Full wwPDB X-ray Structure Validation Report (i)

Jun 10, 2024 – 05:09 PM EDT

PDB ID	:	8T51
Title	:	Crystal structure of Fab 3.10C2 bound to TREM2
Authors	:	Hsu, P.L.; Wallweber, H.
Deposited on	:	2023-06-12
Resolution	:	1.90 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:

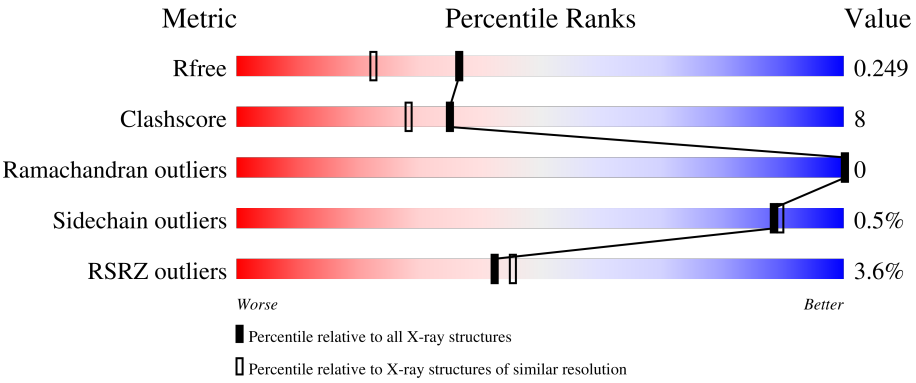
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	222	4% 85% 12% ·
1	C	222	2% 84% 11% 5%
2	B	219	3% 82% 16% ·
2	D	219	3% 79% 19% ··
3	E	20	10% 65% 20% 15%

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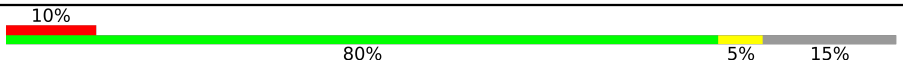
Mol	Chain	Length	Quality of chain
3	F	20	

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	B	301	-	-	-	X
6	GOL	D	304	-	-	X	-
7	ACT	B	309	-	-	X	-
8	PEG	B	305	-	-	-	X
8	PEG	B	306	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7732 atoms, of which 127 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 3.10C2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	2	0
			1624	1027	268	323	6			
1	C	210	Total	C	N	O	S	6	7	0
			1619	1024	266	323	6			

- Molecule 2 is a protein called 3.10C2 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	2	0
			1692	1070	280	336	6			
2	D	217	Total	C	N	O	S	0	3	0
			1691	1070	280	335	6			

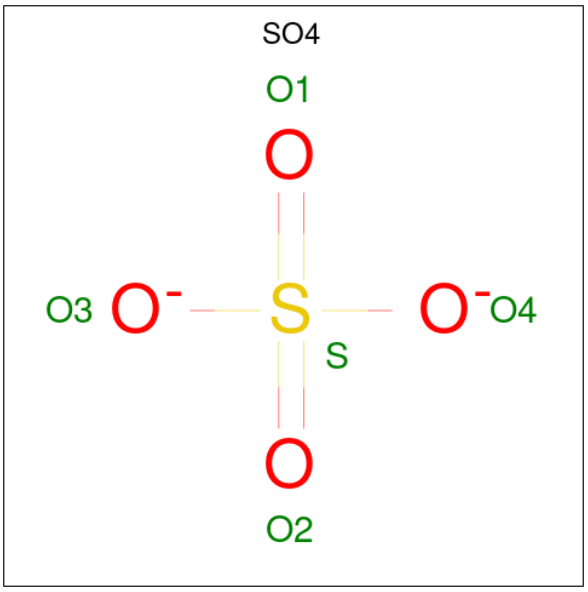
- Molecule 3 is a protein called Triggering receptor expressed on myeloid cells 2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	17	Total	C	N	O	0	1	0
			135	81	25	29			
3	F	17	Total	C	N	O	0	1	0
			146	89	25	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	165	GLU	-	insertion	UNP Q9NZC2
F	165	GLU	-	insertion	UNP Q9NZC2

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

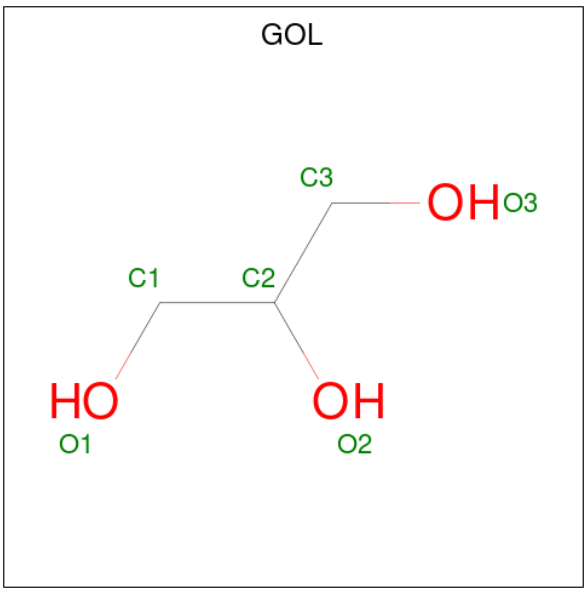


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

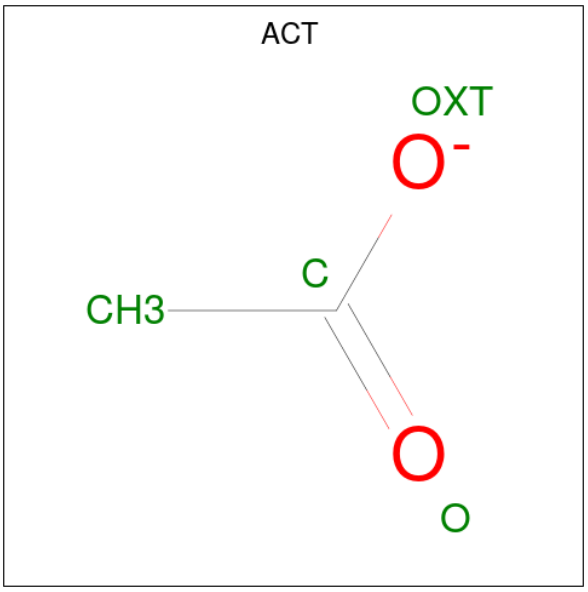
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Zn 3 3	0	0
5	B	2	Total Zn 2 2	0	0
5	E	1	Total Zn 1 1	0	0
5	F	2	Total Zn 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



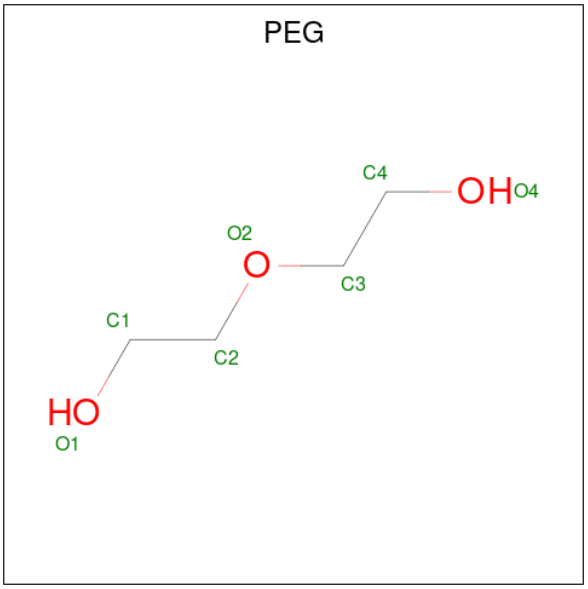
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 14 3 8 3	0	0
6	A	1	Total C H O 14 3 8 3	0	0
6	B	1	Total C H O 14 3 8 3	0	0
6	B	1	Total C H O 14 3 8 3	0	0
6	C	1	Total C H O 14 3 8 3	0	0
6	C	1	Total C H O 14 3 8 3	0	0
6	D	1	Total C H O 14 3 8 3	0	0
6	D	1	Total C H O 14 3 8 3	0	0
6	D	1	Total C H O 14 3 8 3	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 7 2 3 2	0	0
7	B	1	Total C H O 7 2 3 2	0	0
7	B	1	Total C H O 7 2 3 2	0	0
7	C	1	Total C H O 7 2 3 2	0	0
7	D	1	Total C H O 7 2 3 2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			17	4	10	3		
8	B	1	Total	C	H	O	0	0
			17	4	10	3		
8	E	1	Total	C	H	O	0	0
			17	4	10	3		
8	F	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is water.

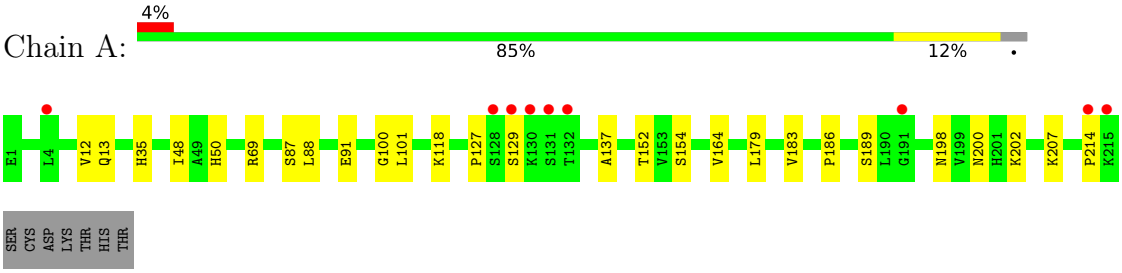
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	132	Total	O	0	5
			137	137		
9	B	106	Total	O	0	2
			108	108		
9	C	139	Total	O	0	5
			144	144		
9	D	127	Total	O	0	4
			131	131		
9	E	15	Total	O	0	0
			15	15		
9	F	13	Total	O	0	0
			13	13		

3 Residue-property plots

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.

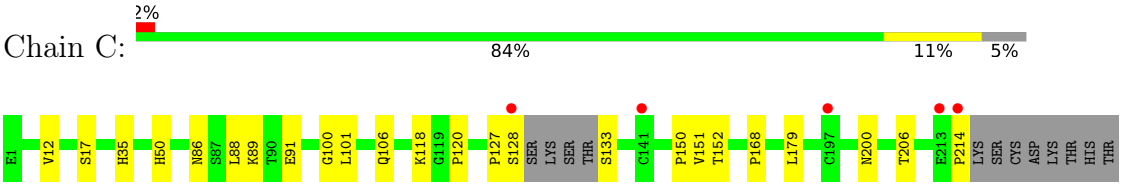
• Molecule 1: 3.10C2 Fab heavy chain

Chain A:



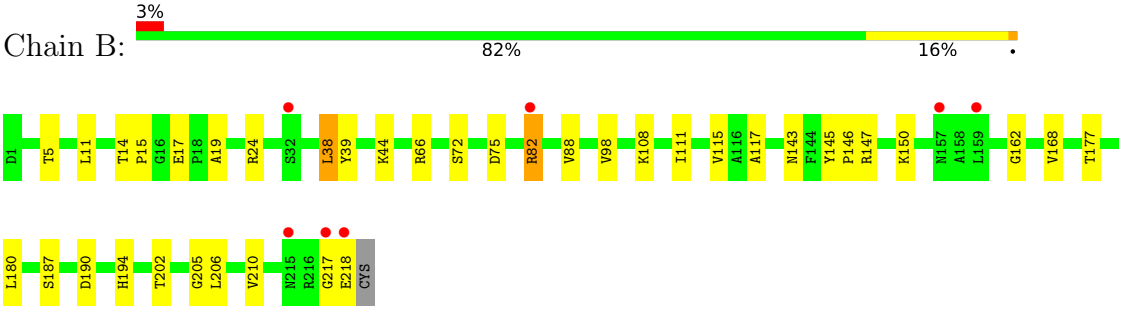
• Molecule 1: 3.10C2 Fab heavy chain

Chain C:



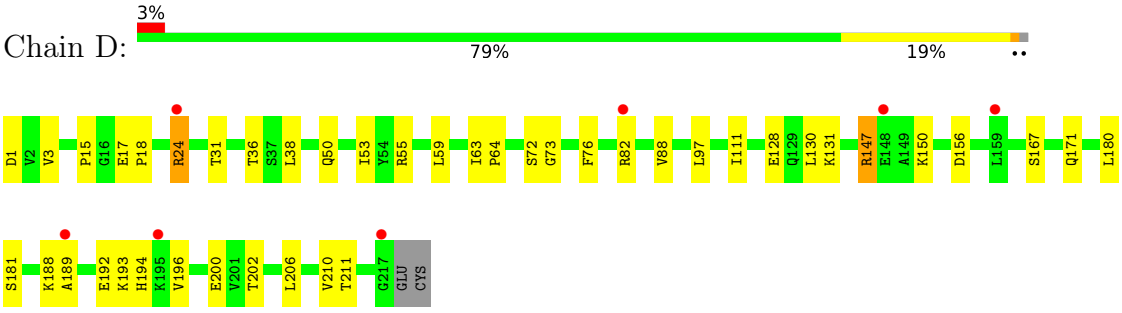
• Molecule 2: 3.10C2 Fab light chain

Chain B:



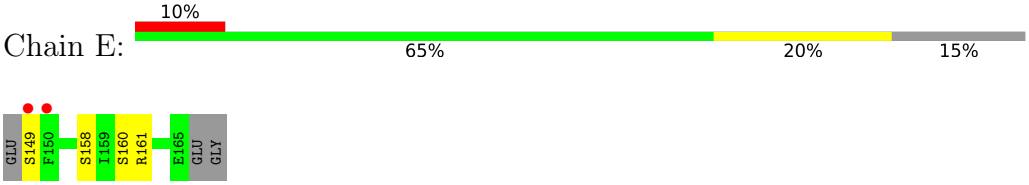
• Molecule 2: 3.10C2 Fab light chain

Chain D:



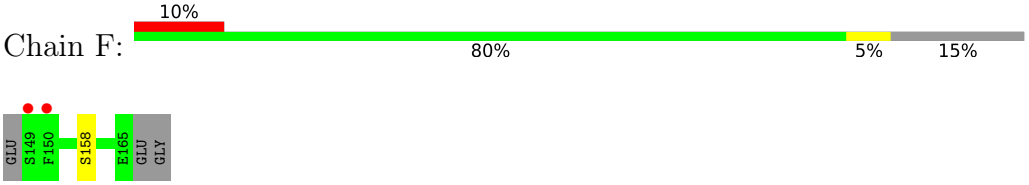
• Molecule 3: Triggering receptor expressed on myeloid cells 2 peptide

Chain E:



• Molecule 3: Triggering receptor expressed on myeloid cells 2 peptide

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.38Å 96.03Å 144.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	1.97 – 1.90 38.95 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (1.97-1.90) 91.5 (38.95-1.78)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.82 (at 1.78Å)	Xtriage
Refinement program	PHENIX v1.2	Depositor
R, R_{free}	0.193 , 0.240 0.217 , 0.249	Depositor DCC
R_{free} test set	4605 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7732	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: ZN, GOL, ACT, PEG, 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	0.55	1/1664 (0.1%)	0.76	2/2267 (0.1%)
1	C	0.53	0/1658	0.71	0/2260
2	B	0.52	0/1730	0.70	1/2352 (0.0%)
2	D	0.60	2/1729 (0.1%)	0.72	0/2351
3	E	0.48	0/135	0.73	0/180
3	F	0.58	0/147	0.51	0/195
All	All	0.55	3/7063 (0.0%)	0.72	3/9605 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	GLU	CD-OE2	5.69	1.31	1.25
2	D	3[A]	VAL	C-N	-5.03	1.22	1.34
2	D	3[B]	VAL	C-N	-5.03	1.22	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	38	LEU	CA-CB-CG	-5.87	101.81	115.30
1	A	13	GLN	CA-CB-CG	5.70	125.94	113.40
1	A	179	LEU	CA-CB-CG	5.19	127.23	115.30

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	1624	0	1592	16	0
1	C	1619	0	1576	16	0
2	B	1692	0	1670	35	1
2	D	1691	0	1673	40	1
3	E	135	0	116	6	0
3	F	146	0	130	1	0
4	A	15	0	0	1	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
6	A	12	16	14	0	0
6	B	12	16	16	1	0
6	C	12	16	16	0	0
6	D	18	24	23	4	0
7	A	4	3	3	0	0
7	B	8	6	6	6	0
7	C	4	3	3	1	0
7	D	4	3	3	0	0
8	B	14	20	20	4	0
8	E	7	10	10	1	0
8	F	7	10	10	0	0
9	A	137	0	0	3	1
9	B	108	0	0	3	0
9	C	144	0	0	6	1
9	D	131	0	0	7	0
9	E	15	0	0	3	1
9	F	13	0	0	0	1
All	All	7605	127	6881	114	4

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 8.

All (114) 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:168[A]:VAL:HG21	7:B:309:ACT:H2	1.39	1.02
2:B:147:ARG:HG2	7:B:309:ACT:H1	1.49	0.92
2:D:194:HIS:ND1	9:D:401:HOH:O	2.05	0.90
2:B:168[B]:VAL:HG11	7:B:309:ACT:H2	1.55	0.88
2:B:88:VAL:HG12	2:B:111:ILE:HG12	1.55	0.88
4:A:302:SO4:O2	9:A:401:HOH:O	1.95	0.83
2:D:38[A]:LEU:HD22	2:D:76:PHE:CG	2.17	0.79
1:C:106:GLN:NE2	9:C:401:HOH:O	2.14	0.79
2:B:88:VAL:CG1	2:B:111:ILE:HG12	2.12	0.79
2:B:108:LYS:HE2	9:B:440:HOH:O	1.83	0.78
1:C:118:LYS:NZ	9:C:403:HOH:O	2.21	0.73
1:A:118:LYS:NZ	9:A:402:HOH:O	2.20	0.73
2:B:117:ALA:H	8:B:306:PEG:H32	1.54	0.72
2:D:82:ARG:NH1	9:D:404:HOH:O	2.23	0.72
2:D:130:LEU:O	2:D:188:LYS:HD2	1.91	0.70
2:D:156:ASP:HA	2:D:196:VAL:HG22	1.74	0.70
1:C:12[A]:VAL:HG11	1:C:88:LEU:HD13	1.74	0.69
2:B:147:ARG:CG	7:B:309:ACT:H1	2.21	0.68
1:A:100:GLY:O	1:A:101:LEU:HB2	1.94	0.67
2:B:115:VAL:O	9:B:401:HOH:O	2.12	0.66
2:D:82:ARG:HH11	2:D:82:ARG:HG3	1.62	0.65
1:A:35:HIS:CD2	1:A:101:LEU:HD13	2.32	0.65
2:B:15:PRO:HD3	2:B:111:ILE:HG23	1.79	0.64
2:B:206:LEU:HD13	2:B:210[A]:VAL:HG13	1.81	0.63
2:B:168[A]:VAL:HG21	7:B:309:ACT:CH3	2.23	0.63
2:B:187:SER:OG	2:B:190:ASP:HB2	2.00	0.62
1:A:164:VAL:HG22	1:A:183:VAL:HG22	1.81	0.62
2:D:72:SER:HA	6:D:304:GOL:H32	1.82	0.62
2:B:168[B]:VAL:HG11	7:B:309:ACT:CH3	2.29	0.61
2:D:73:GLY:H	6:D:304:GOL:C3	2.15	0.60
3:E:161:ARG:NH1	9:E:301:HOH:O	2.28	0.59
2:D:73:GLY:H	6:D:304:GOL:H32	1.67	0.59
3:E:149:SER:N	9:E:302:HOH:O	2.34	0.59
2:B:24:ARG:NH1	2:B:75:ASP:OD2	2.36	0.58
2:B:98:VAL:HG22	3:E:149:SER:HA	1.86	0.58
2:D:50:GLN:OE1	9:D:403:HOH:O	2.17	0.57
2:B:11:LEU:HD21	2:B:19:ALA:HB1	1.86	0.56
1:C:128:SER:HB3	9:D:514:HOH:O	2.05	0.56
2:D:15:PRO:HD3	2:D:111:ILE:HG23	1.86	0.56
1:A:152:THR:OG1	1:A:200:ASN:HB3	2.06	0.56
2:B:168[B]:VAL:HG12	2:B:180:LEU:HD12	1.88	0.56
2:B:117:ALA:H	8:B:306:PEG:C3	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:LYS:O	2:D:192:GLU:HG3	2.07	0.55
2:D:147:ARG:HG2	2:D:147:ARG:HH21	1.73	0.54
1:A:12:VAL:HG11	1:A:88:LEU:HD13	1.88	0.54
1:C:100:GLY:O	1:C:101:LEU:HB2	2.09	0.53
2:D:1:ASP:O	2:D:1:ASP:CG	2.47	0.53
1:A:152:THR:HG23	1:A:202:LYS:HZ3	1.74	0.52
1:A:127:PRO:HD2	1:A:214:PRO:HA	1.91	0.52
2:B:150:LYS:HB3	2:B:202:THR:HB	1.93	0.51
2:B:44:LYS:NZ	6:B:304:GOL:H31	2.26	0.51
2:D:1:ASP:HB2	9:D:517:HOH:O	2.11	0.51
2:D:128:GLU:O	2:D:131:LYS:HG2	2.12	0.50
2:B:108:LYS:HB2	8:B:305:PEG:H21	1.94	0.50
1:C:12[A]:VAL:HG11	1:C:88:LEU:CD1	2.41	0.49
1:C:89:LYS:HB2	1:C:91:GLU:HG2	1.94	0.49
9:A:444:HOH:O	3:E:158:SER:HA	2.12	0.49
2:D:156:ASP:CA	2:D:196:VAL:HG22	2.43	0.49
2:D:200:GLU:HG2	2:D:211:THR:OG1	2.12	0.49
2:B:143:ASN:HB2	9:C:498:HOH:O	2.12	0.48
1:A:129:SER:OG	1:A:137:ALA:HB2	2.14	0.48
2:B:66:ARG:HD2	2:B:82:ARG:O	2.13	0.48
2:B:217:GLY:O	2:B:218:GLU:HB2	2.13	0.47
2:D:73:GLY:N	6:D:304:GOL:H32	2.29	0.47
2:B:72:SER:O	2:B:72:SER:OG	2.28	0.47
2:B:190:ASP:O	2:B:194:HIS:HD2	1.98	0.47
2:D:59:LEU:HG	2:D:63:ILE:HB	1.96	0.46
2:D:147:ARG:HG2	2:D:147:ARG:NH2	2.30	0.46
3:E:160:SER:HB2	8:E:201:PEG:H31	1.97	0.46
2:D:156:ASP:HA	2:D:196:VAL:CG2	2.44	0.46
1:C:17[A]:SER:OG	1:C:86:ASN:OD1	2.24	0.46
2:B:14:THR:O	2:B:17:GLU:HB2	2.16	0.46
2:D:38[A]:LEU:HD22	2:D:76:PHE:CB	2.46	0.46
2:D:82:ARG:NH1	2:D:82:ARG:HG3	2.29	0.46
2:B:205:GLY:O	8:B:306:PEG:H21	2.16	0.45
1:A:152:THR:HG23	1:A:202:LYS:NZ	2.32	0.45
2:D:38[A]:LEU:HD22	2:D:76:PHE:CD1	2.51	0.45
1:A:207:LYS:NZ	9:C:479[B]:HOH:O	2.50	0.45
2:B:143:ASN:ND2	2:B:177:THR:HG21	2.32	0.45
2:B:66:ARG:HD3	9:B:403:HOH:O	2.16	0.45
1:A:35:HIS:CE1	1:A:50:HIS:CD2	3.04	0.44
2:D:196:VAL:O	2:D:196:VAL:HG23	2.17	0.44
2:D:189:ALA:O	2:D:193:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:161:ARG:HD2	9:E:314:HOH:O	2.16	0.44
2:B:38:LEU:HG	2:B:39:TYR:N	2.33	0.44
9:C:453:HOH:O	3:F:158:SER:HA	2.17	0.44
2:D:88:VAL:CG1	9:D:424:HOH:O	2.66	0.43
2:D:36:THR:O	2:D:55:ARG:HA	2.17	0.43
1:C:168:PRO:HD2	2:D:167:SER:OG	2.18	0.43
2:D:180:LEU:HD23	2:D:181:SER:N	2.33	0.43
1:C:120:PRO:HD2	1:C:206:THR:HG21	2.00	0.43
2:D:180:LEU:HD23	2:D:180:LEU:C	2.38	0.43
2:D:31:THR:HG22	2:D:97:LEU:HD13	2.01	0.43
1:C:151[A]:VAL:CG1	1:C:179:LEU:HD21	2.49	0.43
1:C:152:THR:OG1	1:C:200:ASN:HB3	2.19	0.43
7:C:304:ACT:H3	9:D:471:HOH:O	2.19	0.43
1:A:154:SER:OG	1:A:198:ASN:HB2	2.19	0.42
1:A:186:PRO:O	1:A:189:SER:HB3	2.20	0.42
2:D:150:LYS:HB3	2:D:202:THR:HB	2.01	0.42
1:C:151[A]:VAL:HG12	1:C:179:LEU:HD21	2.02	0.42
1:C:127:PRO:HD2	1:C:214:PRO:HA	2.02	0.41
2:B:145:TYR:CG	2:B:146:PRO:HA	2.56	0.41
2:D:53:ILE:HD13	2:D:59:LEU:HA	2.02	0.41
2:D:88:VAL:HG21	2:D:171:GLN:HB3	2.01	0.41
1:C:35:HIS:CE1	1:C:50:HIS:CD2	3.08	0.41
2:D:63:ILE:HA	2:D:64:PRO:HD3	1.95	0.41
2:D:206:LEU:HD13	2:D:210:VAL:HG23	2.02	0.41
2:B:5:THR:OG1	2:B:24:ARG:HB3	2.21	0.41
1:C:133:SER:N	9:C:418:HOH:O	2.53	0.41
2:D:59:LEU:HD11	2:D:63:ILE:CG2	2.51	0.41
1:A:69:ARG:HD2	1:A:87[B]:SER:OG	2.22	0.40
2:D:17:GLU:HB3	2:D:18:PRO:HD2	2.02	0.40
2:B:82:ARG:N	2:B:82:ARG:HD3	2.36	0.40
1:A:48:ILE:HD13	1:A:48:ILE:HA	1.94	0.40

All (4) 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)
9:A:513:HOH:O	9:A:513:HOH:O[2_545]	1.82	0.38
2:B:162:GLY:O	2:D:24:ARG:NH2[4_544]	1.90	0.30
9:C:486:HOH:O	9:C:486:HOH:O[2_545]	1.98	0.22
9:E:308:HOH:O	9:F:312:HOH:O[1_455]	2.16	0.04

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	215/222 (97%)	207 (96%)	8 (4%)	0	100	100
1	C	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
2	B	218/219 (100%)	213 (98%)	5 (2%)	0	100	100
2	D	218/219 (100%)	215 (99%)	3 (1%)	0	100	100
3	E	15/20 (75%)	14 (93%)	1 (7%)	0	100	100
3	F	15/20 (75%)	15 (100%)	0	0	100	100
All	All	894/922 (97%)	872 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	184/189 (97%)	184 (100%)	0	100	100
1	C	184/189 (97%)	183 (100%)	1 (0%)	88	89
2	B	195/194 (100%)	194 (100%)	1 (0%)	88	89
2	D	195/194 (100%)	193 (99%)	2 (1%)	76	76
3	E	14/18 (78%)	14 (100%)	0	100	100
3	F	17/18 (94%)	17 (100%)	0	100	100
All	All	789/802 (98%)	785 (100%)	4 (0%)	88	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	82	ARG
1	C	150	PRO
2	D	24	ARG
2	D	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	143	ASN
2	D	157	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 for Mogul analysis.

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	$\#\|Z\| > 2$
6	GOL	A	305	-	5,5,5	1.91	2 (40%)	5,5,5	1.83	1 (20%)
8	PEG	F	203	-	6,6,6	0.51	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	ACT	B	309	-	3,3,3	1.19	0	3,3,3	1.58	1 (33%)
4	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.09	0
6	GOL	B	303	-	5,5,5	1.13	0	5,5,5	0.54	0
6	GOL	D	303	-	5,5,5	0.70	0	5,5,5	0.88	0
4	SO4	A	302	-	4,4,4	0.13	0	6,6,6	0.12	0
7	ACT	C	304	-	3,3,3	1.11	0	3,3,3	1.46	0
4	SO4	A	303	-	4,4,4	0.16	0	6,6,6	0.12	0
7	ACT	A	306	-	3,3,3	1.09	0	3,3,3	1.33	0
6	GOL	A	308	-	5,5,5	1.23	1 (20%)	5,5,5	1.10	0
4	SO4	A	301	-	4,4,4	0.13	0	6,6,6	0.15	0
8	PEG	B	305	-	6,6,6	0.47	0	5,5,5	0.38	0
8	PEG	B	306	-	6,6,6	0.47	0	5,5,5	0.26	0
6	GOL	C	302	-	5,5,5	1.19	0	5,5,5	1.45	1 (20%)
7	ACT	B	308	-	3,3,3	0.70	0	3,3,3	1.63	1 (33%)
4	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	D	302	-	4,4,4	0.16	0	6,6,6	0.05	0
4	SO4	C	301	-	4,4,4	0.17	0	6,6,6	0.18	0
6	GOL	D	306	-	5,5,5	1.15	0	5,5,5	1.29	1 (20%)
7	ACT	D	305	-	3,3,3	0.90	0	3,3,3	1.53	0
6	GOL	B	304	-	5,5,5	0.50	0	5,5,5	1.06	1 (20%)
6	GOL	D	304	-	5,5,5	1.16	0	5,5,5	1.46	1 (20%)
8	PEG	E	201	-	6,6,6	0.47	0	5,5,5	0.25	0
4	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.27	0
6	GOL	C	303	-	5,5,5	0.55	0	5,5,5	0.97	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
6	GOL	A	305	-	-	0/4/4/4	-
6	GOL	D	306	-	-	0/4/4/4	-
8	PEG	F	203	-	-	0/4/4/4	-
8	PEG	B	305	-	-	3/4/4/4	-
6	GOL	B	304	-	-	2/4/4/4	-
6	GOL	D	304	-	-	4/4/4/4	-
8	PEG	B	306	-	-	1/4/4/4	-
8	PEG	E	201	-	-	3/4/4/4	-
6	GOL	B	303	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	302	-	-	0/4/4/4	-
6	GOL	C	303	-	-	4/4/4/4	-
6	GOL	D	303	-	-	0/4/4/4	-
6	GOL	A	308	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	305	GOL	C1-C2	2.73	1.63	1.51
6	A	305	GOL	O2-C2	-2.70	1.35	1.43
6	A	308	GOL	O2-C2	-2.44	1.36	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	305	GOL	C3-C2-C1	-3.58	97.80	111.70
6	D	304	GOL	C3-C2-C1	-2.80	100.81	111.70
6	C	302	GOL	C3-C2-C1	-2.71	101.17	111.70
6	D	306	GOL	C3-C2-C1	-2.36	102.51	111.70
7	B	308	ACT	O-C-CH3	-2.08	114.25	122.33
7	B	309	ACT	OXT-C-O	2.06	129.64	122.05
6	B	304	GOL	C3-C2-C1	-2.01	103.87	111.70

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	303	GOL	O1-C1-C2-O2
6	C	303	GOL	O1-C1-C2-C3
6	C	303	GOL	C1-C2-C3-O3
6	D	304	GOL	O1-C1-C2-O2
6	D	304	GOL	O1-C1-C2-C3
6	C	303	GOL	O2-C2-C3-O3
8	B	305	PEG	O1-C1-C2-O2
8	E	201	PEG	O1-C1-C2-O2
6	B	304	GOL	O2-C2-C3-O3
6	D	304	GOL	O2-C2-C3-O3
8	B	306	PEG	O1-C1-C2-O2
8	B	305	PEG	C1-C2-O2-C3
8	E	201	PEG	O2-C3-C4-O4
8	E	201	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
6	B	304	GOL	C1-C2-C3-O3
6	D	304	GOL	C1-C2-C3-O3
8	B	305	PEG	O2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	309	ACT	6	0
4	A	302	SO4	1	0
7	C	304	ACT	1	0
8	B	305	PEG	1	0
8	B	306	PEG	3	0
6	B	304	GOL	1	0
6	D	304	GOL	4	0
8	E	201	PEG	1	0

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, 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	215/222 (96%)	0.20	9 (4%)	36	39	21, 28, 46, 114	0
1	C	210/222 (94%)	0.15	5 (2%)	59	62	19, 27, 40, 51	0
2	B	218/219 (99%)	0.07	7 (3%)	47	50	22, 33, 48, 92	0
2	D	217/219 (99%)	0.22	7 (3%)	47	50	19, 30, 47, 62	0
3	E	17/20 (85%)	0.63	2 (11%)	4	5	26, 31, 54, 55	0
3	F	17/20 (85%)	0.38	2 (11%)	4	5	23, 27, 48, 73	0
All	All	894/922 (96%)	0.17	32 (3%)	42	45	19, 29, 46, 114	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	149	SER	5.4
1	A	129	SER	4.9
1	A	131	SER	4.7
2	B	159	LEU	4.6
1	A	130	LYS	3.9
1	C	128	SER	3.8
3	F	149	SER	3.7
1	A	132	THR	3.4
2	B	218	GLU	3.3
1	A	214	PRO	3.1
2	B	217	GLY	3.0
1	C	141	CYS	2.9
2	B	32	SER	2.9
3	E	150	PHE	2.9
1	A	215	LYS	2.9
1	A	191	GLY	2.9
2	D	159	LEU	2.7
3	F	150	PHE	2.6
1	C	197	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	195	LYS	2.5
2	B	157	ASN	2.4
2	D	24	ARG	2.3
1	C	213	GLU	2.3
2	D	217	GLY	2.2
2	B	82	ARG	2.2
2	D	82	ARG	2.2
2	D	148	GLU	2.1
2	D	189	ALA	2.1
1	A	4	LEU	2.1
1	A	128	SER	2.1
2	B	215	ASN	2.1
1	C	214	PRO	2.1

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
8	PEG	E	201	7/7	0.50	0.23	42,52,70,80	0
8	PEG	B	305	7/7	0.62	0.42	57,68,77,77	0
7	ACT	B	308	4/4	0.63	0.29	41,49,49,54	0
4	SO4	B	301	5/5	0.68	0.41	82,91,120,122	0
6	GOL	B	304	6/6	0.69	0.26	44,55,63,66	0
4	SO4	D	301	5/5	0.69	0.27	105,111,115,136	0
8	PEG	F	203	7/7	0.70	0.20	37,47,64,64	0
4	SO4	A	301	5/5	0.72	0.34	90,95,102,119	0
7	ACT	A	306	4/4	0.72	0.33	37,41,44,54	0
6	GOL	D	303	6/6	0.73	0.18	29,39,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	D	304	6/6	0.74	0.35	36,47,58,66	0
6	GOL	B	303	6/6	0.74	0.21	25,31,36,36	0
6	GOL	A	305	6/6	0.75	0.16	38,46,50,55	0
8	PEG	B	306	7/7	0.75	0.43	47,61,77,80	0
4	SO4	A	303	5/5	0.77	0.37	69,73,79,99	0
7	ACT	D	305	4/4	0.77	0.26	56,64,67,70	0
4	SO4	D	302	5/5	0.77	0.28	74,74,97,105	0
6	GOL	A	308	6/6	0.78	0.17	31,39,44,47	0
4	SO4	B	302	5/5	0.78	0.26	58,59,65,65	0
6	GOL	D	306	6/6	0.79	0.20	32,44,51,53	0
6	GOL	C	302	6/6	0.80	0.30	40,49,52,61	0
6	GOL	C	303	6/6	0.82	0.27	42,51,61,61	0
7	ACT	B	309	4/4	0.84	0.41	47,51,57,64	0
7	ACT	C	304	4/4	0.89	0.23	32,33,40,40	0
4	SO4	C	301	5/5	0.92	0.14	64,67,74,85	0
4	SO4	A	302	5/5	0.93	0.14	61,66,68,78	0
5	ZN	B	310	1/1	0.94	0.63	115,115,115,115	0
5	ZN	B	307	1/1	0.95	0.57	98,98,98,98	0
5	ZN	A	307	1/1	0.98	0.20	29,29,29,29	0
5	ZN	E	202	1/1	0.99	0.26	30,30,30,30	0
5	ZN	F	201	1/1	0.99	0.10	39,39,39,39	1
5	ZN	A	304	1/1	0.99	0.08	41,41,41,41	1
5	ZN	A	309	1/1	0.99	0.09	28,28,28,28	0
5	ZN	F	202	1/1	1.00	0.11	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.