



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:29 PM GMT

PDB ID : 1P7K  
Title : Crystal structure of an anti-ssDNA antigen-binding fragment (Fab) bound to 4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid (HEPES)  
Authors : Schuermann, J.P.; Henzl, M.T.; Deutscher, S.L.; Tanner, J.J.  
Deposited on : 2003-05-02  
Resolution : 1.75 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

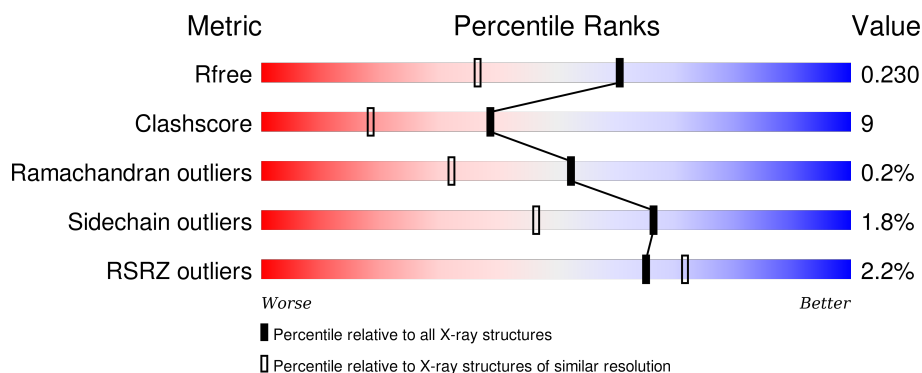
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	214	<div> <div>3%</div> <div>79%</div> <div>21%</div> </div>
1	L	214	<div> <div>87%</div> <div>12%</div> </div>
2	B	224	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
2	H	224	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>•</div> </div>

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
3	SO4	A	806	-	-	-	X
3	SO4	B	809	-	-	-	X
3	SO4	H	801	-	-	X	-
3	SO4	H	802	-	-	X	-
3	SO4	H	805	-	-	-	X
5	1PE	B	1002	-	-	-	X
5	1PE	B	1004	-	-	-	X
5	1PE	H	1001	-	-	-	X
5	1PE	L	1003	-	-	-	X
6	PEG	L	1201	-	-	-	X
7	GOL	A	1108	-	-	-	X
7	GOL	A	1116	-	-	X	-
7	GOL	A	1118	-	-	-	X
7	GOL	A	1120	-	-	-	X
7	GOL	B	1102	-	-	-	X
7	GOL	B	1117	-	-	-	X
7	GOL	H	1101	-	-	-	X
7	GOL	H	1105	-	-	-	X
7	GOL	H	1106	-	-	X	X
7	GOL	L	1103	-	-	X	X
7	GOL	L	1115	-	-	-	X
7	GOL	L	1119	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7565 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 light chain FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	1	0
			1633	1021	273	333	6			
1	A	214	Total	C	N	O	S	0	1	0
			1623	1018	272	327	6			

- Molecule 2 is a protein called antibody heavy chain FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	2	0
			1653	1055	263	324	11			
2	B	217	Total	C	N	O	S	0	3	0
			1636	1045	259	321	11			

There are 22 discrepancies between the modelled and reference sequences:

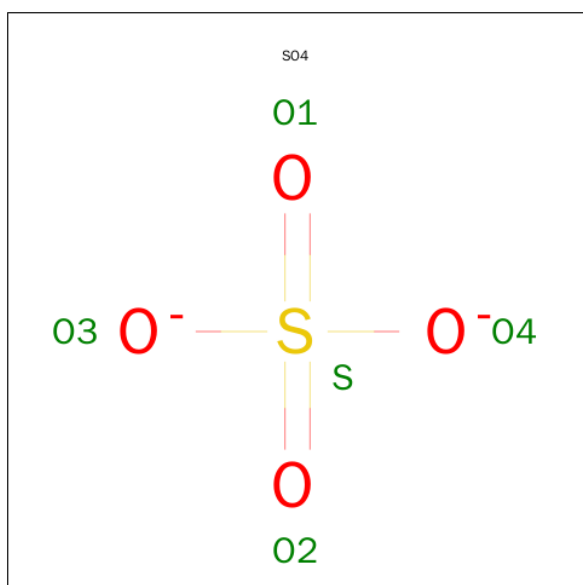
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLN	-	CLONING ARTIFACT	UNP Q9JL75
H	2	VAL	-	CLONING ARTIFACT	UNP Q9JL75
H	3	LYS	-	CLONING ARTIFACT	UNP Q9JL75
H	4	LEU	-	CLONING ARTIFACT	UNP Q9JL75
H	52A	PRO	-	INSERTION	UNP Q9JL75
H	82A	SER	-	INSERTION	UNP Q9JL75
H	82B	SER	-	INSERTION	UNP Q9JL75
H	82C	LEU	-	INSERTION	UNP Q9JL75
H	100A	TYR	-	INSERTION	UNP Q9JL75
H	100B	ALA	-	INSERTION	UNP Q9JL75
H	100C	MET	-	INSERTION	UNP Q9JL75
B	1	GLN	-	CLONING ARTIFACT	UNP Q9JL75
B	2	VAL	-	CLONING ARTIFACT	UNP Q9JL75
B	3	LYS	-	CLONING ARTIFACT	UNP Q9JL75
B	4	LEU	-	CLONING ARTIFACT	UNP Q9JL75
B	52A	PRO	-	INSERTION	UNP Q9JL75

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Chain	Residue	Modelled	Actual	Comment	Reference
B	82A	SER	-	INSERTION	UNP Q9JL75
B	82B	SER	-	INSERTION	UNP Q9JL75
B	82C	LEU	-	INSERTION	UNP Q9JL75
B	100A	TYR	-	INSERTION	UNP Q9JL75
B	100B	ALA	-	INSERTION	UNP Q9JL75
B	100C	MET	-	INSERTION	UNP Q9JL75

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



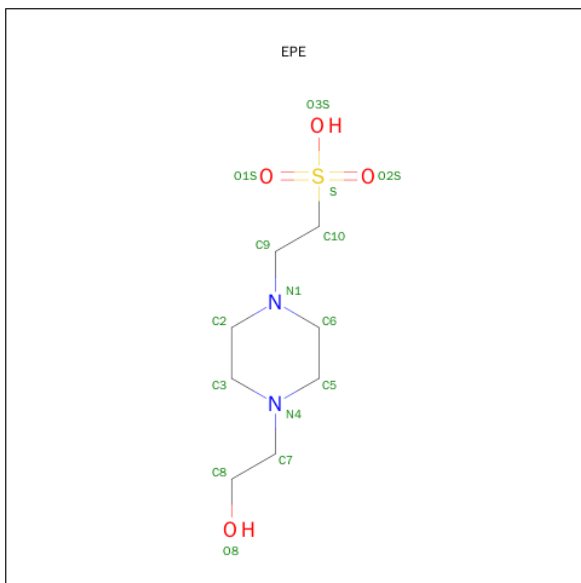
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

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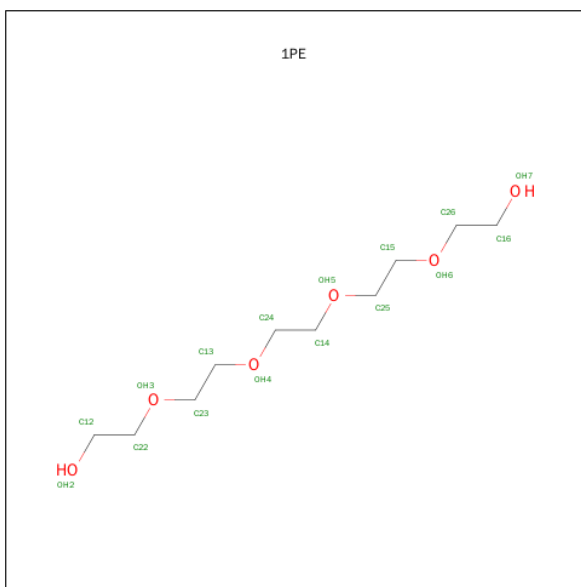
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



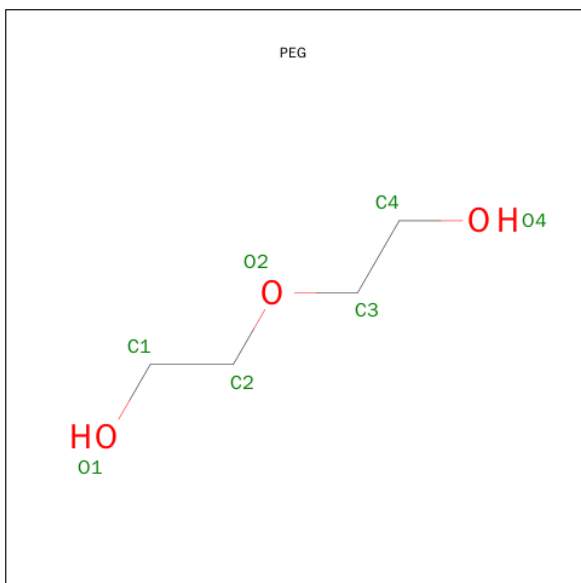
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



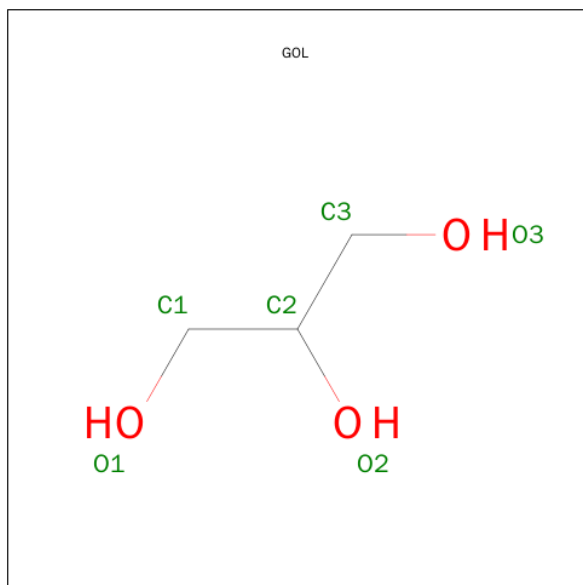
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	L	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			7	4	3		
6	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	L	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	162	Total 162	O 162	0	0
8	B	177	Total 177	O 177	0	0
8	H	195	Total 195	O 195	0	0
8	L	237	Total 237	O 237	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.

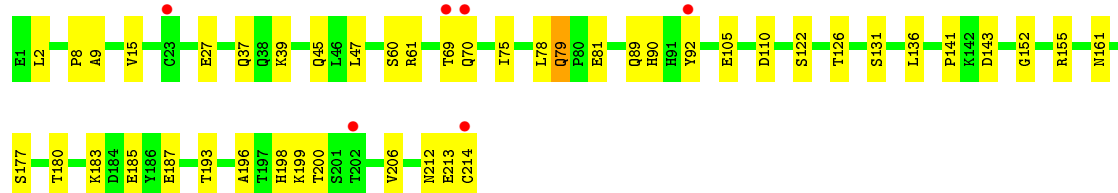
- Molecule 1: antibody light chain FAB

Chain L: 




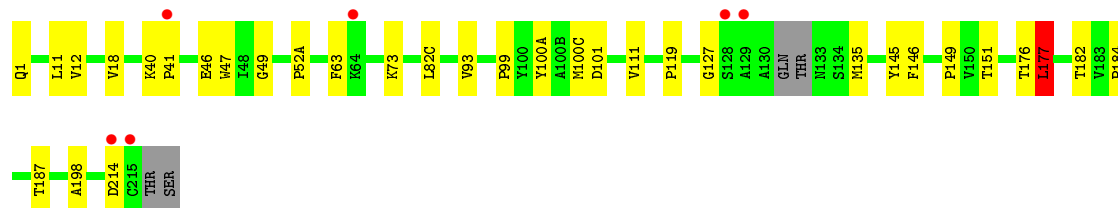
- Molecule 1: antibody light chain FAB

Chain A: 




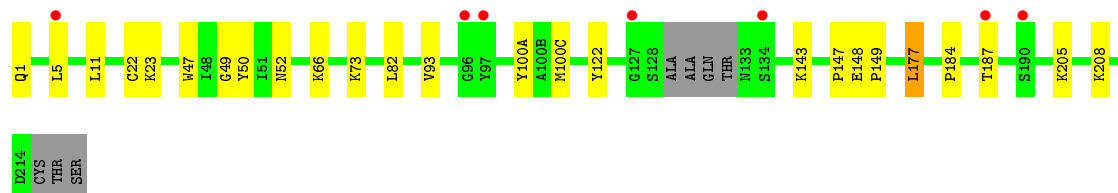
- Molecule 2: antibody heavy chain FAB

Chain H: 



- Molecule 2: antibody heavy chain FAB

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.67 Å   156.70 Å   61.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.14 – 1.75 48.13 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.4 (48.14-1.75) 93.4 (48.13-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.75 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197   ,   0.230 0.197   ,   0.230	Depositor DCC
$R_{free}$ test set	9796 reflections (11.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 97988 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: EPE, GOL, PEG, SO4, IPE

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	0/1660	0.72	0/2257
1	L	0.50	0/1671	0.76	0/2270
2	B	0.45	0/1682	0.76	2/2298 (0.1%)
2	H	0.50	0/1699	0.77	1/2320 (0.0%)
All	All	0.48	0/6712	0.75	3/9145 (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	177	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	22[A]	CYS	CA-CB-SG	5.38	123.68	114.00
2	B	22[B]	CYS	CA-CB-SG	5.38	123.68	114.00

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	1623	0	1529	36	0
1	L	1633	0	1541	29	0
2	B	1636	0	1569	22	0
2	H	1653	0	1595	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	H	25	0	0	0	8
3	L	5	0	0	0	0
4	B	15	0	18	1	0
4	L	15	0	17	2	0
5	B	32	0	44	8	0
5	H	16	0	22	3	0
5	L	16	0	22	2	0
6	H	7	0	10	1	0
6	L	7	0	10	3	0
7	A	24	0	31	11	0
7	B	24	0	32	4	0
7	H	18	0	24	7	0
7	L	30	0	40	14	0
8	A	162	0	0	8	0
8	B	177	0	0	3	0
8	H	195	0	0	3	0
8	L	237	0	0	9	0
All	All	7565	0	6504	120	8

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 9.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ARG:HE	6:L:1201:PEG:H11	1.27	0.99
1:A:8:PRO:HB2	7:A:1116:GOL:H12	1.48	0.94
7:L:1103:GOL:H2	1:A:15:VAL:HG12	1.52	0.91
1:L:9:ALA:H	7:L:1107:GOL:H11	1.38	0.89
5:H:1001:IPE:H251	8:H:1331:HOH:O	1.74	0.86
1:A:9:ALA:H	7:A:1116:GOL:C3	1.92	0.82
1:A:9:ALA:H	7:A:1116:GOL:H31	1.43	0.82
2:B:93:VAL:HG11	2:B:100(C):MET:HB3	1.61	0.81
2:B:73:LYS:HZ1	7:B:1112:GOL:H31	1.43	0.80
1:L:31:SER:HB2	7:L:1103:GOL:O1	1.81	0.79
2:H:1:GLN:HE21	2:H:1:GLN:CA	1.95	0.78
1:L:50:ASN:OD1	7:L:1103:GOL:H11	1.85	0.75
2:H:18:VAL:HG22	2:H:82(C):LEU:HD11	1.68	0.75
8:A:1169:HOH:O	7:B:1117:GOL:H32	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:THR:HG22	7:H:1106:GOL:H32	1.70	0.73
2:H:52(A):PRO:O	2:H:73:LYS:HE2	1.88	0.73
2:H:93:VAL:HG11	2:H:100(C):MET:HB3	1.71	0.72
1:L:42:LYS:O	7:L:1115:GOL:H12	1.90	0.72
1:A:185:GLU:HG2	8:A:1185:HOH:O	1.91	0.71
1:A:9:ALA:HB3	7:A:1116:GOL:H2	1.72	0.71
1:A:212:ASN:C	1:A:214:CYS:H	1.94	0.71
2:B:93:VAL:CG1	2:B:100(C):MET:HB3	2.23	0.69
7:L:1103:GOL:H32	8:A:1198:HOH:O	1.93	0.68
1:A:45:GLN:HG3	8:A:1206:HOH:O	1.93	0.68
2:B:73:LYS:NZ	7:B:1112:GOL:H31	2.08	0.68
1:L:52:LYS:HB3	5:L:1003:1PE:H261	1.74	0.68
1:L:79:GLN:NE2	8:L:1360:HOH:O	2.27	0.66
1:A:90:HIS:HD2	1:A:92:TYR:H	1.42	0.66
2:B:11:LEU:CD2	5:B:1004:1PE:H152	2.26	0.66
2:B:11:LEU:HD21	5:B:1004:1PE:H152	1.79	0.64
1:L:147:LYS:HE2	8:L:1320:HOH:O	1.98	0.63
1:L:9:ALA:N	7:L:1107:GOL:H11	2.11	0.63
1:L:50:ASN:CG	7:L:1103:GOL:H11	2.19	0.62
1:A:198:HIS:HD2	1:A:200:THR:OG1	1.82	0.62
1:A:79[B]:GLN:HG2	8:A:1198:HOH:O	1.98	0.61
1:L:59:PRO:HD3	7:L:1119:GOL:H31	1.83	0.61
1:A:131:SER:OG	1:A:180:THR:HG22	2.01	0.60
7:A:1118:GOL:H11	2:B:122:TYR:OH	2.01	0.60
5:B:1002:1PE:H142	7:B:1111:GOL:H2	1.84	0.60
2:H:1:GLN:CA	2:H:1:GLN:NE2	2.66	0.59
7:L:1110:GOL:H32	2:H:127:GLY:HA2	1.84	0.59
1:A:2:LEU:HG	1:A:27:GLU:HG2	1.85	0.58
1:L:90:HIS:HD2	1:L:92:TYR:H	1.51	0.58
1:A:9:ALA:N	7:A:1116:GOL:H31	2.15	0.57
1:A:61:ARG:NH2	1:A:79[A]:GLN:HG2	2.20	0.57
2:B:52:ASN:HD22	5:B:1002:1PE:H261	1.70	0.57
1:L:155:ARG:NE	6:L:1201:PEG:H11	2.10	0.55
2:B:148:GLU:O	5:B:1004:1PE:H231	2.06	0.55
2:H:177:LEU:HA	7:H:1106:GOL:C1	2.36	0.55
1:A:39:LYS:HE2	1:A:81:GLU:O	2.06	0.55
1:A:69:THR:HG23	1:A:70:GLN:HG2	1.90	0.53
1:L:22:THR:HG23	8:L:1364:HOH:O	2.08	0.53
2:B:100(A):TYR:HB2	4:B:902:EPE:O1S	2.07	0.53
1:L:9:ALA:H	7:L:1107:GOL:C1	2.18	0.53
1:A:193:THR:CG2	1:A:206:VAL:HG13	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:THR:HG22	7:H:1106:GOL:C3	2.36	0.52
1:A:155:ARG:NH2	8:A:1185:HOH:O	2.37	0.52
1:A:212:ASN:C	1:A:214:CYS:N	2.61	0.52
1:L:59:PRO:CD	7:L:1119:GOL:H31	2.38	0.52
1:A:122:SER:O	1:A:126:THR:HG23	2.09	0.52
2:H:151:THR:OG1	2:H:198:ALA:HB3	2.09	0.52
2:H:184:PRO:HB2	2:H:187:THR:HG23	1.93	0.51
1:A:141:PRO:O	1:A:198:HIS:HE1	1.94	0.51
1:L:153:SER:HB2	6:L:1201:PEG:H32	1.92	0.51
2:B:147:PRO:HD3	5:B:1004:1PE:H151	1.93	0.51
2:H:40:LYS:N	7:H:1105:GOL:O3	2.33	0.51
1:L:76:ASN:ND2	8:L:1312:HOH:O	2.43	0.51
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.46	0.51
2:B:184:PRO:HB2	2:B:187:THR:HG23	1.93	0.50
5:H:1001:1PE:H252	8:H:1339:HOH:O	2.12	0.49
2:H:93:VAL:CG1	2:H:100(C):MET:HB3	2.42	0.49
2:H:135:MET:HE3	2:H:182:THR:HG22	1.94	0.49
2:B:205:LYS:HD3	8:B:1273:HOH:O	2.13	0.48
1:A:39:LYS:NZ	1:A:81:GLU:CG	2.77	0.48
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.44	0.48
1:A:75:ILE:HG21	1:A:78:LEU:HD23	1.95	0.48
2:H:63:PHE:CZ	7:H:1101:GOL:H2	2.49	0.48
5:B:1002:1PE:H152	8:B:1223:HOH:O	2.13	0.48
1:L:74:LYS:NZ	8:L:1340:HOH:O	2.46	0.48
1:A:206:VAL:O	7:A:1108:GOL:H2	2.14	0.47
5:H:1001:1PE:H162	6:H:1202:PEG:H41	1.97	0.47
1:A:8:PRO:HA	7:A:1116:GOL:H31	1.97	0.46
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.97	0.46
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.98	0.45
1:A:110:ASP:OD2	1:A:199:LYS:NZ	2.49	0.45
1:A:9:ALA:CB	7:A:1116:GOL:H2	2.45	0.45
1:L:201:SER:HB2	8:L:1285:HOH:O	2.16	0.45
2:B:1:GLN:HG2	2:B:1:GLN:O	2.17	0.45
2:B:50:TYR:CD1	2:B:50:TYR:C	2.90	0.45
1:L:193:THR:CG2	1:L:206:VAL:HG13	2.47	0.45
2:H:46:GLU:HB2	7:H:1105:GOL:H11	1.98	0.45
2:H:12:VAL:O	2:H:111:VAL:HA	2.17	0.45
1:A:161:ASN:HD22	1:A:177:SER:HA	1.81	0.45
2:H:73:LYS:NZ	8:H:1314:HOH:O	2.42	0.45
1:A:9:ALA:H	7:A:1116:GOL:C2	2.30	0.44
2:B:208:LYS:HE3	8:B:1234:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:LEU:HB3	2:B:23:LYS:HB3	1.99	0.44
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.52	0.44
1:A:69:THR:HG22	8:A:1203:HOH:O	2.18	0.44
5:L:1003:1PE:H151	5:L:1003:1PE:H161	1.71	0.44
2:H:11:LEU:HD11	2:H:146:PHE:CZ	2.53	0.44
1:A:183:LYS:O	1:A:187:GLU:HG3	2.17	0.44
1:A:193:THR:HG23	1:A:206:VAL:HG13	2.00	0.43
2:B:177:LEU:C	2:B:177:LEU:HD12	2.38	0.43
4:L:901:EPE:O2S	2:H:99:PRO:HA	2.19	0.43
1:L:161:ASN:HD22	1:L:177:SER:HA	1.83	0.43
1:A:152:GLY:HA2	8:A:1214:HOH:O	2.19	0.43
1:L:38:GLN:NE2	7:L:1115:GOL:H11	2.33	0.43
2:H:11:LEU:HD11	2:H:146:PHE:HZ	1.84	0.42
7:A:1118:GOL:H12	2:B:143:LYS:HD3	2.02	0.42
1:L:31:SER:HB2	7:L:1103:GOL:HO1	1.83	0.42
2:B:66:LYS:O	2:B:82:LEU:HA	2.19	0.42
1:L:42:LYS:NZ	8:L:1427:HOH:O	2.53	0.42
1:L:27:GLU:HG3	8:L:1321:HOH:O	2.20	0.41
4:L:901:EPE:O1S	2:H:100(A):TYR:HB2	2.19	0.41
1:L:199:LYS:HB2	1:L:199:LYS:HE3	1.86	0.41
2:H:177:LEU:HA	7:H:1106:GOL:H12	2.02	0.41
1:L:193:THR:HG23	1:L:206:VAL:HG13	2.02	0.41
2:B:11:LEU:HD23	5:B:1004:1PE:H152	2.00	0.40
1:L:103:LYS:CG	8:L:1392:HOH:O	2.69	0.40

All (8) 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)
3:H:801:SO4:S	3:H:801:SO4:O2[2_655]	1.46	0.74
3:H:801:SO4:S	3:H:801:SO4:O1[2_655]	1.47	0.73
3:H:802:SO4:S	3:H:802:SO4:O4[2_655]	1.47	0.73
3:H:802:SO4:S	3:H:802:SO4:O2[2_655]	1.48	0.72
3:H:802:SO4:S	3:H:802:SO4:O1[2_655]	1.48	0.72
3:H:801:SO4:S	3:H:801:SO4:O4[2_655]	1.48	0.72
3:H:802:SO4:S	3:H:802:SO4:O3[2_655]	1.48	0.72
3:H:801:SO4:S	3:H:801:SO4:O3[2_655]	1.49	0.71



## 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	213/214 (100%)	206 (97%)	6 (3%)	1 (0%)	34	14
1	L	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
2	B	216/224 (96%)	212 (98%)	4 (2%)	0	100	100
2	H	218/224 (97%)	210 (96%)	7 (3%)	1 (0%)	34	14
All	All	859/876 (98%)	836 (97%)	21 (2%)	2 (0%)	52	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
2	H	214	ASP

### 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	177/188 (94%)	171 (97%)	6 (3%)	44	18
1	L	181/188 (96%)	179 (99%)	2 (1%)	80	66
2	B	183/194 (94%)	181 (99%)	2 (1%)	80	66
2	H	185/194 (95%)	181 (98%)	4 (2%)	60	35
All	All	726/764 (95%)	712 (98%)	14 (2%)	66	43

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	105	GLU
2	H	41	PRO
2	H	101	ASP
2	H	149	PRO
2	H	177	LEU
1	A	60	SER
1	A	79[A]	GLN
1	A	79[B]	GLN
1	A	89	GLN
1	A	105	GLU
1	A	143	ASP
2	B	149	PRO
2	B	177	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	70	GLN
1	L	76	ASN
1	L	89	GLN
1	L	90	HIS
1	L	137	ASN
1	L	161	ASN
1	A	40	GLN
1	A	89	GLN
1	A	90	HIS
1	A	137	ASN
1	A	161	ASN
1	A	198	HIS
2	B	171	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

33 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	$\# Z  > 2$
7	GOL	A	1108	-	5,5,5	0.27	0	5,5,5	0.42	0
7	GOL	A	1116	-	5,5,5	0.15	0	5,5,5	0.80	0
7	GOL	A	1118	-	5,5,5	0.22	0	5,5,5	1.73	2 (40%)
7	GOL	A	1120	-	5,5,5	0.25	0	5,5,5	1.14	1 (20%)
3	SO4	A	806	-	4,4,4	0.31	0	6,6,6	0.11	0
5	1PE	B	1002	-	15,15,15	0.72	0	14,14,14	0.78	0
5	1PE	B	1004	-	15,15,15	0.79	0	14,14,14	0.90	0
7	GOL	B	1102	-	5,5,5	0.21	0	5,5,5	1.13	1 (20%)
7	GOL	B	1111	-	5,5,5	0.22	0	5,5,5	0.73	0
7	GOL	B	1112	-	5,5,5	0.16	0	5,5,5	0.32	0
7	GOL	B	1117	-	5,5,5	0.18	0	5,5,5	1.19	1 (20%)
3	SO4	B	807	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SO4	B	809	-	4,4,4	0.29	0	6,6,6	0.06	0
4	EPE	B	902	-	14,15,15	0.80	0	18,20,20	1.43	3 (16%)
5	1PE	H	1001	-	15,15,15	0.71	0	14,14,14	0.80	0
7	GOL	H	1101	-	5,5,5	0.22	0	5,5,5	1.75	2 (40%)
7	GOL	H	1105	-	5,5,5	0.24	0	5,5,5	1.30	1 (20%)
7	GOL	H	1106	-	5,5,5	0.18	0	5,5,5	1.52	1 (20%)
6	PEG	H	1202	-	6,6,6	0.53	0	5,5,5	1.52	1 (20%)
3	SO4	H	801	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	H	802	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	H	803	-	4,4,4	0.21	0	6,6,6	0.18	0
3	SO4	H	804	-	4,4,4	0.27	0	6,6,6	0.15	0
3	SO4	H	805	-	4,4,4	0.28	0	6,6,6	0.10	0
5	1PE	L	1003	-	15,15,15	0.73	0	14,14,14	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	L	1103	-	5,5,5	0.18	0	5,5,5	1.69	2 (40%)
7	GOL	L	1107	-	5,5,5	0.26	0	5,5,5	1.06	1 (20%)
7	GOL	L	1110	-	5,5,5	0.26	0	5,5,5	1.27	0
7	GOL	L	1115	-	5,5,5	0.31	0	5,5,5	1.26	1 (20%)
7	GOL	L	1119	-	5,5,5	0.22	0	5,5,5	0.41	0
6	PEG	L	1201	-	6,6,6	0.60	0	5,5,5	1.62	1 (20%)
3	SO4	L	808	-	4,4,4	0.30	0	6,6,6	0.14	0
4	EPE	L	901	-	14,15,15	0.82	0	18,20,20	1.75	4 (22%)

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
7	GOL	A	1108	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1116	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1118	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1120	-	-	0/4/4/4	0/0/0/0
3	SO4	A	806	-	-	0/0/0/0	0/0/0/0
5	1PE	B	1002	-	-	0/13/13/13	0/0/0/0
5	1PE	B	1004	-	-	0/13/13/13	0/0/0/0
7	GOL	B	1102	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1111	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1112	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1117	-	-	0/4/4/4	0/0/0/0
3	SO4	B	807	-	-	0/0/0/0	0/0/0/0
3	SO4	B	809	-	-	0/0/0/0	0/0/0/0
4	EPE	B	902	-	-	0/9/19/19	0/1/1/1
5	1PE	H	1001	-	-	0/13/13/13	0/0/0/0
7	GOL	H	1101	-	-	0/4/4/4	0/0/0/0
7	GOL	H	1105	-	-	0/4/4/4	0/0/0/0
7	GOL	H	1106	-	-	0/4/4/4	0/0/0/0
6	PEG	H	1202	-	-	0/4/4/4	0/0/0/0
3	SO4	H	801	-	-	0/0/0/0	0/0/0/0
3	SO4	H	802	-	-	0/0/0/0	0/0/0/0
3	SO4	H	803	-	-	0/0/0/0	0/0/0/0
3	SO4	H	804	-	-	0/0/0/0	0/0/0/0
3	SO4	H	805	-	-	0/0/0/0	0/0/0/0
5	1PE	L	1003	-	-	0/13/13/13	0/0/0/0
7	GOL	L	1103	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	L	1107	-	-	0/4/4/4	0/0/0/0
7	GOL	L	1110	-	-	0/4/4/4	0/0/0/0
7	GOL	L	1115	-	-	0/4/4/4	0/0/0/0
7	GOL	L	1119	-	-	0/4/4/4	0/0/0/0
6	PEG	L	1201	-	-	0/4/4/4	0/0/0/0
3	SO4	L	808	-	-	0/0/0/0	0/0/0/0
4	EPE	L	901	-	-	0/9/19/19	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	EPE	O3S-S-O2S	-3.97	102.36	111.61
4	L	901	EPE	O3S-S-O2S	-3.79	102.79	111.61
4	L	901	EPE	O2S-S-C10	-3.26	104.12	106.91
7	H	1101	GOL	C3-C2-C1	-2.69	100.57	111.12
7	L	1103	GOL	C3-C2-C1	-2.59	100.97	111.12
7	L	1107	GOL	C3-C2-C1	-2.12	102.80	111.12
4	B	902	EPE	C5-C6-N1	-2.07	106.92	110.63
7	H	1105	GOL	C3-C2-C1	-2.05	103.09	111.12
7	B	1117	GOL	O2-C2-C3	2.03	117.96	108.65
7	B	1102	GOL	O2-C2-C3	2.06	118.10	108.65
4	L	901	EPE	O2S-S-O1S	2.08	121.04	113.48
7	L	1115	GOL	O2-C2-C3	2.19	118.70	108.65
7	A	1118	GOL	O2-C2-C1	2.22	118.85	108.65
6	H	1202	PEG	O2-C2-C1	2.24	120.75	110.43
6	L	1201	PEG	O2-C2-C1	2.26	120.83	110.43
4	B	902	EPE	O2S-S-O1S	2.28	121.78	113.48
7	H	1101	GOL	O2-C2-C1	2.30	119.19	108.65
7	A	1120	GOL	O2-C2-C3	2.33	119.33	108.65
7	L	1103	GOL	O2-C2-C3	2.65	120.81	108.65
7	H	1106	GOL	O2-C2-C3	2.87	121.80	108.65
7	A	1118	GOL	C3-C2-C1	3.09	123.24	111.12
4	L	901	EPE	O1S-S-C10	3.63	110.00	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1108	GOL	1	0
7	A	1116	GOL	8	0
7	A	1118	GOL	2	0
5	B	1002	1PE	3	0
5	B	1004	1PE	5	0
7	B	1111	GOL	1	0
7	B	1112	GOL	2	0
7	B	1117	GOL	1	0
4	B	902	EPE	1	0
5	H	1001	1PE	3	0
7	H	1101	GOL	1	0
7	H	1105	GOL	2	0
7	H	1106	GOL	4	0
6	H	1202	PEG	1	0
3	H	801	SO4	0	4
3	H	802	SO4	0	4
5	L	1003	1PE	2	0
7	L	1103	GOL	6	0
7	L	1107	GOL	3	0
7	L	1110	GOL	1	0
7	L	1115	GOL	2	0
7	L	1119	GOL	2	0
6	L	1201	PEG	3	0
4	L	901	EPE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	214/214 (100%)	0.22	6 (2%) 56 62	17, 29, 42, 50	0
1	L	213/214 (99%)	0.04	0 100 100	13, 23, 35, 49	0
2	B	217/224 (96%)	0.26	7 (3%) 51 57	17, 26, 44, 48	0
2	H	220/224 (98%)	0.04	6 (2%) 58 64	13, 23, 36, 56	1 (0%)
All	All	864/876 (98%)	0.14	19 (2%) 65 72	13, 25, 41, 56	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	4.3
2	H	129	ALA	4.0
2	B	97	TYR	3.9
2	B	187	THR	3.6
2	B	5	LEU	3.3
2	H	128	SER	3.1
1	A	23	CYS	3.0
1	A	214	CYS	2.9
1	A	202	THR	2.8
2	H	215	CYS	2.8
2	H	64	LYS	2.7
1	A	70	GLN	2.7
2	B	190	SER	2.7
2	H	214	ASP	2.5
2	B	127	GLY	2.4
2	B	96	GLY	2.2
2	B	134	SER	2.1
1	A	92	TYR	2.1
2	H	41	PRO	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	1PE	B	1004	16/16	0.71	0.40	20.48	56,57,62,63	0
7	GOL	A	1108	6/6	0.52	0.26	13.31	58,59,59,59	0
7	GOL	H	1105	6/6	0.81	0.26	10.63	50,51,52,55	0
7	GOL	L	1119	6/6	0.80	0.27	9.31	60,61,63,65	0
7	GOL	B	1117	6/6	0.81	0.20	8.92	58,59,59,60	0
5	1PE	B	1002	16/16	0.75	0.22	7.99	63,64,68,69	0
7	GOL	L	1115	6/6	0.64	0.25	7.94	52,55,55,56	0
5	1PE	H	1001	16/16	0.69	0.21	7.81	62,64,67,68	0
7	GOL	H	1106	6/6	0.80	0.28	7.35	45,46,48,48	0
5	1PE	L	1003	16/16	0.77	0.25	7.28	68,69,70,71	0
7	GOL	L	1103	6/6	0.73	0.28	7.04	65,65,66,67	0
6	PEG	L	1201	7/7	0.81	0.17	5.77	54,56,56,57	0
3	SO4	A	806	5/5	0.87	0.23	4.76	80,80,80,81	0
7	GOL	B	1102	6/6	0.62	0.18	4.53	49,51,52,53	0
7	GOL	A	1118	6/6	0.86	0.15	4.10	40,42,44,45	0
7	GOL	H	1101	6/6	0.72	0.25	3.91	40,41,42,42	0
3	SO4	B	809	5/5	0.95	0.16	3.62	64,65,65,66	0
3	SO4	H	805	5/5	0.94	0.15	2.45	69,69,69,70	0
7	GOL	A	1120	6/6	0.78	0.18	2.01	52,54,55,56	0
7	GOL	L	1110	6/6	0.78	0.23	1.18	61,62,62,62	0
3	SO4	H	803	5/5	0.98	0.12	1.09	41,43,44,44	0
3	SO4	H	801	5/5	0.98	0.12	0.83	22,22,23,23	4
4	EPE	L	901	15/15	0.96	0.13	0.83	23,40,48,48	0
4	EPE	B	902	15/15	0.93	0.16	0.34	45,52,57,57	0
3	SO4	H	804	5/5	0.97	0.09	-0.77	52,52,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	A	1116	6/6	0.79	0.29	-	60,61,62,62	0
3	SO4	B	807	5/5	0.94	0.20	-	52,52,53,53	0
3	SO4	H	802	5/5	0.89	0.30	-	32,32,34,36	4
7	GOL	L	1107	6/6	0.78	0.22	-	41,45,46,48	0
7	GOL	B	1111	6/6	0.82	0.15	-	65,65,65,65	0
7	GOL	B	1112	6/6	0.77	0.15	-	66,66,67,68	0
3	SO4	L	808	5/5	0.93	0.12	-	59,60,60,61	0
6	PEG	H	1202	7/7	0.83	0.22	-	45,45,46,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.