



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:42 AM GMT

PDB ID : 3CFE
Title : Crystal structure of purple-fluorescent antibody EP2-25C10
Authors : Debler, E.W.; Heine, A.; Wilson, I.A.
Deposited on : 2008-03-03
Resolution : 2.99 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

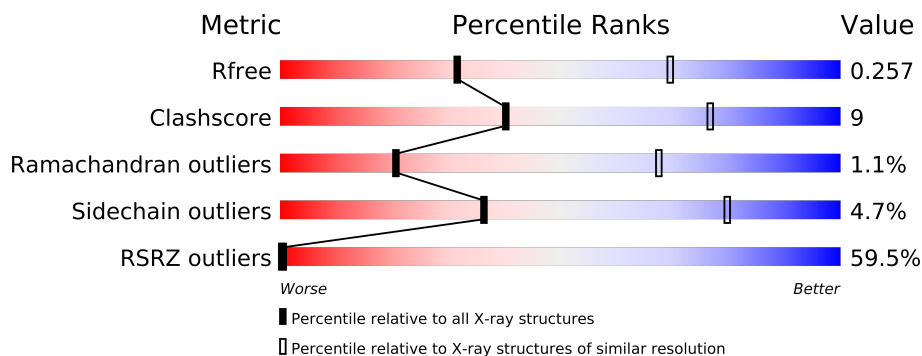
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.99 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	214	
1	L	214	
2	B	220	
2	H	220	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6677 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

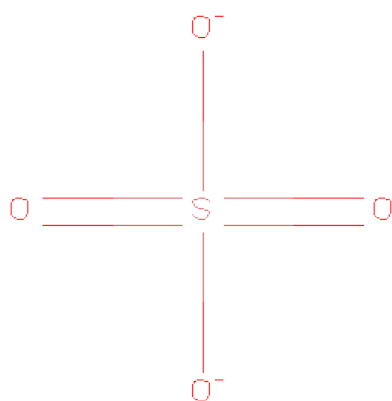
- Molecule 1 is a protein called PURPLE-FLUORESCENT ANTIBODY EP2-25C10-KAPPA LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1650	1021	279	344	6			
1	A	213	Total	C	N	O	S	0	0	0
			1650	1021	279	344	6			

- Molecule 2 is a protein called PURPLE-FLUORESCENT ANTIBODY EP2-25C10-IGG2B HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1667	1046	276	338	7			
2	B	219	Total	C	N	O	S	0	0	0
			1667	1046	276	338	7			

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

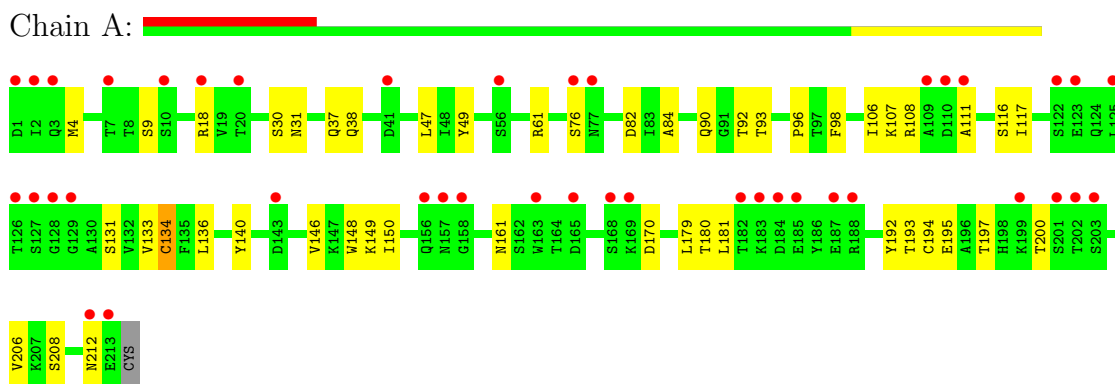
3 Residue-property plots

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.

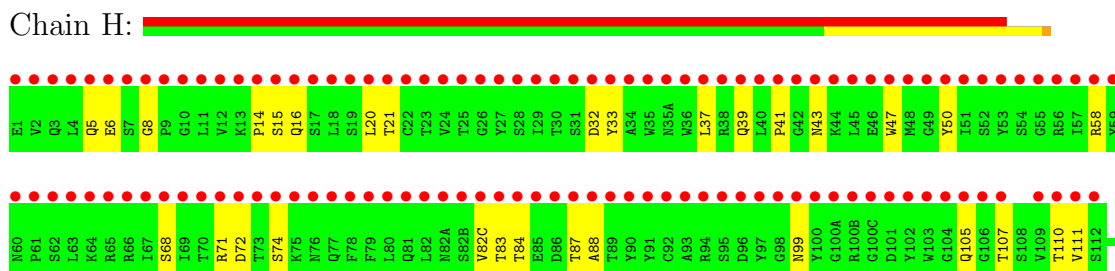
• Molecule 1: PURPLE-FLUORESCENT ANTIBODY EP2-25C10-KAPPA LIGHT CHAIN

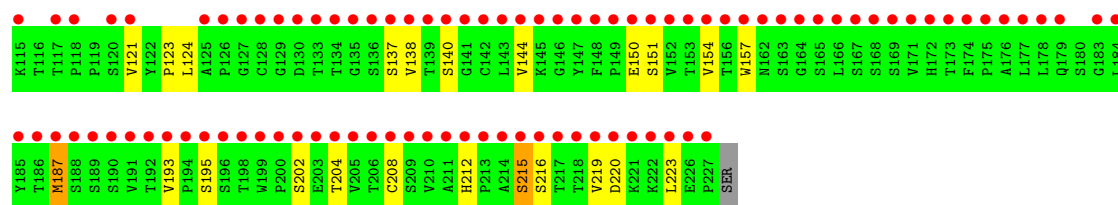


• Molecule 1: PURPLE-FLUORESCENT ANTIBODY EP2-25C10-KAPPA LIGHT CHAIN



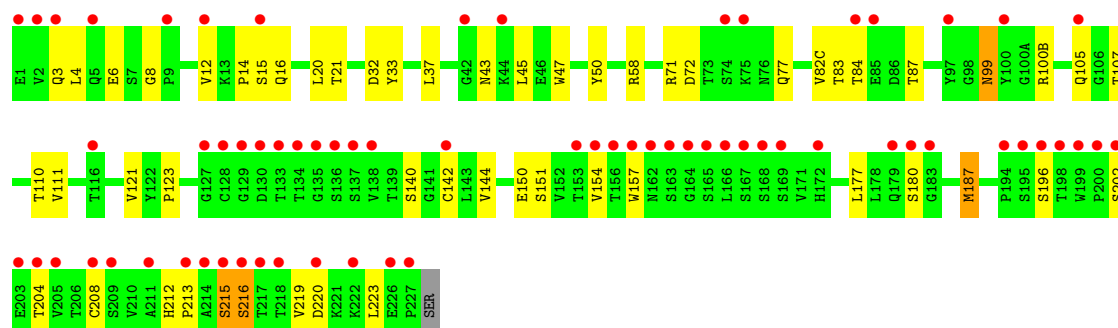
• Molecule 2: PURPLE-FLUORESCENT ANTIBODY EP2-25C10-IGG2B HEAVY CHAIN





● Molecule 2: PURPLE-FLUORESCENT ANTIBODY EP2-25C10-IGG2B HEAVY CHAIN

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.13Å 59.46Å 149.37Å 90.00° 100.37° 90.00°	Depositor
Resolution (Å)	24.46 – 2.99 23.11 – 2.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.46-2.99) 85.4 (23.11-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.99Å)	Xtriage
Refinement program	REFMAC 5.3.0017	Depositor
R, R_{free}	0.211 , 0.255 0.215 , 0.257	Depositor DCC
R_{free} test set	960 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 25.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 19902 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.9619e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/1684	0.72	0/2288
1	L	0.70	0/1684	0.73	0/2288
2	B	0.71	0/1711	0.78	2/2341 (0.1%)
2	H	0.70	0/1711	0.77	1/2341 (0.0%)
All	All	0.70	0/6790	0.75	3/9258 (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	H	58	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	58	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	B	142	CYS	CA-CB-SG	-5.48	104.13	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1650	0	1578	33	0
1	L	1650	0	1578	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1667	0	1608	34	1
2	H	1667	0	1608	32	1
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	L	10	0	0	3	0
4	A	6	0	8	0	0
4	H	6	0	8	0	0
4	L	6	0	8	0	0
All	All	6677	0	6396	123	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:154:VAL:HG21	2:B:187:MET:CE	1.81	1.09
2:H:154:VAL:HG21	2:H:187:MET:CE	1.92	0.99
2:B:154:VAL:HG21	2:B:187:MET:HE2	1.42	0.98
2:H:154:VAL:HG21	2:H:187:MET:HE1	1.55	0.85
2:B:154:VAL:HG21	2:B:187:MET:HE1	1.58	0.83
2:H:154:VAL:HG21	2:H:187:MET:HE2	1.60	0.81
1:L:92:THR:HG23	1:L:93:THR:HG23	1.66	0.77
2:B:154:VAL:CG2	2:B:187:MET:HE2	2.15	0.75
1:L:192:TYR:O	1:L:208:SER:HB2	1.90	0.71
1:A:92:THR:HG23	1:A:93:THR:HG23	1.72	0.70
1:L:55:HIS:ND1	3:L:303:SO4:O4	2.17	0.69
1:A:131:SER:OG	1:A:180:THR:HG23	1.95	0.67
2:H:121:VAL:HG21	2:H:219:VAL:HG22	1.75	0.67
1:A:192:TYR:O	1:A:208:SER:HB2	1.96	0.66
1:A:90:GLN:OE1	1:A:92:THR:HG22	1.96	0.65
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.79	0.64
2:H:121:VAL:HG21	2:H:219:VAL:CG2	2.29	0.63
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.82	0.62
2:B:121:VAL:HG21	2:B:219:VAL:HG22	1.80	0.62
2:B:14:PRO:O	2:B:15:SER:HB3	2.00	0.62
2:B:121:VAL:HG21	2:B:219:VAL:CG2	2.31	0.61
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.83	0.59
2:H:154:VAL:CG2	2:H:187:MET:HE2	2.31	0.59
2:H:84:THR:HG22	2:H:111:VAL:O	2.01	0.59
1:L:149:LYS:HB2	1:L:193:THR:HB	1.85	0.59
2:B:212:HIS:ND1	2:B:215:SER:HB3	2.18	0.58
2:H:14:PRO:O	2:H:15:SER:HB3	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.86	0.58
2:B:32:ASP:O	2:B:33:TYR:HB2	2.03	0.58
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.86	0.58
1:A:149:LYS:HB2	1:A:193:THR:HB	1.86	0.57
2:B:87:THR:HG23	2:B:110:THR:HA	1.85	0.57
2:B:154:VAL:CG2	2:B:187:MET:CE	2.71	0.57
2:H:87:THR:HG23	2:H:110:THR:HA	1.86	0.57
2:H:39:GLN:O	2:H:88:ALA:HB1	2.06	0.56
1:L:150:ILE:HD11	1:L:179:LEU:HD21	1.87	0.56
1:L:90:GLN:OE1	1:L:92:THR:HG22	2.05	0.55
2:B:84:THR:HG22	2:B:111:VAL:O	2.06	0.55
1:L:107:LYS:HA	1:L:140:TYR:OH	2.08	0.54
1:A:170:ASP:OD1	1:A:170:ASP:C	2.46	0.54
1:L:24:ARG:NH1	3:L:302:SO4:O3	2.41	0.53
1:L:106:ILE:HG22	1:L:107:LYS:O	2.09	0.53
1:L:111:ALA:C	1:L:200:THR:HG21	2.29	0.53
2:H:212:HIS:ND1	2:H:215:SER:HB3	2.24	0.52
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.44	0.52
2:B:83:THR:C	2:B:111:VAL:HG11	2.30	0.51
1:A:106:ILE:HG22	1:A:107:LYS:O	2.10	0.51
2:B:83:THR:O	2:B:111:VAL:HG11	2.11	0.51
2:H:32:ASP:O	2:H:33:TYR:HB2	2.09	0.51
2:H:140:SER:HB3	2:H:223:LEU:HD13	1.93	0.50
2:B:150:GLU:CG	2:B:151:SER:HA	2.41	0.50
2:H:83:THR:O	2:H:111:VAL:HG11	2.12	0.50
2:B:16:GLN:O	2:B:82(C):VAL:HG22	2.12	0.50
2:B:21:THR:HG21	2:B:77:GLN:NE2	2.27	0.49
2:B:72:ASP:OD1	2:B:72:ASP:C	2.50	0.49
1:L:131:SER:OG	1:L:180:THR:HG23	2.13	0.49
1:L:193:THR:HG22	1:L:194:CYS:N	2.27	0.49
1:L:61:ARG:HD2	1:L:76:SER:O	2.13	0.49
2:B:213:PRO:O	2:B:216:SER:N	2.34	0.49
1:L:55:HIS:HA	3:L:303:SO4:O4	2.13	0.48
1:A:193:THR:HG22	1:A:194:CYS:N	2.28	0.48
1:A:133:VAL:CG1	1:A:134:CYS:N	2.76	0.48
2:H:6:GLU:HA	2:H:21:THR:O	2.14	0.48
1:A:136:LEU:HD21	1:A:146:VAL:HG22	1.96	0.48
2:H:137:SER:HB2	2:H:193:VAL:O	2.14	0.47
2:H:208:CYS:O	2:H:220:ASP:HA	2.15	0.47
2:B:157:TRP:CZ3	2:B:208:CYS:HB3	2.50	0.47
1:L:136:LEU:HD21	1:L:146:VAL:HG22	1.97	0.47
2:H:16:GLN:O	2:H:82(C):VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:ARG:HD2	1:A:76:SER:O	2.15	0.46
1:A:92:THR:HG23	1:A:93:THR:N	2.30	0.46
1:A:96:PRO:HD2	2:B:47:TRP:CE3	2.50	0.46
2:H:138:VAL:HG23	2:H:195:SER:HB3	1.98	0.46
2:B:208:CYS:O	2:B:220:ASP:HA	2.14	0.46
1:A:92:THR:CG2	1:A:93:THR:N	2.78	0.45
1:L:96:PRO:HD2	2:H:47:TRP:CE3	2.51	0.45
2:B:6:GLU:HA	2:B:21:THR:O	2.16	0.45
1:A:136:LEU:N	1:A:136:LEU:HD12	2.31	0.45
2:B:144:VAL:HB	2:B:187:MET:HG3	1.99	0.45
2:B:140:SER:HB3	2:B:223:LEU:HD13	1.97	0.45
2:H:123:PRO:HB2	2:H:223:LEU:HD23	1.99	0.45
1:L:96:PRO:HD2	2:H:47:TRP:CD2	2.51	0.45
2:H:83:THR:C	2:H:111:VAL:HG11	2.37	0.45
1:A:161:ASN:O	2:B:177:LEU:HD11	2.16	0.45
2:H:154:VAL:CG2	2:H:187:MET:CE	2.79	0.44
1:A:117:ILE:HD12	1:A:194:CYS:HB2	1.99	0.44
2:B:4:LEU:HD12	2:B:4:LEU:N	2.32	0.44
1:A:136:LEU:HD21	1:A:146:VAL:CG2	2.48	0.44
1:L:136:LEU:N	1:L:136:LEU:HD12	2.32	0.44
1:A:111:ALA:C	1:A:200:THR:HG21	2.38	0.44
1:A:96:PRO:HD2	2:B:47:TRP:CD2	2.53	0.44
1:L:170:ASP:OD1	1:L:170:ASP:C	2.56	0.44
1:L:92:THR:CG2	1:L:93:THR:N	2.81	0.43
2:H:150:GLU:CG	2:H:151:SER:HA	2.48	0.43
1:A:107:LYS:HA	1:A:140:TYR:OH	2.18	0.43
1:L:136:LEU:HD21	1:L:146:VAL:CG2	2.48	0.43
1:A:134:CYS:HB2	1:A:148:TRP:CZ2	2.53	0.43
1:L:193:THR:CG2	1:L:194:CYS:N	2.82	0.43
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.51	0.43
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.00	0.43
1:A:4:MET:SD	1:A:90:GLN:HB3	2.59	0.42
2:B:123:PRO:HB2	2:B:223:LEU:HD23	2.01	0.42
1:A:193:THR:CG2	1:A:194:CYS:N	2.82	0.42
1:L:18:ARG:HA	1:L:76:SER:HA	2.01	0.42
1:A:38:GLN:O	1:A:84:ALA:HB1	2.19	0.42
1:L:192:TYR:O	1:L:208:SER:CB	2.66	0.42
1:L:193:THR:HA	1:L:208:SER:HB3	2.02	0.42
1:L:133:VAL:CG1	1:L:134:CYS:N	2.83	0.42
2:H:157:TRP:CZ3	2:H:208:CYS:HB3	2.55	0.42
2:H:121:VAL:CG2	2:H:219:VAL:CG2	2.97	0.41
1:L:4:MET:SD	1:L:90:GLN:HB3	2.60	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.02	0.41
1:L:92:THR:HG23	1:L:93:THR:N	2.35	0.41
2:B:12:VAL:O	2:B:111:VAL:HA	2.19	0.41
2:H:144:VAL:HB	2:H:187:MET:HG3	2.03	0.41
1:A:18:ARG:HA	1:A:76:SER:HA	2.02	0.41
1:A:98:PHE:CD2	2:B:45:LEU:HD23	2.56	0.41
1:A:49:TYR:CE2	2:B:100(B):ARG:NH1	2.89	0.41
2:H:72:ASP:C	2:H:72:ASP:OD1	2.60	0.41
2:H:123:PRO:O	2:H:124:LEU:HD23	2.21	0.40
1:A:30:SER:O	1:A:31:ASN:HB2	2.21	0.40
2:H:32:ASP:OD1	2:H:33:TYR:N	2.54	0.40
2:B:3:GLN:C	2:B:4:LEU:HD12	2.42	0.40

All (1) 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	Distance(Å)	Clash(Å)
2:H:5:GLN:NE2	2:B:196:SER:O[2_546]	2.19	0.01

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	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	38	84
1	L	211/214 (99%)	201 (95%)	8 (4%)	2 (1%)	25	73
2	B	217/220 (99%)	205 (94%)	9 (4%)	3 (1%)	16	60
2	H	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	16	60
All	All	856/868 (99%)	810 (95%)	37 (4%)	9 (1%)	21	67

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	99	ASN
2	B	99	ASN

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Mol	Chain	Res	Type
1	L	212	ASN
2	H	202	SER
1	A	212	ASN
2	B	202	SER
2	B	180	SER
1	L	83	ILE
2	H	41	PRO

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	191/192 (100%)	185 (97%)	6 (3%)	52	89
1	L	191/192 (100%)	184 (96%)	7 (4%)	45	86
2	B	193/194 (100%)	182 (94%)	11 (6%)	29	71
2	H	193/194 (100%)	181 (94%)	12 (6%)	26	67
All	All	768/772 (100%)	732 (95%)	36 (5%)	36	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	SER
1	L	108	ARG
1	L	116	SER
1	L	134	CYS
1	L	143	ASP
1	L	181	LEU
1	L	197	THR
2	H	37	LEU
2	H	43	ASN
2	H	50	TYR
2	H	68	SER
2	H	71	ARG
2	H	74	SER
2	H	105	GLN
2	H	107	THR

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Mol	Chain	Res	Type
2	H	187	MET
2	H	204	THR
2	H	215	SER
2	H	216	SER
1	A	9	SER
1	A	108	ARG
1	A	116	SER
1	A	134	CYS
1	A	181	LEU
1	A	197	THR
2	B	37	LEU
2	B	43	ASN
2	B	50	TYR
2	B	71	ARG
2	B	99	ASN
2	B	105	GLN
2	B	107	THR
2	B	187	MET
2	B	204	THR
2	B	215	SER
2	B	216	SER

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

Mol	Chain	Res	Type
1	L	38	GLN
2	H	39	GLN
2	H	43	ASN
1	A	38	GLN
1	A	157	ASN
2	B	39	GLN
2	B	43	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

8 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	A	301	-	4,4,4	0.25	0	6,6,6	0.22	0
3	SO4	A	304	-	4,4,4	0.22	0	6,6,6	0.14	0
4	GOL	A	403	-	5,5,5	0.45	0	5,5,5	0.46	0
3	SO4	B	305	-	4,4,4	0.15	0	6,6,6	0.28	0
4	GOL	H	401	-	5,5,5	0.48	0	5,5,5	1.00	0
3	SO4	L	302	-	4,4,4	0.29	0	6,6,6	0.10	0
3	SO4	L	303	-	4,4,4	0.24	0	6,6,6	0.33	0
4	GOL	L	402	-	5,5,5	0.46	0	5,5,5	1.00	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	A	301	-	-	0/0/0/0	0/0/0/0
3	SO4	A	304	-	-	0/0/0/0	0/0/0/0
4	GOL	A	403	-	-	0/4/4/4	0/0/0/0
3	SO4	B	305	-	-	0/0/0/0	0/0/0/0
4	GOL	H	401	-	-	0/4/4/4	0/0/0/0
3	SO4	L	302	-	-	0/0/0/0	0/0/0/0
3	SO4	L	303	-	-	0/0/0/0	0/0/0/0
4	GOL	L	402	-	-	0/4/4/4	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.

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	213/214 (99%)	0.97	41 (19%) 2 1	19, 21, 23, 24	0
1	L	213/214 (99%)	5.58	201 (94%) 0 0	19, 21, 23, 24	0
2	B	219/220 (99%)	1.46	67 (30%) 1 0	18, 21, 24, 25	0
2	H	219/220 (99%)	6.33	210 (95%) 0 0	18, 21, 23, 24	0
All	All	864/868 (99%)	3.59	519 (60%) 0 0	18, 21, 23, 25	0

All (519) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	142	CYS	21.8
1	L	193	THR	20.3
2	H	7	SER	19.5
2	H	8	GLY	18.2
2	H	141	GLY	17.8
2	H	3	GLN	17.2
2	H	144	VAL	17.2
2	H	6	GLU	17.1
2	H	9	PRO	16.6
2	H	4	LEU	16.2
1	L	191	SER	15.2
1	L	192	TYR	13.5
1	L	189	HIS	13.5
2	H	2	VAL	13.1
1	L	23	CYS	13.1
1	L	190	ASN	13.0
1	L	118	PHE	12.9
2	H	68	SER	12.4
2	H	5	GLN	12.0
2	H	100(C)	GLY	11.8
2	H	146	GLY	11.8

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Mol	Chain	Res	Type	RSRZ
2	H	152	VAL	11.6
1	L	116	SER	11.6
2	H	143	LEU	11.4
2	H	151	SER	11.2
2	H	36	TRP	11.1
1	L	138	ASN	10.9
1	L	178	THR	10.9
2	H	140	SER	10.7
2	H	59	TYR	10.7
1	L	4	MET	10.6
1	L	134	CYS	10.6
1	L	88	CYS	10.5
2	H	22	CYS	10.5
2	H	149	PRO	10.4
1	L	208	SER	10.4
2	H	67	ILE	10.2
2	H	92	CYS	10.0
2	H	69	ILE	9.8
2	H	70	THR	9.7
2	H	35(A)	ASN	9.6
2	H	139	THR	9.4
2	H	57	ILE	9.3
2	H	145	LYS	9.3
2	H	49	GLY	9.2
1	L	35	TRP	9.2
1	L	188	ARG	9.1
1	L	86	TYR	9.1
2	H	147	TYR	9.1
1	L	22	SER	9.0
1	L	184	ASP	9.0
2	H	212	HIS	8.9
2	H	10	GLY	8.9
2	H	23	THR	8.9
2	H	103	TRP	8.9
2	H	100(A)	GLY	8.9
1	L	161	ASN	8.9
2	H	187	MET	8.8
1	L	36	TYR	8.8
2	H	1	GLU	8.8
2	H	37	LEU	8.8
1	L	202	THR	8.8
2	H	50	TYR	8.7

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Mol	Chain	Res	Type	RSRZ
1	L	112	ALA	8.7
2	H	176	ALA	8.6
2	H	102	TYR	8.6
2	H	100(B)	ARG	8.6
1	L	120	PRO	8.6
2	H	188	SER	8.5
2	H	35	TRP	8.5
1	L	117	ILE	8.4
2	H	150	GLU	8.4
1	L	135	PHE	8.4
2	H	48	MET	8.3
1	L	176	SER	8.3
1	L	130	ALA	8.2
1	L	163	TRP	8.2
1	L	114	THR	8.2
1	L	13	ALA	8.2
1	L	148	TRP	8.1
1	L	187	GLU	8.1
1	L	175	MET	8.0
1	L	5	THR	8.0
2	H	175	PRO	8.0
1	L	177	SER	8.0
1	L	3	GLN	8.0
2	H	58	ARG	8.0
2	H	214	ALA	8.0
1	L	119	PRO	7.9
2	H	208	CYS	7.9
1	L	139	PHE	7.8
2	H	189	SER	7.8
1	L	195	GLU	7.8
1	L	8	THR	7.8
1	L	6	GLN	7.7
2	H	173	THR	7.7
2	H	80	LEU	7.7
2	H	82	LEU	7.7
1	L	19	VAL	7.6
2	H	101	ASP	7.6
1	L	121	SER	7.6
2	H	33	TYR	7.6
2	H	90	TYR	7.6
2	H	56	ARG	7.5
1	L	209	PHE	7.5

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Mol	Chain	Res	Type	RSRZ
2	B	128	CYS	7.5
1	L	172	THR	7.4
2	H	186	THR	7.4
2	H	202	SER	7.4
1	L	84	ALA	7.4
2	H	71	ARG	7.4
2	H	195	SER	7.3
2	H	66	ARG	7.3
1	L	115	VAL	7.3
1	L	15	LEU	7.3
2	H	165	SER	7.3
2	H	51	ILE	7.3
1	L	186	TYR	7.3
2	H	157	TRP	7.3
1	L	133	VAL	7.2
2	H	153	THR	7.2
2	H	162	ASN	7.2
1	L	174	SER	7.2
2	H	177	LEU	7.1
2	H	31	SER	7.1
2	H	190	SER	7.1
1	L	34	ASN	7.1
1	L	20	THR	7.1
2	H	12	VAL	7.0
1	L	136	LEU	7.0
2	H	192	THR	7.0
1	L	183	LYS	7.0
1	L	14	SER	7.0
1	L	206	VAL	7.0
1	L	109	ALA	6.9
2	H	21	THR	6.9
2	H	47	TRP	6.9
2	H	174	PHE	6.8
2	B	133	THR	6.8
1	L	173	TYR	6.8
1	L	51	THR	6.8
2	H	193	VAL	6.8
2	H	91	TYR	6.8
1	L	149	LYS	6.8
1	L	110	ASP	6.7
2	H	73	THR	6.7
2	B	134	THR	6.7

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Mol	Chain	Res	Type	RSRZ
1	L	194	CYS	6.7
2	B	164	GLY	6.7
2	H	34	ALA	6.7
1	L	167	ASP	6.7
2	H	88	ALA	6.7
1	L	137	ASN	6.6
1	L	140	TYR	6.6
2	B	163	SER	6.6
1	L	164	THR	6.6
1	L	63	SER	6.6
2	H	164	GLY	6.6
1	L	210	ASN	6.6
2	H	168	SER	6.6
2	H	127	GLY	6.6
2	H	148	PHE	6.6
1	L	2	ILE	6.5
2	H	171	VAL	6.5
1	L	171	SER	6.5
1	L	106	ILE	6.5
2	H	172	HIS	6.5
2	B	165	SER	6.5
2	H	79	PHE	6.5
1	L	9	SER	6.5
2	H	154	VAL	6.5
1	L	11	LEU	6.4
2	H	27	TYR	6.4
2	H	32	ASP	6.4
2	B	167	SER	6.4
2	H	20	LEU	6.4
1	L	151	ASP	6.4
1	L	113	PRO	6.4
2	H	104	GLY	6.3
1	L	159	VAL	6.3
2	H	29	ILE	6.3
2	H	82(C)	VAL	6.3
1	L	131	SER	6.3
2	H	136	SER	6.3
1	L	146	VAL	6.2
1	L	162	SER	6.2
1	L	196	ALA	6.1
2	H	167	SER	6.1
2	H	81	GLN	6.1

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Mol	Chain	Res	Type	RSRZ
1	L	158	GLY	6.1
2	H	52	SER	6.1
1	L	132	VAL	6.1
1	L	16	GLY	6.1
1	L	205	ILE	6.1
2	H	78	PHE	6.0
1	L	111	ALA	6.0
1	L	207	LYS	6.0
2	H	19	SER	6.0
1	L	179	LEU	6.0
2	H	138	VAL	5.9
2	H	55	GLY	5.9
1	L	12	SER	5.9
2	H	216	SER	5.9
2	H	200	PRO	5.9
1	L	166	GLN	5.9
2	H	24	VAL	5.9
1	A	129	GLY	5.9
1	L	54	LEU	5.9
1	L	200	THR	5.8
1	L	64	GLY	5.8
1	L	180	THR	5.8
1	L	7	THR	5.8
2	H	95	SER	5.8
2	H	77	GLN	5.8
2	H	45	LEU	5.7
2	H	93	ALA	5.7
2	H	28	SER	5.7
2	H	184	LEU	5.7
2	H	223	LEU	5.7
1	L	185	GLU	5.7
2	H	60	ASN	5.7
2	H	130	ASP	5.7
2	H	74	SER	5.7
2	H	215	SER	5.7
2	H	205	VAL	5.6
2	B	135	GLY	5.6
1	L	147	LYS	5.6
1	L	89	GLN	5.6
1	L	47	LEU	5.6
2	B	204	THR	5.5
2	H	213	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	166	LEU	5.5
2	H	54	SER	5.5
1	L	85	THR	5.5
1	L	98	PHE	5.5
2	H	129	GLY	5.4
1	L	17	ASP	5.4
2	H	107	THR	5.4
2	H	196	SER	5.3
2	H	82(A)	ASN	5.3
2	H	163	SER	5.3
1	L	1	ASP	5.3
2	H	169	SER	5.3
1	L	160	LEU	5.3
1	L	24	ARG	5.2
2	H	53	TYR	5.2
2	H	25	THR	5.2
1	L	25	ALA	5.2
1	L	170	ASP	5.2
2	B	202	SER	5.2
1	L	102	THR	5.2
2	H	191	VAL	5.1
1	L	10	SER	5.1
1	L	52	SER	5.1
1	L	203	SER	5.1
2	H	15	SER	5.1
1	L	197	THR	5.1
1	L	153	SER	5.1
2	H	38	ARG	5.1
1	L	129	GLY	5.1
2	H	94	ARG	5.1
2	H	166	LEU	5.0
1	L	21	ILE	5.0
2	H	63	LEU	5.0
1	L	204	PRO	5.0
2	B	130	ASP	5.0
2	B	194	PRO	4.9
2	B	136	SER	4.9
1	L	62	PHE	4.9
1	L	46	LEU	4.9
1	L	144	ILE	4.9
2	H	76	ASN	4.9
1	L	66	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	H	134	THR	4.8
2	H	39	GLN	4.8
2	H	89	THR	4.8
1	L	58	VAL	4.8
1	L	55	HIS	4.8
2	H	18	LEU	4.8
2	H	87	THR	4.8
2	H	198	THR	4.8
1	L	100	GLY	4.8
1	L	71	TYR	4.8
2	H	100	TYR	4.7
1	L	87	PHE	4.7
2	H	227	PRO	4.7
2	H	30	THR	4.7
1	L	82	ASP	4.7
1	L	65	SER	4.7
2	H	199	TRP	4.6
1	L	124	GLN	4.6
1	L	150	ILE	4.6
1	A	126	THR	4.6
2	B	195	SER	4.6
1	L	143	ASP	4.6
1	L	152	GLY	4.6
2	B	169	SER	4.5
1	L	48	ILE	4.5
2	H	26	GLY	4.5
2	B	220	ASP	4.5
2	H	99	ASN	4.5
2	B	203	GLU	4.5
1	L	72	SER	4.5
2	H	72	ASP	4.4
2	H	14	PRO	4.4
1	A	202	THR	4.4
1	L	33	LEU	4.4
2	H	183	GLY	4.4
1	A	168	SER	4.4
1	L	145	ASN	4.3
1	L	104	LEU	4.3
2	H	137	SER	4.3
1	L	49	TYR	4.3
2	H	211	ALA	4.3
2	B	180	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	75	ILE	4.3
2	H	219	VAL	4.3
1	L	168	SER	4.3
1	L	198	HIS	4.3
2	H	65	ARG	4.3
2	B	211	ALA	4.3
1	L	83	ILE	4.3
2	H	128	CYS	4.3
2	H	218	THR	4.2
2	H	178	LEU	4.2
1	L	74	THR	4.2
2	H	105	GLN	4.2
2	H	133	THR	4.2
1	L	91	GLY	4.2
2	H	210	VAL	4.2
2	H	185	TYR	4.1
2	H	11	LEU	4.1
1	L	50	TYR	4.1
2	H	62	SER	4.1
2	H	43	ASN	4.1
1	L	78	LEU	4.1
1	L	37	GLN	4.1
2	H	64	LYS	4.1
2	H	217	THR	4.0
1	A	187	GLU	4.0
2	B	74	SER	4.0
1	L	123	GLU	4.0
1	L	181	LEU	4.0
2	H	40	LEU	3.9
2	B	168	SER	3.9
2	H	42	GLY	3.9
1	L	90	GLN	3.8
1	A	1	ASP	3.8
1	L	199	LYS	3.7
1	A	188	ARG	3.7
1	L	81	ASP	3.7
2	B	183	GLY	3.7
1	A	7	THR	3.7
2	B	216	SER	3.7
1	L	126	THR	3.6
2	H	126	PRO	3.6
2	B	1	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	141	PRO	3.6
2	H	82(B)	SER	3.6
2	H	46	GLU	3.6
2	H	194	PRO	3.6
2	B	129	GLY	3.6
2	B	3	GLN	3.5
2	B	218	THR	3.5
1	L	122	SER	3.5
1	L	97	THR	3.5
1	L	165	ASP	3.5
2	B	137	SER	3.5
2	H	61	PRO	3.5
2	H	203	GLU	3.4
1	A	163	TRP	3.4
1	A	184	ASP	3.4
1	L	29	ILE	3.4
1	L	96	PRO	3.4
1	L	73	LEU	3.4
1	A	18	ARG	3.4
2	H	156	THR	3.4
1	L	57	GLY	3.4
2	B	179	GLN	3.4
1	L	99	GLY	3.4
1	L	60	SER	3.3
1	A	76	SER	3.3
1	A	41	ASP	3.3
2	H	85	GLU	3.3
2	H	97	TYR	3.3
2	B	214	ALA	3.3
2	H	135	GLY	3.3
2	H	16	GLN	3.3
1	A	156	GLN	3.3
2	B	162	ASN	3.3
2	B	196	SER	3.2
1	L	107	LYS	3.2
2	H	44	LYS	3.2
2	H	96	ASP	3.2
2	H	111	VAL	3.2
2	H	121	VAL	3.2
2	H	206	THR	3.2
1	L	76	SER	3.2
2	B	2	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	110	THR	3.2
1	L	128	GLY	3.2
2	B	222	LYS	3.1
1	L	211	ARG	3.1
1	A	212	ASN	3.1
1	A	201	SER	3.1
2	B	213	PRO	3.1
1	L	31	ASN	3.1
1	L	79	ASP	3.1
1	L	32	TYR	3.1
1	L	142	LYS	3.1
1	L	101	GLY	3.1
1	L	30	SER	3.0
1	L	182	THR	3.0
2	H	204	THR	3.0
1	L	18	ARG	3.0
2	B	153	THR	3.0
2	B	9	PRO	3.0
1	L	108	ARG	3.0
2	H	98	GLY	3.0
2	B	5	GLN	2.9
2	H	226	GLU	2.9
1	L	92	THR	2.9
1	L	157	ASN	2.9
1	A	109	ALA	2.8
1	L	61	ARG	2.8
1	A	203	SER	2.8
2	H	83	THR	2.8
1	A	127	SER	2.8
2	H	13	LYS	2.8
2	B	142	CYS	2.8
1	A	2	ILE	2.8
1	A	169	LYS	2.8
2	H	86	ASP	2.8
1	L	45	LYS	2.8
2	H	209	SER	2.8
1	L	94	LEU	2.8
2	H	106	GLY	2.7
2	B	217	THR	2.7
2	H	125	ALA	2.7
1	A	3	GLN	2.7
1	A	182	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	100	TYR	2.7
2	H	84	THR	2.7
1	L	67	SER	2.7
2	B	42	GLY	2.7
2	B	208	CYS	2.6
2	H	112	SER	2.6
2	B	15	SER	2.6
2	B	84	THR	2.6
1	A	128	GLY	2.6
1	L	212	ASN	2.6
1	A	77	ASN	2.6
2	B	138	VAL	2.6
2	B	116	THR	2.6
1	L	201	SER	2.5
1	L	125	LEU	2.5
2	H	220	ASP	2.5
1	A	123	GLU	2.5
1	L	43	THR	2.5
2	H	221	LYS	2.5
1	A	111	ALA	2.5
2	B	215	SER	2.5
1	L	53	ARG	2.4
2	H	179	GLN	2.4
2	H	109	VAL	2.4
2	H	117	THR	2.4
2	B	127	GLY	2.4
2	B	154	VAL	2.4
1	L	59	PRO	2.4
1	A	125	LEU	2.4
1	A	157	ASN	2.4
1	A	122	SER	2.4
1	L	95	PRO	2.4
2	H	115	LYS	2.4
1	A	110	ASP	2.4
1	L	44	VAL	2.4
1	A	213	GLU	2.4
2	B	85	GLU	2.4
2	B	209	SER	2.3
2	B	205	VAL	2.3
1	A	165	ASP	2.3
1	L	38	GLN	2.3
1	L	103	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	77	ASN	2.3
1	A	143	ASP	2.3
2	B	226	GLU	2.3
1	A	158	GLY	2.3
2	B	105	GLN	2.2
1	A	199	LYS	2.2
2	B	44	LYS	2.2
1	L	41	ASP	2.2
1	L	93	THR	2.2
2	B	157	TRP	2.2
2	H	120	SER	2.2
1	L	28	ASP	2.2
1	L	169	LYS	2.2
2	H	118	PRO	2.2
1	A	185	GLU	2.2
1	L	39	LYS	2.2
1	A	56	SER	2.1
2	B	200	PRO	2.1
2	B	75	LYS	2.1
1	L	27	GLN	2.1
1	L	105	GLU	2.1
1	A	10	SER	2.1
2	B	199	TRP	2.1
2	H	75	LYS	2.1
1	A	20	THR	2.1
2	B	198	THR	2.1
2	H	41	PRO	2.1
2	H	17	SER	2.1
2	B	12	VAL	2.1
2	B	227	PRO	2.1
2	B	97	TYR	2.1
1	A	183	LYS	2.1
2	B	172	HIS	2.0
2	B	156	THR	2.0
1	L	56	SER	2.0
2	H	222	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	304	5/5	0.23	-	79,79,80,80	0
4	GOL	H	401	6/6	0.31	-	35,39,40,41	0
4	GOL	A	403	6/6	0.16	-	27,33,33,33	0
3	SO4	A	301	5/5	0.14	-	67,67,68,69	0
4	GOL	L	402	6/6	0.49	-	33,34,35,36	0
3	SO4	B	305	5/5	0.20	-	74,75,76,77	0
3	SO4	L	303	5/5	0.33	-	82,82,83,83	0
3	SO4	L	302	5/5	0.24	-	69,69,69,70	0

6.5 Other polymers

There are no such residues in this entry.