



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 7TQA / pdb_00007tqa
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

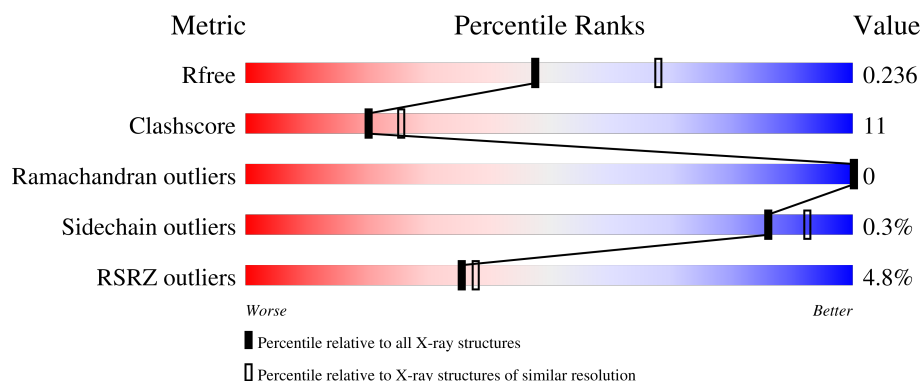
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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	7% 77% 17% 6%
1	C	231	6% 73% 22% 6%
1	H	231	7% 69% 22% 9%
2	B	219	87% 13%
2	D	219	2% 80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	L	219	5% 68% 31%

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
1	H	210	Total	C	N	O	S	0	3	0
			1578	1002	254	314	8			
1	C	218	Total	C	N	O	S	0	2	0
			1645	1048	266	322	9			
1	A	216	Total	C	N	O	S	0	0	0
			1609	1024	255	322	8			

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

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

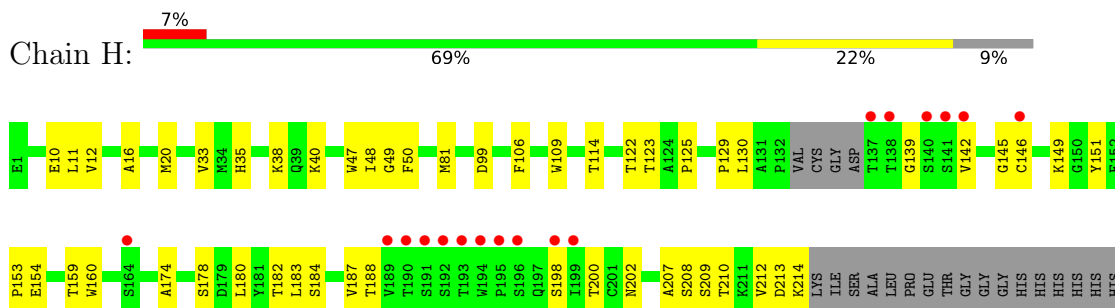
- Molecule 5 is water.

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		

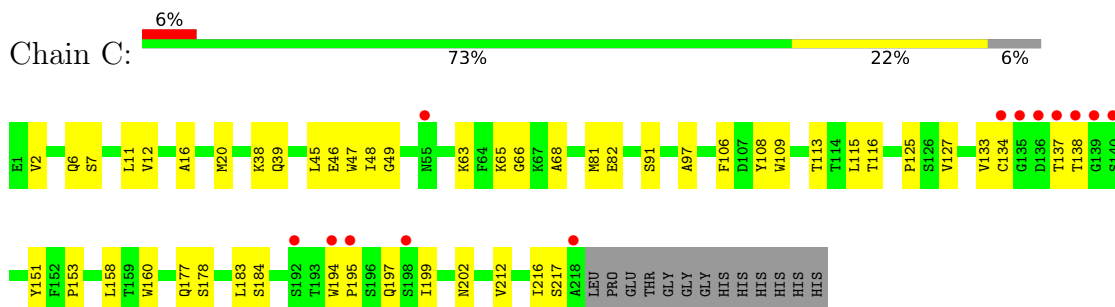
3 Residue-property plots [i](#)

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.

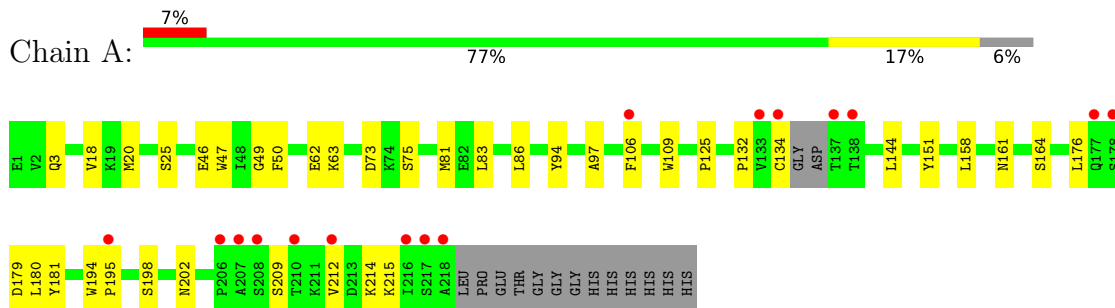
- Molecule 1: Fab S9.6 heavy chain



- Molecule 1: Fab S9.6 heavy chain

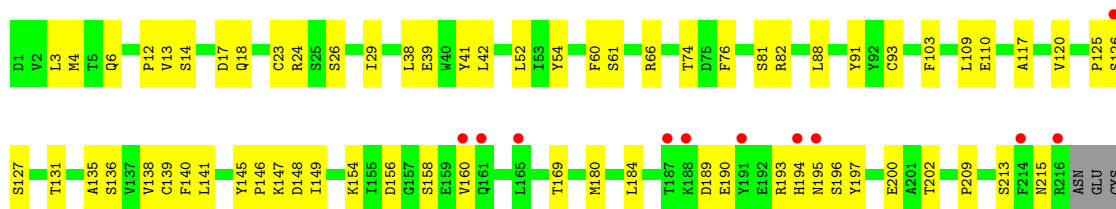


- Molecule 1: Fab S9.6 heavy chain

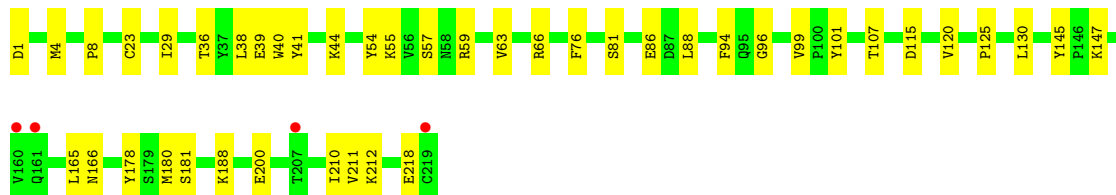
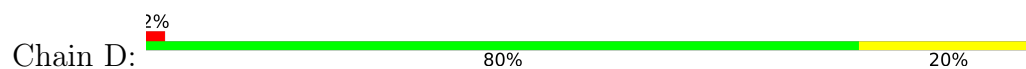


- Molecule 2: Fab S9.6 light chain

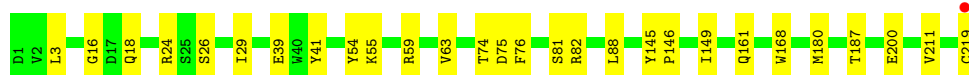
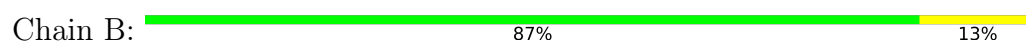




● Molecule 2: Fab S9.6 light chain



● Molecule 2: Fab S9.6 light chain



4 Data and refinement statistics

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)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.179 , 0.235 0.182 , 0.236	Depositor DCC
R_{free} test set	2899 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.030 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10314	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage'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: SO4, GOL

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	0.37	0/1652	0.60	1/2260 (0.0%)
1	C	0.38	0/1689	0.59	0/2305
1	H	0.34	0/1619	0.55	0/2208
2	B	0.40	0/1725	0.63	1/2343 (0.0%)
2	D	0.38	0/1712	0.61	1/2328 (0.0%)
2	L	0.37	0/1669	0.59	0/2272
All	All	0.37	0/10066	0.60	3/13716 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	55	LYS	CB-CA-C	8.39	123.80	111.89
1	A	209	SER	N-CA-C	7.85	118.62	108.34
2	B	55	LYS	CB-CA-C	5.31	119.44	111.89

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	35	0
1	C	1645	0	1581	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1578	0	1479	48	0
2	B	1686	0	1595	21	0
2	D	1673	0	1579	33	0
2	L	1631	0	1522	56	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	2	0
5	L	61	0	0	3	0
All	All	10306	8	9285	217	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 11.

All (217) 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
2:D:59:ARG:HG2	2:D:63:VAL:HB	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:4:MET:HE3	2:D:23:CYS:SG	2.39	0.61
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:147:LYS:C	2:L:147:LYS:HD2	2.27	0.60
2:L:190:GLU:HA	2:L:197:TYR:OH	2.02	0.60
1:H:106:PHE:CE2	1:H:109:TRP:CZ2	2.90	0.59
2:B:168:TRP:CZ2	2:B:180:MET:HE2	2.38	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
1:C:20:MET:HE1	1:C:81:MET:HE3	1.86	0.57
1:C:20:MET:CE	1:C:81:MET:HE3	2.35	0.57
2:L:13:VAL:CG2	2:L:109:LEU:HD21	2.34	0.57
1:H:198:SER:C	1:H:200:THR:H	2.12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:40:LYS:NZ	5:H:401:HOH:O	2.39	0.55
1:C:6:GLN:HG2	5:C:422:HOH:O	2.04	0.55
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
1:C:39:GLN:HB2	1:C:45:LEU:HD23	1.88	0.55
1:H:20:MET:HE1	1:H:81:MET:HE3	1.88	0.54
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:OE2	2:D:218:GLU:N	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
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:A:20:MET:HE1	1:A:81:MET:HE3	1.94	0.49
2:L:4:MET:HE3	2:L:93:CYS:SG	2.53	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
2:D:88:LEU:C	2:D:88:LEU:HD12	2.38	0.49
2:L:141:LEU:HD22	2:L:180:MET:HE3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:149:ILE:CG2	2:B:180:MET:HE3	2.44	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
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
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:C:137:THR:O	1:C:138:THR:C	2.57	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:198:SER:C	1:H:200:THR:N	2.73	0.46
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:N	2:L:141:LEU:HD12	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
1:C:106:PHE:CD1	2:D:41:TYR:OH	2.70	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
2:L:88:LEU:C	2:L:88:LEU:HD12	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:PRO:O	2:D:107:THR:OG1	2.29	0.45
2:L:193:ARG:O	2:L:195:ASN:N	2.49	0.45
1:C:177:GLN:O	1:C:178:SER:HB2	2.17	0.45
2:D:166:ASN:HB3	2:D:180:MET:HE3	1.98	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
2:L:4:MET:HE3	2:L:23:CYS:SG	2.57	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
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:50:PHE:C	1:H:50:PHE:CD2	2.96	0.44
1:H:125:PRO:CB	1:H:151:TYR:HB3	2.40	0.44
1:H:139:GLY:HA2	2:B:161:GLN:CB	2.28	0.44
2:L:149:ILE:HG21	2:L:180:MET:CE	2.48	0.44
1:A:20:MET:HE1	1:A:83:LEU:HD11	1.99	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:B:88:LEU:C	2:B:88:LEU:HD12	2.44	0.43
2:D:115:ASP:HA	2:D:145:TYR:O	2.18	0.43
2:B:149:ILE:HG21	2:B:180:MET:HE3	2.00	0.43
1:A:81:MET:HE1	1:A:94:TYR:CD1	2.54	0.43
1:A:179:ASP:C	1:A:180:LEU:HD22	2.44	0.43
1:H:183:LEU:HD23	1:H:183:LEU:C	2.44	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:20:MET:CE	1:H:81:MET:HE3	2.49	0.42
1:H:178:SER:HB2	1:H:180:LEU:CD1	2.49	0.42
1:C:194:TRP:O	1:C:195:PRO:C	2.61	0.42
2:B:200:GLU:HG2	2:B:211:VAL:HG22	2.02	0.42
1:C:133:VAL:O	1:C:134:CYS:C	2.62	0.42
2:L:12:PRO:HA	2:L:110:GLU:O	2.20	0.41
2:L:60:PHE:O	2:L:61:SER:C	2.63	0.41
1:C:183:LEU:HD23	1:C:183:LEU:C	2.45	0.41
1:H:122:THR:HG22	1:H:123:THR:N	2.34	0.41
1:A:3:GLN:HB2	1:A:25:SER:OG	2.20	0.41
2:L:138:VAL:HG12	2:L:139:CYS:N	2.35	0.41
1:H:106:PHE:CE2	2:L:41:TYR:CZ	3.09	0.41
1:A:50:PHE:CD2	1:A:50:PHE:C	2.99	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
1:H:187:VAL:O	1:H:187:VAL:HG13	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
1:A:20:MET:HE1	1:A:83:LEU:CD1	2.52	0.40
2:B:24:ARG:HH11	2:B:75:ASP:CG	2.29	0.40

There are no symmetry-related clashes.

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	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 ⓘ

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%)	177 (100%)	0	100	100
1	C	181/198 (91%)	179 (99%)	2 (1%)	65	80
1	H	172/198 (87%)	172 (100%)	0	100	100
2	B	193/196 (98%)	193 (100%)	0	100	100
2	D	191/196 (97%)	190 (100%)	1 (0%)	81	89
2	L	182/196 (93%)	182 (100%)	0	100	100
All	All	1096/1182 (93%)	1093 (100%)	3 (0%)	86	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	197	GLN
1	C	217	SER
2	D	57	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	161	ASN
1	H	170	HIS
2	L	35	ASN
1	C	197	GLN
2	D	47	GLN
2	D	162	ASN
2	B	58	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 oligosaccharides 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	H	302	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	B	302	-	4,4,4	0.22	0	6,6,6	0.21	0
3	SO4	D	302	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SO4	B	303	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	B	301	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	B	304	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	B	305	-	4,4,4	0.25	0	6,6,6	0.06	0
4	GOL	C	301	-	5,5,5	0.10	0	5,5,5	0.28	0
3	SO4	C	302	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	H	301	-	4,4,4	0.21	0	6,6,6	0.21	0
3	SO4	L	301	-	4,4,4	0.26	0	6,6,6	0.06	0
3	SO4	D	301	-	4,4,4	0.24	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	D	302	SO4	1	0
3	C	302	SO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	216/231 (93%)	0.26	16 (7%)	20 23	29, 46, 84, 116	0
1	C	218/231 (94%)	0.13	13 (5%)	27 30	17, 42, 85, 140	2 (0%)
1	H	210/231 (90%)	0.25	17 (8%)	18 20	14, 44, 94, 128	3 (1%)
2	B	219/219 (100%)	-0.17	1 (0%)	87 88	18, 39, 61, 86	1 (0%)
2	D	219/219 (100%)	-0.04	4 (1%)	67 70	30, 43, 63, 101	0
2	L	216/219 (98%)	0.27	11 (5%)	33 36	17, 45, 90, 120	1 (0%)
All	All	1298/1350 (96%)	0.12	62 (4%)	35 38	14, 43, 82, 140	7 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	146[A]	CYS	6.9
1	H	195	PRO	6.2
1	H	194	TRP	5.5
1	A	106	PHE	4.2
2	L	188	LYS	3.9
1	H	193	THR	3.9
1	C	134	CYS	3.8
1	H	138	THR	3.8
2	D	219	CYS	3.7
1	C	136	ASP	3.7
1	A	195	PRO	3.6
1	H	196	SER	3.6
1	H	189	VAL	3.4
1	C	139	GLY	3.4
1	H	192	SER	3.3
1	C	138	THR	3.2
2	L	195	ASN	3.2
1	C	195	PRO	3.2
1	A	134	CYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	216	ARG	3.1
1	A	212	VAL	3.0
1	A	138	THR	3.0
1	A	210	THR	3.0
1	C	194	TRP	3.0
1	H	191	SER	2.9
1	A	217	SER	2.9
1	C	218	ALA	2.9
2	L	187	THR	2.9
2	L	191	TYR	2.8
2	L	126	SER	2.8
2	L	160	VAL	2.8
1	H	190	THR	2.7
2	L	194	HIS	2.6
2	L	214	PHE	2.6
1	H	198	SER	2.6
1	H	164	SER	2.6
1	H	142	VAL	2.5
1	A	216	ILE	2.5
1	H	137	THR	2.4
2	B	219	CYS	2.4
1	C	135	GLY	2.4
1	C	140	SER	2.4
1	C	192	SER	2.4
1	H	141	SER	2.4
1	A	207	ALA	2.3
1	A	137	THR	2.3
1	H	199	ILE	2.3
1	A	133	VAL	2.3
2	D	160	VAL	2.3
1	A	206	PRO	2.3
1	C	55	ASN	2.3
1	C	137	THR	2.2
2	D	161	GLN	2.2
1	A	177	GLN	2.2
1	A	178	SER	2.2
1	C	198	SER	2.2
2	D	207	THR	2.2
2	L	165	LEU	2.1
2	L	161	GLN	2.1
1	A	208	SER	2.1
1	A	218	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	140	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	301	5/5	0.55	0.13	111,114,116,116	0
3	SO4	B	305	5/5	0.69	0.15	122,122,123,123	0
3	SO4	H	301	5/5	0.74	0.14	103,107,112,113	0
3	SO4	C	302	5/5	0.76	0.12	139,141,142,143	0
3	SO4	H	302	5/5	0.79	0.14	100,100,104,111	0
3	SO4	B	303	5/5	0.80	0.13	92,92,94,96	0
3	SO4	B	304	5/5	0.82	0.12	118,120,120,123	0
3	SO4	A	301	5/5	0.82	0.21	149,150,151,152	0
3	SO4	D	301	5/5	0.86	0.10	99,100,105,107	0
3	SO4	L	301	5/5	0.87	0.12	115,115,117,119	0
4	GOL	C	301	6/6	0.87	0.11	78,94,100,101	0
3	SO4	D	302	5/5	0.89	0.10	89,91,92,98	0
3	SO4	B	302	5/5	0.90	0.11	95,98,100,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.