Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 03:13 AM EDT

PDB ID	:	7LR4
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 (i) 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 (1)) were used in the production of this report:

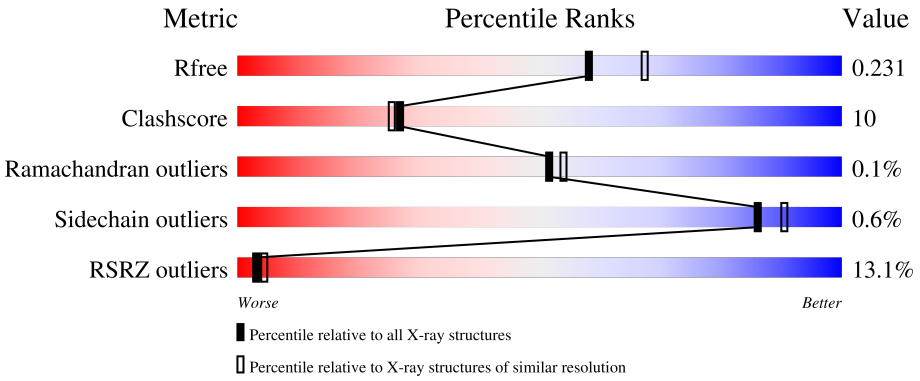
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	12% 77% 19% .
1	H	226	6% 83% 14% .
2	B	214	20% 79% 19% ..
2	L	214	3% 83% 16%
3	C	123	20% 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	-
5	MES	H	303	-	-	-	X

2 Entry composition (i)

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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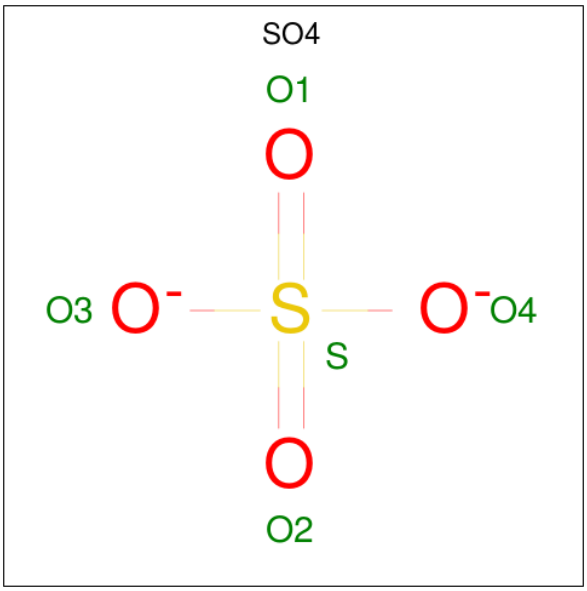
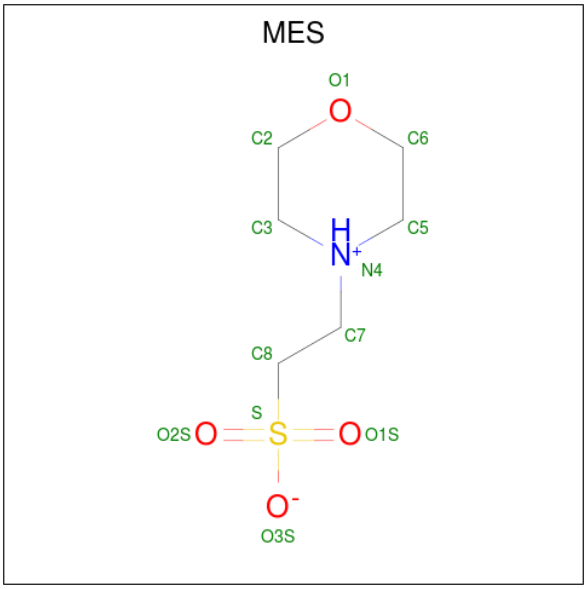
Chain	Residue	Modelled	Actual	Comment	Reference
C	624	HIS	-	expression tag	UNP Q4YCF6
D	516	THR	ASN	engineered mutation	UNP Q4YCF6
D	533	ASN	SER	engineered mutation	UNP Q4YCF6
D	539	GLN	ASN	engineered mutation	UNP Q4YCF6
D	619	HIS	-	expression tag	UNP Q4YCF6
D	620	HIS	-	expression tag	UNP Q4YCF6
D	621	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 (three-letter code: SO4) (formula: O_4S).



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 (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 6 is water.

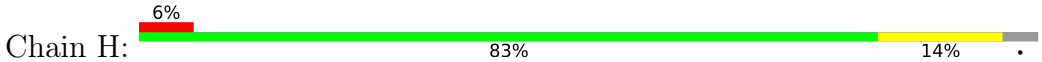
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	115	Total	O	0	0
			115	115		
6	L	111	Total	O	0	0
			111	111		
6	A	50	Total	O	0	0
			50	50		
6	B	47	Total	O	0	0
			47	47		
6	C	18	Total	O	0	0
			18	18		
6	D	13	Total	O	0	0
			13	13		

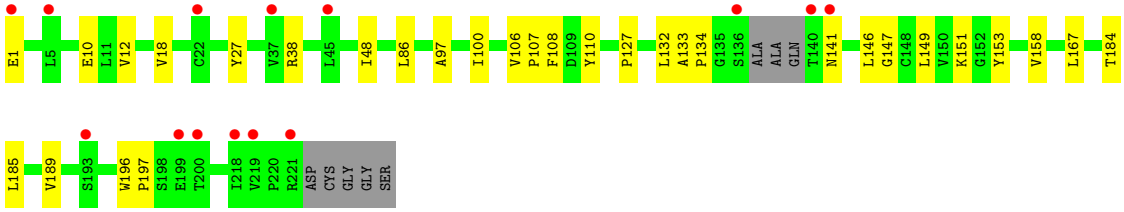
3 Residue-property plots (i)

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

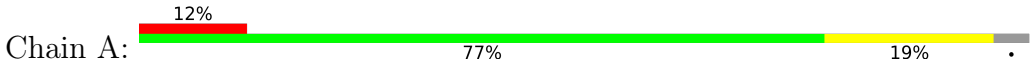
Chain H:

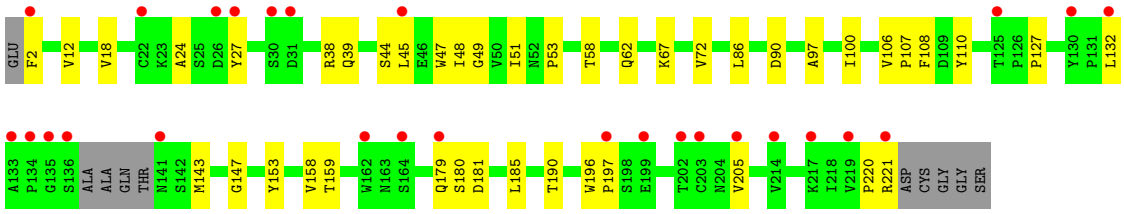




• Molecule 1: D3_2/1.12 Fab heavy chain

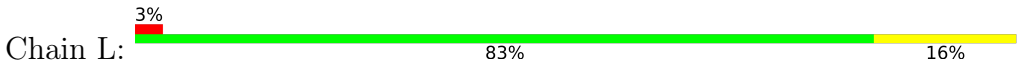
Chain A:

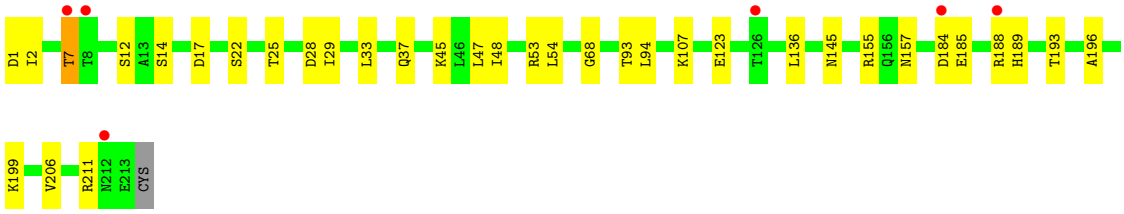




• Molecule 2: D3_2/1.12 Fab light chain

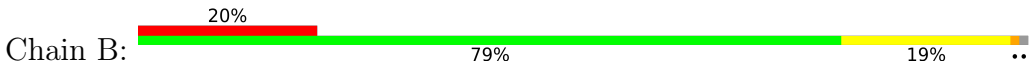
Chain L:

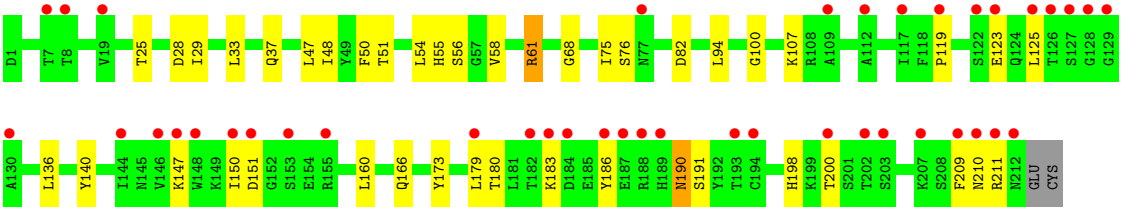




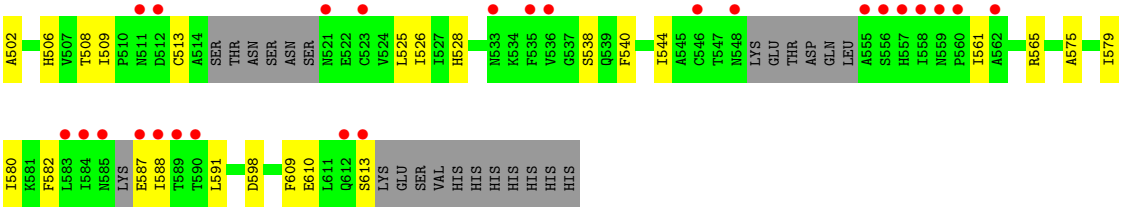
• Molecule 2: D3_2/1.12 Fab light chain

Chain B:

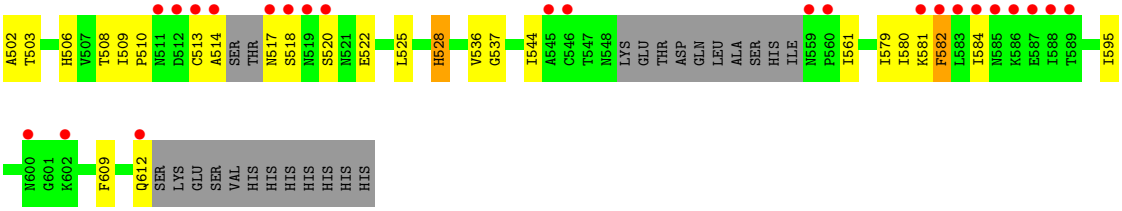




• Molecule 3: Hapless 2



• Molecule 3: Hapless 2



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.07 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.189 , 0.231 0.189 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (2.94%)	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)	0.33 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 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	0.26	0/1693	0.46	0/2318
1	H	0.26	0/1710	0.47	0/2341
2	B	0.25	0/1685	0.45	0/2288
2	L	0.26	0/1703	0.46	0/2312
3	C	0.25	0/794	0.43	0/1075
3	D	0.26	0/788	0.44	0/1067
All	All	0.26	0/8373	0.46	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

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	35	0
1	H	1664	0	1613	30	0
2	B	1650	0	1583	35	0
2	L	1668	0	1594	25	0
3	C	780	0	767	20	0
3	D	774	0	760	21	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	7	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	165	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 10.

All (165) 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
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
1:H:1:GLU:N	6:H:406:HOH:O	2.27	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
4:H:302:SO4:O1	6:H:402:HOH:O	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:L:107:LYS:NZ	6:L:306:HOH:O	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:PHE:O	2:B:51:THR:HB	2.08	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
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
3:D:525:LEU:HD21	3:D:609:PHE:HZ	1.75	0.51
2:L:1:ASP:N	6:L:302:HOH:O	2.12	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
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
3:D:517:ASN:O	3:D:518:SER:HB2	2.13	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:185:LEU:HD12	1:H:185:LEU:C	2.36	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
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
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:A:220:PRO:O	1:A:221:ARG:HB2	2.18	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:N	3:C:588:ILE:HD12	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
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
3:C:587:GLU:C	3:C:588:ILE:HD12	2.39	0.42
1:H:27:TYR:CZ	1:H:100:ILE:HD11	2.55	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:143:MET:HE2	1:A:190:THR:HG22	2.02	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

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 (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	213/226 (94%)	207 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	26
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%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	7	THR

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	192/197 (98%)	192 (100%)	0	100	100
1	H	194/197 (98%)	194 (100%)	0	100	100
2	B	190/192 (99%)	187 (98%)	3 (2%)	62	69
2	L	192/192 (100%)	191 (100%)	1 (0%)	88	92
3	C	89/112 (80%)	89 (100%)	0	100	100
3	D	89/112 (80%)	87 (98%)	2 (2%)	52	57
All	All	946/1002 (94%)	940 (99%)	6 (1%)	86	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	33	LEU
2	B	56	SER
2	B	61	ARG
2	B	190	ASN
3	D	528	HIS

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Mol	Chain	Res	Type
3	D	582	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	B	301	-	4,4,4	0.15	0	6,6,6	0.08	0
5	MES	H	303	-	12,12,12	2.33	1 (8%)	14,16,16	2.11	6 (42%)
4	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	H	302	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.05	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	-7.81	1.66	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	303	MES	C7-N4-C5	4.20	121.99	111.23
5	H	303	MES	O1S-S-C8	3.68	111.35	106.92
5	H	303	MES	C6-C5-N4	-2.86	105.77	110.10
5	H	303	MES	O2S-S-C8	2.28	109.66	106.92
5	H	303	MES	C2-C3-N4	2.28	113.55	110.10
5	H	303	MES	C7-N4-C3	-2.01	106.10	111.23

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
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
5	H	303	MES	1	0
4	H	302	SO4	2	0
4	B	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, 95^{th} 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%)	1.09	27 (12%) 3 5	46, 67, 121, 178	0
1	H	218/226 (96%)	0.89	14 (6%) 19 24	37, 52, 94, 142	0
2	B	212/214 (99%)	1.21	42 (19%) 1 1	48, 80, 141, 170	0
2	L	213/214 (99%)	0.65	6 (2%) 53 59	38, 56, 91, 142	0
3	C	99/123 (80%)	1.67	25 (25%) 0 0	44, 76, 154, 197	0
3	D	99/123 (80%)	1.70	24 (24%) 0 0	47, 77, 152, 193	0
All	All	1057/1126 (93%)	1.09	138 (13%) 3 4	37, 66, 130, 197	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	585	ASN	9.7
3	D	583	LEU	8.8
3	C	588	ILE	8.7
1	H	140	THR	8.7
1	A	135	GLY	8.4
3	D	514	ALA	8.2
3	D	518	SER	7.5
3	C	613	SER	7.1
3	C	589	THR	7.1
2	L	7	THR	6.9
1	A	136	SER	6.8
1	A	27	TYR	6.8
3	D	612	GLN	6.7
3	C	555	ALA	6.6
3	C	557	HIS	6.3
3	D	586	LYS	6.2
3	C	587	GLU	6.2
1	H	141	ASN	6.1
3	D	588	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
3	D	587	GLU	5.9
3	C	558	ILE	5.8
2	B	127	SER	5.8
3	C	556	SER	5.8
3	D	581	LYS	5.7
2	B	209	PHE	5.6
3	D	589	THR	5.6
2	B	150	ILE	5.6
2	B	182	THR	5.5
3	C	584	ILE	5.3
2	B	194	CYS	5.3
3	C	512	ASP	5.0
3	D	559	ASN	5.0
1	A	179	GLN	4.9
1	A	219	VAL	4.8
3	C	521	ASN	4.8
1	A	26	ASP	4.8
1	H	221	ARG	4.7
3	D	584	ILE	4.7
3	C	590	THR	4.7
1	A	141	ASN	4.7
3	D	512	ASP	4.6
2	B	200	THR	4.6
2	B	153	SER	4.5
2	B	122	SER	4.4
1	H	219	VAL	4.4
2	B	155	ARG	4.4
3	C	546	CYS	4.3
3	D	517	ASN	4.3
3	D	520	SER	4.2
2	B	183	LYS	4.2
2	B	130	ALA	4.2
1	H	136	SER	4.1
3	C	560	PRO	4.1
1	A	199	GLU	4.1
2	B	202	THR	4.0
2	B	186	TYR	4.0
2	B	125	LEU	3.9
1	H	193	SER	3.9
2	B	203	SER	3.7
3	D	582	PHE	3.7
2	B	187	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
3	D	513	CYS	3.6
1	A	221	ARG	3.6
3	D	602	LYS	3.5
1	A	130	TYR	3.5
1	A	214	VAL	3.5
1	A	205	VAL	3.4
3	D	511	ASN	3.4
1	H	1	GLU	3.4
1	A	134	PRO	3.3
2	B	129	GLY	3.3
3	C	548	ASN	3.2
2	B	119	PRO	3.2
2	B	184	ASP	3.2
2	B	148	TRP	3.2
3	C	535	PHE	3.2
2	B	188	ARG	3.1
1	A	202	THR	3.1
3	C	511	ASN	3.0
1	A	162	TRP	3.0
1	H	200	THR	3.0
2	L	126	THR	3.0
1	H	5	LEU	2.8
1	A	132	LEU	2.8
3	D	519	ASN	2.8
3	D	600	ASN	2.7
2	B	211	ARG	2.7
3	D	546	CYS	2.7
2	L	184	ASP	2.7
2	L	212	ASN	2.7
3	C	612	GLN	2.6
2	L	188	ARG	2.6
2	B	128	GLY	2.6
2	B	210	ASN	2.6
1	A	31	ASP	2.6
2	B	144	ILE	2.6
3	C	559	ASN	2.6
2	B	179	LEU	2.5
1	A	2	PHE	2.5
2	B	7	THR	2.5
2	B	146	VAL	2.5
1	H	199	GLU	2.5
1	H	22	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	203	CYS	2.4
2	B	109	ALA	2.4
2	B	126	THR	2.4
1	H	37	VAL	2.4
3	C	523	CYS	2.4
2	B	212	ASN	2.4
3	C	585	ASN	2.4
3	D	545	ALA	2.4
2	B	151	ASP	2.4
3	C	536	VAL	2.3
1	H	218	ILE	2.3
1	A	22	CYS	2.3
1	A	217	LYS	2.3
3	C	533	ASN	2.3
2	B	189	HIS	2.3
1	H	45	LEU	2.3
2	B	19	VAL	2.3
3	C	562	ALA	2.3
3	D	560	PRO	2.3
3	C	583	LEU	2.2
1	A	197	PRO	2.2
1	A	45	LEU	2.1
1	A	133	ALA	2.1
1	A	164	SER	2.1
1	A	30	SER	2.1
2	B	8	THR	2.1
2	B	77	ASN	2.1
2	B	112	ALA	2.1
2	B	123	GLU	2.1
2	B	117	ILE	2.0
2	B	207	LYS	2.0
2	L	8	THR	2.0
2	B	193	THR	2.0
2	B	147	LYS	2.0
1	A	125	THR	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, 95^{th} 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
5	MES	H	303	12/12	0.58	0.44	161,200,225,240	0
4	SO4	H	302	5/5	0.65	0.26	146,161,164,170	0
4	SO4	B	302	5/5	0.77	0.28	133,136,137,144	0
4	SO4	A	302	5/5	0.88	0.33	125,128,130,135	0
4	SO4	A	301	5/5	0.90	0.14	98,99,102,106	0
4	SO4	H	301	5/5	0.94	0.16	72,79,84,88	0
4	SO4	B	301	5/5	0.95	0.19	68,88,92,94	0

6.5 Other polymers (i)

There are no such residues in this entry.