Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:26 PM GMT

PDB ID	:	1FL5
Title	:	THE UNLIGANDED GERMLINE PRECURSOR TO THE SULFIDE OXIDASE CATALYTIC ANTIBODY 28B4.
Authors	:	Yin, J.; Mundorff, E.C.; Yang, P.L.; Wendt, K.U.; Hanway, D.; Stevens, R.C.; Schultz, P.G.
Deposited on	:	2000-08-11
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

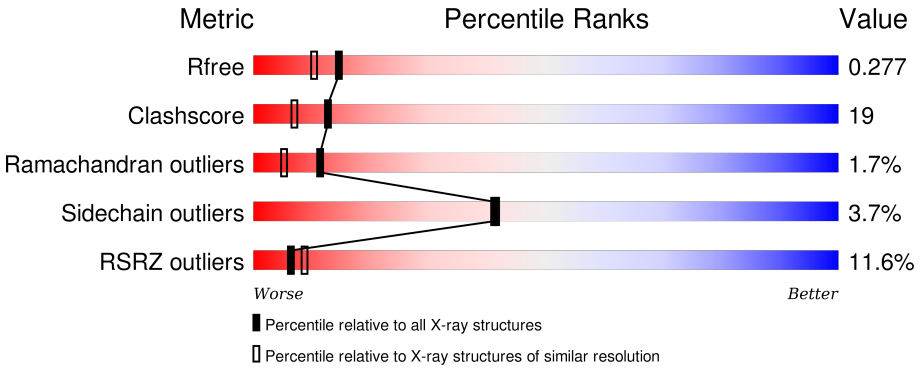
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	217	18%, 62%, 35%
1	L	217	8%, 72%, 24%
2	B	219	12%, 74%, 25%
2	H	219	9%, 74%, 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6922 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

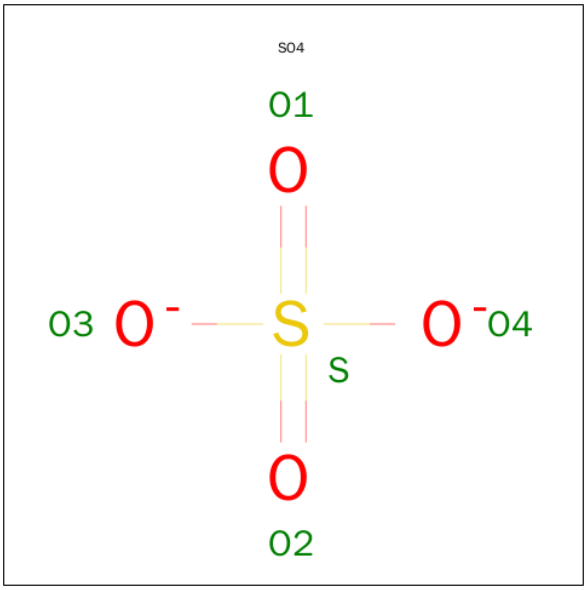
- Molecule 1 is a protein called ANTIBODY GERMLINE PRECURSOR TO ANTIBODY 28B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1674	1050	285	334	5			
1	A	217	Total	C	N	O	S	0	0	0
			1674	1050	285	334	5			

- Molecule 2 is a protein called ANTIBODY GERMLINE PRECURSOR TO ANTIBODY 28B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1645	1035	275	328	7			
2	B	219	Total	C	N	O	S	0	0	0
			1645	1035	275	328	7			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

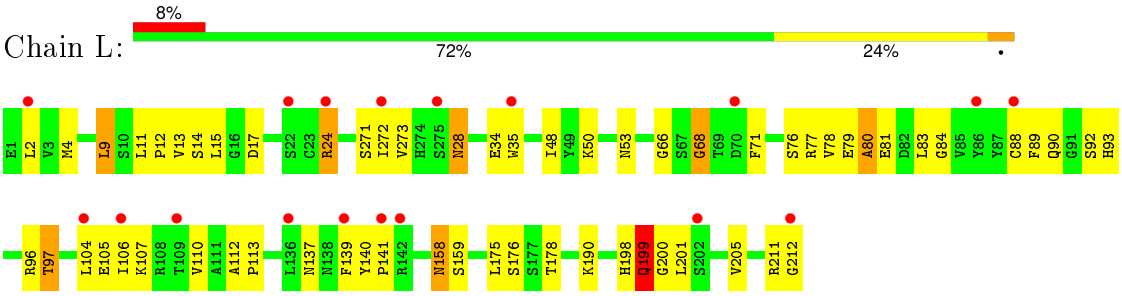
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	57	Total O 57 57	0	0
4	B	66	Total O 66 66	0	0
4	H	93	Total O 93 93	0	0
4	L	58	Total O 58 58	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

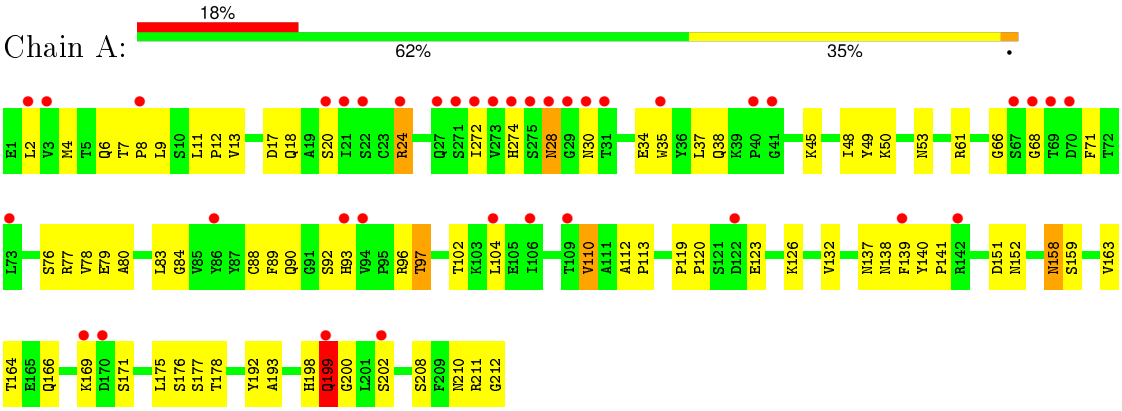
- Molecule 1: ANTIBODY GERMLINE PRECURSOR TO ANTIBODY 28B4

Chain L:



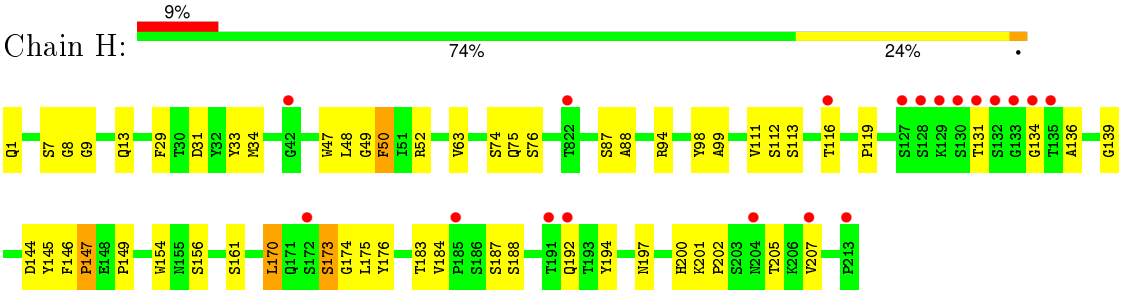
- Molecule 1: ANTIBODY GERMLINE PRECURSOR TO ANTIBODY 28B4

Chain A:



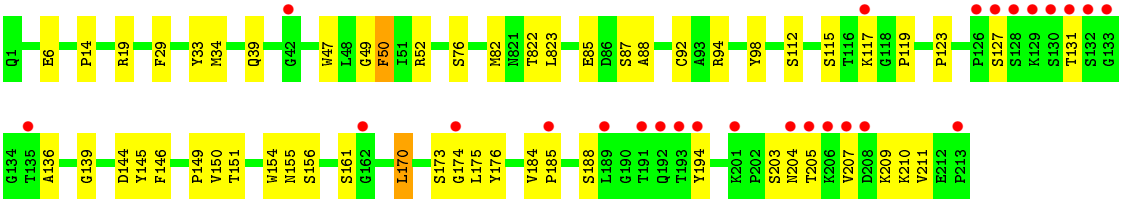
- Molecule 2: ANTIBODY GERMLINE PRECURSOR TO ANTIBODY 28B4

Chain H:



- Molecule 2: ANTIBODY GERMLINE PRECURSOR TO ANTIBODY 28B4

Chain B:


Q1 E6 P14 R19 F29 Y33 M34 Q39 G42 W47 L48 G49 F50 I51 R52 S76 M82 N821 T822 L823 E85 D86 S87 A88 C92 A93 R94 Y98 S112 S115 T116 K117 G118 P119 P123 P126 S127 S128 K129 S130 T131 S132 G133
G134 T135 A136 G139 D144 Y145 F146 P149 V150 T151 W154 N155 S156 S161 G162 L170 S173 G174 L175 Y176 V184 P185 S188 L189 G190 T191 Q192 T193 Y194 K201 P202 S203 N204 T205 K206 V207 D208 K209 K210 V211 E212 P213

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	36.42Å 69.65Å 85.31Å 74.56° 80.18° 77.55°	Depositor
Resolution (Å)	20.00 – 2.10 19.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-2.10) 87.0 (19.92-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.01Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.226 , 0.268 0.237 , 0.277	Depositor DCC
R_{free} test set	4399 reflections (10.11%)	DCC
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 49575 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6922	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0/1710	0.72	0/2316
1	L	0.44	0/1710	0.73	0/2316
2	B	0.55	0/1685	0.75	0/2294
2	H	0.56	0/1685	0.76	0/2294
All	All	0.50	0/6790	0.74	0/9220

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	1674	0	1641	78	0
1	L	1674	0	1641	70	0
2	B	1645	0	1599	58	0
2	H	1645	0	1599	62	0
3	B	5	0	0	0	0
3	H	5	0	0	0	0
4	A	57	0	0	14	0
4	B	66	0	0	13	0
4	H	93	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	58	0	0	11	0
All	All	6922	0	6480	253	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 19.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:HE1	2:B:94:ARG:HG3	1.38	1.03
2:H:7:SER:HB2	2:B:204:ASN:O	1.59	1.02
2:H:34:MET:HE1	2:H:94:ARG:HG3	1.43	1.01
2:H:188:SER:HA	4:H:861:HOH:O	1.62	1.00
1:L:90:GLN:NE2	1:L:93:HIS:H	1.63	0.96
1:A:90:GLN:NE2	1:A:93:HIS:H	1.65	0.93
1:L:273:VAL:HG23	4:L:289:HOH:O	1.68	0.92
2:H:8:GLY:H	2:B:204:ASN:HB2	1.35	0.88
2:H:34:MET:CE	2:H:94:ARG:HA	2.03	0.88
2:H:34:MET:HE2	2:H:94:ARG:HA	1.55	0.88
1:L:13:VAL:HB	4:L:326:HOH:O	1.72	0.88
2:B:207:VAL:HG12	4:B:866:HOH:O	1.76	0.86
1:A:28:ASN:ND2	1:A:28:ASN:H	1.73	0.84
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.60	0.84
2:B:34:MET:HE2	2:B:94:ARG:HA	1.59	0.83
2:B:34:MET:CE	2:B:94:ARG:HA	2.08	0.82
1:A:177:SER:HB2	4:A:325:HOH:O	1.79	0.82
2:H:74:SER:HB3	1:A:126:LYS:HD2	1.59	0.82
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.62	0.81
2:H:74:SER:HB3	1:A:126:LYS:CD	2.11	0.80
1:L:28:ASN:ND2	1:L:28:ASN:H	1.77	0.80
1:A:175:LEU:HD21	4:A:325:HOH:O	1.82	0.79
1:A:18:GLN:HG2	4:A:324:HOH:O	1.82	0.79
2:H:188:SER:HB2	4:H:908:HOH:O	1.82	0.78
1:L:12:PRO:O	1:L:13:VAL:HG13	1.86	0.76
1:A:28:ASN:H	1:A:28:ASN:HD22	1.35	0.74
2:B:175:LEU:HD23	4:B:861:HOH:O	1.87	0.74
1:L:68:GLY:HA2	4:L:289:HOH:O	1.88	0.74
1:A:12:PRO:O	1:A:13:VAL:HG13	1.88	0.74
1:A:90:GLN:NE2	1:A:93:HIS:N	2.36	0.73
2:B:156:SER:HA	4:B:855:HOH:O	1.87	0.73
1:L:90:GLN:NE2	1:L:93:HIS:N	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:GLN:HG2	1:A:123:GLU:OE1	1.90	0.71
2:B:34:MET:HE1	2:B:94:ARG:CG	2.18	0.70
1:A:158:ASN:ND2	4:A:287:HOH:O	2.23	0.70
2:H:156:SER:H	2:H:197:ASN:HD21	1.37	0.69
1:L:90:GLN:HE21	1:L:92:SER:N	1.91	0.69
2:H:174:GLY:N	4:H:877:HOH:O	2.24	0.68
2:H:173:SER:HB2	4:H:877:HOH:O	1.93	0.68
1:L:199:GLN:O	1:L:199:GLN:HG3	1.93	0.68
2:H:147:PRO:HD2	4:H:889:HOH:O	1.93	0.68
1:L:28:ASN:HD22	1:L:28:ASN:H	1.41	0.68
2:H:34:MET:HE1	2:H:94:ARG:CG	2.22	0.67
2:H:74:SER:CB	1:A:126:LYS:HD2	2.25	0.67
1:A:20:SER:HB3	4:A:324:HOH:O	1.94	0.67
2:B:144:ASP:HB3	2:B:175:LEU:HD12	1.77	0.66
2:H:112:SER:HG	2:H:146:PHE:HZ	1.43	0.66
2:B:85:GLU:HG2	4:B:856:HOH:O	1.95	0.66
2:B:170:LEU:HD11	2:B:174:GLY:HA2	1.78	0.65
1:L:80:ALA:HB3	4:L:320:HOH:O	1.97	0.65
2:H:31:ASP:HB3	4:H:909:HOH:O	1.95	0.65
1:A:199:GLN:O	1:A:199:GLN:HG3	1.97	0.65
1:L:158:ASN:CG	4:L:299:HOH:O	2.36	0.64
1:L:211:ARG:HH11	1:L:211:ARG:HG2	1.63	0.64
2:B:155:ASN:HA	4:B:845:HOH:O	1.98	0.64
1:A:158:ASN:CG	4:A:287:HOH:O	2.38	0.62
2:H:33:TYR:O	2:H:34:MET:HE3	1.99	0.62
2:H:187:SER:HB2	4:H:915:HOH:O	1.98	0.62
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.34	0.62
1:L:83:LEU:HD22	1:L:104:LEU:O	2.00	0.62
1:A:83:LEU:HD22	1:A:104:LEU:O	2.00	0.62
1:L:272:ILE:HG21	4:L:293:HOH:O	1.99	0.62
1:A:90:GLN:HE22	1:A:93:HIS:N	1.97	0.61
2:H:8:GLY:N	2:B:204:ASN:HB2	2.13	0.61
2:H:144:ASP:HB3	2:H:175:LEU:HD12	1.83	0.60
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.36	0.60
1:L:90:GLN:HE21	1:L:92:SER:H	1.49	0.60
1:A:90:GLN:HE21	1:A:92:SER:N	1.98	0.60
1:L:104:LEU:HD23	1:L:104:LEU:C	2.23	0.60
1:A:192:TYR:O	1:A:208:SER:HB2	2.02	0.59
2:H:192:GLN:NE2	4:H:908:HOH:O	2.35	0.59
2:B:139:GLY:HA2	2:B:154:TRP:CH2	2.37	0.59
2:B:170:LEU:HD23	2:B:176:TYR:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:OE1	2:B:39:GLN:NE2	2.27	0.58
2:H:170:LEU:HD11	2:H:174:GLY:HA2	1.86	0.58
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.39	0.57
2:B:209:LYS:HB2	4:B:866:HOH:O	2.05	0.57
1:A:78:VAL:HG12	1:A:79:GLU:N	2.19	0.57
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.40	0.56
1:L:90:GLN:HE22	1:L:93:HIS:N	2.01	0.56
1:L:81:GLU:HG3	4:L:320:HOH:O	2.05	0.56
1:L:78:VAL:HG12	1:L:79:GLU:N	2.19	0.56
2:H:87:SER:O	2:H:88:ALA:HB2	2.04	0.56
1:A:274:HIS:HB2	1:A:30:ASN:O	2.06	0.56
1:A:112:ALA:HB2	1:A:200:GLY:O	2.04	0.56
2:H:33:TYR:O	2:H:34:MET:CE	2.54	0.56
2:B:144:ASP:HB3	2:B:175:LEU:CD1	2.36	0.56
2:B:82:MET:HE2	2:B:823:LEU:HD21	1.88	0.56
1:L:110:VAL:HG11	1:L:199:GLN:O	2.06	0.56
2:H:200:HIS:CE1	4:H:889:HOH:O	2.58	0.55
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.87	0.55
1:A:90:GLN:HE21	1:A:92:SER:H	1.55	0.55
1:L:90:GLN:NE2	1:L:92:SER:N	2.55	0.54
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.41	0.54
2:B:188:SER:HB3	4:B:848:HOH:O	2.06	0.54
1:L:158:ASN:ND2	4:L:299:HOH:O	2.39	0.54
2:H:205:THR:HG22	2:H:207:VAL:HG23	1.89	0.54
1:A:210:ASN:C	1:A:212:GLY:H	2.11	0.54
1:A:210:ASN:O	1:A:212:GLY:N	2.40	0.54
1:L:28:ASN:ND2	1:L:28:ASN:N	2.53	0.54
1:A:113:PRO:HB3	1:A:139:PHE:HB3	1.88	0.54
1:L:211:ARG:O	1:L:212:GLY:C	2.43	0.54
2:B:184:VAL:HG11	2:B:194:TYR:CE2	2.42	0.54
1:A:97:THR:HG21	4:A:283:HOH:O	2.08	0.53
2:B:205:THR:HG22	2:B:207:VAL:HG23	1.89	0.53
2:H:34:MET:HA	2:H:34:MET:HE2	1.89	0.53
2:B:29:PHE:CD2	2:B:76:SER:HA	2.44	0.53
1:L:2:LEU:HD11	4:L:293:HOH:O	2.09	0.53
1:A:50:LYS:HE2	2:B:98:TYR:CD2	2.44	0.52
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.90	0.52
2:H:7:SER:CB	2:B:204:ASN:O	2.48	0.52
1:A:61:ARG:HG3	4:A:300:HOH:O	2.07	0.52
1:L:50:LYS:HE2	2:H:98:TYR:CD2	2.45	0.52
2:H:144:ASP:HB3	2:H:175:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:MET:HB3	2:B:823:LEU:HD21	1.91	0.51
1:L:4:MET:HE2	1:L:90:GLN:HB2	1.91	0.51
2:H:147:PRO:CD	4:H:889:HOH:O	2.54	0.51
2:H:8:GLY:HA2	2:B:203:SER:O	2.10	0.51
1:A:2:LEU:HD22	1:A:97:THR:HG21	1.92	0.51
2:H:13:GLN:HG3	4:B:875:HOH:O	2.11	0.51
2:H:184:VAL:HG11	2:H:194:TYR:CE2	2.46	0.51
2:B:123:PRO:HB2	2:B:211:VAL:HG13	1.92	0.51
2:B:34:MET:HA	2:B:34:MET:HE2	1.92	0.51
2:H:34:MET:HE1	2:H:94:ARG:HA	1.92	0.50
1:A:90:GLN:NE2	1:A:92:SER:N	2.59	0.50
1:A:4:MET:HE2	1:A:90:GLN:HB2	1.92	0.50
2:B:33:TYR:O	2:B:34:MET:HE3	2.11	0.50
2:H:75:GLN:NE2	1:A:123:GLU:OE1	2.45	0.50
2:B:174:GLY:N	4:B:857:HOH:O	2.42	0.50
1:L:80:ALA:HA	1:L:106:ILE:HD11	1.93	0.50
1:L:35:TRP:CH2	1:L:88:CYS:HB3	2.46	0.50
1:A:198:HIS:O	1:A:200:GLY:N	2.44	0.50
2:B:33:TYR:O	2:B:34:MET:CE	2.60	0.49
2:H:134:GLY:HA3	4:H:888:HOH:O	2.12	0.49
2:H:146:PHE:C	4:H:889:HOH:O	2.50	0.49
2:H:200:HIS:NE2	4:H:889:HOH:O	2.34	0.49
1:L:14:SER:N	1:L:107:LYS:HG2	2.28	0.49
1:A:110:VAL:HG11	1:A:199:GLN:O	2.13	0.49
2:B:33:TYR:CE2	2:B:52:ARG:HG2	2.48	0.49
1:L:211:ARG:O	1:L:212:GLY:O	2.31	0.49
2:B:87:SER:O	2:B:88:ALA:HB2	2.11	0.49
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.47	0.49
1:A:198:HIS:C	1:A:200:GLY:H	2.16	0.49
2:H:111:VAL:O	2:H:112:SER:HB3	2.13	0.48
2:H:9:GLY:O	2:B:204:ASN:ND2	2.47	0.48
2:B:822:THR:HG22	2:B:822:THR:O	2.13	0.48
1:A:66:GLY:HA3	1:A:71:PHE:HA	1.96	0.48
1:A:35:TRP:CH2	1:A:88:CYS:HB3	2.48	0.48
1:L:15:LEU:HD23	4:L:316:HOH:O	2.13	0.48
2:B:19:ARG:HD2	4:B:841:HOH:O	2.14	0.48
1:L:112:ALA:HB2	1:L:200:GLY:O	2.13	0.48
2:B:210:LYS:NZ	2:B:210:LYS:HB3	2.29	0.47
2:H:147:PRO:N	4:H:889:HOH:O	2.46	0.47
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.49	0.47
2:H:29:PHE:CD2	2:H:76:SER:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:SER:HG	2:B:146:PHE:HZ	1.62	0.47
1:L:113:PRO:HD3	1:L:198:HIS:CD2	2.50	0.47
1:L:198:HIS:O	1:L:200:GLY:N	2.46	0.47
1:L:211:ARG:NH1	1:L:211:ARG:HG2	2.28	0.47
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.50	0.47
1:L:140:TYR:CD1	1:L:141:PRO:HA	2.50	0.47
2:H:50:PHE:C	2:H:50:PHE:CD1	2.89	0.47
1:A:159:SER:HA	1:A:178:THR:O	2.15	0.47
1:L:90:GLN:HG3	4:L:293:HOH:O	2.16	0.46
1:L:80:ALA:HA	1:L:106:ILE:CD1	2.44	0.46
1:A:163:VAL:HG12	1:A:164:THR:O	2.15	0.46
1:A:83:LEU:HD13	1:A:84:GLY:N	2.31	0.46
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.98	0.46
2:H:170:LEU:HD23	2:H:176:TYR:CZ	2.50	0.46
1:A:48:ILE:HA	1:A:53:ASN:O	2.16	0.46
2:H:48:LEU:HD22	2:H:63:VAL:HG11	1.98	0.46
4:H:900:HOH:O	2:B:117:LYS:HG3	2.16	0.45
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.97	0.45
1:L:198:HIS:C	1:L:200:GLY:H	2.19	0.45
1:A:8:PRO:O	1:A:102:THR:HG23	2.16	0.45
2:B:119:PRO:CB	2:B:145:TYR:HB3	2.40	0.45
1:A:11:LEU:C	1:A:11:LEU:HD23	2.36	0.45
1:L:14:SER:CA	1:L:107:LYS:HG2	2.47	0.45
1:L:159:SER:HA	1:L:178:THR:O	2.16	0.45
1:A:175:LEU:HD23	1:A:176:SER:N	2.32	0.45
2:H:116:THR:HG21	2:H:202:PRO:O	2.17	0.45
1:A:78:VAL:CG1	1:A:79:GLU:N	2.80	0.45
1:A:193:ALA:CB	1:A:208:SER:HB3	2.47	0.45
1:L:89:PHE:CZ	1:L:96:ARG:HB3	2.52	0.44
1:L:96:ARG:C	1:L:97:THR:HG22	2.37	0.44
1:A:89:PHE:CZ	1:A:96:ARG:HB3	2.52	0.44
1:A:37:LEU:O	1:A:45:LYS:HG2	2.17	0.44
2:B:170:LEU:HD12	4:B:879:HOH:O	2.17	0.44
1:L:78:VAL:CG1	1:L:79:GLU:N	2.80	0.44
1:L:9:LEU:O	1:L:9:LEU:HD13	2.17	0.44
1:L:190:LYS:NZ	1:L:212:GLY:HA2	2.31	0.44
1:A:6:GLN:HB3	4:A:331:HOH:O	2.18	0.44
1:L:11:LEU:C	1:L:11:LEU:HD23	2.38	0.44
2:H:33:TYR:CE2	2:H:52:ARG:HG2	2.53	0.44
1:A:76:SER:O	1:A:77:ARG:HB2	2.18	0.44
1:A:151:ASP:O	1:A:152:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.83	0.43
1:A:175:LEU:HD23	1:A:175:LEU:C	2.39	0.43
2:B:170:LEU:HD23	2:B:176:TYR:CE1	2.53	0.43
2:H:201:LYS:HB2	2:H:202:PRO:HD3	1.98	0.43
1:L:17:ASP:O	1:L:78:VAL:HG23	2.18	0.43
1:A:28:ASN:ND2	1:A:28:ASN:N	2.52	0.43
2:H:119:PRO:CB	2:H:145:TYR:HB3	2.42	0.43
1:A:210:ASN:C	1:A:212:GLY:N	2.71	0.43
1:A:24:ARG:NH1	1:A:24:ARG:HG2	2.33	0.43
2:B:139:GLY:HA2	2:B:154:TRP:HH2	1.79	0.43
1:A:28:ASN:N	1:A:28:ASN:HD22	2.10	0.43
1:L:76:SER:O	1:L:77:ARG:HB2	2.19	0.43
1:A:17:ASP:O	1:A:78:VAL:HG23	2.19	0.42
1:A:119:PRO:HG3	2:B:127:SER:HB2	2.01	0.42
1:A:96:ARG:C	1:A:97:THR:HG22	2.40	0.42
1:L:190:LYS:NZ	1:L:212:GLY:CA	2.82	0.42
1:L:83:LEU:CD2	1:L:105:GLU:HA	2.50	0.42
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.54	0.42
1:A:7:THR:HG23	4:A:302:HOH:O	2.19	0.42
1:A:193:ALA:HB2	1:A:208:SER:HB3	2.01	0.42
2:H:183:THR:O	2:H:184:VAL:CG1	2.68	0.42
1:L:83:LEU:HD13	1:L:84:GLY:N	2.35	0.42
1:L:175:LEU:HD23	1:L:176:SER:N	2.35	0.42
1:A:169:LYS:HD3	4:A:322:HOH:O	2.19	0.42
2:B:209:LYS:CA	4:B:866:HOH:O	2.67	0.42
1:L:28:ASN:HD22	1:L:28:ASN:N	2.10	0.42
1:L:190:LYS:HZ2	1:L:212:GLY:HA2	1.85	0.42
2:B:50:PHE:CD1	2:B:50:PHE:C	2.93	0.42
1:L:24:ARG:HG2	1:L:24:ARG:NH1	2.35	0.42
1:L:2:LEU:C	1:L:2:LEU:HD23	2.40	0.41
1:L:15:LEU:HD13	1:L:79:GLU:HA	2.02	0.41
2:H:136:ALA:O	2:H:184:VAL:HG22	2.21	0.41
1:L:107:LYS:HA	1:L:140:TYR:OH	2.20	0.41
1:L:175:LEU:HD23	1:L:175:LEU:C	2.41	0.41
1:L:2:LEU:HD22	1:L:97:THR:HG21	2.01	0.41
1:L:24:ARG:HH11	1:L:24:ARG:HG2	1.86	0.41
2:B:150:VAL:CG1	2:B:151:THR:N	2.84	0.41
1:A:272:ILE:HG21	1:A:90:GLN:HG3	2.03	0.41
1:A:202:SER:HB2	4:A:293:HOH:O	2.20	0.41
2:H:170:LEU:HD23	2:H:176:TYR:CE1	2.56	0.41
2:H:112:SER:OG	2:H:146:PHE:HZ	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLU:HG2	2:B:92:CYS:SG	2.61	0.41
1:A:90:GLN:OE1	1:A:97:THR:HG23	2.21	0.41
1:A:13:VAL:HG23	4:A:311:HOH:O	2.19	0.41
2:H:202:PRO:HB2	4:H:889:HOH:O	2.21	0.41
2:B:170:LEU:HD21	2:B:174:GLY:O	2.19	0.41
2:H:139:GLY:HA2	2:H:154:TRP:HH2	1.83	0.41
1:A:49:TYR:O	1:A:53:ASN:HB2	2.21	0.41
1:L:48:ILE:HA	1:L:53:ASN:O	2.21	0.41
1:L:2:LEU:HD12	1:L:93:HIS:CD2	2.56	0.40
1:A:212:GLY:HA2	4:A:321:HOH:O	2.21	0.40
2:B:14:PRO:HD3	2:B:112:SER:C	2.41	0.40
1:A:166:GLN:HG3	1:A:171:SER:O	2.21	0.40
2:B:185:PRO:HD2	2:B:188:SER:OG	2.22	0.40
2:B:136:ALA:O	2:B:184:VAL:HG22	2.22	0.40
2:B:209:LYS:CB	4:B:866:HOH:O	2.65	0.40
1:A:13:VAL:HG21	1:A:104:LEU:HD11	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	215/217 (99%)	195 (91%)	14 (6%)	6 (3%)	6 2
1	L	215/217 (99%)	196 (91%)	15 (7%)	4 (2%)	10 4
2	B	217/219 (99%)	197 (91%)	18 (8%)	2 (1%)	21 15
2	H	217/219 (99%)	198 (91%)	16 (7%)	3 (1%)	14 7
All	All	864/872 (99%)	786 (91%)	63 (7%)	15 (2%)	11 5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY
1	L	68	GLY
2	H	173	SER
1	A	211	ARG
2	B	173	SER
1	L	271	SER
2	H	131	THR
1	A	199	GLN
2	B	131	THR
1	L	80	ALA
1	L	199	GLN
1	A	80	ALA
2	H	99	ALA
1	A	138	ASN
1	A	110	VAL

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	192/192 (100%)	184 (96%)	8 (4%)	36	35
1	L	192/192 (100%)	184 (96%)	8 (4%)	36	35
2	B	184/184 (100%)	179 (97%)	5 (3%)	52	56
2	H	184/184 (100%)	177 (96%)	7 (4%)	40	40
All	All	752/752 (100%)	724 (96%)	28 (4%)	41	41

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LEU
1	L	24	ARG
1	L	28	ASN
1	L	34	GLU
1	L	97	THR
1	L	137	ASN
1	L	158	ASN

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Mol	Chain	Res	Type
1	L	199	GLN
2	H	1	GLN
2	H	50	PHE
2	H	113	SER
2	H	147	PRO
2	H	149	PRO
2	H	161	SER
2	H	170	LEU
1	A	9	LEU
1	A	24	ARG
1	A	28	ASN
1	A	34	GLU
1	A	97	THR
1	A	137	ASN
1	A	158	ASN
1	A	199	GLN
2	B	50	PHE
2	B	115	SER
2	B	149	PRO
2	B	161	SER
2	B	170	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	274	HIS
1	L	28	ASN
1	L	30	ASN
1	L	53	ASN
1	L	90	GLN
1	L	93	HIS
1	L	137	ASN
1	L	138	ASN
1	L	210	ASN
2	H	192	GLN
2	H	197	ASN
2	H	199	ASN
1	A	274	HIS
1	A	28	ASN
1	A	30	ASN
1	A	38	GLN
1	A	90	GLN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	138	ASN
2	B	39	GLN
2	B	199	ASN
2	B	204	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	B	302	-	4,4,4	0.14	0	6,6,6	0.24	0
3	SO4	H	301	-	4,4,4	0.23	0	6,6,6	0.66	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
3	SO4	B	302	-	-	0/0/0/0	0/0/0/0
3	SO4	H	301	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

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	217/217 (100%)	0.99	38 (17%) 2 3	19, 43, 61, 66	0
1	L	217/217 (100%)	0.70	18 (8%) 14 19	19, 43, 59, 65	0
2	B	219/219 (100%)	0.76	26 (11%) 6 8	15, 33, 69, 85	0
2	H	219/219 (100%)	0.59	19 (8%) 13 17	15, 32, 68, 85	0
All	All	872/872 (100%)	0.76	101 (11%) 6 9	15, 38, 63, 85	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	SER	11.4
2	H	128	SER	9.9
2	B	133	GLY	7.8
2	B	132	SER	7.4
2	H	131	THR	7.0
2	B	129	LYS	6.7
2	B	130	SER	6.4
2	H	133	GLY	6.4
2	B	131	THR	6.2
2	H	132	SER	5.6
2	B	191	THR	5.4
2	B	127	SER	5.2
1	A	94	VAL	4.9
2	H	191	THR	4.8
1	A	28	ASN	4.7
2	H	130	SER	4.6
2	B	207	VAL	4.4
2	H	129	LYS	4.3
2	B	192	GLN	4.2
1	A	70	ASP	4.0
2	H	135	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	29	GLY	3.8
1	A	3	VAL	3.7
2	H	127	SER	3.7
2	H	192	GLN	3.7
1	A	275	SER	3.6
2	H	204	ASN	3.6
1	A	104	LEU	3.5
1	L	24	ARG	3.4
2	B	204	ASN	3.4
1	A	86	TYR	3.3
1	A	27	GLN	3.3
1	A	202	SER	3.3
2	B	189	LEU	3.2
1	A	169	LYS	3.2
2	B	174	GLY	3.2
1	L	142	ARG	3.2
2	B	185	PRO	3.2
2	B	213	PRO	3.1
1	L	275	SER	3.0
1	A	68	GLY	3.0
2	B	201	LYS	3.0
1	A	30	ASN	3.0
1	A	106	ILE	2.9
1	L	109	THR	2.9
1	A	40	PRO	2.9
2	H	207	VAL	2.9
2	H	172	SER	2.9
1	L	2	LEU	2.9
2	B	206	LYS	2.9
2	B	205	THR	2.9
1	A	21	ILE	2.8
1	L	88	CYS	2.8
2	B	208	ASP	2.8
1	L	86	TYR	2.7
2	B	126	PRO	2.7
2	B	117	LYS	2.7
2	H	134	GLY	2.7
1	A	93	HIS	2.7
1	L	104	LEU	2.7
1	L	136	LEU	2.6
1	A	67	SER	2.6
1	A	20	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	185	PRO	2.5
1	L	35	TRP	2.5
1	A	273	VAL	2.5
2	H	822	THR	2.5
2	H	116	THR	2.5
1	A	274	HIS	2.4
1	A	199	GLN	2.4
1	A	69	THR	2.4
2	B	42	GLY	2.4
2	B	193	THR	2.4
2	H	213	PRO	2.3
1	A	272	ILE	2.3
1	A	2	LEU	2.3
2	H	42	GLY	2.3
1	L	141	PRO	2.3
1	A	139	PHE	2.2
1	L	272	ILE	2.2
1	L	202	SER	2.2
1	A	22	SER	2.2
1	L	212	GLY	2.2
1	A	41	GLY	2.2
1	A	73	LEU	2.2
1	A	8	PRO	2.2
2	B	162	GLY	2.1
2	B	135	THR	2.1
1	L	106	ILE	2.1
1	A	24	ARG	2.1
1	A	142	ARG	2.1
1	L	70	ASP	2.1
1	L	22	SER	2.1
2	B	194	TYR	2.1
1	A	122	ASP	2.1
1	A	271	SER	2.0
1	A	31	THR	2.0
1	A	35	TRP	2.0
1	L	139	PHE	2.0
1	A	109	THR	2.0
1	A	170	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	H	301	5/5	0.95	0.14	0.92	37,38,40,41	0
3	SO4	B	302	5/5	0.98	0.13	0.05	35,36,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.