



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:18 AM UTC

PDB ID : 7LR4 / pdb_00007lr4
Title : Complex of Fab 2/1.12 with domain 3 of P. berghei HAP2
Authors : Feng, J.; Dong, X.C.; Su, Y.; Lu, X.F.; Springer, T.A.
Deposited on : 2021-02-15
Resolution : 2.10 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

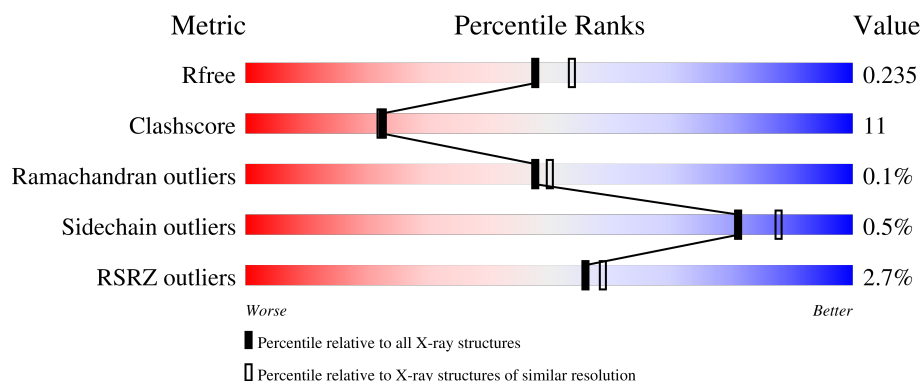
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	226	2% 75% 20% .
1	H	226	% 83% 14% .
2	B	214	4% 79% 19% ..
2	L	214	% 84% 15%
3	C	123	6% 61% 20% 20%

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Mol	Chain	Length	Quality of chain
3	D	123	

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	H	302	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8592 atoms, of which 13 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 D3_2/1.12 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	1	0
			1664	1052	274	331	7			
1	A	216	Total	C	N	O	S	0	1	0
			1647	1044	272	324	7			

- Molecule 2 is a protein called D3_2/1.12 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	1	0
			1668	1036	281	345	6			
2	B	212	Total	C	N	O	S	0	0	0
			1650	1026	279	339	6			

- Molecule 3 is a protein called Hapless 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	0	1	0
			780	501	129	144	6			
3	D	99	Total	C	N	O	S	0	0	0
			774	494	129	145	6			

There are 18 discrepancies between the modelled and reference sequences:

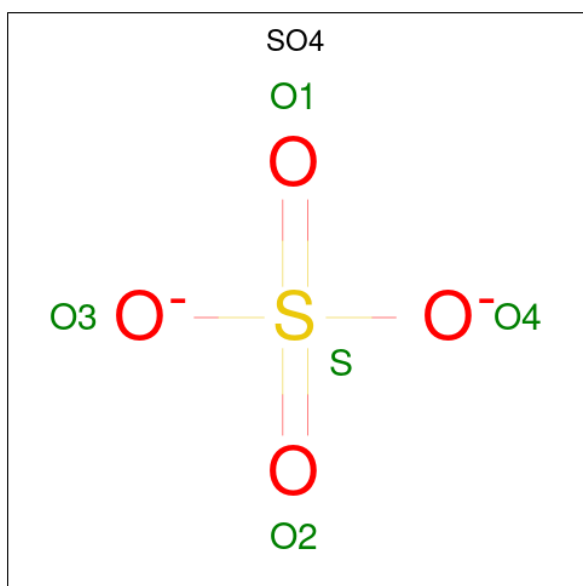
Chain	Residue	Modelled	Actual	Comment	Reference
C	516	THR	ASN	engineered mutation	UNP Q4YCF6
C	533	ASN	SER	engineered mutation	UNP Q4YCF6
C	539	GLN	ASN	engineered mutation	UNP Q4YCF6
C	619	HIS	-	expression tag	UNP Q4YCF6
C	620	HIS	-	expression tag	UNP Q4YCF6
C	621	HIS	-	expression tag	UNP Q4YCF6
C	622	HIS	-	expression tag	UNP Q4YCF6
C	623	HIS	-	expression tag	UNP Q4YCF6

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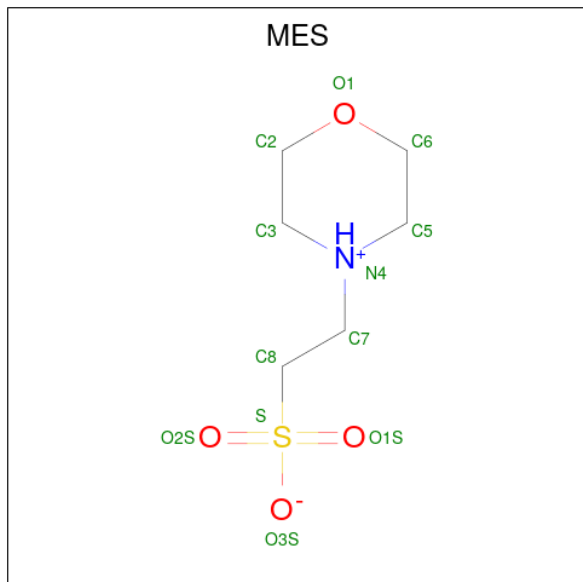
Chain	Residue	Modelled	Actual	Comment	Reference
C	624	HIS	-	expression tag	UNP Q4YCF6
D	516	THR	ASN	engineered mutation	UNP Q4YCF6
D	533	ASN	SER	engineered mutation	UNP Q4YCF6
D	539	GLN	ASN	engineered mutation	UNP Q4YCF6
D	619	HIS	-	expression tag	UNP Q4YCF6
D	620	HIS	-	expression tag	UNP Q4YCF6
D	621	HIS	-	expression tag	UNP Q4YCF6
D	622	HIS	-	expression tag	UNP Q4YCF6
D	623	HIS	-	expression tag	UNP Q4YCF6
D	624	HIS	-	expression tag	UNP Q4YCF6

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



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
								0	0

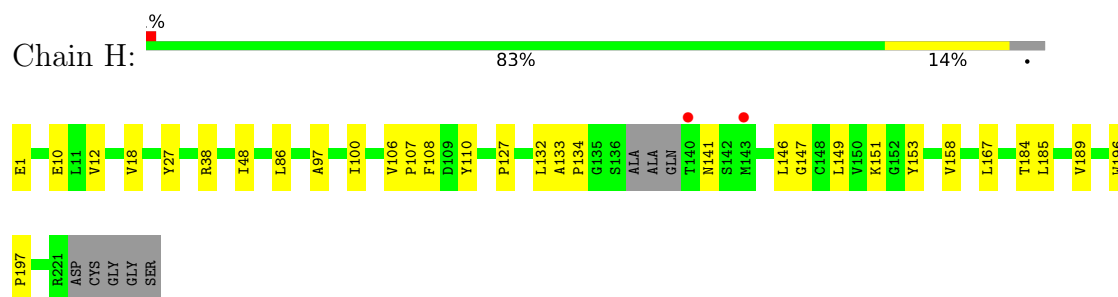
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	115	Total	O		
			115	115	0	0
6	L	111	Total	O		
			111	111	0	0
6	A	50	Total	O		
			50	50	0	0
6	B	47	Total	O		
			47	47	0	0
6	C	18	Total	O		
			18	18	0	0
6	D	13	Total	O		
			13	13	0	0

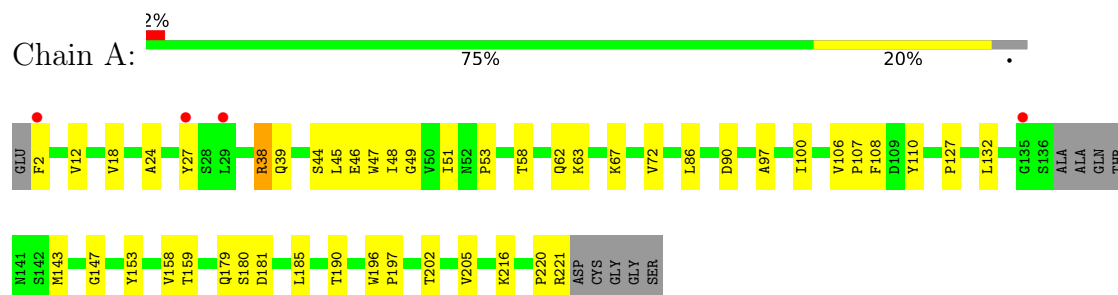
3 Residue-property plots [i](#)

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.

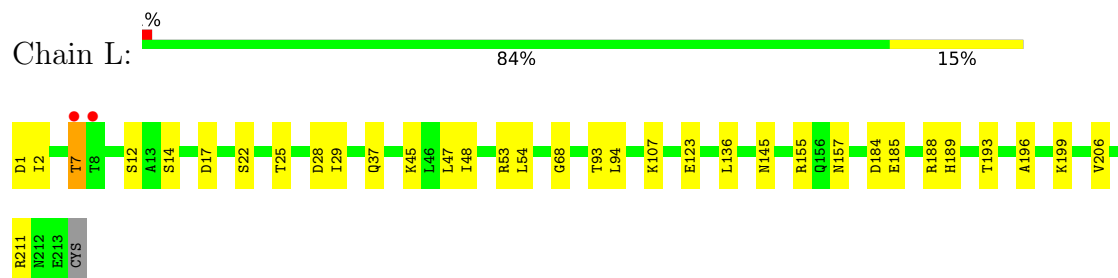
- Molecule 1: D3_2/1.12 Fab heavy chain



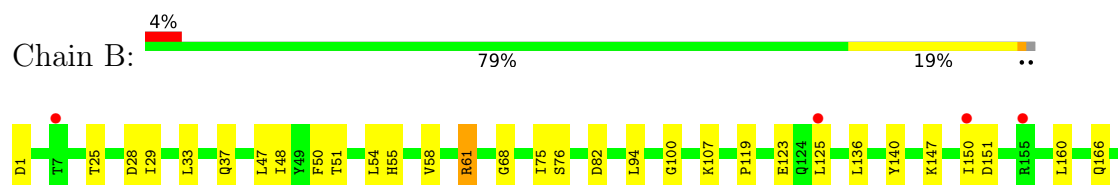
- Molecule 1: D3_2/1.12 Fab heavy chain

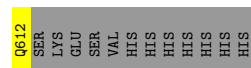


- Molecule 2: D3_2/1.12 Fab light chain



- Molecule 2: D3_2/1.12 Fab light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.88Å 187.10Å 74.37Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	47.69 – 2.10 47.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.69-2.10) 98.4 (47.69-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.189 , 0.231 0.196 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8592	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, MES

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	0.12	0/1693	0.30	0/2318
1	H	0.13	0/1710	0.32	0/2341
2	B	0.10	0/1685	0.28	0/2288
2	L	0.13	0/1703	0.33	0/2312
3	C	0.10	0/794	0.24	0/1075
3	D	0.11	0/788	0.23	0/1067
All	All	0.12	0/8373	0.30	0/11401

There are no bond length outliers.

There are no bond angle outliers.

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	1647	0	1602	38	0
1	H	1664	0	1613	30	0
2	B	1650	0	1583	36	0
2	L	1668	0	1594	25	0
3	C	780	0	767	20	0
3	D	774	0	760	22	0
4	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	2	0
4	H	10	0	0	2	0
5	H	12	13	12	1	0
6	A	50	0	0	3	1
6	B	47	0	0	8	0
6	C	18	0	0	3	0
6	D	13	0	0	2	0
6	H	115	0	0	11	2
6	L	111	0	0	6	3
All	All	8579	13	7931	170	3

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 (170) 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)
3:D:514:ALA:HB1	3:D:518:SER:HB3	1.52	0.91
3:C:544[B]:ILE:HD11	3:C:561:ILE:HG21	1.57	0.87
3:D:506:HIS:HB2	3:D:528:HIS:HB2	1.59	0.84
1:H:12:VAL:HG11	1:H:18:VAL:HG22	1.61	0.82
2:L:7:THR:HG23	2:L:22:SER:HB2	1.61	0.82
2:B:150:ILE:HD11	2:B:179:LEU:HD21	1.62	0.81
2:L:123[A]:GLU:OE2	6:L:301:HOH:O	2.05	0.73
1:H:141:ASN:ND2	6:H:404:HOH:O	2.22	0.73
4:H:302:SO4:O4	6:H:401:HOH:O	2.07	0.73
1:H:151:LYS:HB2	6:H:498:HOH:O	1.89	0.72
1:A:12:VAL:HG11	1:A:18[A]:VAL:HG22	1.70	0.71
1:H:146:LEU:HG	6:H:490:HOH:O	1.89	0.71
1:H:106:VAL:HG22	1:H:107:PRO:HA	1.71	0.71
1:A:143:MET:HE2	1:A:190:THR:HG22	1.72	0.71
2:L:7:THR:CG2	2:L:22:SER:HB2	2.22	0.69
3:D:502:ALA:N	6:D:701:HOH:O	2.26	0.68
1:H:127:PRO:HB3	1:H:153:TYR:HB3	1.76	0.68
2:L:1:ASP:N	6:L:302:HOH:O	2.12	0.67
1:H:106:VAL:CG2	1:H:107:PRO:HA	2.26	0.66
1:A:12:VAL:HG11	1:A:18[B]:VAL:HG12	1.78	0.66
5:H:303:MES:S	6:H:405:HOH:O	2.54	0.65
2:L:53:ARG:NH1	6:L:305:HOH:O	2.30	0.65
1:H:134:PRO:HD3	6:H:490:HOH:O	1.97	0.64
1:A:2:PHE:N	6:A:405:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:302:SO4:O1	6:H:402:HOH:O	2.13	0.63
2:B:48:ILE:HG12	2:B:54:LEU:HD23	1.81	0.63
2:L:185:GLU:OE1	6:L:303:HOH:O	2.15	0.63
1:A:97:ALA:HB1	1:A:108:PHE:HB3	1.81	0.63
1:A:44:SER:HB2	6:A:401:HOH:O	1.98	0.63
1:A:12:VAL:HG11	1:A:18[B]:VAL:CG1	2.27	0.62
1:H:149:LEU:HG	6:H:498:HOH:O	2.00	0.62
3:C:502:ALA:N	6:C:701:HOH:O	2.30	0.62
1:H:133:ALA:HA	6:H:490:HOH:O	1.99	0.62
1:A:62:GLN:NE2	6:A:404:HOH:O	2.28	0.62
3:C:506:HIS:HB2	3:C:528:HIS:HB2	1.81	0.62
3:D:525:LEU:HD21	3:D:609:PHE:CZ	2.35	0.62
1:H:12:VAL:HG11	1:H:18:VAL:CG2	2.30	0.61
2:L:94:LEU:HD11	3:D:579:ILE:HD12	1.82	0.61
2:B:54:LEU:HD13	2:B:58:VAL:HG23	1.82	0.61
3:D:522:GLU:HG2	3:D:581:LYS:HG2	1.82	0.61
1:A:38:ARG:HB2	1:A:48:ILE:HD11	1.84	0.60
1:H:38:ARG:HB2	1:H:48:ILE:HD11	1.84	0.59
2:L:107:LYS:NZ	6:L:306:HOH:O	2.35	0.59
1:H:100:ILE:HD12	1:H:110:TYR:CD2	2.38	0.59
1:A:51:ILE:HD13	1:A:72:VAL:HG23	1.86	0.58
2:L:37:GLN:OE1	2:L:45:LYS:HE2	2.03	0.58
2:B:147:LYS:HB3	6:B:413:HOH:O	2.01	0.58
2:B:151:ASP:OD1	2:B:191:SER:OG	2.21	0.58
1:H:1:GLU:N	6:H:406:HOH:O	2.27	0.58
2:B:190:ASN:O	2:B:211:ARG:N	2.34	0.58
1:A:18[A]:VAL:HG23	1:A:86:LEU:HD11	1.86	0.57
1:A:179:GLN:HE22	2:B:180:THR:HG21	1.69	0.57
1:H:100:ILE:HD12	1:H:110:TYR:CG	2.40	0.56
2:L:28:ASP:OD1	2:L:68:GLY:HA2	2.05	0.56
2:L:189:HIS:O	2:L:211:ARG:HD3	2.05	0.56
3:C:587:GLU:N	3:C:613:SER:HG	2.02	0.56
2:B:125:LEU:O	2:B:183:LYS:HD2	2.06	0.56
3:D:503:THR:HG23	6:D:711:HOH:O	2.05	0.56
1:H:10:GLU:HG3	1:H:18:VAL:HG11	1.88	0.56
2:B:150:ILE:HG22	6:B:431:HOH:O	2.06	0.56
2:L:155:ARG:NH1	2:L:157:ASN:O	2.39	0.55
1:A:106:VAL:CG2	1:A:107:PRO:HA	2.36	0.55
2:B:76:SER:N	6:B:403:HOH:O	2.18	0.55
2:B:28:ASP:OD1	2:B:68:GLY:HA2	2.06	0.55
2:B:107:LYS:HD2	2:B:140:TYR:OH	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:VAL:HG23	1:H:86:LEU:HD11	1.89	0.54
2:L:14:SER:O	2:L:17:ASP:HB2	2.08	0.54
1:A:51:ILE:HG13	1:A:58:THR:HG22	1.90	0.54
4:B:302:SO4:O3	6:B:402:HOH:O	2.17	0.54
1:A:67:LYS:HE2	1:A:90:ASP:OD1	2.07	0.54
3:D:517:ASN:ND2	3:D:518:SER:O	2.41	0.54
2:B:190:ASN:O	2:B:210:ASN:HA	2.07	0.53
2:L:184:ASP:O	2:L:188:ARG:HG3	2.09	0.53
2:B:123:GLU:HB2	6:B:442:HOH:O	2.07	0.53
1:A:53:PRO:HB3	1:A:72:VAL:HG11	1.91	0.53
3:C:525:LEU:HD23	3:C:544[A]:ILE:HD13	1.90	0.53
2:L:193:THR:HG23	2:L:206:VAL:HG13	1.91	0.52
1:A:24:ALA:HB1	1:A:27:TYR:CE2	2.44	0.52
2:B:50:PHE:O	2:B:51:THR:HB	2.08	0.52
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.91	0.52
2:B:75:ILE:HA	6:B:403:HOH:O	2.10	0.52
1:A:132:LEU:HB2	1:A:147:GLY:CA	2.40	0.52
1:A:127:PRO:HB3	1:A:153:TYR:HB3	1.92	0.52
3:C:509:ILE:HD11	3:C:609:PHE:HB2	1.92	0.52
2:B:1:ASP:N	6:B:401:HOH:O	2.08	0.51
3:D:525:LEU:HD21	3:D:609:PHE:HZ	1.75	0.51
3:D:525:LEU:HD23	3:D:544:ILE:HD13	1.93	0.51
2:B:48:ILE:HG12	2:B:54:LEU:CD2	2.41	0.51
3:C:544[B]:ILE:CD1	3:C:561:ILE:HG21	2.35	0.51
2:L:12:SER:HB3	2:L:107:LYS:HG2	1.93	0.51
1:H:185:LEU:HD12	1:H:185:LEU:C	2.36	0.51
2:B:186:TYR:CZ	2:B:211:ARG:HD3	2.46	0.50
1:H:196:TRP:CG	1:H:197:PRO:HA	2.46	0.50
1:H:196:TRP:CD1	1:H:197:PRO:HA	2.46	0.50
2:B:25:THR:HG21	2:B:29:ILE:HD13	1.92	0.50
3:C:525:LEU:CD2	3:C:544[A]:ILE:HD13	2.41	0.50
1:A:143:MET:CE	1:A:190:THR:HG22	2.41	0.50
2:L:14:SER:HB2	2:L:17:ASP:OD2	2.12	0.49
2:B:190:ASN:N	2:B:190:ASN:OD1	2.46	0.49
2:B:54:LEU:HD22	2:B:58:VAL:HG21	1.93	0.49
1:A:179:GLN:HA	2:B:160:LEU:HD11	1.95	0.49
1:H:27:TYR:CE2	1:H:100:ILE:HD11	2.48	0.49
3:D:517:ASN:O	3:D:518:SER:HB2	2.13	0.49
2:B:54:LEU:HD13	2:B:58:VAL:CG2	2.43	0.49
3:C:561:ILE:HG12	3:C:580:ILE:CD1	2.43	0.49
1:A:12:VAL:HG11	1:A:18[A]:VAL:CG2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:591:LEU:HD23	3:C:610:GLU:HG2	1.94	0.48
1:A:196:TRP:CG	1:A:197:PRO:HA	2.48	0.48
4:B:301:SO4:O2	6:B:404:HOH:O	2.19	0.48
2:B:55:HIS:O	2:B:58:VAL:HG13	2.13	0.48
3:D:508:THR:O	3:D:525:LEU:HD12	2.13	0.48
1:A:132:LEU:HB2	1:A:147:GLY:HA3	1.95	0.47
1:A:106:VAL:HG23	1:A:107:PRO:HA	1.95	0.47
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.96	0.47
3:C:587:GLU:C	3:C:588:ILE:HD12	2.39	0.47
1:A:159:THR:O	1:A:205:VAL:HA	2.14	0.47
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.49	0.47
3:C:525:LEU:HD21	3:C:609:PHE:CZ	2.50	0.47
2:L:25:THR:HG21	2:L:29:ILE:HD13	1.96	0.46
2:L:48:ILE:HG12	2:L:54:LEU:CD2	2.45	0.46
1:A:180:SER:OG	1:A:181:ASP:N	2.47	0.46
2:B:119:PRO:HB3	2:B:209:PHE:CE1	2.50	0.46
1:A:44:SER:HB3	2:B:100:GLY:HA2	1.98	0.46
3:C:508:THR:HB	3:C:526:ILE:HB	1.98	0.46
1:H:12:VAL:HG21	1:H:18:VAL:CG2	2.45	0.45
3:D:595:ILE:HD12	3:D:595:ILE:N	2.32	0.45
1:H:12:VAL:HG21	1:H:86:LEU:HD13	1.99	0.45
1:A:46:GLU:OE2	1:A:63:LYS:NZ	2.45	0.45
3:C:528:HIS:CE1	3:C:575:ALA:HB2	2.52	0.45
2:B:94:LEU:HD11	3:C:579:ILE:HD12	1.99	0.44
1:A:185:LEU:C	1:A:185:LEU:HD12	2.42	0.44
2:B:136:LEU:HD12	2:B:136:LEU:N	2.32	0.44
3:C:565:ARG:HG2	6:C:714:HOH:O	2.17	0.44
3:D:514:ALA:HB3	3:D:520:SER:HB2	2.00	0.44
1:H:97:ALA:HB1	1:H:108:PHE:HB3	2.00	0.44
2:B:198:HIS:CE1	2:B:200:THR:HG23	2.53	0.44
2:L:48:ILE:HG12	2:L:54:LEU:HD23	1.99	0.43
2:L:136:LEU:HD12	2:L:136:LEU:N	2.32	0.43
3:D:514:ALA:CB	3:D:518:SER:HB3	2.34	0.43
3:C:598:ASP:HB2	6:C:708:HOH:O	2.18	0.43
3:C:588:ILE:HD12	3:C:588:ILE:N	2.33	0.43
3:D:509:ILE:HD11	3:D:609:PHE:HB2	2.00	0.43
1:H:12:VAL:HG21	1:H:18:VAL:HG21	2.00	0.43
1:A:220:PRO:O	1:A:221:ARG:HB2	2.18	0.43
2:B:61:ARG:NH2	2:B:82:ASP:OD2	2.52	0.43
1:A:179:GLN:NE2	2:B:180:THR:HG21	2.33	0.42
1:H:27:TYR:CZ	1:H:100:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:CG2	1:A:185:LEU:HD21	2.49	0.42
2:B:186:TYR:CE2	2:B:211:ARG:HD3	2.55	0.42
3:D:587:GLU:C	3:D:588:ILE:HD12	2.44	0.42
3:D:536:VAL:HG12	3:D:537:GLY:O	2.19	0.42
1:H:132:LEU:HB2	1:H:147:GLY:CA	2.49	0.42
3:D:580:ILE:HG22	3:D:582:PHE:H	1.85	0.42
3:C:538:SER:HB2	3:C:540:PHE:CE2	2.55	0.42
3:D:544:ILE:HG22	3:D:561:ILE:HD12	2.01	0.41
2:L:199:LYS:HE3	6:L:307:HOH:O	2.19	0.41
3:D:584:ILE:HG21	3:D:612:GLN:HB2	2.02	0.41
2:L:145:ASN:O	2:L:196:ALA:HA	2.20	0.41
1:A:153:TYR:CE2	1:A:158:VAL:HG13	2.55	0.41
2:B:29:ILE:HD11	2:B:33:LEU:HB2	2.03	0.41
3:C:513:CYS:HB3	3:C:582:PHE:CD2	2.54	0.41
1:H:153:TYR:CE2	1:H:158:VAL:HG13	2.55	0.41
2:B:166:GLN:HB2	2:B:173:TYR:CZ	2.56	0.41
1:H:167:LEU:HD13	1:H:189:VAL:HG21	2.02	0.41
2:L:2:ILE:CD1	2:L:93:THR:HG22	2.50	0.41
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.01	0.41
3:D:510:PRO:HG2	3:D:513:CYS:SG	2.61	0.40
1:A:100:ILE:HD12	1:A:110:TYR:CD1	2.56	0.40
1:H:184:THR:HG23	6:H:498:HOH:O	2.22	0.40
1:A:202:THR:HG23	1:A:216:LYS:C	2.47	0.40

All (3) 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)
6:H:455:HOH:O	6:L:395:HOH:O[1_655]	1.92	0.28
6:L:388:HOH:O	6:A:404:HOH:O[2_545]	1.98	0.22
6:H:455:HOH:O	6:L:310:HOH:O[1_655]	1.99	0.21

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	213/226 (94%)	207 (97%)	6 (3%)	0	100	100
1	H	215/226 (95%)	203 (94%)	12 (6%)	0	100	100
2	B	210/214 (98%)	205 (98%)	5 (2%)	0	100	100
2	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	24	22
3	C	92/123 (75%)	88 (96%)	4 (4%)	0	100	100
3	D	93/123 (76%)	84 (90%)	9 (10%)	0	100	100
All	All	1035/1126 (92%)	992 (96%)	42 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	7	THR

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	192/197 (98%)	191 (100%)	1 (0%)	81	88
1	H	194/197 (98%)	194 (100%)	0	100	100
2	B	190/192 (99%)	188 (99%)	2 (1%)	65	74
2	L	192/192 (100%)	192 (100%)	0	100	100
3	C	89/112 (80%)	89 (100%)	0	100	100
3	D	89/112 (80%)	87 (98%)	2 (2%)	45	53
All	All	946/1002 (94%)	941 (100%)	5 (0%)	81	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG

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Mol	Chain	Res	Type
2	B	61	ARG
2	B	190	ASN
3	D	528	HIS
3	D	582	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	74	GLN
2	L	157	ASN
1	A	39	GLN
1	A	74	GLN
2	B	38	GLN
2	B	77	ASN
2	B	124	GLN
2	B	138	ASN
2	B	145	ASN
2	B	210	ASN
3	C	573	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](#)

7 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	301	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	B	301	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	H	301	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.06	0
5	MES	H	303	-	12,12,12	2.37	1 (8%)	15,16,16	1.93	4 (26%)
4	SO4	H	302	-	4,4,4	0.23	0	6,6,6	0.08	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
5	MES	H	303	-	-	5/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	303	MES	C8-S	-7.98	1.66	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	303	MES	C7-N4-C5	4.03	121.99	111.24
5	H	303	MES	O1S-S-C8	3.06	111.35	106.73
5	H	303	MES	C6-C5-N4	-2.87	105.77	110.12
5	H	303	MES	C2-C3-N4	2.26	113.55	110.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	303	MES	C8-C7-N4-C5
5	H	303	MES	N4-C7-C8-S
5	H	303	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
5	H	303	MES	C7-C8-S-O2S
5	H	303	MES	C7-C8-S-O3S

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	SO4	1	0
4	B	302	SO4	1	0
5	H	303	MES	1	0
4	H	302	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	216/226 (95%)	0.31	4 (1%)	66 69	28, 67, 121, 178	1 (0%)
1	H	218/226 (96%)	-0.11	2 (0%)	81 83	33, 51, 94, 142	1 (0%)
2	B	212/214 (99%)	0.41	8 (3%)	44 46	48, 80, 141, 170	0
2	L	213/214 (99%)	-0.06	2 (0%)	81 83	38, 56, 91, 142	1 (0%)
3	C	99/123 (80%)	0.64	7 (7%)	22 23	31, 76, 154, 197	1 (1%)
3	D	99/123 (80%)	0.71	6 (6%)	27 29	47, 77, 152, 193	0
All	All	1057/1126 (93%)	0.24	29 (2%)	56 59	28, 65, 130, 197	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	588	ILE	4.0
3	D	582	PHE	3.5
2	L	7	THR	3.3
1	A	27	TYR	3.3
2	B	209	PHE	2.9
3	C	514	ALA	2.8
3	D	535	PHE	2.7
1	A	2	PHE	2.7
2	B	125	LEU	2.7
3	D	583	LEU	2.6
3	C	555	ALA	2.6
2	B	150	ILE	2.5
3	C	513	CYS	2.5
1	H	140	THR	2.5
3	D	514	ALA	2.4
2	B	190	ASN	2.4
1	A	29	LEU	2.3
1	A	135	GLY	2.3
3	D	588	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	7	THR	2.2
2	B	155	ARG	2.1
1	H	143	MET	2.1
3	D	611	LEU	2.1
2	L	8	THR	2.1
2	B	193	THR	2.1
2	B	192	TYR	2.0
3	C	584	ILE	2.0
3	C	585	ASN	2.0
3	C	600	ASN	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
4	SO4	H	302	5/5	0.75	0.15	146,161,164,170	0
4	SO4	A	301	5/5	0.79	0.12	98,99,102,106	0
4	SO4	A	302	5/5	0.82	0.11	125,128,130,135	0
4	SO4	B	302	5/5	0.87	0.11	133,136,137,144	0
5	MES	H	303	12/12	0.88	0.22	161,200,225,240	0
4	SO4	B	301	5/5	0.93	0.07	68,88,92,94	0
4	SO4	H	301	5/5	0.97	0.07	72,79,84,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.