Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 06:10 AM EDT

PDB ID	:	6HSW
Title	:	A CE15 glucuronoyl esterase from Teredinibacter turnerae T7901
Authors	:	Mazurkewich, S.; Lo Leggio, L.; Navarro Poulsen, J.C.; Larsbrink, J.
Deposited on	:	2018-10-02
Resolution	:	2.15 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 (i)) were used in the production of this report:

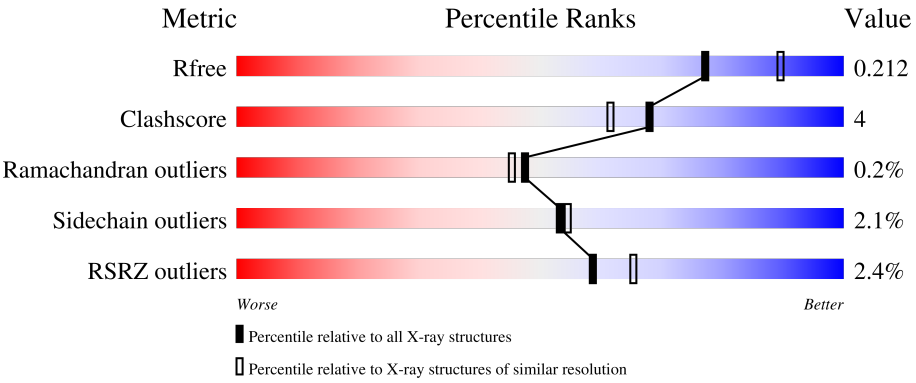
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

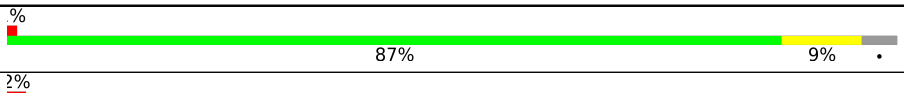
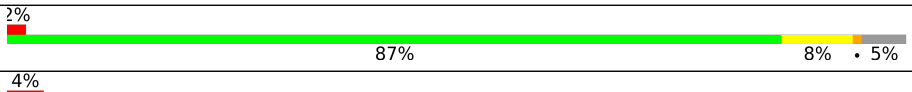
The reported resolution of this entry is 2.15 Å.

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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	440	
1	B	440	
1	C	440	

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	EDO	C	507	-	-	-	X
4	GOL	B	515	-	-	-	X
4	GOL	B	516	-	-	-	X
4	GOL	B	517	-	-	-	X
4	GOL	B	518	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20325 atoms, of which 9602 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 Carbohydrate esterase family 15 domain protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	422	Total	C	H	N	O	S	Se	0	4	0
			6377	2052	3126	586	606	1	6			
1	B	420	Total	C	H	N	O	S	Se	0	7	0
			6347	2043	3113	577	606	1	7			
1	C	420	Total	C	H	N	O	S	Se	0	3	0
			6310	2033	3092	575	603	1	6			

There are 60 discrepancies between the modelled and reference sequences:

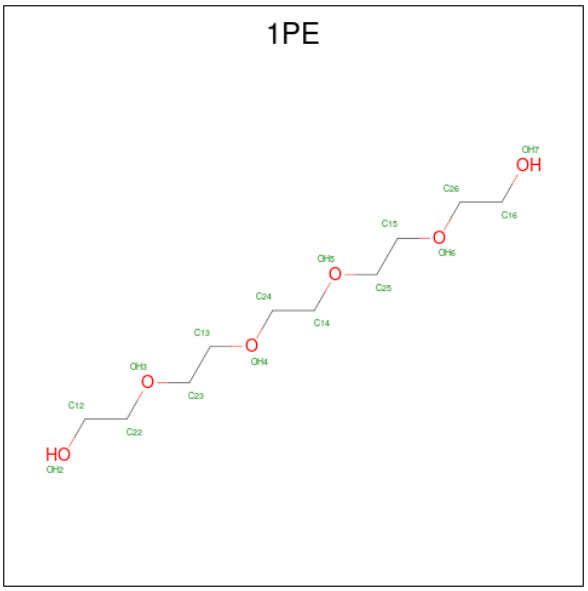
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MSE	-	initiating methionine	UNP C5BN23
A	-19	GLY	-	expression tag	UNP C5BN23
A	-18	SER	-	expression tag	UNP C5BN23
A	-17	SER	-	expression tag	UNP C5BN23
A	-16	HIS	-	expression tag	UNP C5BN23
A	-15	HIS	-	expression tag	UNP C5BN23
A	-14	HIS	-	expression tag	UNP C5BN23
A	-13	HIS	-	expression tag	UNP C5BN23
A	-12	HIS	-	expression tag	UNP C5BN23
A	-11	HIS	-	expression tag	UNP C5BN23
A	-10	SER	-	expression tag	UNP C5BN23
A	-9	SER	-	expression tag	UNP C5BN23
A	-8	GLU	-	expression tag	UNP C5BN23
A	-7	ASN	-	expression tag	UNP C5BN23
A	-6	LEU	-	expression tag	UNP C5BN23
A	-5	TYR	-	expression tag	UNP C5BN23
A	-4	PHE	-	expression tag	UNP C5BN23
A	-3	GLN	-	expression tag	UNP C5BN23
A	-2	GLY	-	expression tag	UNP C5BN23
A	-1	HIS	-	expression tag	UNP C5BN23
B	-20	MSE	-	initiating methionine	UNP C5BN23
B	-19	GLY	-	expression tag	UNP C5BN23
B	-18	SER	-	expression tag	UNP C5BN23

Continued on next page...

Continued from previous page...

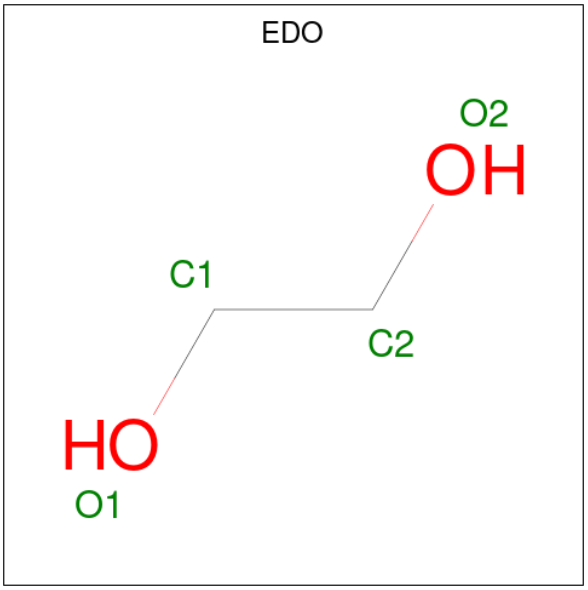
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP C5BN23
B	-16	HIS	-	expression tag	UNP C5BN23
B	-15	HIS	-	expression tag	UNP C5BN23
B	-14	HIS	-	expression tag	UNP C5BN23
B	-13	HIS	-	expression tag	UNP C5BN23
B	-12	HIS	-	expression tag	UNP C5BN23
B	-11	HIS	-	expression tag	UNP C5BN23
B	-10	SER	-	expression tag	UNP C5BN23
B	-9	SER	-	expression tag	UNP C5BN23
B	-8	GLU	-	expression tag	UNP C5BN23
B	-7	ASN	-	expression tag	UNP C5BN23
B	-6	LEU	-	expression tag	UNP C5BN23
B	-5	TYR	-	expression tag	UNP C5BN23
B	-4	PHE	-	expression tag	UNP C5BN23
B	-3	GLN	-	expression tag	UNP C5BN23
B	-2	GLY	-	expression tag	UNP C5BN23
B	-1	HIS	-	expression tag	UNP C5BN23
C	-20	MSE	-	initiating methionine	UNP C5BN23
C	-19	GLY	-	expression tag	UNP C5BN23
C	-18	SER	-	expression tag	UNP C5BN23
C	-17	SER	-	expression tag	UNP C5BN23
C	-16	HIS	-	expression tag	UNP C5BN23
C	-15	HIS	-	expression tag	UNP C5BN23
C	-14	HIS	-	expression tag	UNP C5BN23
C	-13	HIS	-	expression tag	UNP C5BN23
C	-12	HIS	-	expression tag	UNP C5BN23
C	-11	HIS	-	expression tag	UNP C5BN23
C	-10	SER	-	expression tag	UNP C5BN23
C	-9	SER	-	expression tag	UNP C5BN23
C	-8	GLU	-	expression tag	UNP C5BN23
C	-7	ASN	-	expression tag	UNP C5BN23
C	-6	LEU	-	expression tag	UNP C5BN23
C	-5	TYR	-	expression tag	UNP C5BN23
C	-4	PHE	-	expression tag	UNP C5BN23
C	-3	GLN	-	expression tag	UNP C5BN23
C	-2	GLY	-	expression tag	UNP C5BN23
C	-1	HIS	-	expression tag	UNP C5BN23

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			38	10	22	6		
2	B	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



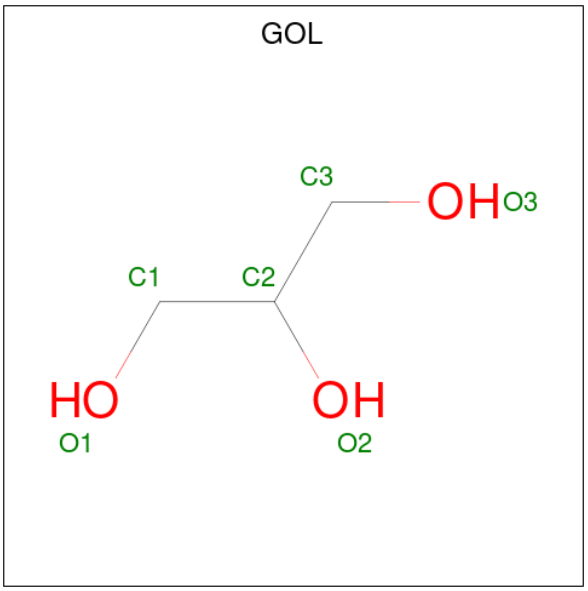
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

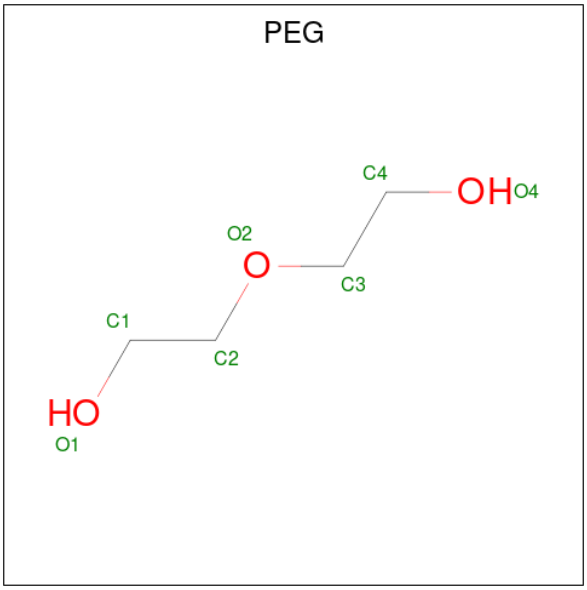


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 13 3 7 3	0	0
4	B	1	Total C H O 12 3 6 3	0	0
4	B	1	Total C H O 13 3 7 3	0	0
4	B	1	Total C H O 13 3 7 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 13 3 7 3	0	0
4	B	1	Total C H O 13 3 7 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Br 1 1	0	0
5	C	1	Total Br 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C H O 17 4 10 3	0	0

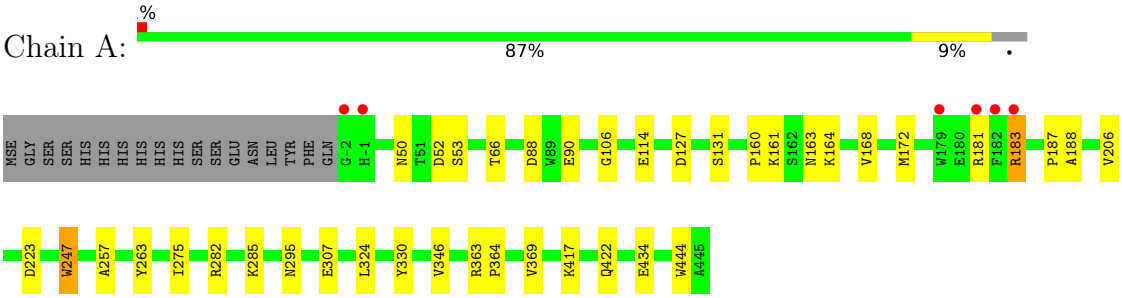
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	281	Total O 281 281	0	0
7	B	308	Total O 308 308	0	0
7	C	232	Total O 232 232	0	0

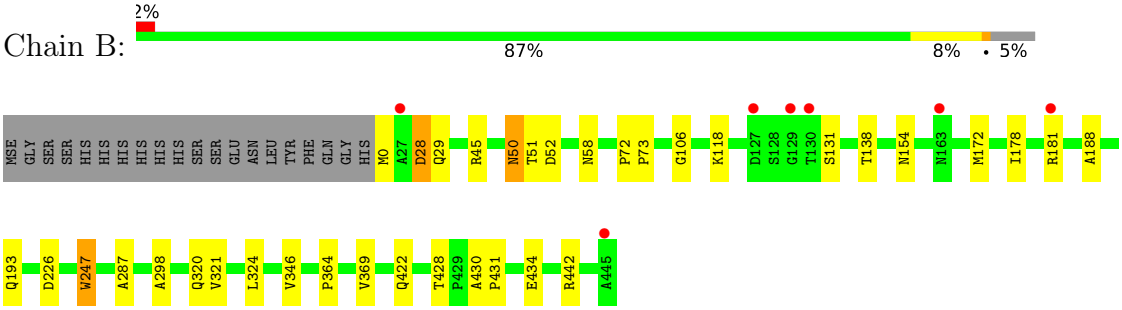
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

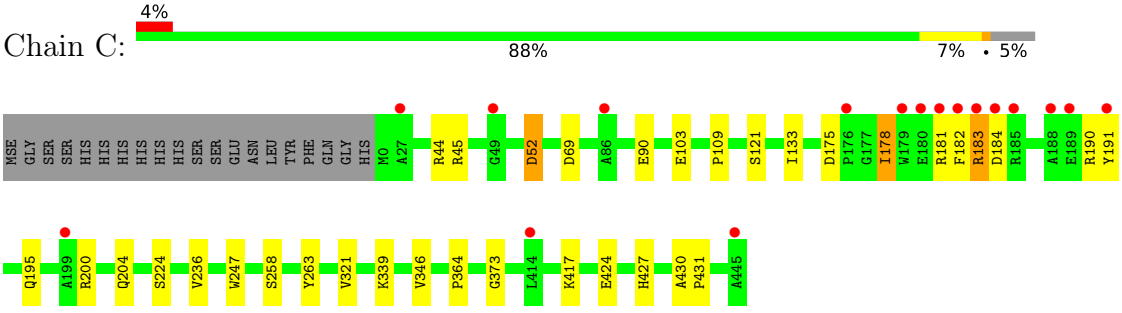
• Molecule 1: Carbohydrate esterase family 15 domain protein



• Molecule 1: Carbohydrate esterase family 15 domain protein



• Molecule 1: Carbohydrate esterase family 15 domain protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.17Å 121.17Å 198.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.81 – 2.15 46.37 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.81-2.15) 90.9 (46.37-2.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.48 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.164 , 0.212 0.164 , 0.212	Depositor DCC
R_{free} test set	969 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20325	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: PEG, GOL, BR, 1PE, EDO

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	0.54	0/3348	0.64	1/4552 (0.0%)
1	B	0.57	0/3350	0.66	0/4561
1	C	0.51	0/3317	0.63	0/4516
All	All	0.54	0/10015	0.64	1/13629 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	ASP	CB-CG-OD1	5.29	123.06	118.30

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	3251	3126	3114	26	1
1	B	3234	3113	3086	26	0
1	C	3218	3092	3078	22	1
2	A	16	22	22	4	0
2	B	16	22	22	1	0
3	A	28	42	42	1	0
3	B	28	42	42	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	24	36	36	2	0
4	A	18	24	24	1	0
4	B	54	65	71	9	0
4	C	6	8	8	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	C	7	10	10	1	0
7	A	281	0	0	4	0
7	B	308	0	0	4	0
7	C	232	0	0	3	0
All	All	10723	9602	9555	75	1

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 4.

All (75) 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:C:424:GLU:OE2	7:C:601:HOH:O	2.02	0.77
1:A:163:ASN:ND2	7:A:602:HOH:O	2.18	0.76
1:C:90:GLU:OE2	7:C:602:HOH:O	2.05	0.74
1:A:90:GLU:OE2	7:A:601:HOH:O	2.08	0.71
1:A:282:ARG:HA	1:A:285:LYS:HD2	1.71	0.71
1:C:182:PHE:O	1:C:184:ASP:N	2.25	0.69
1:C:69[A]:ASP:OD2	7:C:603:HOH:O	2.10	0.68
1:A:164:LYS:NZ	7:A:605:HOH:O	2.28	0.67
1:C:52:ASP:N	1:C:52:ASP:OD1	2.28	0.66
1:B:346:VAL:HG11	4:B:518:GOL:H11	1.86	0.57
1:A:172:MSE:HE2	1:A:257:ALA:HB2	1.87	0.57
1:A:187:PRO:HG2	2:A:501:1PE:H241	1.89	0.55
1:A:285:LYS:HE3	1:A:307:GLU:O	2.07	0.54
1:A:50:ASN:ND2	1:A:52:ASP:OD1	2.34	0.52
1:A:187:PRO:O	1:A:188:ALA:HB3	2.09	0.52
1:C:103:GLU:OE1	1:C:339:LYS:NZ	2.42	0.52
1:A:364:PRO:HA	1:A:417:LYS:O	2.10	0.52
4:B:518:GOL:H32	7:B:831:HOH:O	2.09	0.52
1:C:175:ASP:O	1:C:178:ILE:HG13	2.10	0.51
1:B:188:ALA:HB3	4:B:514:GOL:H11	1.93	0.51
1:C:45:ARG:HA	3:C:506:EDO:H11	1.92	0.51
1:C:321:VAL:HG21	1:C:346:VAL:HG22	1.92	0.51
1:A:187:PRO:HG3	2:A:501:1PE:H242	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:514:GOL:H31	1:C:44:ARG:NE	2.26	0.50
1:A:114:GLU:HG2	7:A:837:HOH:O	2.12	0.49
4:B:518:GOL:C3	7:B:831:HOH:O	2.61	0.48
1:B:321:VAL:HG12	4:B:518:GOL:O2	2.14	0.48
1:A:223:ASP:OD2	1:A:282:ARG:NH1	2.42	0.47
1:B:188:ALA:H	4:B:514:GOL:H32	1.80	0.47
1:B:320:GLN:HA	4:B:518:GOL:H2	1.96	0.47
1:B:51:THR:OG1	1:C:373:GLY:HA3	2.15	0.46
1:C:258:SER:OG	6:C:502:PEG:H41	2.16	0.46
1:C:109:PRO:HG2	1:C:236:VAL:HG11	1.98	0.46
1:B:106:GLY:HA3	1:B:247:TRP:HA	1.98	0.45
1:B:58:ASN:HB2	2:B:502:1PE:H141	1.99	0.45
1:B:172:MSE:HE1	1:B:287:ALA:N	2.32	0.45
1:B:50:ASN:HB2	1:B:52:ASP:OD1	2.16	0.45
1:B:138[B]:THR:HG22	1:B:154:ASN:OD1	2.17	0.45
1:B:51:THR:HG22	1:B:51:THR:O	2.17	0.44
1:A:187:PRO:HG2	2:A:501:1PE:C24	2.46	0.44
1:C:200:ARG:O	1:C:204:GLN:HG3	2.17	0.44
1:A:160:PRO:HB3	1:A:206:VAL:HG13	2.00	0.44
1:A:168:VAL:O	1:A:275:ILE:HA	2.18	0.43
1:A:187:PRO:CG	2:A:501:1PE:H242	2.48	0.43
1:A:369:VAL:O	1:A:422:GLN:HA	2.18	0.43
1:B:0[B]:MSE:HE3	1:B:28:ASP:H	1.82	0.43
1:C:364:PRO:HA	1:C:417:LYS:O	2.18	0.43
1:B:369:VAL:O	1:B:422:GLN:HA	2.18	0.43
1:B:434:GLU:OE1	7:B:601:HOH:O	2.22	0.43
1:A:183[A]:ARG:HD2	1:A:183[A]:ARG:C	2.39	0.43
1:A:434:GLU:HA	3:A:505:EDO:H22	1.99	0.42
1:C:182:PHE:O	1:C:184:ASP:OD1	2.37	0.42
1:B:45:ARG:HE	3:C:505:EDO:C2	2.32	0.42
1:B:442:ARG:HB2	3:B:505:EDO:C1	2.49	0.42
1:C:183:ARG:HG3	1:C:191:TYR:CE1	2.54	0.42
1:B:50:ASN:OD1	1:B:50:ASN:N	2.52	0.42
1:B:51:THR:CG2	1:C:427:HIS:H	2.33	0.42
1:C:263:TYR:CD2	1:C:263:TYR:C	2.91	0.42
1:B:430:ALA:HB3	1:B:431:PRO:HD3	2.02	0.42
1:A:263:TYR:CD2	1:A:263:TYR:C	2.91	0.42
1:B:430:ALA:N	1:B:431:PRO:CD	2.83	0.41
1:B:72:PRO:HA	1:B:73:PRO:HD3	1.94	0.41
1:A:324:LEU:O	1:A:330:TYR:HA	2.20	0.41
1:A:444:TRP:O	4:A:509:GOL:H2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLN:HA	1:C:195:GLN:OE1	2.21	0.41
1:B:0[A]:MSE:HG3	1:B:29:GLN:H	1.86	0.41
1:C:430:ALA:HB3	1:C:431:PRO:HD3	2.03	0.41
1:C:133:ILE:HD12	1:C:133:ILE:C	2.41	0.41
4:B:518:GOL:O2	7:B:602:HOH:O	2.22	0.41
1:A:106:GLY:HA3	1:A:247:TRP:HA	2.02	0.40
1:A:131:SER:CB	1:A:161:LYS:HB2	2.51	0.40
1:B:298:ALA:O	1:B:364:PRO:HD2	2.21	0.40
1:A:295:ASN:HA	1:A:363:ARG:CZ	2.51	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:OD1	1:C:121:SER:OG[5_565]	2.09	0.11

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	424/440 (96%)	415 (98%)	9 (2%)	0	100	100
1	B	424/440 (96%)	414 (98%)	9 (2%)	1 (0%)	47	45
1	C	421/440 (96%)	410 (97%)	10 (2%)	1 (0%)	47	45
All	All	1269/1320 (96%)	1239 (98%)	28 (2%)	2 (0%)	47	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	ARG
1	B	131	SER

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	329/335 (98%)	322 (98%)	7 (2%)	53	54
1	B	330/335 (98%)	322 (98%)	8 (2%)	49	49
1	C	327/335 (98%)	321 (98%)	6 (2%)	59	60
All	All	986/1005 (98%)	965 (98%)	21 (2%)	53	54

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	66	THR
1	A	181	ARG
1	A	183[A]	ARG
1	A	183[B]	ARG
1	A	247	TRP
1	A	346	VAL
1	B	28	ASP
1	B	50	ASN
1	B	118	LYS
1	B	178	ILE
1	B	181	ARG
1	B	193	GLN
1	B	247	TRP
1	B	428	THR
1	C	52	ASP
1	C	178	ILE
1	C	181	ARG
1	C	190	ARG
1	C	224	SER
1	C	247	TRP

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

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 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
3	EDO	B	504	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	B	507	-	3,3,3	0.50	0	2,2,2	0.40	0
3	EDO	C	507	-	3,3,3	0.40	0	2,2,2	0.52	0
4	GOL	C	509	-	5,5,5	1.04	0	5,5,5	0.90	0
4	GOL	A	510	-	5,5,5	1.19	1 (20%)	5,5,5	0.96	0
3	EDO	B	509	-	3,3,3	0.47	0	2,2,2	0.09	0
4	GOL	A	511	-	5,5,5	0.99	0	5,5,5	1.13	0
3	EDO	A	507	-	3,3,3	0.73	0	2,2,2	0.62	0
3	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.38	0
4	GOL	B	515	-	5,5,5	0.92	0	5,5,5	1.02	0
4	GOL	B	514	-	5,5,5	0.57	0	5,5,5	0.80	0
3	EDO	A	508	-	3,3,3	0.54	0	2,2,2	0.25	0
4	GOL	B	517	-	5,5,5	1.14	0	5,5,5	0.89	0
4	GOL	B	513	-	5,5,5	1.48	1 (20%)	5,5,5	0.57	0
3	EDO	A	506	-	3,3,3	0.57	0	2,2,2	0.10	0
3	EDO	B	503	-	3,3,3	0.48	0	2,2,2	0.39	0
2	1PE	A	501	-	15,15,15	0.62	0	14,14,14	0.94	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	C	505	-	3,3,3	0.39	0	2,2,2	0.43	0
3	EDO	A	504	-	3,3,3	0.71	0	2,2,2	0.19	0
4	GOL	B	518	-	5,5,5	2.30	3 (60%)	5,5,5	0.51	0
3	EDO	C	508	-	3,3,3	0.46	0	2,2,2	0.31	0
4	GOL	A	509	-	5,5,5	1.55	2 (40%)	5,5,5	0.86	0
6	PEG	C	502	-	6,6,6	0.51	0	5,5,5	0.60	0
4	GOL	B	516	-	5,5,5	1.15	0	5,5,5	1.01	0
3	EDO	C	506	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	C	504	-	3,3,3	0.49	0	2,2,2	0.18	0
4	GOL	B	510	-	5,5,5	0.62	0	5,5,5	1.28	1 (20%)
3	EDO	A	503	-	3,3,3	0.51	0	2,2,2	0.48	0
4	GOL	B	512	-	5,5,5	0.77	0	5,5,5	1.26	1 (20%)
3	EDO	A	505	-	3,3,3	0.99	0	2,2,2	0.81	0
3	EDO	B	505	-	3,3,3	0.66	0	2,2,2	0.27	0
3	EDO	C	503	-	3,3,3	0.54	0	2,2,2	0.48	0
4	GOL	B	511	-	5,5,5	0.87	0	5,5,5	1.14	0
3	EDO	B	508	-	3,3,3	0.40	0	2,2,2	0.38	0
2	1PE	B	502	-	15,15,15	0.53	0	14,14,14	0.45	0
3	EDO	B	506	-	3,3,3	0.49	0	2,2,2	0.47	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	EDO	B	504	-	-	1/1/1/1	-
3	EDO	B	507	-	-	1/1/1/1	-
3	EDO	C	507	-	-	0/1/1/1	-
4	GOL	C	509	-	-	2/4/4/4	-
4	GOL	A	510	-	-	2/4/4/4	-
3	EDO	B	509	-	-	1/1/1/1	-
4	GOL	A	511	-	-	1/4/4/4	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
4	GOL	B	515	-	-	2/4/4/4	-
4	GOL	B	514	-	-	2/4/4/4	-
3	EDO	A	508	-	-	0/1/1/1	-
4	GOL	B	517	-	-	0/4/4/4	-
4	GOL	B	513	-	-	4/4/4/4	-
3	EDO	A	506	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	503	-	-	1/1/1/1	-
2	1PE	A	501	-	-	10/13/13/13	-
3	EDO	C	505	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
4	GOL	B	518	-	-	0/4/4/4	-
3	EDO	C	508	-	-	1/1/1/1	-
4	GOL	A	509	-	-	0/4/4/4	-
6	PEG	C	502	-	-	3/4/4/4	-
4	GOL	B	516	-	-	3/4/4/4	-
3	EDO	C	506	-	-	1/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
4	GOL	B	510	-	-	2/4/4/4	-
3	EDO	A	503	-	-	0/1/1/1	-
4	GOL	B	512	-	-	0/4/4/4	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
4	GOL	B	511	-	-	2/4/4/4	-
3	EDO	B	508	-	-	1/1/1/1	-
2	1PE	B	502	-	-	7/13/13/13	-
3	EDO	B	506	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	518	GOL	O2-C2	-3.75	1.32	1.43
4	A	509	GOL	C3-C2	2.65	1.62	1.51
4	B	518	GOL	C1-C2	2.45	1.61	1.51
4	B	518	GOL	C3-C2	2.34	1.61	1.51
4	A	510	GOL	C1-C2	2.19	1.60	1.51
4	A	509	GOL	C1-C2	2.04	1.60	1.51
4	B	513	GOL	O2-C2	-2.04	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	1PE	OH4-C24-C14	2.35	120.99	110.39
4	B	510	GOL	C3-C2-C1	-2.27	102.88	111.70
4	B	512	GOL	C3-C2-C1	-2.21	103.13	111.70

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	511	GOL	O1-C1-C2-O2
4	B	511	GOL	O1-C1-C2-C3
4	B	514	GOL	O1-C1-C2-C3
4	B	516	GOL	C1-C2-C3-O3
4	B	516	GOL	O2-C2-C3-O3
4	C	509	GOL	O1-C1-C2-C3
2	B	502	1PE	OH4-C13-C23-OH3
2	A	501	1PE	OH4-C13-C23-OH3
2	A	501	1PE	OH2-C12-C22-OH3
4	A	510	GOL	O1-C1-C2-C3
4	B	510	GOL	C1-C2-C3-O3
4	B	513	GOL	O1-C1-C2-C3
4	B	513	GOL	C1-C2-C3-O3
4	B	515	GOL	O1-C1-C2-C3
4	B	514	GOL	O1-C1-C2-O2
2	B	502	1PE	OH2-C12-C22-OH3
3	A	506	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
3	B	508	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	C	505	EDO	O1-C1-C2-O2
4	B	515	GOL	O1-C1-C2-O2
2	A	501	1PE	OH6-C15-C25-OH5
2	A	501	1PE	OH7-C16-C26-OH6
6	C	502	PEG	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
4	B	513	GOL	O2-C2-C3-O3
4	B	516	GOL	O1-C1-C2-O2
4	C	509	GOL	O1-C1-C2-O2
3	C	506	EDO	O1-C1-C2-O2
2	A	501	1PE	C23-C13-OH4-C24
2	A	501	1PE	C25-C15-OH6-C26
4	A	510	GOL	O1-C1-C2-O2
2	A	501	1PE	C16-C26-OH6-C15
3	A	505	EDO	O1-C1-C2-O2
3	B	505	EDO	O1-C1-C2-O2
6	C	502	PEG	C1-C2-O2-C3
2	A	501	1PE	OH5-C14-C24-OH4
3	B	504	EDO	O1-C1-C2-O2
3	B	506	EDO	O1-C1-C2-O2
3	B	507	EDO	O1-C1-C2-O2
2	B	502	1PE	OH5-C14-C24-OH4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	513	GOL	O1-C1-C2-O2
6	C	502	PEG	C4-C3-O2-C2
3	C	508	EDO	O1-C1-C2-O2
2	A	501	1PE	C12-C22-OH3-C23
4	B	510	GOL	O2-C2-C3-O3
2	B	502	1PE	C23-C13-OH4-C24
2	B	502	1PE	C14-C24-OH4-C13
2	B	502	1PE	OH6-C15-C25-OH5
4	A	511	GOL	C1-C2-C3-O3
2	A	501	1PE	C13-C23-OH3-C22
3	B	509	EDO	O1-C1-C2-O2
2	B	502	1PE	C15-C25-OH5-C14

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	514	GOL	3	0
2	A	501	1PE	4	0
3	C	505	EDO	1	0
4	B	518	GOL	6	0
4	A	509	GOL	1	0
6	C	502	PEG	1	0
3	C	506	EDO	1	0
3	A	505	EDO	1	0
3	B	505	EDO	1	0
2	B	502	1PE	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	416/440 (94%)	-0.27	6 (1%)	75	80	27, 41, 70, 119	0
1	B	414/440 (94%)	-0.24	7 (1%)	70	75	26, 36, 71, 142	0
1	C	414/440 (94%)	-0.04	17 (4%)	37	45	31, 45, 86, 118	0
All	All	1244/1320 (94%)	-0.18	30 (2%)	59	65	26, 41, 75, 142	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	TRP	6.8
1	B	130	THR	6.0
1	C	182	PHE	5.3
1	A	-1	HIS	4.0
1	C	27	ALA	4.0
1	C	183	ARG	3.9
1	C	184	ASP	3.9
1	C	188	ALA	3.9
1	B	127	ASP	3.8
1	B	129	GLY	3.6
1	C	185	ARG	3.5
1	B	445	ALA	3.4
1	A	181	ARG	3.1
1	B	27[A]	ALA	3.1
1	A	182	PHE	3.0
1	C	176	PRO	3.0
1	B	163	ASN	3.0
1	C	191	TYR	2.9
1	A	-2	GLY	2.8
1	C	180	GLU	2.8
1	C	181	ARG	2.7
1	C	49	GLY	2.6
1	C	86	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	445	ALA	2.5
1	C	199	ALA	2.3
1	B	181	ARG	2.3
1	A	179	TRP	2.3
1	C	189	GLU	2.2
1	A	183[A]	ARG	2.1
1	C	414	LEU	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
3	EDO	C	505	4/4	0.35	0.21	97,117,141,141	0
4	GOL	A	509	6/6	0.60	0.22	57,70,81,85	0
3	EDO	B	505	4/4	0.64	0.40	65,78,98,98	0
4	GOL	B	515	6/6	0.68	0.47	65,80,114,114	0
3	EDO	B	504	4/4	0.71	0.28	92,110,126,126	0
3	EDO	A	505	4/4	0.72	0.17	52,63,71,71	0
4	GOL	A	511	6/6	0.73	0.27	89,169,211,211	0
4	GOL	B	516	6/6	0.77	0.43	62,75,90,104	0
3	EDO	C	507	4/4	0.78	0.56	86,120,144,144	0
3	EDO	A	507	4/4	0.79	0.18	42,73,81,87	0
4	GOL	B	517	6/6	0.79	0.43	67,87,110,110	0
3	EDO	B	506	4/4	0.81	0.27	72,87,95,95	0
2	1PE	A	501	16/16	0.83	0.25	59,78,87,100	0
6	PEG	C	502	7/7	0.84	0.25	47,72,92,92	0
4	GOL	C	509	6/6	0.85	0.49	83,135,185,185	0
3	EDO	A	506	4/4	0.85	0.16	60,73,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	504	4/4	0.87	0.52	76,92,95,110	0
2	1PE	B	502	16/16	0.87	0.29	59,82,105,125	0
4	GOL	B	513	6/6	0.87	0.17	63,76,84,92	0
3	EDO	A	504	4/4	0.87	0.17	63,75,83,83	0
3	EDO	B	509	4/4	0.88	0.39	53,64,82,82	0
4	GOL	B	510	6/6	0.88	0.22	50,68,100,100	0
3	EDO	B	507	4/4	0.89	0.24	60,73,79,81	0
4	GOL	B	511	6/6	0.89	0.22	55,68,83,90	0
3	EDO	C	503	4/4	0.90	0.28	50,62,64,75	0
4	GOL	B	512	6/6	0.90	0.27	58,70,75,81	0
3	EDO	C	508	4/4	0.91	0.34	58,79,96,102	0
4	GOL	A	510	6/6	0.91	0.10	56,68,82,82	0
3	EDO	B	508	4/4	0.93	0.24	56,67,77,77	0
4	GOL	B	518	6/6	0.93	0.28	35,50,62,62	0
3	EDO	A	502	4/4	0.94	0.38	48,61,74,74	0
3	EDO	A	508	4/4	0.94	0.11	53,65,79,79	0
5	BR	C	501	1/1	0.94	0.20	121,121,121,121	0
4	GOL	B	514	6/6	0.94	0.14	54,65,78,93	0
3	EDO	C	506	4/4	0.95	0.44	52,65,78,91	0
3	EDO	A	503	4/4	0.95	0.36	56,68,68,74	0
3	EDO	B	503	4/4	0.96	0.38	46,59,74,74	0
5	BR	B	501	1/1	0.99	0.04	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.