



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 01:54 PM EDT

PDB ID : 2AI0
Title : Anti-Cocaine Antibody 7.5.21, Crystal Form III
Authors : Pozharski, E.; Hewagama, A.; Shanafelt, A.; Ringe, D.; Petsko, G.A.
Deposited on : 2005-07-28
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

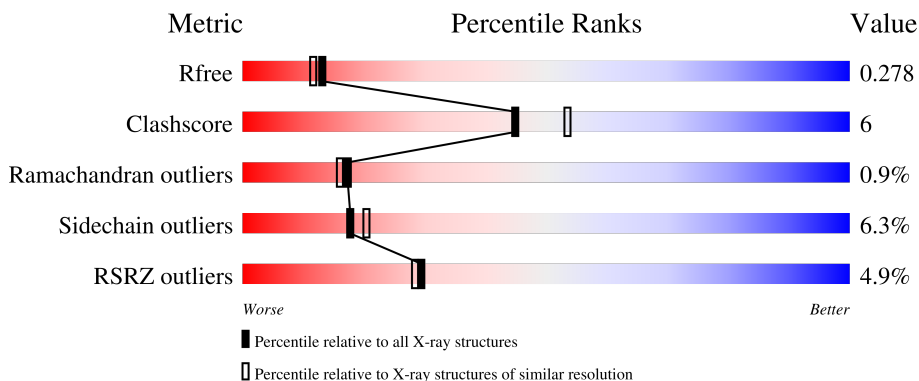
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	L	217	 3% 77% 20%
1	M	217	 3% 82% 15%
1	N	217	 6% 72% 24%
1	O	217	 0% 84% 14%
2	H	224	 4% 79% 14%

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Mol	Chain	Length	Quality of chain
2	I	224	
2	J	224	
2	K	224	

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
3	SO4	K	619	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14074 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 Immunoglobulin Light Chain kappa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	217	Total 1689	C 1056	N 290	O 336	S 7	0	0	0
1	M	214	Total 1668	C 1043	N 286	O 332	S 7	0	0	0
1	N	216	Total 1681	C 1052	N 288	O 334	S 7	0	0	0
1	O	217	Total 1689	C 1056	N 290	O 336	S 7	0	0	0

- Molecule 2 is a protein called Immunoglobulin Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	216	Total 1629	C 1028	N 276	O 318	S 7	0	0	0
2	I	223	Total 1691	C 1071	N 284	O 329	S 7	0	0	0
2	J	223	Total 1691	C 1071	N 284	O 329	S 7	0	0	0
2	K	218	Total 1646	C 1041	N 278	O 320	S 7	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	L	1	5	4	1	0	0
3	L	1	5	4	1	0	0
3	L	1	5	4	1	0	0
3	L	1	5	4	1	0	0
3	H	1	5	4	1	0	0
3	H	1	5	4	1	0	0
3	H	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	M	1	5	4	1	0	0
3	I	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0

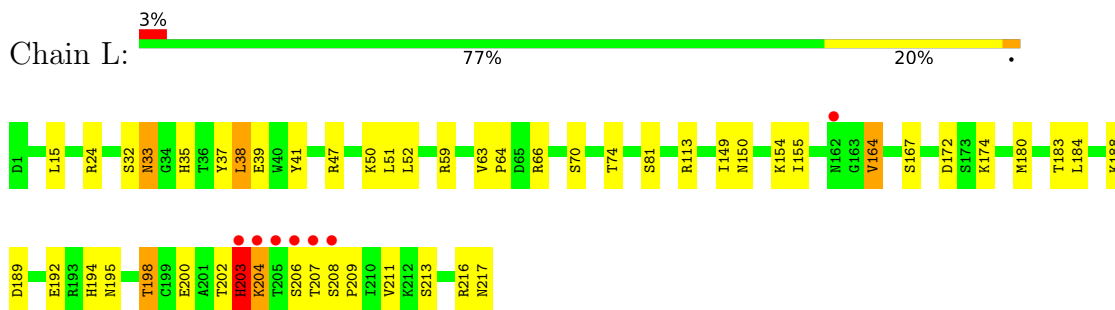
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	85	Total O 85 85	0	0
5	H	56	Total O 56 56	0	0
5	M	86	Total O 86 86	0	0
5	I	57	Total O 57 57	0	0
5	N	48	Total O 48 48	0	0
5	J	44	Total O 44 44	0	0
5	O	79	Total O 79 79	0	0
5	K	76	Total O 76 76	0	0

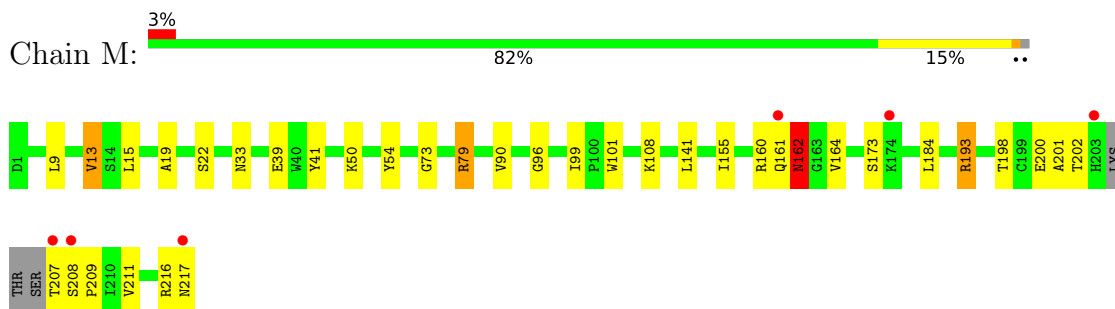
3 Residue-property plots [i](#)

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.

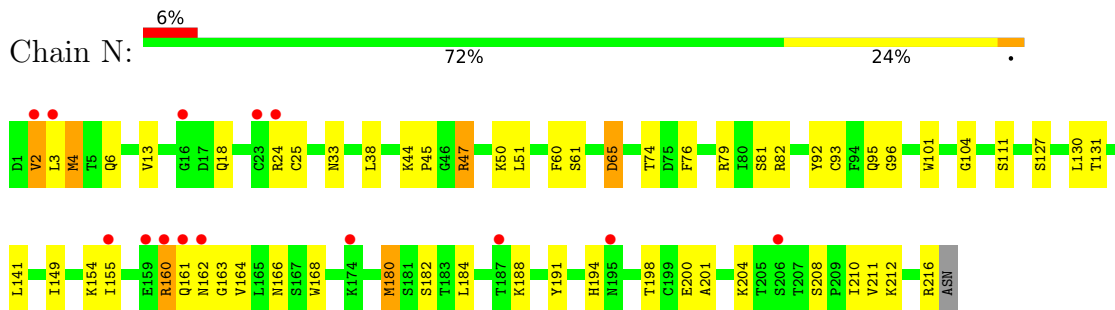
- Molecule 1: Immunoglobulin Light Chain kappa



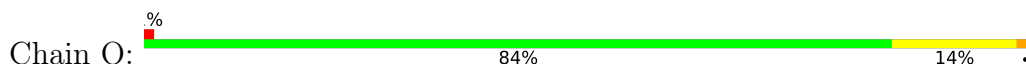
- Molecule 1: Immunoglobulin Light Chain kappa

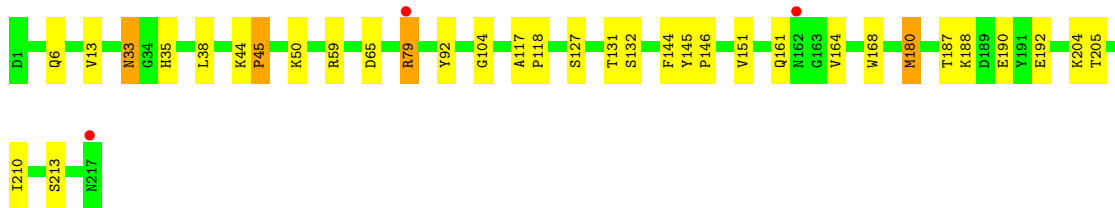


- Molecule 1: Immunoglobulin Light Chain kappa

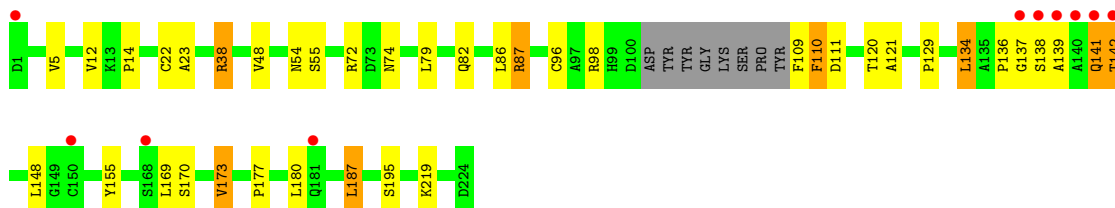
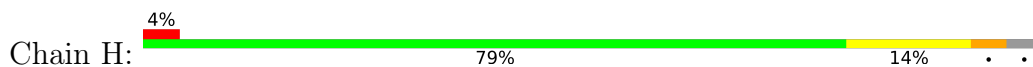


- Molecule 1: Immunoglobulin Light Chain kappa

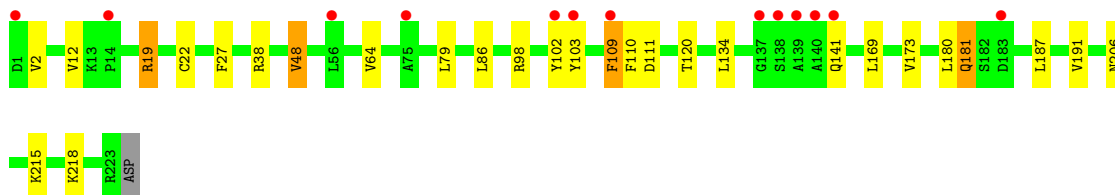
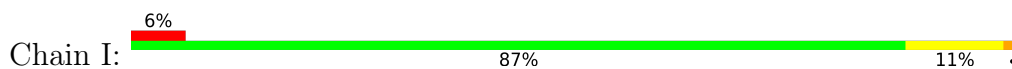




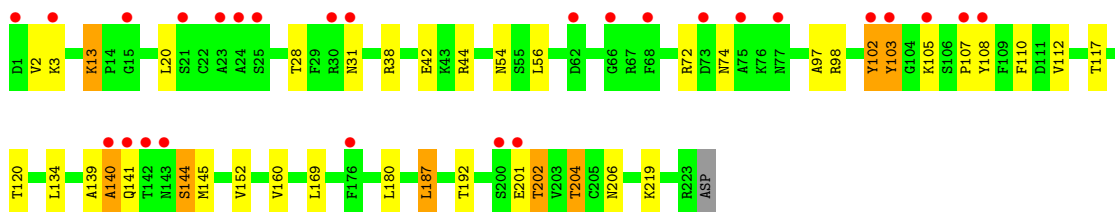
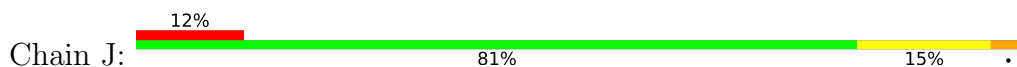
- Molecule 2: Immunoglobulin Heavy Chain



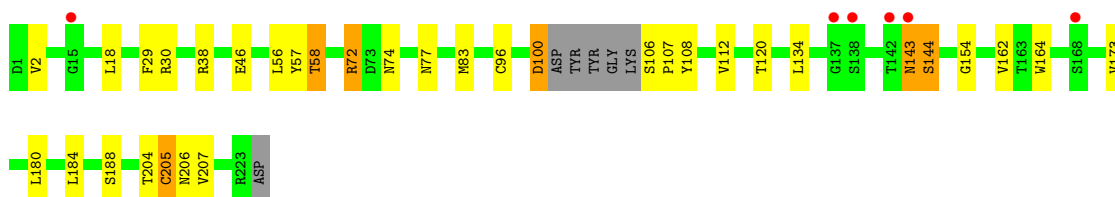
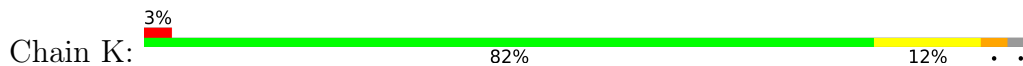
- Molecule 2: Immunoglobulin Heavy Chain



- Molecule 2: Immunoglobulin Heavy Chain



- Molecule 2: Immunoglobulin Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.98Å 216.35Å 58.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.20 38.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (129.10-2.20) 97.8 (38.49-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.20Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.279 0.221 , 0.278	Depositor DCC
R_{free} test set	5097 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14074	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.76 % 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 8.1065e-03. 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	L	0.52	0/1729	0.63	1/2344 (0.0%)
1	M	0.49	0/1707	0.63	1/2312 (0.0%)
1	N	0.47	0/1721	0.60	0/2333
1	O	0.53	0/1729	0.63	0/2344
2	H	0.54	1/1670 (0.1%)	0.69	2/2279 (0.1%)
2	I	0.48	0/1737	0.66	1/2372 (0.0%)
2	J	0.63	2/1737 (0.1%)	0.65	1/2372 (0.0%)
2	K	0.57	1/1689 (0.1%)	0.71	2/2306 (0.1%)
All	All	0.53	4/13719 (0.0%)	0.65	8/18662 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	13	LYS	CE-NZ	9.21	1.72	1.49
2	J	13	LYS	CD-CE	7.78	1.70	1.51
2	H	96	CYS	CB-SG	-6.55	1.71	1.82
2	K	96	CYS	CB-SG	-5.83	1.72	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	72	ARG	NE-CZ-NH2	-8.00	116.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	72	ARG	NE-CZ-NH1	7.72	124.16	120.30
2	J	13	LYS	CD-CE-NZ	-6.25	97.33	111.70
2	H	187	LEU	CA-CB-CG	6.24	129.65	115.30
2	I	109	PHE	N-CA-C	5.70	126.38	111.00
1	L	38	LEU	CA-CB-CG	-5.51	102.64	115.30
2	H	134	LEU	CA-CB-CG	5.20	127.25	115.30
1	M	193	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	143	ASN	Peptide

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	L	1689	0	1632	27	0
1	M	1668	0	1606	19	0
1	N	1681	0	1626	39	0
1	O	1689	0	1632	15	0
2	H	1629	0	1595	21	0
2	I	1691	0	1651	15	0
2	J	1691	0	1651	27	0
2	K	1646	0	1612	17	0
3	H	15	0	0	0	0
3	I	10	0	0	0	0
3	J	10	0	0	0	0
3	K	20	0	0	2	0
3	L	20	0	0	1	0
3	M	30	0	0	1	0
3	N	15	0	0	1	0
3	O	15	0	0	0	0
4	I	6	0	8	0	0
4	L	12	0	16	1	0
4	N	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	56	0	0	0	0
5	I	57	0	0	0	0
5	J	44	0	0	0	0
5	K	76	0	0	1	0
5	L	85	0	0	1	0
5	M	86	0	0	1	0
5	N	48	0	0	1	0
5	O	79	0	0	0	0
All	All	14074	0	13037	172	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 6.

All (172) 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:J:13:LYS:CE	2:J:13:LYS:NZ	1.72	1.53
1:N:101:TRP:CH2	2:J:107:PRO:O	2.18	0.96
2:H:98:ARG:O	2:H:110:PHE:HA	1.68	0.93
2:I:98:ARG:O	2:I:110:PHE:HA	1.74	0.87
1:M:79:ARG:HH11	1:M:79:ARG:HG2	1.40	0.85
1:M:41:TYR:OH	2:I:109:PHE:O	1.95	0.85
1:M:79:ARG:HH11	1:M:79:ARG:CG	1.90	0.84
1:N:101:TRP:HH2	2:J:107:PRO:O	1.59	0.83
1:L:172:ASP:OD1	1:L:174:LYS:HG2	1.79	0.82
1:L:203:HIS:HB2	1:L:206:SER:HB3	1.61	0.82
1:N:4:MET:CE	1:N:25:CYS:HB3	2.10	0.81
2:K:30:ARG:NH1	3:K:619:SO4:O1	2.16	0.78
1:N:50:LYS:HE2	3:N:615:SO4:O2	1.84	0.78
1:M:90:VAL:HG22	1:M:108:LYS:HG2	1.65	0.77
2:I:19:ARG:HG3	2:I:19:ARG:HH11	1.50	0.75
1:O:187:THR:OG1	1:O:190:GLU:HG3	1.91	0.71
1:N:160:ARG:HH11	1:N:160:ARG:CG	2.05	0.68
1:M:155:ILE:HD11	1:M:184:LEU:HD21	1.75	0.68
1:M:208:SER:HB2	1:M:209:PRO:HD2	1.74	0.68
2:J:13:LYS:NZ	2:J:13:LYS:CD	2.57	0.67
2:J:141:GLN:HG3	2:J:144:SER:HB2	1.77	0.67
1:N:4:MET:HE1	1:N:25:CYS:HB3	1.77	0.67
1:N:38:LEU:HD22	1:N:76:PHE:CG	2.30	0.67
2:K:18:LEU:HB3	2:K:83:MET:HE3	1.77	0.67
2:K:30:ARG:NH1	3:K:619:SO4:S	2.67	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:160:ARG:HH11	1:N:160:ARG:HG3	1.58	0.66
1:M:79:ARG:HG2	1:M:79:ARG:NH1	2.06	0.66
1:L:195:ASN:HD21	1:L:217:ASN:H	1.45	0.65
2:J:152:VAL:HB	2:J:187:LEU:HD23	1.79	0.65
1:L:50:LYS:HE3	1:L:51:LEU:O	1.97	0.64
1:N:168:TRP:CZ2	1:N:180:MET:HE2	2.32	0.64
1:N:130:LEU:O	1:N:188:LYS:HE2	1.97	0.64
2:K:58:THR:HG21	5:K:640:HOH:O	1.97	0.64
2:I:173:VAL:HG12	2:I:191:VAL:HG23	1.80	0.63
2:J:201:GLU:O	2:J:202:THR:HB	1.98	0.63
2:J:102:TYR:O	2:J:103:TYR:HB2	1.99	0.63
2:I:98:ARG:HD2	2:I:111:ASP:OD1	1.99	0.62
2:I:19:ARG:HG3	2:I:19:ARG:NH1	2.13	0.61
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.83	0.61
1:L:198:THR:HB	1:L:213:SER:OG	2.01	0.61
1:L:200:GLU:HG3	1:L:211:VAL:HG22	1.81	0.60
1:M:193:ARG:NH2	3:M:604:SO4:O3	2.34	0.60
1:N:4:MET:HB2	1:N:104:GLY:HA2	1.83	0.60
1:O:44:LYS:HB3	1:O:45:PRO:HD2	1.84	0.60
1:M:202:THR:HG22	5:M:700:HOH:O	2.02	0.60
2:K:100:ASP:HB2	2:K:106:SER:HB3	1.84	0.59
1:L:41:TYR:OH	2:H:109:PHE:O	2.20	0.59
2:I:102:TYR:CG	2:I:103:TYR:N	2.69	0.59
1:M:200:GLU:HG3	1:M:211:VAL:HG22	1.85	0.58
1:N:101:TRP:CZ3	2:J:107:PRO:O	2.56	0.58
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.33	0.58
2:H:54:ASN:O	2:H:55:SER:CB	2.51	0.58
2:H:38:ARG:HG2	2:H:48:VAL:HG21	1.86	0.58
1:N:6:GLN:HE21	1:N:104:GLY:HA3	1.67	0.58
2:J:152:VAL:HB	2:J:187:LEU:CD2	2.34	0.58
1:N:65:ASP:OD2	1:N:65:ASP:N	2.37	0.57
1:N:6:GLN:HE22	1:N:92:TYR:HA	1.68	0.57
2:H:14:PRO:HB3	2:H:87:ARG:HD2	1.87	0.56
1:N:44:LYS:HB3	1:N:45:PRO:HD2	1.85	0.56
2:K:72:ARG:CD	2:K:74:ASN:OD1	2.54	0.56
1:N:96:GLY:HA3	2:J:108:TYR:O	2.05	0.56
1:M:160:ARG:C	1:M:162:ASN:H	2.09	0.55
1:L:66:ARG:HB2	1:L:81:SER:O	2.06	0.55
1:M:39:GLU:HG3	1:M:54:TYR:HA	1.89	0.55
1:N:18:GLN:NE2	1:N:79:ARG:HD3	2.22	0.55
1:N:201:ALA:HB3	1:N:210:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:168:TRP:CD1	1:O:180:MET:HG3	2.43	0.54
2:J:42:GLU:OE1	2:J:44:ARG:NH2	2.40	0.54
2:I:22:CYS:HB3	2:I:79:LEU:HB3	1.90	0.54
2:K:72:ARG:HD3	2:K:74:ASN:OD1	2.09	0.53
2:J:31:ASN:HB2	2:J:105:LYS:HE2	1.90	0.53
2:J:72:ARG:NH1	2:J:74:ASN:OD1	2.42	0.53
1:L:202:THR:HG22	5:L:732:HOH:O	2.08	0.53
1:N:127:SER:O	1:N:131:THR:HG23	2.09	0.53
1:M:160:ARG:HG3	1:M:162:ASN:HB2	1.90	0.52
1:O:59:ARG:NE	1:O:65:ASP:HA	2.25	0.52
1:N:51:LEU:HD23	1:N:60:PHE:CD1	2.45	0.52
2:H:109:PHE:O	2:H:110:PHE:O	2.28	0.52
1:O:6:GLN:HE21	1:O:104:GLY:HA3	1.75	0.52
2:I:2:VAL:HG13	2:I:27:PHE:CD2	2.44	0.52
2:J:98:ARG:O	2:J:110:PHE:HA	2.10	0.51
2:K:106:SER:HA	2:K:108:TYR:H	1.75	0.51
2:K:143:ASN:N	2:K:144:SER:HB3	2.26	0.51
1:L:59:ARG:HD3	1:L:64:PRO:O	2.11	0.50
1:N:200:GLU:HG3	1:N:211:VAL:HG22	1.92	0.50
1:L:167:SER:OG	2:H:177:PRO:HD2	2.10	0.50
1:L:189:ASP:HB2	3:L:612:SO4:O4	2.12	0.49
2:I:48:VAL:CG2	2:I:64:VAL:HG11	2.42	0.49
1:L:208:SER:O	1:L:209:PRO:C	2.49	0.49
1:M:141:LEU:HD23	1:M:201:ALA:HB2	1.95	0.49
2:J:204:THR:HB	2:J:219:LYS:HA	1.94	0.49
1:L:52:LEU:HA	1:L:63:VAL:HG21	1.93	0.48
2:J:42:GLU:HB2	2:J:44:ARG:NH1	2.29	0.48
1:M:79:ARG:CG	1:M:79:ARG:NH1	2.60	0.48
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.94	0.48
2:J:97:ALA:HB1	2:J:110:PHE:HB3	1.96	0.48
1:N:6:GLN:NE2	1:N:93:CYS:H	2.11	0.48
1:N:82:ARG:HH12	4:N:703:GOL:H12	1.79	0.48
1:N:155:ILE:HD11	1:N:184:LEU:HD21	1.94	0.48
2:H:129:PRO:HB3	2:H:155:TYR:HB3	1.95	0.47
1:L:194:HIS:O	1:L:216:ARG:HD3	2.14	0.47
2:H:139:ALA:O	2:H:141:GLN:HG3	2.13	0.47
1:O:151:VAL:HG21	1:O:180:MET:SD	2.54	0.47
2:H:98:ARG:HD2	2:H:111:ASP:OD1	2.15	0.46
2:H:72:ARG:HD3	2:H:74:ASN:OD1	2.14	0.46
2:I:181:GLN:O	2:I:181:GLN:HG2	2.15	0.46
1:N:194:HIS:O	1:N:216:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:117:ALA:HB1	1:O:210:ILE:HD11	1.97	0.46
2:K:162:VAL:HG22	2:K:207:VAL:HG22	1.97	0.46
1:L:155:ILE:HD11	1:L:184:LEU:HD21	1.97	0.46
1:N:160:ARG:CG	1:N:160:ARG:NH1	2.70	0.46
2:I:12:VAL:HG21	2:I:86:LEU:HD13	1.97	0.46
1:L:113:ARG:HH22	4:L:702:GOL:H32	1.81	0.46
1:N:2:VAL:HG13	1:N:95:GLN:NE2	2.31	0.46
1:O:50:LYS:HE2	1:O:50:LYS:HB2	1.59	0.45
2:K:72:ARG:HD2	2:K:74:ASN:OD1	2.15	0.45
1:M:13:VAL:HG11	1:M:19:ALA:HB2	1.99	0.45
2:J:145:MET:HB3	2:J:192:THR:HG22	1.97	0.45
2:H:136:PRO:HD3	2:H:148:LEU:CD2	2.46	0.45
1:N:166:ASN:ND2	1:N:182:SER:OG	2.49	0.45
2:J:31:ASN:HB2	2:J:105:LYS:CE	2.47	0.45
1:N:154:LYS:HB2	1:N:198:THR:HB	1.99	0.45
1:O:6:GLN:HE22	1:O:92:TYR:HA	1.81	0.45
1:L:24:ARG:HA	1:L:74:THR:O	2.16	0.44
2:H:137:GLY:O	2:H:139:ALA:N	2.50	0.44
1:L:32:SER:HA	2:K:57:TYR:CD1	2.52	0.44
2:H:54:ASN:O	2:H:55:SER:HB3	2.16	0.44
2:H:170:SER:O	2:H:173:VAL:HG13	2.18	0.44
1:M:99:ILE:HG12	1:M:101:TRP:CH2	2.53	0.44
2:J:139:ALA:O	2:J:140:ALA:HB3	2.18	0.44
1:O:33:ASN:ND2	1:O:35:HIS:H	2.15	0.44
2:J:2:VAL:HG11	2:J:112:VAL:HG21	2.00	0.43
1:L:188:LYS:O	1:L:192:GLU:HG2	2.18	0.43
1:N:47:ARG:HD2	5:N:745:HOH:O	2.19	0.43
1:N:81:SER:O	1:N:82:ARG:HG3	2.17	0.43
1:L:216:ARG:O	1:L:217:ASN:HB2	2.17	0.43
1:N:13:VAL:O	1:N:111:SER:HA	2.18	0.43
1:N:25:CYS:SG	1:N:74:THR:HA	2.59	0.43
1:O:188:LYS:O	1:O:192:GLU:HG2	2.19	0.43
1:N:191:TYR:CZ	1:N:216:ARG:HD2	2.54	0.42
1:N:60:PHE:CG	1:N:61:SER:N	2.88	0.42
2:J:42:GLU:HB2	2:J:44:ARG:HH12	1.85	0.42
2:J:42:GLU:CB	2:J:44:ARG:HH12	2.32	0.42
1:M:96:GLY:HA2	1:M:101:TRP:CD1	2.54	0.42
1:N:168:TRP:CZ2	1:N:180:MET:CE	3.02	0.42
1:L:33:ASN:ND2	1:L:35:HIS:H	2.18	0.42
2:J:102:TYR:O	2:J:103:TYR:CB	2.68	0.42
1:L:154:LYS:HB2	1:L:198:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:212:LYS:HD3	1:N:212:LYS:HA	1.86	0.42
2:J:20:LEU:HD22	2:J:117:THR:HG21	2.02	0.42
1:L:203:HIS:HB3	1:L:204:LYS:H	1.54	0.41
1:M:207:THR:HA	1:M:208:SER:HA	1.66	0.41
1:L:149:ILE:CG2	1:L:180:MET:HE3	2.50	0.41
2:H:12:VAL:O	2:H:121:ALA:HA	2.21	0.41
2:K:154:GLY:HA2	2:K:184:LEU:HB3	2.02	0.41
1:O:118:PRO:HB3	1:O:144:PHE:HB3	2.03	0.41
2:K:2:VAL:HG11	2:K:112:VAL:HG21	2.02	0.41
2:I:102:TYR:CD1	2:I:103:TYR:HB2	2.56	0.41
1:O:79:ARG:CZ	1:O:79:ARG:HB2	2.51	0.41
1:O:127:SER:O	1:O:131:THR:HG23	2.21	0.41
2:I:206:ASN:HB3	2:I:215:LYS:HE2	2.03	0.41
2:J:3:LYS:HE2	2:J:3:LYS:HB3	1.94	0.41
1:O:145:TYR:CG	1:O:146:PRO:HA	2.56	0.41
2:K:38:ARG:HD2	2:K:46:GLU:OE1	2.20	0.41
2:K:29:PHE:HB2	2:K:77:ASN:HD22	1.86	0.41
2:H:5:VAL:HG13	2:H:23:ALA:HB3	2.02	0.40
2:I:48:VAL:HG22	2:I:64:VAL:HG21	2.03	0.40
1:L:37:TYR:O	1:L:39:GLU:OE1	2.39	0.40
1:L:164:VAL:HA	1:L:183:THR:O	2.22	0.40
2:H:12:VAL:HG21	2:H:86:LEU:CD1	2.50	0.40
1:N:141:LEU:HD23	1:N:149:ILE:HD13	2.03	0.40
2:K:164:TRP:CZ3	2:K:205:CYS:HB3	2.56	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	L	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	29 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	210/217 (97%)	202 (96%)	5 (2%)	3 (1%)	11	8
1	N	214/217 (99%)	203 (95%)	9 (4%)	2 (1%)	17	16
1	O	215/217 (99%)	206 (96%)	8 (4%)	1 (0%)	29	31
2	H	212/224 (95%)	203 (96%)	6 (3%)	3 (1%)	11	8
2	I	221/224 (99%)	211 (96%)	10 (4%)	0	100	100
2	J	221/224 (99%)	211 (96%)	6 (3%)	4 (2%)	8	5
2	K	214/224 (96%)	204 (95%)	8 (4%)	2 (1%)	17	16
All	All	1722/1764 (98%)	1644 (96%)	62 (4%)	16 (1%)	17	16

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	110	PHE
1	O	45	PRO
2	H	138	SER
1	N	33	ASN
2	J	102	TYR
2	J	103	TYR
2	J	202	THR
2	K	144	SER
1	M	162	ASN
2	J	140	ALA
2	H	142	THR
1	M	161	GLN
1	L	203	HIS
1	M	73	GLY
1	N	163	GLY
2	K	107	PRO

5.3.2 Protein sidechains [i](#)

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	L	194/194 (100%)	183 (94%)	11 (6%)	20	24
1	M	191/194 (98%)	178 (93%)	13 (7%)	16	17
1	N	193/194 (100%)	180 (93%)	13 (7%)	16	18
1	O	194/194 (100%)	183 (94%)	11 (6%)	20	24
2	H	184/191 (96%)	171 (93%)	13 (7%)	14	16
2	I	190/191 (100%)	179 (94%)	11 (6%)	20	23
2	J	190/191 (100%)	177 (93%)	13 (7%)	16	17
2	K	186/191 (97%)	175 (94%)	11 (6%)	19	23
All	All	1522/1540 (99%)	1426 (94%)	96 (6%)	18	20

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	15	LEU
1	L	33	ASN
1	L	38	LEU
1	L	47	ARG
1	L	70	SER
1	L	150	ASN
1	L	164	VAL
1	L	198	THR
1	L	203	HIS
1	L	204	LYS
1	L	207	THR
2	H	38	ARG
2	H	82	GLN
2	H	87	ARG
2	H	120	THR
2	H	134	LEU
2	H	141	GLN
2	H	142	THR
2	H	169	LEU
2	H	173	VAL
2	H	180	LEU
2	H	187	LEU
2	H	195	SER
2	H	219	LYS
1	M	9	LEU
1	M	13	VAL
1	M	15	LEU

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Mol	Chain	Res	Type
1	M	22	SER
1	M	33	ASN
1	M	50	LYS
1	M	79	ARG
1	M	162	ASN
1	M	164	VAL
1	M	173	SER
1	M	198	THR
1	M	216	ARG
1	M	217	ASN
2	I	19	ARG
2	I	38	ARG
2	I	48	VAL
2	I	120	THR
2	I	134	LEU
2	I	141	GLN
2	I	169	LEU
2	I	180	LEU
2	I	181	GLN
2	I	187	LEU
2	I	218	LYS
1	N	2	VAL
1	N	3	LEU
1	N	4	MET
1	N	24	ARG
1	N	47	ARG
1	N	65	ASP
1	N	160	ARG
1	N	161	GLN
1	N	162	ASN
1	N	164	VAL
1	N	180	MET
1	N	204	LYS
1	N	208	SER
2	J	28	THR
2	J	38	ARG
2	J	54	ASN
2	J	56	LEU
2	J	120	THR
2	J	134	LEU
2	J	144	SER
2	J	160	VAL

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Mol	Chain	Res	Type
2	J	169	LEU
2	J	180	LEU
2	J	187	LEU
2	J	204	THR
2	J	206	ASN
1	O	13	VAL
1	O	33	ASN
1	O	38	LEU
1	O	79	ARG
1	O	132	SER
1	O	161	GLN
1	O	164	VAL
1	O	180	MET
1	O	204	LYS
1	O	205	THR
1	O	213	SER
2	K	56	LEU
2	K	58	THR
2	K	100	ASP
2	K	120	THR
2	K	134	LEU
2	K	173	VAL
2	K	180	LEU
2	K	188	SER
2	K	204	THR
2	K	205	CYS
2	K	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	33	ASN
1	L	166	ASN
1	L	194	HIS
1	L	195	ASN
1	M	33	ASN
1	M	166	ASN
1	M	215	ASN
1	N	6	GLN
1	N	18	GLN
1	N	166	ASN
2	J	54	ASN

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Mol	Chain	Res	Type
2	J	78	ASN
1	O	6	GLN
1	O	33	ASN
1	O	35	HIS
1	O	166	ASN
1	O	195	ASN
2	K	77	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

31 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	$\# Z > 2$
3	SO4	M	608	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	I	620	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	M	614	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	O	627	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	L	612	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	N	613	-	4,4,4	0.12	0	6,6,6	0.15	0
3	SO4	K	619	-	4,4,4	0.12	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	H	610	-	4,4,4	0.14	0	6,6,6	0.15	0
4	GOL	L	704	-	5,5,5	0.34	0	5,5,5	0.35	0
3	SO4	I	618	-	4,4,4	0.11	0	6,6,6	0.23	0
4	GOL	N	703	-	5,5,5	0.41	0	5,5,5	0.28	0
4	GOL	L	702	-	5,5,5	0.40	0	5,5,5	0.38	0
3	SO4	L	625	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	L	609	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	L	602	-	4,4,4	0.22	0	6,6,6	0.37	0
3	SO4	M	604	-	4,4,4	0.20	0	6,6,6	0.28	0
3	SO4	O	611	-	4,4,4	0.11	0	6,6,6	0.25	0
3	SO4	H	605	-	4,4,4	0.15	0	6,6,6	0.40	0
4	GOL	I	701	-	5,5,5	0.33	0	5,5,5	0.41	0
3	SO4	N	615	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	M	622	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	K	626	-	4,4,4	0.18	0	6,6,6	0.26	0
3	SO4	J	616	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	H	623	-	4,4,4	0.17	0	6,6,6	0.19	0
3	SO4	O	607	-	4,4,4	0.19	0	6,6,6	0.41	0
3	SO4	K	617	-	4,4,4	0.12	0	6,6,6	0.23	0
3	SO4	K	621	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	M	603	-	4,4,4	0.09	0	6,6,6	0.39	0
3	SO4	J	624	-	4,4,4	0.13	0	6,6,6	0.22	0
3	SO4	M	606	-	4,4,4	0.12	0	6,6,6	0.23	0
3	SO4	N	601	-	4,4,4	0.22	0	6,6,6	0.42	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	GOL	L	702	-	-	4/4/4/4	-
4	GOL	N	703	-	-	0/4/4/4	-
4	GOL	I	701	-	-	4/4/4/4	-
4	GOL	L	704	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	702	GOL	C1-C2-C3-O3
4	L	702	GOL	O2-C2-C3-O3
4	I	701	GOL	O1-C1-C2-C3
4	I	701	GOL	C1-C2-C3-O3
4	L	702	GOL	O1-C1-C2-C3
4	I	701	GOL	O2-C2-C3-O3
4	L	702	GOL	O1-C1-C2-O2
4	I	701	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	612	SO4	1	0
3	K	619	SO4	2	0
4	N	703	GOL	1	0
4	L	702	GOL	1	0
3	M	604	SO4	1	0
3	N	615	SO4	1	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	L	217/217 (100%)	0.27	7 (3%) 47 45	33, 41, 52, 66	0
1	M	214/217 (98%)	0.28	6 (2%) 53 51	39, 47, 61, 70	0
1	N	216/217 (99%)	0.41	14 (6%) 18 17	41, 52, 61, 65	0
1	O	217/217 (100%)	-0.02	3 (1%) 75 73	39, 47, 56, 64	0
2	H	216/224 (96%)	0.28	10 (4%) 32 31	33, 42, 56, 70	0
2	I	223/224 (99%)	0.45	13 (5%) 23 22	41, 50, 62, 79	0
2	J	223/224 (99%)	0.74	27 (12%) 4 3	42, 52, 61, 66	0
2	K	218/224 (97%)	0.25	6 (2%) 53 51	38, 45, 56, 66	0
All	All	1744/1764 (98%)	0.34	86 (4%) 29 28	33, 47, 60, 79	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	205	THR	8.6
2	I	139	ALA	8.5
1	L	204	LYS	7.9
2	I	102	TYR	7.4
2	H	139	ALA	6.9
2	I	138	SER	5.8
1	L	206	SER	4.9
1	L	207	THR	4.6
2	J	141	GLN	4.5
2	K	143	ASN	4.4
2	H	137	GLY	4.4
2	K	137	GLY	4.4
2	H	138	SER	4.3
2	J	66	GLY	4.2
2	J	201	GLU	4.2
2	J	24	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	140	ALA	4.1
1	L	203	HIS	4.0
1	N	162	ASN	4.0
2	J	30	ARG	3.9
1	L	208	SER	3.8
2	J	102	TYR	3.7
2	H	142	THR	3.7
2	J	3	LYS	3.7
2	J	1	ASP	3.7
2	K	138	SER	3.6
2	J	103	TYR	3.6
2	H	141	GLN	3.6
2	J	140	ALA	3.4
2	J	108	TYR	3.3
2	I	75	ALA	3.3
1	N	195	ASN	3.3
1	M	217	ASN	3.2
2	J	21	SER	3.1
2	J	105	LYS	3.1
2	J	142	THR	3.1
2	J	143	ASN	3.1
1	M	203	HIS	3.1
2	J	23	ALA	3.0
2	J	68	PHE	3.0
1	N	161	GLN	3.0
1	N	187	THR	2.8
2	J	15	GLY	2.8
1	N	3	LEU	2.8
2	H	168	SER	2.6
2	J	77	ASN	2.6
1	N	160	ARG	2.5
1	N	2	VAL	2.5
2	I	109	PHE	2.5
2	J	31	ASN	2.5
1	N	206	SER	2.5
2	I	137	GLY	2.5
2	J	62	ASP	2.5
1	N	24	ARG	2.5
1	N	16	GLY	2.5
1	N	174	LYS	2.5
2	I	141	GLN	2.4
2	J	200	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	181	GLN	2.4
2	I	14	PRO	2.3
1	O	217	ASN	2.3
2	J	25	SER	2.3
2	H	150	CYS	2.3
1	O	162	ASN	2.3
2	K	142	THR	2.2
2	I	183	ASP	2.2
2	J	73	ASP	2.2
2	J	75	ALA	2.2
2	J	107	PRO	2.2
2	I	140	ALA	2.2
2	I	103	TYR	2.2
2	I	56	LEU	2.1
1	L	162	ASN	2.1
2	K	168	SER	2.1
2	J	176	PHE	2.1
2	K	15	GLY	2.1
1	N	23	CYS	2.1
1	M	174	LYS	2.1
1	N	159	GLU	2.1
2	I	1	ASP	2.1
2	H	1	ASP	2.0
1	M	161	GLN	2.0
1	N	155	ILE	2.0
1	M	207	THR	2.0
1	M	208	SER	2.0
1	O	79	ARG	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 monosaccharides 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(Å ²)	Q<0.9
3	SO4	O	627	5/5	0.54	0.31	153,153,153,153	0
4	GOL	L	702	6/6	0.82	0.24	73,75,75,75	0
3	SO4	L	625	5/5	0.83	0.20	62,62,62,63	5
3	SO4	J	624	5/5	0.84	0.40	48,50,52,52	5
4	GOL	L	704	6/6	0.84	0.20	59,59,60,60	0
3	SO4	H	623	5/5	0.85	0.39	56,56,57,58	5
3	SO4	I	620	5/5	0.86	0.13	98,98,98,98	0
3	SO4	K	626	5/5	0.86	0.37	87,87,87,88	0
4	GOL	I	701	6/6	0.86	0.14	53,55,56,56	0
4	GOL	N	703	6/6	0.86	0.18	90,91,92,92	0
3	SO4	M	622	5/5	0.87	0.19	64,64,65,65	5
3	SO4	J	616	5/5	0.90	0.10	58,58,59,59	5
3	SO4	N	615	5/5	0.90	0.15	56,56,56,57	5
3	SO4	K	621	5/5	0.92	0.17	87,87,88,89	0
3	SO4	O	611	5/5	0.92	0.25	70,71,71,72	0
3	SO4	N	613	5/5	0.93	0.18	75,75,76,76	0
3	SO4	L	612	5/5	0.93	0.20	76,76,76,77	0
3	SO4	M	614	5/5	0.94	0.13	50,50,51,51	5
3	SO4	K	619	5/5	0.94	0.29	70,70,71,71	0
3	SO4	L	609	5/5	0.96	0.18	68,68,68,68	0
3	SO4	N	601	5/5	0.96	0.15	42,43,46,47	0
3	SO4	I	618	5/5	0.96	0.22	70,71,72,72	0
3	SO4	M	606	5/5	0.97	0.11	58,59,60,61	0
3	SO4	K	617	5/5	0.98	0.34	34,35,35,35	5
3	SO4	M	608	5/5	0.98	0.19	76,76,76,76	0
3	SO4	H	610	5/5	0.98	0.19	63,64,64,65	0
3	SO4	L	602	5/5	0.98	0.06	40,41,43,44	0
3	SO4	M	603	5/5	0.98	0.13	46,46,47,48	0
3	SO4	O	607	5/5	0.98	0.10	57,57,58,60	0
3	SO4	M	604	5/5	0.98	0.11	52,53,53,54	0
3	SO4	H	605	5/5	0.98	0.13	46,47,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.