



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:07 AM GMT

PDB ID : 2VXS
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

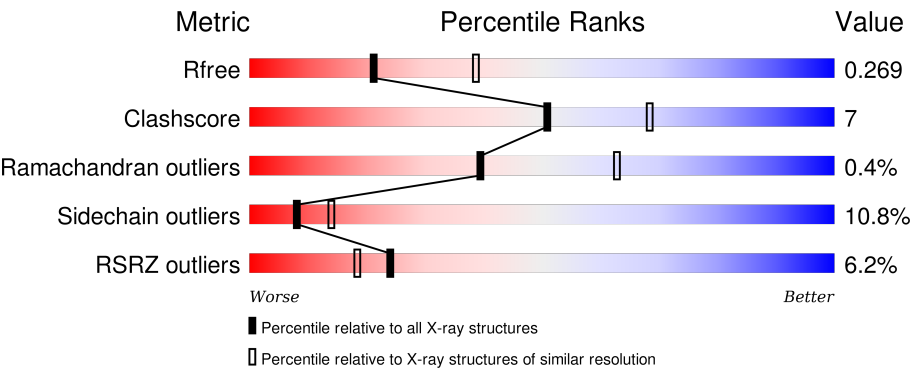
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

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 2.63 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}	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>8%</div><div>42%</div><div>18%</div><div>•</div><div>37%</div></div>
1	B	137	<div><div>4%</div><div>42%</div><div>14%</div><div>•</div><div>42%</div></div>
1	C	137	<div><div>9%</div><div>47%</div><div>9%</div><div>•</div><div>42%</div></div>
1	D	137	<div><div>7%</div><div>44%</div><div>12%</div><div>•</div><div>44%</div></div>
2	H	225	<div><div>4%</div><div>80%</div><div>14%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
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	B	1129	-	-	X	-
4	SO4	D	1129	-	-	-	X
4	SO4	I	1218	-	-	-	X
4	SO4	L	1212	-	-	-	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 (three-letter code: SO4) (formula: O₄S).



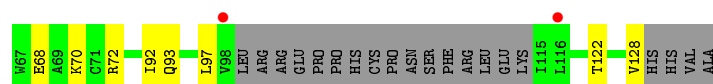
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total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

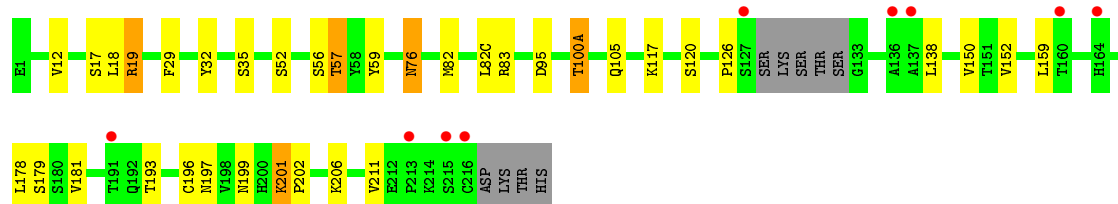
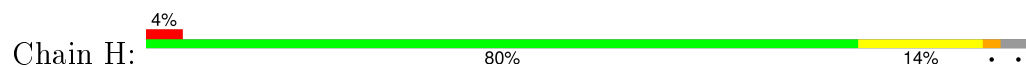
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total O 9 9	0	0
5	B	15	Total O 15 15	0	0
5	C	4	Total O 4 4	0	0
5	D	2	Total O 2 2	0	0
5	H	19	Total O 19 19	0	0
5	I	52	Total O 52 52	0	0
5	J	7	Total O 7 7	0	0
5	K	28	Total O 28 28	0	0
5	L	17	Total O 17 17	0	0
5	M	31	Total O 31 31	0	0
5	N	10	Total O 10 10	0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

- Molecule 1: INTERLEUKIN-17A

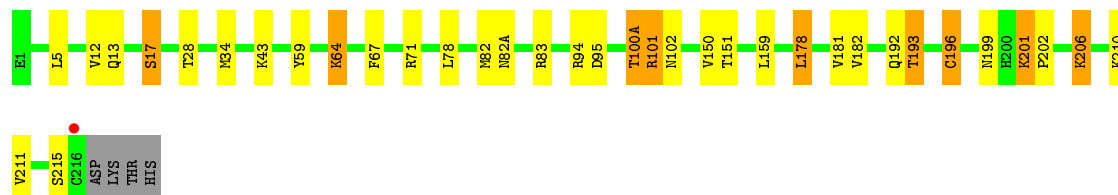
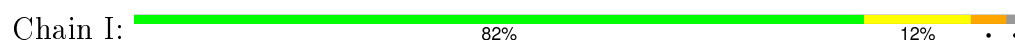




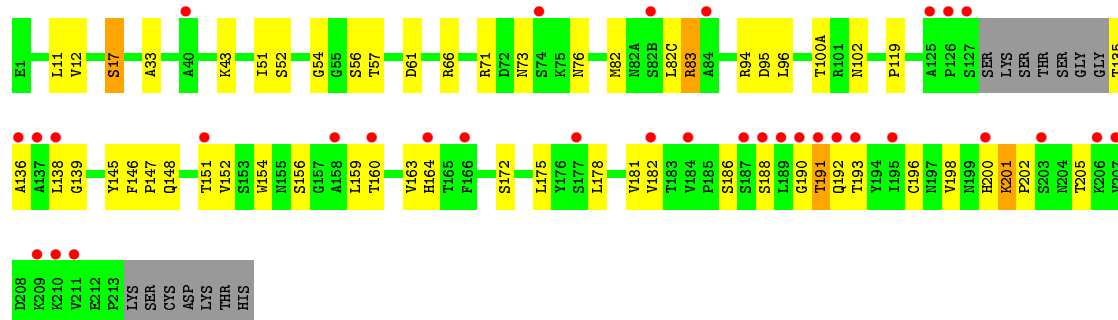
• Molecule 2: FAB FRAGMENT



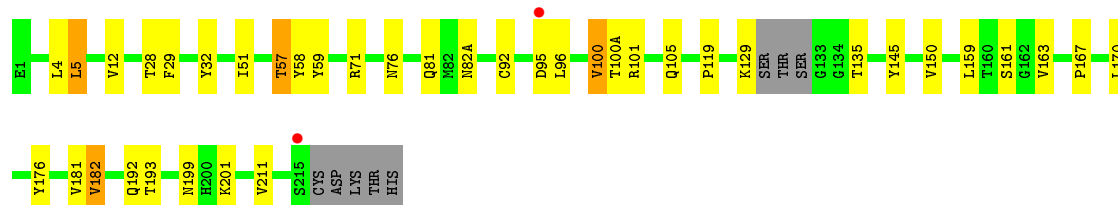
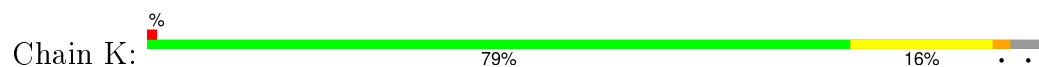
• Molecule 2: FAB FRAGMENT




• Molecule 2: FAB FRAGMENT

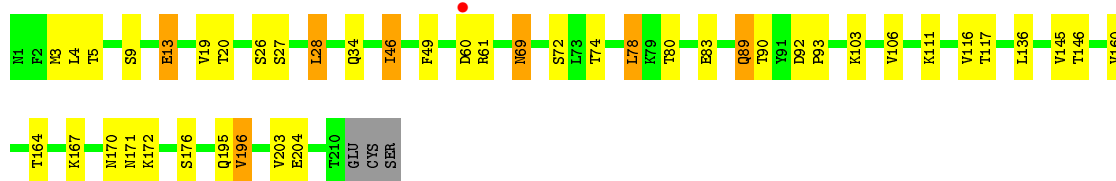


• Molecule 2: FAB FRAGMENT




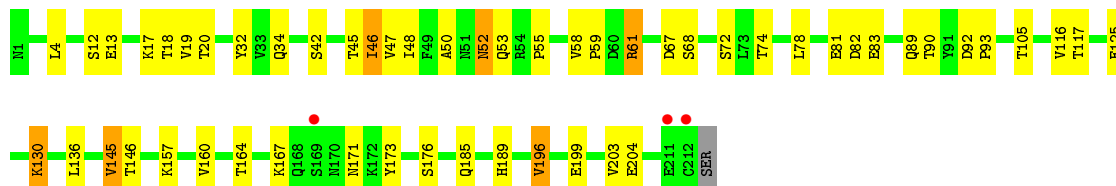
• Molecule 3: FAB FRAGMENT

Chain L:  78% 17% ..




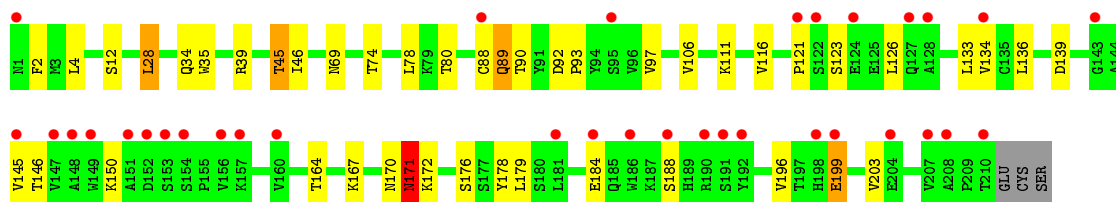
• Molecule 3: FAB FRAGMENT

Chain M:  75% 22% ..




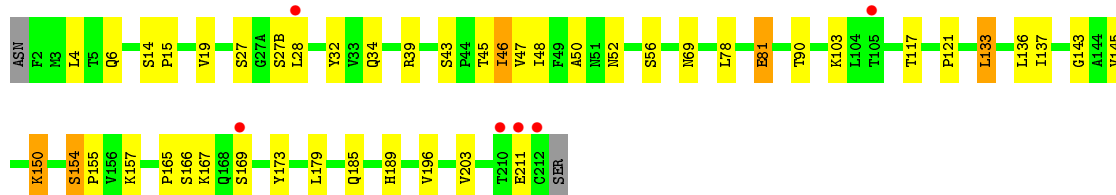
• Molecule 3: FAB FRAGMENT

Chain N:  78% 19% ..



• Molecule 3: FAB FRAGMENT

Chain O:  78% 19% ..



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 – 2.63 101.85 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (204.12-2.63) 99.9 (101.85-2.63)	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 (5.28%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 79218 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/694	0.65	0/946
1	B	0.46	0/648	0.58	0/881
1	C	0.46	0/655	0.63	0/889
1	D	0.44	0/627	0.58	0/856
2	H	0.59	0/1629	0.66	0/2216
2	I	0.63	1/1656 (0.1%)	0.73	0/2255
2	J	0.49	0/1600	0.64	0/2179
2	K	0.56	0/1634	0.69	0/2222
3	L	0.56	0/1647	0.65	0/2251
3	M	0.58	0/1662	0.65	0/2271
3	N	0.48	0/1647	0.58	0/2251
3	O	0.52	0/1657	0.62	0/2264
All	All	0.54	1/15756 (0.0%)	0.65	0/21481

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	196	CYS	CB-SG	-5.95	1.72	1.81

There are no bond angle outliers.

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	679	0	651	16	0
1	B	635	0	613	14	0
1	C	642	0	624	8	0
1	D	612	0	584	7	0
2	H	1594	0	1570	18	0
2	I	1620	0	1590	21	0
2	J	1565	0	1541	27	0
2	K	1599	0	1579	25	0
3	L	1606	0	1547	18	1
3	M	1621	0	1557	27	1
3	N	1606	0	1547	21	0
3	O	1616	0	1553	27	0
4	A	5	0	0	1	0
4	B	10	0	0	2	0
4	C	5	0	0	0	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
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	211	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 (211) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	2:H:19:ARG:HG2	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
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
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
3:O:121:PRO:HD3	3:O:133:LEU:CD1	2.32	0.59
2:J:71:ARG:HE	2:J:73:ASN:HD21	1.50	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
2:J:135:THR:N	2:J:186:SER:HG	2.01	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:ARG:HG2	2:H:19:ARG:NH1	2.16	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
3:M:46:ILE:HD13	3:M:46:ILE:C	2.27	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
3:N:78:LEU:HD11	3:N:106:VAL:HG22	1.91	0.53
1:C:61:ARG:NH2	1:C:66:ILE:HG12	2.24	0.53
2:K:5:LEU:HD23	2:K:105:GLN:HE22	1.72	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
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
2:J:94:ARG:HH21	2:J:102:ASN:ND2	2.08	0.52
3:O:167:LYS:HE3	3:O:173:TYR:CZ	2.45	0.52
3:N:116:VAL:HG21	3:N:196:VAL:CG1	2.40	0.52
2:I:94:ARG:HD3	2:I:102:ASN:HD22	1.75	0.51
3:L:28:LEU:H	3:L:69:ASN:HD21	1.58	0.51
2:J:66:ARG:HD3	2:J:83:ARG:NH2	2.26	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
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:M:185:GLN:O	3:M:189:HIS:HD2	1.94	0.50
3:L:4:LEU:HD11	3:L:90:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:52:ASN:C	3:M:52:ASN:HD22	2.15	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:K:100:VAL:HG23	2:K:100:VAL:O	2.13	0.49
2:J:33:ALA:HB3	2:J:95:ASP:HB2	1.94	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
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:111:LYS:HD2	3:N:199:GLU:HG3	1.94	0.48
3:N:92:ASP:HB2	3:N:93:PRO:CD	2.43	0.48
2:K:95:ASP:O	2:K:96:LEU:CB	2.59	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
3:L:13:GLU:HB2	3:L:19:VAL:HG12	1.96	0.48
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
3:M:59:PRO:HB2	3:M:61:ARG:HG3	1.95	0.47
2:K:167:PRO:HG2	3:O:166:SER:OG	2.13	0.47
3:L:46:ILE:HD11	3:L:49:PHE:HD2	1.79	0.47
1:A:94:GLN:NE2	1:A:94:GLN:HA	2.28	0.47
3:L:83:GLU:HG2	3:L:167:LYS:HE3	1.96	0.47
1:D:42:ASP:OD2	2:K:32:TYR:OH	2.19	0.47
1:A:119:VAL:HG21	1:B:119:VAL:HG11	1.97	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
1:A:36:ASN:O	1:A:39:ARG:HG3	2.15	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:CG	2:H:19:ARG:HH11	2.24	0.47
2:H:95:ASP:OD1	2:H:100(A):THR:HG22	2.15	0.46
2:J:52:SER:HB3	2:J:56:SER:HB2	1.97	0.46
2:H:150:VAL:CG2	2:H:178:LEU:HD21	2.46	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
2:I:101:ARG:HE	3:M:46:ILE:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:81:GLU:CD	3:M:81:GLU:H	2.17	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: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
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	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: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
2:J:94:ARG:HE	2:J:102:ASN:ND2	2.15	0.44
1:D:40:SER:O	2:K:28:THR:HG23	2.17	0.44
3:N:167:LYS:HE2	3:N:171:ASN:O	2.17	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
2:K:170:LEU:HD13	2:K:176:TYR:CZ	2.52	0.44
2:K:105:GLN:HA	3:O:43:SER:HG	1.83	0.44
3:O:121:PRO:HD3	3:O:133:LEU:HD12	1.98	0.44
2:H:57:THR:HG23	2:H:59:TYR:HE2	1.81	0.44
1:D:128:VAL:O	1:D:128:VAL:HG12	2.17	0.44
2:K:100:VAL:CG2	2:K:100:VAL:O	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: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
3:N:35:TRP:CZ3	3:N:88:CYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:SER:HB3	2:H:56:SER:HB2	2.01	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:A:73:HIS:HB3	4:A:1130:SO4:O1	2.19	0.42
3:O:154:SER:HA	3:O:155:PRO:HD3	1.84	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:O:81:GLU:CD	3:O:81:GLU:H	2.23	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: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
3:M:61:ARG:NH2	3:M:82:ASP:CG	2.74	0.41
2:K:119:PRO:HB3	2:K:145:TYR:HB3	2.02	0.41
3:O:185:GLN:O	3:O:189:HIS:HD2	2.02	0.41
2:I:95:ASP:OD1	2:I:100(A):THR:HB	2.19	0.41
2:H:199:ASN:ND2	2:H:206:LYS:HG3	2.34	0.41
1:D:37:PRO:O	1:D:39:ARG:N	2.53	0.41
3:O:143:GLY:O	3:O:165:PRO:HG2	2.20	0.41
2:I:17:SER:HB2	2:I:82(A):ASN:HD22	1.86	0.41
1:A:74:LEU:O	1:A:88:ASN:HA	2.21	0.41
3:M:12:SER:HB3	3:M:105:THR:HB	2.02	0.41
2:H:201:LYS:N	2:H:202:PRO:CD	2.84	0.41
2:J:12:VAL:HG11	2:J:82(C):LEU:HD12	2.03	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
2:H:12:VAL:CG2	2:H:18:LEU:HD22	2.50	0.41
3:M:136:LEU:HD23	3:M:176:SER:HB3	2.03	0.41
1:A:38:LYS:HB2	1:A:44:TYR:CE1	2.55	0.41
2:I:193:THR:HB	2:I:210:LYS:HE3	2.02	0.41
2:I:67:PHE:CZ	2:I:82:MET:HG2	2.56	0.41
2:K:181:VAL:CG2	3:O:136:LEU:CD1	2.97	0.40
2:J:135:THR:HG22	2:J:136:ALA:N	2.36	0.40
3:M:116:VAL:HG21	3:M:196:VAL:HG13	2.02	0.40
2:H:17:SER:HA	2:H:82:MET:O	2.21	0.40
3:O:47:VAL:HG12	3:O:48:ILE:HG12	2.02	0.40
1:D:58:ASP:HA	1:D:59:PRO:HD2	1.83	0.40
3:N:2:PHE:CZ	3:N:97:VAL:HB	2.56	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
2:J:11:LEU:HB2	2:J:147:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:46:ILE:HD13	3:L:49:PHE:HB3	2.04	0.40
2:I:199:ASN:HD22	2:I:206:LYS:CG	2.34	0.40
1:B:73:HIS:HB3	4:B:1129:SO4:O2	2.21	0.40
1:C:63:PRO:HD2	1:C:98:VAL:HG12	2.03	0.40
1:C:42:ASP:HB3	1:C:46:ARG:HD3	2.02	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 ⓘ

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	82/137 (60%)	77 (94%)	3 (4%)	2 (2%)	7	12
1	B	74/137 (54%)	74 (100%)	0	0	100	100
1	C	74/137 (54%)	71 (96%)	2 (3%)	1 (1%)	14	26
1	D	73/137 (53%)	69 (94%)	3 (4%)	1 (1%)	14	26
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%)	19	37
2	K	213/225 (95%)	208 (98%)	5 (2%)	0	100	100
3	L	211/216 (98%)	201 (95%)	9 (4%)	1 (0%)	34	57
3	M	213/216 (99%)	202 (95%)	11 (5%)	0	100	100
3	N	211/216 (98%)	200 (95%)	9 (4%)	2 (1%)	21	40
3	O	212/216 (98%)	202 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2001/2312 (86%)	1915 (96%)	77 (4%)	9 (0%)	39	63

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
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%)	68 (88%)	9 (12%)	7	11
1	B	73/128 (57%)	62 (85%)	11 (15%)	3	5
1	C	74/128 (58%)	67 (90%)	7 (10%)	11	19
1	D	71/128 (56%)	65 (92%)	6 (8%)	13	24
2	H	178/187 (95%)	162 (91%)	16 (9%)	12	21
2	I	181/187 (97%)	160 (88%)	21 (12%)	7	11
2	J	175/187 (94%)	154 (88%)	21 (12%)	6	10
2	K	178/187 (95%)	159 (89%)	19 (11%)	8	14
3	L	184/188 (98%)	162 (88%)	22 (12%)	6	10
3	M	186/188 (99%)	161 (87%)	25 (13%)	5	8
3	N	184/188 (98%)	172 (94%)	12 (6%)	21	40
3	O	186/188 (99%)	166 (89%)	20 (11%)	8	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1747/2012 (87%)	1558 (89%)	189 (11%)	8 14

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	39	ARG
1	A	93	GLN
1	A	94	GLN
1	A	111	ARG
1	A	112	LEU
1	A	116	LEU
1	A	119	VAL
1	A	124	VAL
1	B	39	ARG
1	B	45	ASN
1	B	56	ASN
1	B	58	ASP
1	B	61	ARG
1	B	72	ARG
1	B	87	MET
1	B	93	GLN
1	B	95	GLU
1	B	96	ILE
1	B	97	LEU
1	C	42	ASP
1	C	56	ASN
1	C	58	ASP
1	C	80	ASP
1	C	99	LEU
1	C	111	ARG
1	C	116	LEU
1	D	53	LEU
1	D	55	ARG
1	D	68	GLU
1	D	70	LYS
1	D	72	ARG
1	D	93	GLN
2	H	19	ARG
2	H	35	SER
2	H	57	THR
2	H	76	ASN

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Mol	Chain	Res	Type
2	H	83	ARG
2	H	100(A)	THR
2	H	105	GLN
2	H	117	LYS
2	H	120	SER
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	13	GLN
2	I	17	SER
2	I	43	LYS
2	I	64	LYS
2	I	71	ARG
2	I	83	ARG
2	I	100(A)	THR
2	I	101	ARG
2	I	151	THR
2	I	159	LEU
2	I	178	LEU
2	I	182	VAL
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	215	SER
2	J	17	SER
2	J	43	LYS
2	J	57	THR
2	J	61	ASP
2	J	76	ASN
2	J	83	ARG
2	J	96	LEU
2	J	100(A)	THR
2	J	138	LEU

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Mol	Chain	Res	Type
2	J	148	GLN
2	J	151	THR
2	J	159	LEU
2	J	160	THR
2	J	164	HIS
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	K	4	LEU
2	K	5	LEU
2	K	12	VAL
2	K	57	THR
2	K	58	TYR
2	K	92	CYS
2	K	100	VAL
2	K	100(A)	THR
2	K	101	ARG
2	K	129	LYS
2	K	135	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	13	GLU
3	L	20	THR
3	L	27	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

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Mol	Chain	Res	Type
3	L	89	GLN
3	L	103	LYS
3	L	111	LYS
3	L	117	THR
3	L	145	VAL
3	L	146	THR
3	L	160	VAL
3	L	164	THR
3	L	172	LYS
3	L	196	VAL
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	72	SER
3	M	74	THR
3	M	78	LEU
3	M	83	GLU
3	M	89	GLN
3	M	117	THR
3	M	130	LYS
3	M	145	VAL
3	M	146	THR
3	M	157	LYS
3	M	160	VAL
3	M	164	THR
3	M	196	VAL
3	M	199	GLU
3	M	203	VAL
3	M	204	GLU
3	N	12	SER
3	N	28	LEU
3	N	45	THR
3	N	46	ILE
3	N	74	THR
3	N	89	GLN

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Mol	Chain	Res	Type
3	N	123	SER
3	N	145	VAL
3	N	146	THR
3	N	164	THR
3	N	171	ASN
3	N	203	VAL
3	O	6	GLN
3	O	19	VAL
3	O	27	SER
3	O	27(B)	SER
3	O	45	THR
3	O	46	ILE
3	O	52	ASN
3	O	56	SER
3	O	78	LEU
3	O	81	GLU
3	O	103	LYS
3	O	117	THR
3	O	133	LEU
3	O	145	VAL
3	O	150	LYS
3	O	154	SER
3	O	157	LYS
3	O	169	SER
3	O	203	VAL
3	O	211	GLU

Some 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	86	HIS
1	B	93	GLN
1	C	56	ASN
1	D	93	GLN
2	H	13	GLN
2	H	76	ASN
2	H	82(A)	ASN
2	H	105	GLN
2	H	148	GLN
2	H	199	ASN

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

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1130	-	4,4,4	0.25	0	6,6,6	0.15	0
4	SO4	B	1129	-	4,4,4	0.22	0	6,6,6	0.37	0
4	SO4	B	1130	-	4,4,4	0.27	0	6,6,6	0.19	0
4	SO4	C	1129	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	D	1129	-	4,4,4	0.22	0	6,6,6	0.25	0
4	SO4	I	1217	-	4,4,4	0.14	0	6,6,6	0.17	0
4	SO4	I	1218	-	4,4,4	0.25	0	6,6,6	0.38	0
4	SO4	L	1211	-	4,4,4	0.19	0	6,6,6	0.37	0
4	SO4	L	1212	-	4,4,4	0.17	0	6,6,6	0.11	0
4	SO4	M	1213	-	4,4,4	0.11	0	6,6,6	0.22	0
4	SO4	N	1211	-	4,4,4	0.11	0	6,6,6	0.18	0
4	SO4	O	1213	-	4,4,4	0.18	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1130	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1129	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1130	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1129	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1129	-	-	0/0/0/0	0/0/0/0
4	SO4	I	1217	-	-	0/0/0/0	0/0/0/0
4	SO4	I	1218	-	-	0/0/0/0	0/0/0/0
4	SO4	L	1211	-	-	0/0/0/0	0/0/0/0
4	SO4	L	1212	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1213	-	-	0/0/0/0	0/0/0/0
4	SO4	N	1211	-	-	0/0/0/0	0/0/0/0
4	SO4	O	1213	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1130	SO4	1	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%)	0.94	11 (12%) 5 3	33, 51, 62, 64	0
1	B	80/137 (58%)	0.78	5 (6%) 23 18	35, 50, 63, 65	0
1	C	80/137 (58%)	1.10	12 (15%) 3 1	34, 50, 63, 65	0
1	D	77/137 (56%)	0.96	10 (12%) 5 2	34, 48, 64, 65	0
2	H	216/225 (96%)	0.57	9 (4%) 40 33	29, 39, 47, 65	0
2	I	221/225 (98%)	0.51	1 (0%) 91 90	29, 39, 48, 79	0
2	J	211/225 (93%)	1.17	33 (15%) 3 1	31, 39, 46, 56	0
2	K	217/225 (96%)	0.44	2 (0%) 85 83	30, 39, 47, 66	0
3	L	213/216 (98%)	0.46	1 (0%) 91 90	32, 45, 55, 62	0
3	M	215/216 (99%)	0.48	3 (1%) 78 74	33, 45, 55, 80	0
3	N	213/216 (98%)	1.03	34 (15%) 3 1	33, 46, 55, 62	0
3	O	214/216 (99%)	0.53	6 (2%) 56 50	33, 45, 55, 74	0
All	All	2043/2312 (88%)	0.69	127 (6%) 24 18	29, 43, 58, 80	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	127	SER	7.6
2	J	210	LYS	6.4
2	J	187	SER	6.2
3	N	184	GLU	6.0
2	J	189	LEU	5.4
3	M	212	CYS	5.3
2	J	191	THR	5.1
3	N	127	GLN	4.9
2	H	127	SER	4.6
2	J	125	ALA	4.6
3	N	207	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	113	GLU	4.5
3	N	151	ALA	4.5
2	J	190	GLY	4.5
3	N	156	VAL	4.4
2	J	193	THR	4.3
1	D	36	ASN	4.3
1	A	112	LEU	4.3
2	J	136	ALA	4.2
2	J	137	ALA	4.2
1	D	57	GLU	4.2
2	J	184	VAL	4.2
2	H	216	CYS	4.1
1	D	98	VAL	4.1
3	N	143	GLY	4.1
3	N	204	GLU	4.1
3	O	211	GLU	4.0
2	H	215	SER	4.0
3	N	153	SER	3.9
3	N	191	SER	3.9
2	I	216	CYS	3.8
1	D	66	ILE	3.7
2	J	40	ALA	3.7
3	O	212	CYS	3.5
1	A	99	LEU	3.4
3	N	208	ALA	3.4
1	C	96	ILE	3.4
2	J	211	VAL	3.4
1	C	113	GLU	3.3
2	J	195	ILE	3.3
3	N	124	GLU	3.3
3	N	128	ALA	3.3
2	J	164	HIS	3.3
1	C	37	PRO	3.3
2	J	158	ALA	3.1
3	N	1	ASN	3.1
1	D	59	PRO	3.1
2	J	203	SER	3.1
1	C	57	GLU	3.1
1	B	36	ASN	3.1
3	N	181	LEU	3.0
2	K	215	SER	3.0
3	N	145	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	J	182	VAL	2.9
1	D	116	LEU	2.9
2	J	126	PRO	2.9
3	N	188	SER	2.9
3	N	186	TRP	2.8
3	N	122	SER	2.8
1	C	79	ALA	2.8
2	J	207	VAL	2.8
1	C	99	LEU	2.8
2	J	200	HIS	2.8
1	A	96	ILE	2.8
1	B	62	TYR	2.7
1	C	65	VAL	2.7
1	A	62	TYR	2.7
1	C	62	TYR	2.7
3	N	192	TYR	2.7
1	D	65	VAL	2.7
3	N	190	ARG	2.7
2	H	191	THR	2.7
2	J	160	THR	2.7
3	M	169	SER	2.7
3	N	134	VAL	2.7
3	M	211	GLU	2.7
3	O	169	SER	2.7
3	N	157	LYS	2.6
2	J	151	THR	2.6
2	H	164	HIS	2.6
3	N	152	ASP	2.6
2	J	82(B)	SER	2.6
3	N	210	THR	2.5
1	C	54	HIS	2.5
2	J	188	SER	2.5
1	C	94	GLN	2.5
1	C	58	ASP	2.5
1	D	56	ASN	2.4
1	C	66	ILE	2.4
3	N	147	VAL	2.4
3	O	210	THR	2.4
1	B	97	LEU	2.4
1	B	56	ASN	2.4
2	J	138	LEU	2.4
1	A	79	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	84	ALA	2.3
2	H	136	ALA	2.3
1	A	60	GLU	2.3
1	A	54	HIS	2.3
3	L	60	ASP	2.3
3	N	160	VAL	2.3
3	N	149	TRP	2.2
3	O	28	LEU	2.2
2	J	209	LYS	2.2
2	H	160	THR	2.2
3	O	105	THR	2.2
1	D	63	PRO	2.2
2	J	192	GLN	2.2
1	D	54	HIS	2.2
3	N	154	SER	2.1
3	N	121	PRO	2.1
2	J	74	SER	2.1
3	N	198	HIS	2.1
3	N	95	SER	2.1
3	N	199	GLU	2.1
2	H	213	PRO	2.1
3	N	88	CYS	2.1
1	A	65	VAL	2.1
2	J	177	SER	2.1
1	A	66	ILE	2.1
2	J	206	LYS	2.0
1	B	57	GLU	2.0
1	A	97	LEU	2.0
2	J	166	PHE	2.0
2	K	95	ASP	2.0
2	H	137	ALA	2.0
3	N	148	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	D	1129	5/5	0.92	0.44	7.69	67,69,69,70	0
4	SO4	L	1212	5/5	0.90	0.29	3.74	85,85,85,85	0
4	SO4	I	1218	5/5	0.92	0.29	2.17	74,74,76,77	0
4	SO4	A	1130	5/5	0.90	0.26	1.42	66,68,68,68	0
4	SO4	B	1129	5/5	0.95	0.26	0.51	53,53,55,55	0
4	SO4	C	1129	5/5	0.96	0.24	0.23	80,80,80,81	0
4	SO4	L	1211	5/5	0.92	0.19	-0.65	65,65,66,67	0
4	SO4	N	1211	5/5	0.86	0.22	-	93,94,94,94	0
4	SO4	O	1213	5/5	0.93	0.26	-	69,69,69,70	0
4	SO4	I	1217	5/5	0.94	0.29	-	74,74,75,75	0
4	SO4	B	1130	5/5	0.92	0.31	-	82,82,83,84	0
4	SO4	M	1213	5/5	0.97	0.12	-	68,70,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.