	SO4	D	1129	5/5	0.90	0.26	67,69,69,70	0
4	SO4	C	1129	5/5	0.91	0.23	80,80,80,81	0
4	SO4	L	1211	5/5	0.91	0.16	65,65,66,67	0
4	SO4	O	1213	5/5	0.91	0.21	69,69,69,70	0
4	SO4	I	1217	5/5	0.92	0.16	74,74,75,75	0
4	SO4	B	1129	5/5	0.93	0.23	53,53,55,55	0
4	SO4	M	1213	5/5	0.96	0.13	68,70,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.