



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2023 – 06:28 AM EST

PDB ID : 7TQA
Title : Crystal Structure of monoclonal S9.6 Fab
Authors : Bou-Nader, C.; Zhang, J.
Deposited on : 2022-01-26
Resolution : 2.33 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)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

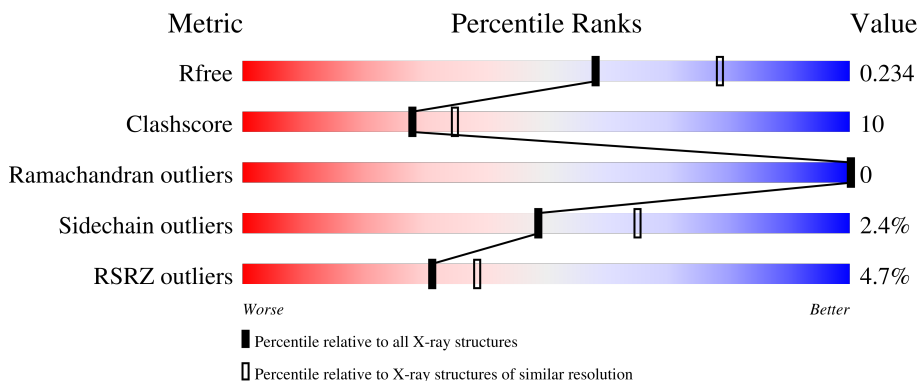
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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.



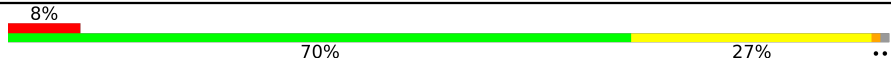
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	231	4% 78% 15% 6%
1	C	231	6% 73% 20% 6%
1	H	231	7% 69% 22% 9%
2	B	219	87% 12%
2	D	219	% 82% 17%

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Mol	Chain	Length	Quality of chain
2	L	219	 <p>8% 70% 27% ..</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10314 atoms, of which 8 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 Fab S9.6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	210	Total 1578	C 1002	N 254	O 314	S 8	0	3	0
1	C	218	Total 1645	C 1048	N 266	O 322	S 9	0	2	0
1	A	216	Total 1609	C 1024	N 255	O 322	S 8	0	0	0

- Molecule 2 is a protein called Fab S9.6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	216	Total 1631	C 1023	N 270	O 332	S 6	0	1	0
2	D	219	Total 1673	C 1048	N 276	O 343	S 6	0	0	0
2	B	219	Total 1686	C 1054	N 282	O 344	S 6	0	1	0

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	C	1	14	3	8	3	0	0

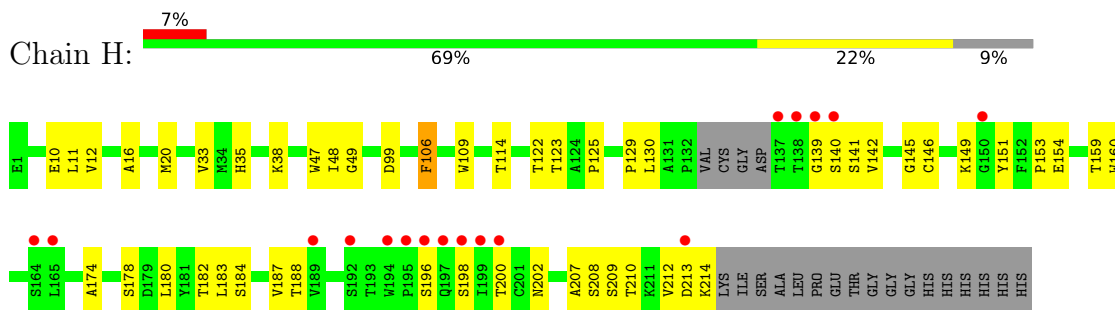
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	78	Total	O	0	0
			78	78		
5	L	61	Total	O	0	0
			61	61		
5	C	67	Total	O	0	0
			67	67		
5	D	61	Total	O	0	0
			61	61		
5	A	65	Total	O	0	0
			65	65		
5	B	86	Total	O	0	0
			86	86		

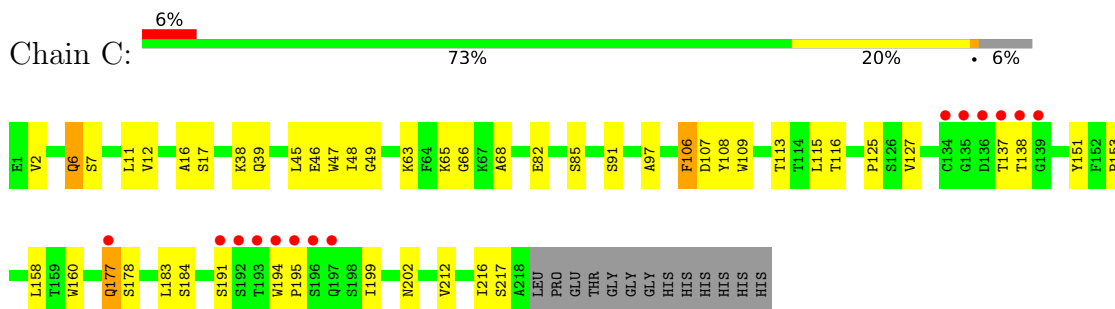
3 Residue-property plots [i](#)

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.

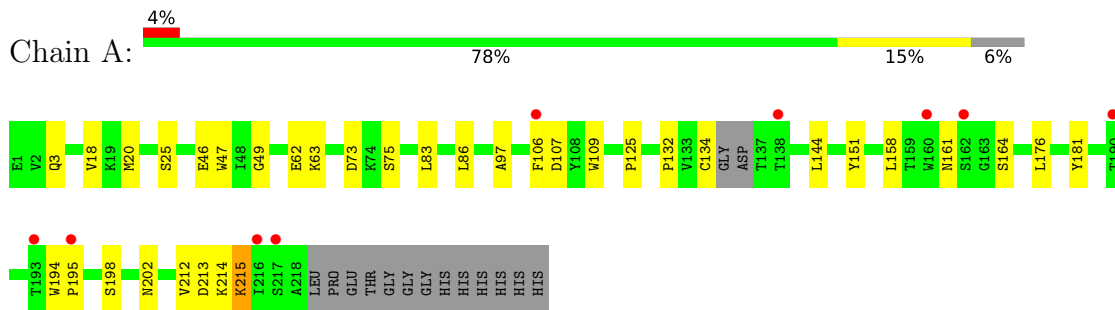
- Molecule 1: Fab S9.6 heavy chain



- Molecule 1: Fab S9.6 heavy chain

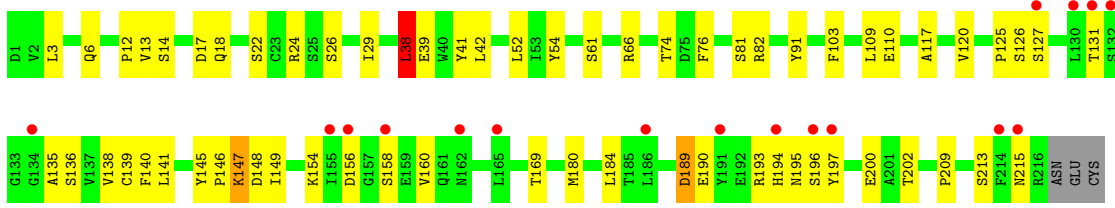


- Molecule 1: Fab S9.6 heavy chain

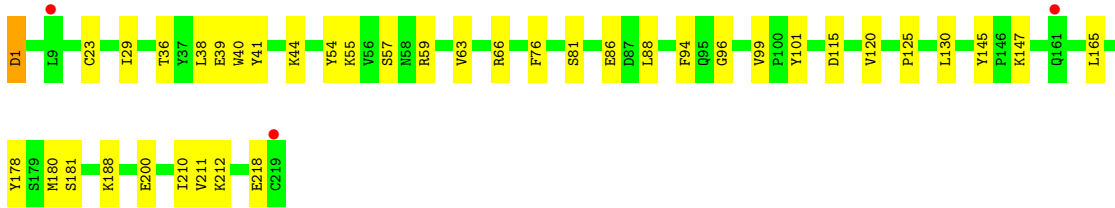
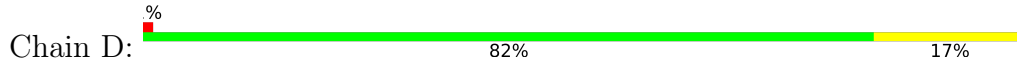


- Molecule 2: Fab S9.6 light chain

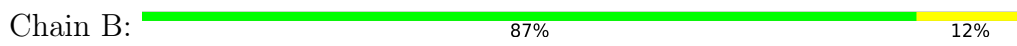




● Molecule 2: Fab S9.6 light chain



● Molecule 2: Fab S9.6 light chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	96.65Å 96.65Å 140.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.70 – 2.33 45.70 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.70-2.33) 99.6 (45.70-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.32Å)	Xtrriage
Refinement program	PHENIX 1.14 3260	Depositor
R, R_{free}	0.179 , 0.235 0.179 , 0.234	Depositor DCC
R_{free} test set	2897 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.030 for h,-h-k,-l 0.016 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10314	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 [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	A	0.45	0/1652	0.63	1/2260 (0.0%)
1	C	0.44	0/1689	0.64	1/2305 (0.0%)
1	H	0.42	0/1619	0.60	0/2208
2	B	0.45	0/1725	0.63	0/2343
2	D	0.44	0/1712	0.61	1/2328 (0.0%)
2	L	0.44	0/1669	0.59	1/2272 (0.0%)
All	All	0.44	0/10066	0.62	4/13716 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	55	LYS	CB-CA-C	6.70	123.80	110.40
1	C	107	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	107	ASP	CB-CG-OD1	5.44	123.19	118.30
2	L	38	LEU	CA-CB-CG	-5.41	102.87	115.30

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	1609	0	1521	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1645	0	1581	34	0
1	H	1578	0	1479	43	0
2	B	1686	0	1595	16	0
2	D	1673	0	1579	30	0
2	L	1631	0	1522	51	0
3	A	5	0	0	0	0
3	B	25	0	0	0	0
3	C	5	0	0	1	0
3	D	10	0	0	1	0
3	H	10	0	0	0	0
3	L	5	0	0	0	0
4	C	6	8	8	0	0
5	A	65	0	0	1	0
5	B	86	0	0	0	0
5	C	67	0	0	1	0
5	D	61	0	0	2	0
5	H	78	0	0	1	0
5	L	61	0	0	3	0
All	All	10306	8	9285	190	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 10.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:CE2	1:A:109:TRP:CZ2	2.41	1.08
1:C:177:GLN:HG3	2:D:165:LEU:HD21	1.38	1.05
1:H:139:GLY:HA2	2:B:161:GLN:HB2	1.40	0.99
1:H:125:PRO:HB3	1:H:151:TYR:HB3	1.58	0.86
1:A:106:PHE:CE2	1:A:109:TRP:HZ2	1.89	0.85
2:B:24:ARG:HD2	2:B:75:ASP:OD1	1.77	0.85
1:A:125:PRO:HB3	1:A:151:TYR:HB3	1.63	0.80
2:L:202:THR:HG23	5:L:416:HOH:O	1.86	0.75
1:C:194:TRP:HD1	1:C:199:ILE:HD13	1.52	0.73
1:A:194:TRP:HB3	1:A:195:PRO:HD3	1.70	0.73
1:H:130:LEU:HB2	1:H:145:GLY:CA	2.21	0.70
2:L:202:THR:HG22	2:L:209:PRO:HB3	1.74	0.70
1:C:194:TRP:CD1	1:C:199:ILE:HD13	2.27	0.69
2:L:127:SER:O	2:L:131:THR:HG23	1.92	0.69
2:L:6:GLN:NE2	2:L:91:TYR:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:ARG:HG2	2:D:63:VAL:HB	1.76	0.68
2:D:200:GLU:HG2	2:D:211:VAL:HG22	1.76	0.67
1:C:65:LYS:HD2	1:C:66:GLY:H	1.59	0.67
1:A:106:PHE:HE2	1:A:109:TRP:CZ2	2.05	0.67
1:A:202:ASN:HD22	1:A:212:VAL:HG12	1.59	0.67
1:C:106:PHE:CE1	1:C:109:TRP:CZ2	2.83	0.66
1:C:7:SER:HA	3:C:302:SO4:O2	1.96	0.66
1:H:200:THR:HA	1:H:214:LYS:O	1.96	0.65
1:H:122:THR:CG2	1:H:208:SER:HB3	2.27	0.65
1:A:198:SER:HB2	1:A:214:LYS:HE3	1.78	0.65
2:L:196:SER:H	2:L:215:ASN:CB	2.09	0.65
1:A:106:PHE:CE2	2:B:41:TYR:CZ	2.86	0.64
2:L:200:GLU:HG3	2:L:209:PRO:HB2	1.80	0.64
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.32	0.64
1:A:106:PHE:HE2	1:A:109:TRP:HZ2	1.36	0.63
2:L:136:SER:HA	2:L:184:LEU:O	1.97	0.63
2:L:196:SER:H	2:L:215:ASN:HB3	1.62	0.63
1:A:106:PHE:CE2	1:A:109:TRP:CE2	2.87	0.62
1:C:106:PHE:CE1	2:D:41:TYR:CZ	2.88	0.62
2:L:42:LEU:HB2	2:L:52:LEU:HD11	1.82	0.62
2:L:156:ASP:OD2	2:L:193:ARG:HB3	2.00	0.62
1:H:130:LEU:HB2	1:H:145:GLY:HA3	1.81	0.61
2:B:39:GLU:HG3	2:B:54:TYR:HA	1.81	0.61
2:L:135:ALA:HB1	2:L:190:GLU:HG3	1.83	0.60
2:L:190:GLU:HA	2:L:197:TYR:OH	2.02	0.60
2:L:149:ILE:HG21	2:L:180:MET:HE2	1.82	0.59
1:H:106:PHE:CE2	1:H:109:TRP:CZ2	2.90	0.59
2:L:29:ILE:HG22	2:L:29:ILE:O	2.03	0.58
2:L:14:SER:HB2	2:L:17:ASP:OD2	2.02	0.58
2:D:130:LEU:HB3	2:D:188:LYS:HE2	1.86	0.58
2:B:24:ARG:HA	2:B:74:THR:O	2.03	0.58
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.39	0.58
1:C:177:GLN:HG3	2:D:165:LEU:CD2	2.24	0.58
2:D:29:ILE:HD11	2:D:76:PHE:CZ	2.39	0.57
2:L:13:VAL:CG2	2:L:109:LEU:HD21	2.34	0.57
2:D:210:ILE:HD12	2:D:210:ILE:N	2.20	0.57
1:A:134:CYS:SG	2:B:219:CYS:HA	2.45	0.57
2:B:3:LEU:HB2	2:B:26:SER:HB3	1.87	0.56
2:L:39:GLU:HG3	2:L:54:TYR:HA	1.87	0.56
1:H:183:LEU:HD23	1:H:184:SER:N	2.20	0.55
1:C:6:GLN:HG2	5:C:422:HOH:O	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:LEU:HB2	1:H:153:PRO:HG3	1.87	0.55
1:A:106:PHE:CZ	1:A:109:TRP:CZ2	2.94	0.55
1:H:178:SER:O	1:H:180:LEU:HD12	2.07	0.55
2:L:147:LYS:HD2	2:L:147:LYS:C	2.27	0.55
1:C:39:GLN:HB2	1:C:45:LEU:HD23	1.88	0.55
1:H:149:LYS:HA	1:H:182:THR:HG23	1.89	0.54
2:D:120:VAL:O	2:D:212:LYS:HE3	2.07	0.54
2:D:218:GLU:N	2:D:218:GLU:OE2	2.41	0.54
1:C:65:LYS:HD2	1:C:66:GLY:N	2.21	0.54
1:C:2:VAL:HG11	1:C:108:TYR:CD2	2.43	0.54
2:D:1:ASP:OD1	5:D:401:HOH:O	2.18	0.53
1:A:125:PRO:CB	1:A:151:TYR:HB3	2.35	0.53
2:L:195:ASN:HA	2:L:215:ASN:HB2	1.90	0.53
1:A:18:VAL:HG12	1:A:86:LEU:HD11	1.91	0.53
2:D:99:VAL:HG13	3:D:302:SO4:O2	2.10	0.52
1:H:154:GLU:OE2	1:H:174:ALA:HB3	2.08	0.52
2:L:66:ARG:HD2	2:L:82:ARG:O	2.09	0.52
2:D:125:PRO:HA	5:D:407:HOH:O	2.09	0.52
2:D:96:GLY:HA2	2:D:101:TYR:CD1	2.45	0.52
1:C:106:PHE:CE1	1:C:109:TRP:HZ2	2.28	0.52
1:H:198:SER:C	1:H:200:THR:H	2.12	0.52
2:L:190:GLU:O	2:L:194:HIS:HA	2.10	0.52
1:H:129:PRO:HD2	2:L:126:SER:OG	2.10	0.51
2:L:195:ASN:CB	2:L:215:ASN:HB2	2.41	0.51
2:D:29:ILE:HD11	2:D:76:PHE:CE1	2.46	0.50
2:L:24:ARG:HA	2:L:74:THR:O	2.11	0.50
1:C:12:VAL:CG1	1:C:16:ALA:HB3	2.42	0.50
1:A:132:PRO:HD3	1:A:144:LEU:HD23	1.93	0.49
1:C:46:GLU:OE2	1:C:63:LYS:HD3	2.12	0.49
1:A:161:ASN:O	1:A:164:SER:HB3	2.12	0.49
2:D:44:LYS:HE2	2:D:86:GLU:O	2.13	0.49
1:H:122:THR:HG21	1:H:208:SER:HB3	1.95	0.49
2:L:154:LYS:HA	2:L:158:SER:O	2.13	0.49
1:C:160:TRP:HZ3	1:C:216:ILE:HD13	1.78	0.48
2:D:39:GLU:HG3	2:D:54:TYR:HA	1.94	0.48
1:C:38:LYS:HB2	1:C:48:ILE:HD11	1.95	0.48
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.95	0.48
2:L:194:HIS:O	2:L:215:ASN:O	2.32	0.48
1:H:146[B]:CYS:HB2	1:H:160:TRP:CH2	2.49	0.48
1:H:159:THR:OG1	1:H:202:ASN:HB2	2.13	0.48
1:C:106:PHE:HE1	2:D:41:TYR:CZ	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:HG12	1:C:16:ALA:HB3	1.95	0.47
1:A:73:ASP:OD1	1:A:75:SER:HB2	2.14	0.47
2:L:195:ASN:CA	2:L:215:ASN:HB2	2.43	0.47
1:A:20:MET:HE1	1:A:83:LEU:HD11	1.96	0.47
1:A:20:MET:HE1	1:A:83:LEU:CD1	2.44	0.47
2:B:29:ILE:HD11	2:B:76:PHE:CE1	2.49	0.47
2:L:3:LEU:HB2	2:L:26:SER:HB3	1.97	0.47
1:H:106:PHE:HZ	2:L:103:PHE:CZ	2.33	0.47
2:L:109:LEU:HD23	2:L:110:GLU:N	2.30	0.47
1:C:194:TRP:HB3	1:C:195:PRO:HD3	1.95	0.47
1:C:127:VAL:HB	1:C:212:VAL:HG11	1.97	0.47
1:H:20:MET:HB3	5:H:436:HOH:O	2.14	0.46
1:H:35:HIS:CD2	1:H:99:ASP:HB2	2.50	0.46
2:L:141:LEU:HD12	2:L:141:LEU:N	2.30	0.46
2:L:141:LEU:HD22	2:L:180:MET:CE	2.46	0.46
1:C:158:LEU:HA	1:C:202:ASN:O	2.16	0.46
1:H:210:THR:HG22	1:H:212:VAL:HG23	1.97	0.46
1:A:20:MET:HB3	5:A:442:HOH:O	2.14	0.46
1:C:68:ALA:HA	1:C:82:GLU:O	2.15	0.46
2:D:130:LEU:O	2:D:188:LYS:HE3	2.15	0.46
2:B:16:GLY:O	2:B:82:ARG:HD3	2.15	0.46
1:H:208:SER:O	1:H:209:SER:OG	2.32	0.46
1:H:142:VAL:O	1:H:188:THR:HA	2.15	0.45
2:L:18:GLN:HA	2:L:81:SER:O	2.17	0.45
1:H:210:THR:CG2	1:H:212:VAL:HG23	2.46	0.45
2:B:59:ARG:HG2	2:B:63:VAL:HB	1.97	0.45
2:D:29:ILE:HG13	2:D:36:THR:HG23	1.99	0.45
1:A:97:ALA:HB1	1:A:106:PHE:HB2	1.97	0.45
1:A:62:GLU:OE1	1:A:62:GLU:HA	2.17	0.45
1:H:10:GLU:HG2	1:H:114[B]:THR:O	2.16	0.45
1:C:177:GLN:O	1:C:178:SER:HB2	2.17	0.45
2:L:193:ARG:O	2:L:195:ASN:N	2.49	0.45
1:H:10:GLU:HG2	1:H:114[A]:THR:O	2.16	0.44
2:L:147:LYS:HE3	2:L:148:ASP:OD2	2.17	0.44
1:A:106:PHE:CD2	1:A:109:TRP:NE1	2.84	0.44
2:L:13:VAL:HG21	2:L:109:LEU:HD21	1.99	0.44
2:L:160:VAL:O	2:L:160:VAL:HG13	2.16	0.44
2:L:189:ASP:OD2	2:L:189:ASP:N	2.47	0.44
1:H:106:PHE:HZ	2:L:103:PHE:HZ	1.66	0.44
1:A:106:PHE:CE2	2:B:41:TYR:CE2	3.05	0.44
1:A:198:SER:CB	1:A:214:LYS:HE3	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:HD23	1:C:184:SER:N	2.32	0.44
2:D:180:MET:HG2	2:D:181:SER:N	2.32	0.44
1:A:158:LEU:HA	1:A:202:ASN:O	2.18	0.44
1:H:125:PRO:CB	1:H:151:TYR:HB3	2.40	0.44
2:D:88:LEU:C	2:D:88:LEU:HD12	2.38	0.44
1:H:139:GLY:HA2	2:B:161:GLN:CB	2.28	0.44
1:C:11:LEU:HD22	1:C:153:PRO:HD3	2.00	0.43
2:L:38:LEU:HD13	2:L:76:PHE:CD1	2.53	0.43
2:L:117:ALA:CB	2:B:187:THR:HG21	2.48	0.43
2:L:200:GLU:CG	2:L:209:PRO:HB2	2.47	0.43
1:H:153:PRO:HD2	1:H:207:ALA:CB	2.48	0.43
2:B:18:GLN:HG3	2:B:81:SER:HA	1.99	0.43
2:D:115:ASP:HA	2:D:145:TYR:O	2.18	0.43
1:C:137:THR:O	1:C:138:THR:C	2.57	0.43
1:H:122:THR:HG22	1:H:123:THR:N	2.34	0.43
2:L:169:THR:HB	5:L:431:HOH:O	2.18	0.42
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.55	0.42
2:D:38:LEU:HD13	2:D:76:PHE:CD1	2.54	0.42
1:A:176:LEU:HD13	1:A:181:TYR:CZ	2.54	0.42
1:A:214:LYS:HG2	1:A:215:LYS:N	2.35	0.42
2:L:38:LEU:HD13	2:L:76:PHE:CE1	2.55	0.42
2:L:197:TYR:O	2:L:213:SER:HB2	2.19	0.42
1:C:106:PHE:CD1	2:D:41:TYR:OH	2.70	0.42
1:C:6:GLN:HG2	1:C:113:THR:OG1	2.20	0.42
2:D:147:LYS:HB3	2:D:178:TYR:CD2	2.54	0.42
1:H:178:SER:HB2	1:H:180:LEU:CD1	2.49	0.42
2:B:200:GLU:HG2	2:B:211:VAL:HG22	2.02	0.42
2:L:12:PRO:HA	2:L:110:GLU:O	2.20	0.41
2:L:138:VAL:HG12	2:L:139:CYS:N	2.35	0.41
1:A:3:GLN:HB2	1:A:25:SER:OG	2.20	0.41
1:H:106:PHE:CE2	2:L:41:TYR:CZ	3.09	0.41
1:H:198:SER:C	1:H:200:THR:N	2.73	0.41
1:H:178:SER:HB2	1:H:180:LEU:HD13	2.02	0.41
2:D:29:ILE:CD1	2:D:38:LEU:HD12	2.51	0.41
1:H:12:VAL:HG12	1:H:16:ALA:HB3	2.02	0.41
1:H:33:VAL:HB	1:H:99:ASP:HB3	2.03	0.41
2:L:120:VAL:HA	2:L:140:PHE:O	2.21	0.41
1:C:125:PRO:HB3	1:C:151:TYR:HB3	2.02	0.41
2:B:145:TYR:CG	2:B:146:PRO:HA	2.56	0.41
1:C:97:ALA:HB1	1:C:106:PHE:HB2	2.03	0.41
1:H:151:TYR:OH	1:H:174:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:VAL:HG13	1:H:187:VAL:O	2.20	0.40
2:L:145:TYR:CG	2:L:146:PRO:HA	2.57	0.40
2:D:94:PHE:CZ	2:D:101:TYR:HB3	2.56	0.40
1:A:46:GLU:OE2	1:A:63:LYS:HD3	2.20	0.40
2:D:23:CYS:HB2	2:D:40:TRP:CH2	2.56	0.40
1:H:106:PHE:CE2	1:H:109:TRP:HZ2	2.38	0.40
1:H:202:ASN:ND2	1:H:213:ASP:OD1	2.51	0.40
2:L:125:PRO:HD2	5:L:412:HOH:O	2.21	0.40
2:D:66:ARG:HB2	2:D:81:SER:O	2.20	0.40
1:C:91:SER:HA	1:C:115:LEU:O	2.22	0.40
1:C:116:THR:HG21	1:C:153:PRO:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/231 (92%)	192 (91%)	20 (9%)	0	100	100
1	C	218/231 (94%)	205 (94%)	13 (6%)	0	100	100
1	H	209/231 (90%)	196 (94%)	13 (6%)	0	100	100
2	B	218/219 (100%)	212 (97%)	6 (3%)	0	100	100
2	D	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
2	L	215/219 (98%)	204 (95%)	11 (5%)	0	100	100
All	All	1289/1350 (96%)	1221 (95%)	68 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	177/198 (89%)	175 (99%)	2 (1%)	73	85
1	C	181/198 (91%)	174 (96%)	7 (4%)	32	45
1	H	172/198 (87%)	168 (98%)	4 (2%)	50	66
2	B	193/196 (98%)	187 (97%)	6 (3%)	40	55
2	D	191/196 (97%)	189 (99%)	2 (1%)	76	87
2	L	182/196 (93%)	177 (97%)	5 (3%)	44	60
All	All	1096/1182 (93%)	1070 (98%)	26 (2%)	49	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	106	PHE
1	H	140	SER
1	H	141	SER
1	H	196	SER
2	L	22	SER
2	L	38	LEU
2	L	61	SER
2	L	147	LYS
2	L	189	ASP
1	C	6	GLN
1	C	17	SER
1	C	85	SER
1	C	106	PHE
1	C	177	GLN
1	C	191	SER
1	C	217	SER
2	D	1	ASP
2	D	57	SER
1	A	213	ASP
1	A	215	LYS
2	B	22	SER
2	B	23	CYS

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Mol	Chain	Res	Type
2	B	24	ARG
2	B	38	LEU
2	B	127	SER
2	B	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	162	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](#)

13 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	C	302	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	L	301	-	4,4,4	0.15	0	6,6,6	0.07	0
4	GOL	C	301	-	5,5,5	0.11	0	5,5,5	0.29	0
3	SO4	B	302	-	4,4,4	0.12	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	301	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	H	302	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	H	301	-	4,4,4	0.12	0	6,6,6	0.21	0
3	SO4	A	301	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	B	303	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.11	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	C	301	-	-	0/4/4/4	-

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	SO4	1	0
3	D	302	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	A	216/231 (93%)	0.35	9 (4%) 36 43	29, 46, 84, 116	0
1	C	218/231 (94%)	0.33	14 (6%) 19 25	27, 42, 85, 140	0
1	H	210/231 (90%)	0.41	17 (8%) 12 16	26, 45, 94, 128	0
2	B	219/219 (100%)	0.10	1 (0%) 91 94	27, 39, 61, 86	0
2	D	219/219 (100%)	0.10	3 (1%) 75 80	30, 43, 63, 101	0
2	L	216/219 (98%)	0.43	17 (7%) 12 17	26, 45, 90, 120	0
All	All	1298/1350 (96%)	0.28	61 (4%) 31 38	26, 43, 82, 140	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	195	PRO	5.7
1	H	196	SER	5.2
2	D	219	CYS	4.6
1	C	134	CYS	4.4
2	L	214	PHE	4.2
2	L	194	HIS	4.0
1	H	198	SER	3.9
1	H	197	GLN	3.9
1	C	177	GLN	3.8
1	H	192	SER	3.7
1	H	165	LEU	3.7
1	H	138	THR	3.7
2	L	156	ASP	3.6
1	C	138	THR	3.5
1	C	192	SER	3.5
1	A	138	THR	3.5
1	A	193	THR	3.4
1	C	139	GLY	3.4
2	L	132	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	L	158	SER	3.3
1	C	194	TRP	3.3
1	A	195	PRO	3.3
1	H	189	VAL	3.1
1	H	139	GLY	3.1
1	A	106	PHE	2.9
1	A	217	SER	2.9
2	L	155	ILE	2.8
2	D	161	GLN	2.8
1	C	191	SER	2.8
1	A	190	THR	2.8
1	C	137	THR	2.7
2	L	215	ASN	2.7
1	H	194	TRP	2.7
1	H	137	THR	2.7
1	C	195	PRO	2.7
1	C	197	GLN	2.7
2	L	165	LEU	2.6
1	C	193	THR	2.6
2	B	219	CYS	2.5
2	L	196	SER	2.5
1	C	136	ASP	2.5
1	A	160	TRP	2.5
1	C	135	GLY	2.5
2	L	186	LEU	2.4
2	L	197	TYR	2.4
1	A	162	SER	2.4
1	H	150	GLY	2.4
1	H	164	SER	2.2
1	H	140	SER	2.2
2	L	191	TYR	2.2
2	L	127	SER	2.2
1	H	213	ASP	2.2
2	L	130	LEU	2.2
2	L	131	THR	2.1
1	H	199	ILE	2.1
2	L	162	ASN	2.1
2	D	9	LEU	2.1
1	H	200	THR	2.1
2	L	134	GLY	2.0
1	A	216	ILE	2.0
1	C	196	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	B	301	5/5	0.70	0.21	111,114,116,116	0
4	GOL	C	301	6/6	0.70	0.19	78,94,100,101	0
3	SO4	C	302	5/5	0.74	0.30	139,141,142,143	0
3	SO4	A	301	5/5	0.76	0.37	149,150,151,152	0
3	SO4	B	305	5/5	0.80	0.17	122,122,123,123	0
3	SO4	H	301	5/5	0.83	0.26	103,107,112,113	0
3	SO4	H	302	5/5	0.84	0.18	100,100,104,111	0
3	SO4	B	304	5/5	0.89	0.21	118,120,120,123	0
3	SO4	D	301	5/5	0.90	0.22	99,100,105,107	0
3	SO4	B	303	5/5	0.91	0.14	92,92,94,96	0
3	SO4	D	302	5/5	0.93	0.20	89,91,92,98	0
3	SO4	B	302	5/5	0.93	0.15	95,98,100,105	0
3	SO4	L	301	5/5	0.93	0.19	115,115,117,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.