Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 11:59 AM JST

PDB ID	:	7CI0
Title	:	Microbial Hormone-sensitive lipase E53 mutant S162A
Authors	:	Yang, X.; Li, Z.; Xu, X.; Li, J.
Deposited on	:	2020-07-06
Resolution	:	1.70 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:

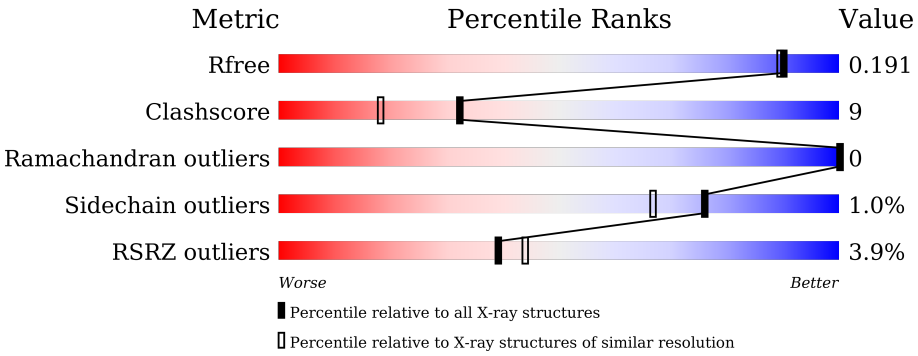
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	314	3% 90% 8% ·
1	B	314	3% 89% 9% ··
1	C	314	3% 91% 7% ·
1	D	314	7% 90% 8% ·

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PGE	C	411	-	-	X	-
3	6NA	A	404	-	-	X	-
5	EDO	B	2703	-	-	X	-
5	EDO	B	2711	-	-	-	X
5	EDO	D	804	-	-	X	-
6	DMS	A	407	-	-	X	-
6	DMS	B	2707	-	-	X	-
6	DMS	C	406	-	-	X	-
6	DMS	C	415	-	-	X	-
6	DMS	D	805	-	-	X	-
6	DMS	D	806	-	-	X	-
6	DMS	D	810	-	-	X	-
7	DIO	A	409	-	-	-	X
7	DIO	C	409	-	-	-	X
8	GOL	A	415	-	-	X	-
8	GOL	B	2713	-	X	X	-
8	GOL	C	407	-	X	-	-
8	GOL	C	412	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 20348 atoms, of which 9467 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.

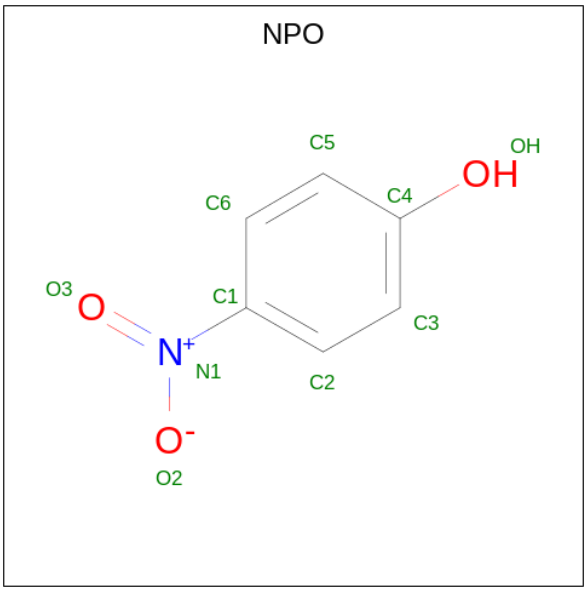
- Molecule 1 is a protein called Lipase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	H	N	O	S	0	0	0
			4533	1443	2257	390	431	12			
1	B	309	Total	C	H	N	O	S	0	0	0
			4553	1447	2271	391	432	12			
1	C	309	Total	C	H	N	O	S	0	0	0
			4546	1446	2266	391	431	12			
1	D	309	Total	C	H	N	O	S	0	0	0
			4564	1451	2274	391	436	12			

There are 4 discrepancies between the modelled and reference sequences:

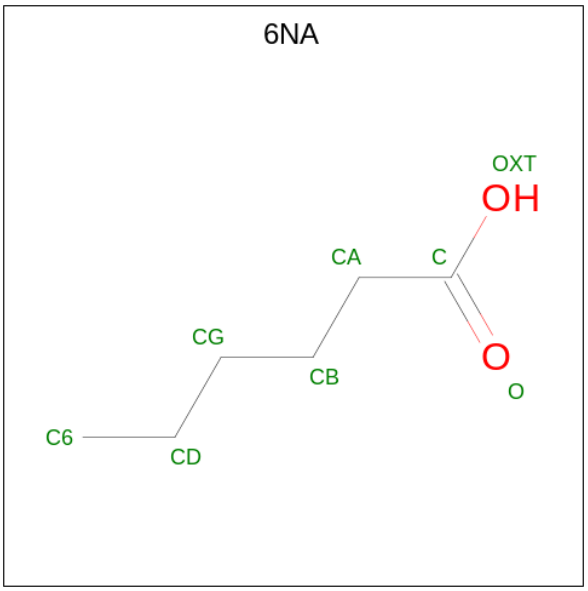
Chain	Residue	Modelled	Actual	Comment	Reference
A	162	ALA	SER	engineered mutation	UNP A0A074MDU6
B	162	ALA	SER	engineered mutation	UNP A0A074MDU6
C	162	ALA	SER	engineered mutation	UNP A0A074MDU6
D	162	ALA	SER	engineered mutation	UNP A0A074MDU6

- Molecule 2 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



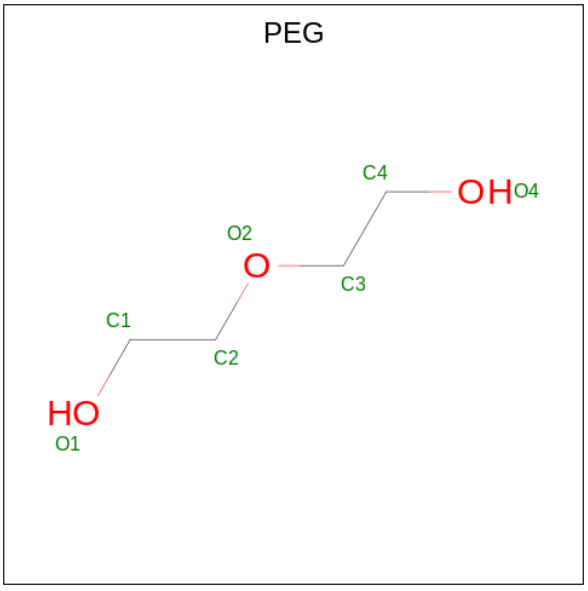
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	A	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	A	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	B	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	B	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	C	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	C	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	C	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	D	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	D	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	D	1	Total	C	H	N	O	0	0
			15	6	5	1	3		

- Molecule 3 is HEXANOIC ACID (three-letter code: 6NA) (formula: $C_6H_{12}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			19	6	11	2		
3	A	1	Total	C	H	O	0	0
			19	6	11	2		
3	B	1	Total	C	H	O	0	0
			19	6	11	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



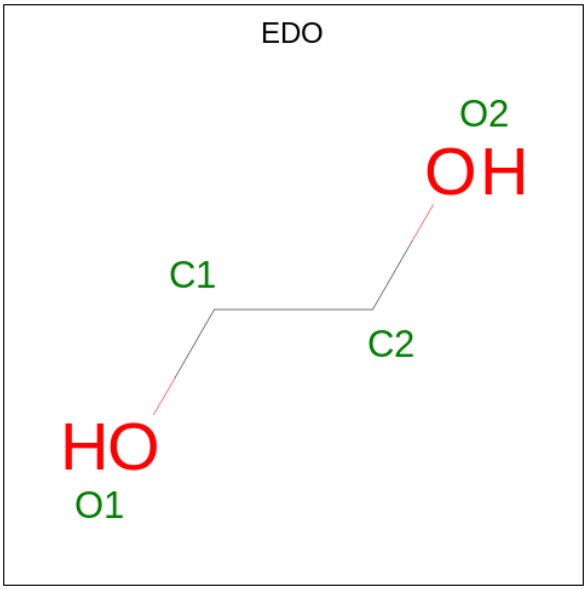
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

Continued on next page...

Continued from previous page...

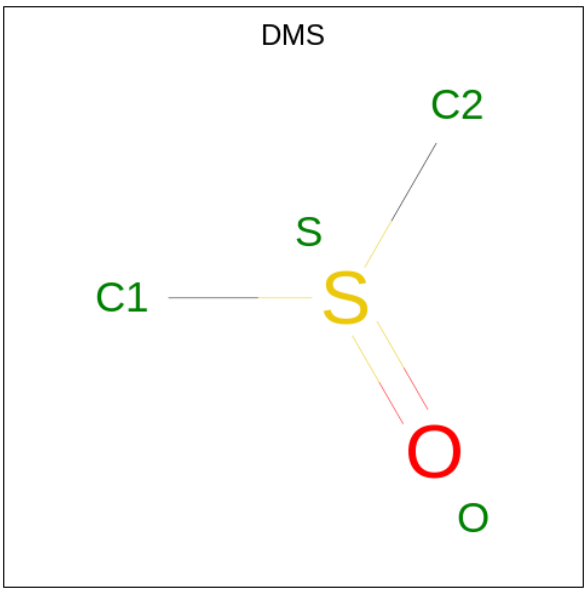
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



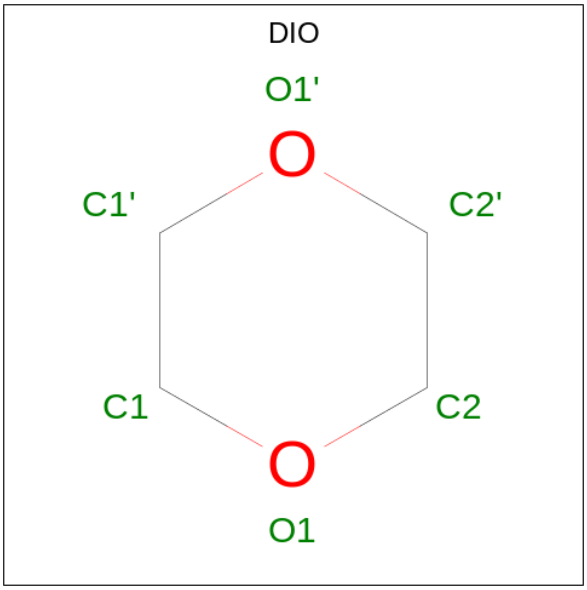
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			8	2	4	1	1		
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

Continued on next page...

Continued from previous page...

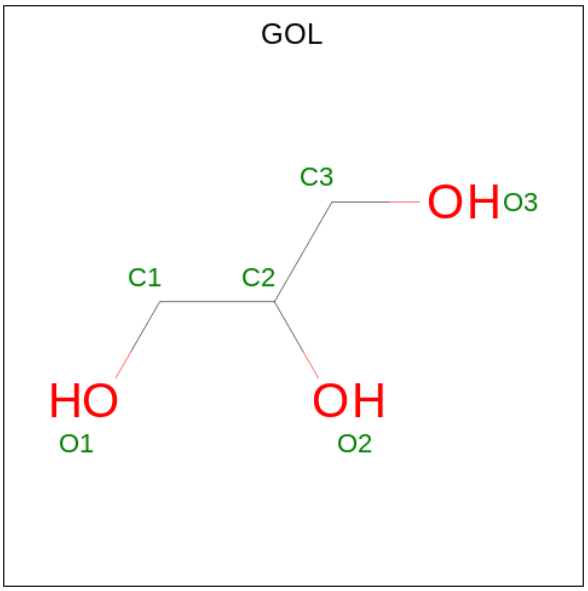
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



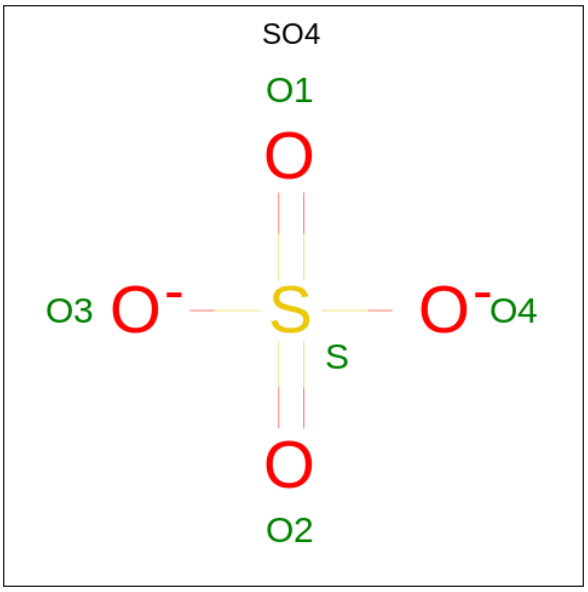
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	4	8	2		
7	A	1	Total	C	H	O	0	0
			14	4	8	2		
7	A	1	Total	C	H	O	0	0
			14	4	8	2		
7	B	1	Total	C	H	O	0	0
			14	4	8	2		
7	C	1	Total	C	H	O	0	0
			14	4	8	2		
7	C	1	Total	C	H	O	0	0
			14	4	8	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



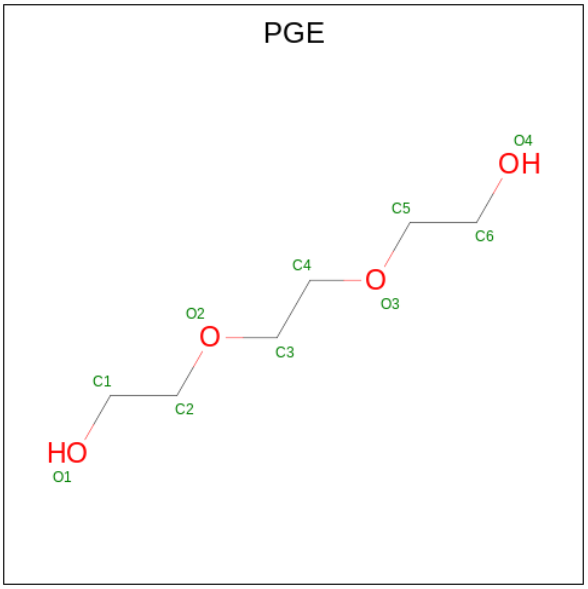
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 12 3 6 3	0	0
8	A	1	Total C H O 13 3 7 3	0	0
8	A	1	Total C H O 14 3 8 3	0	0
8	A	1	Total C H O 14 3 8 3	0	0
8	B	1	Total C H O 12 3 6 3	0	0
8	C	1	Total C H O 13 3 7 3	0	0
8	C	1	Total C H O 14 3 8 3	0	0
8	C	1	Total C H O 12 3 6 3	0	0
8	D	1	Total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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

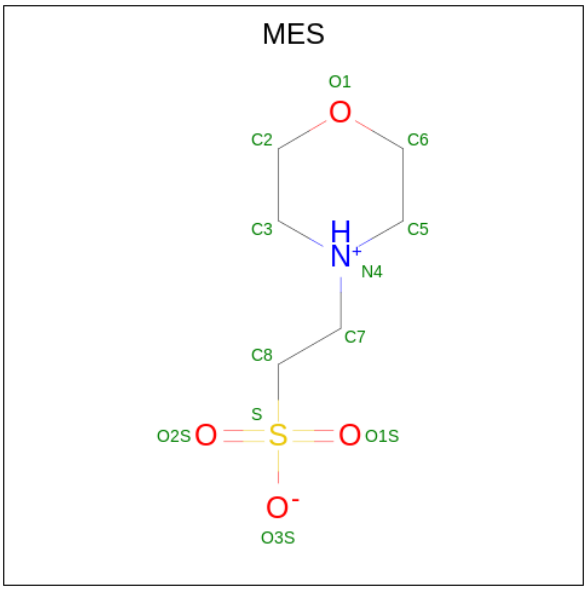


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C H O 23 6 13 4	0	0
10	C	1	Total C H O 22 6 12 4	0	0

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Na 1 1	0	0

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	1	Total C H N O S 24 6 12 1 4 1	0	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	383	Total O 383 383	0	0
13	B	307	Total O 307 307	0	0
13	C	366	Total O 366 366	0	0

Continued on next page...

Continued from previous page...

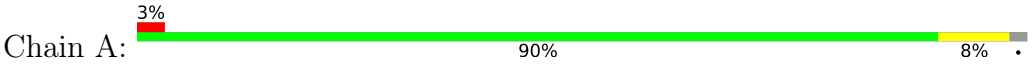
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	305	Total O 305 305	0	0

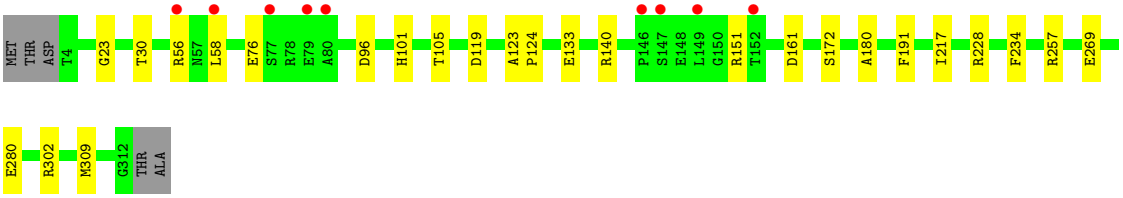
3 Residue-property plots (i)

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: Lipase

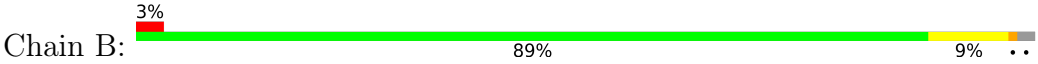
Chain A:

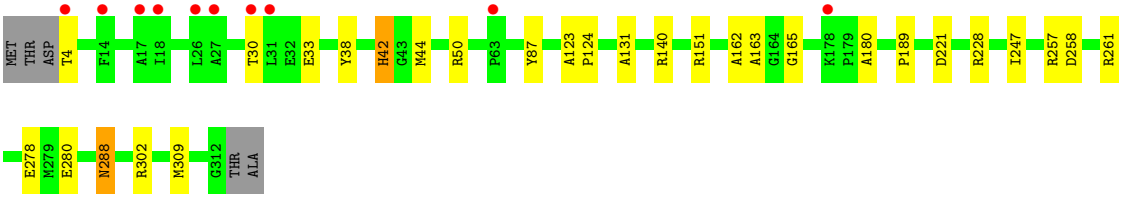




• Molecule 1: Lipase

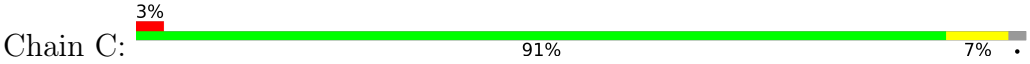
Chain B:

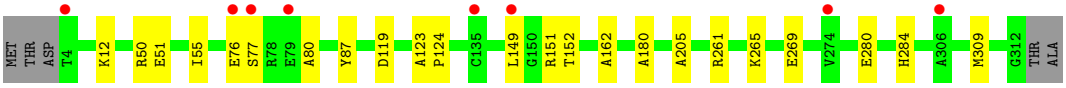




• Molecule 1: Lipase

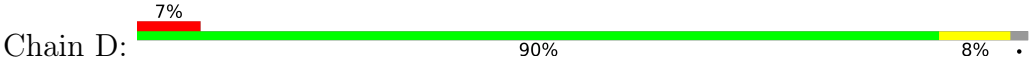
Chain C:

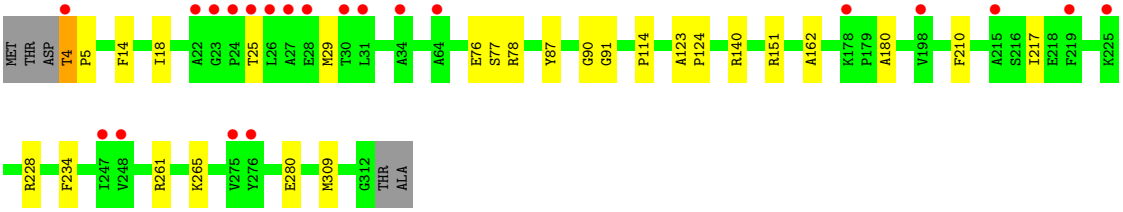




• Molecule 1: Lipase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	70.40Å 129.77Å 220.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 1.70 48.66 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.35-1.70) 99.8 (48.66-1.70)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.14_3247, PHENIX 1.14_3247	Depositor
R, R_{free}	0.171 , 0.191 0.171 , 0.191	Depositor DCC
R_{free} test set	11063 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20348	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.62% 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: SO4, DMS, EDO, NA, MES, PGE, GOL, PEG, 6NA, DIO, NPO

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	0.47	0/2327	0.59	0/3178
1	B	0.55	2/2333 (0.1%)	0.58	0/3185
1	C	0.45	0/2331	0.61	1/3182 (0.0%)
1	D	0.51	0/2341	0.58	1/3195 (0.0%)
All	All	0.49	2/9332 (0.0%)	0.59	2/12740 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	GLU	CD-OE2	-5.86	1.19	1.25
1	B	280	GLU	CD-OE1	-5.86	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	210	PHE	C-N-CA	6.09	136.94	121.70
1	C	50	ARG	NE-CZ-NH1	-5.55	117.53	120.30

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	2276	2257	2250	38	0
1	B	2282	2271	2266	39	0
1	C	2280	2266	2261	35	0
1	D	2290	2274	2273	48	0
2	A	30	15	13	1	0
2	B	20	10	10	2	0
2	C	30	15	15	0	0
2	D	30	15	14	1	0
3	A	16	22	22	11	0
3	B	8	11	11	5	0
4	A	7	10	10	0	0
4	D	7	10	10	0	0
5	A	8	12	12	1	0
5	B	20	30	30	9	0
5	C	8	12	12	2	0
5	D	4	6	6	7	0
6	A	8	12	12	6	0
6	B	12	18	18	8	0
6	C	16	22	24	15	0
6	D	20	30	30	22	0
7	A	18	24	24	0	0
7	B	6	8	8	2	0
7	C	12	16	16	2	0
8	A	24	29	32	5	0
8	B	6	6	7	6	0
8	C	18	21	23	10	0
8	D	6	8	8	0	0
9	A	5	0	0	0	0
9	B	10	0	0	0	0
9	C	5	0	0	0	0
9	D	5	0	0	0	0
10	B	10	13	14	0	0
10	C	10	12	14	6	0
11	B	1	0	0	0	0
12	D	12	12	12	0	0
13	A	383	0	0	7	1
13	B	307	0	0	8	1
13	C	366	0	0	5	1
13	D	305	0	0	6	1
All	All	10881	9467	9457	167	2

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 (167) 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:B:162:ALA:HB1	5:B:2703:EDO:H11	1.44	1.00
1:C:76:GLU:H	6:C:406:DMS:H22	1.23	0.99
1:C:151:ARG:HH22	8:C:410:GOL:H2	1.26	0.98
10:C:411:PGE:H2	1:D:265:LYS:HZ1	1.36	0.91
1:B:30:THR:HG23	1:B:33:GLU:H	1.40	0.86
2:B:2702:NPO:O2	5:B:2703:EDO:H12	1.78	0.83
1:B:50:ARG:NH1	13:B:2802:HOH:O	2.13	0.82
1:C:51:GLU:H	6:C:408:DMS:H23	1.44	0.82
1:D:261:ARG:HH12	6:D:806:DMS:H13	1.46	0.81
1:B:257:ARG:HH12	3:B:2705:6NA:HGC1	1.47	0.80
6:D:806:DMS:O	13:D:901:HOH:O	1.99	0.79
7:B:2714:DIO:O1	13:B:2801:HOH:O	2.01	0.79
1:D:90:GLY:H	5:D:804:EDO:H11	1.49	0.78
1:A:140:ARG:HH11	6:A:407:DMS:H12	1.48	0.78
1:C:261:ARG:HH22	8:C:412:GOL:H12	1.47	0.78
1:D:90:GLY:H	5:D:804:EDO:C1	1.99	0.75
1:D:180:ALA:HA	6:D:805:DMS:H21	1.69	0.75
1:C:51:GLU:H	6:C:408:DMS:C2	2.00	0.74
1:A:180:ALA:HA	6:A:407:DMS:H11	1.69	0.74
1:D:140:ARG:HD3	6:D:805:DMS:H22	1.70	0.74
1:D:140:ARG:HH11	6:D:805:DMS:C2	2.02	0.73
8:C:412:GOL:H32	13:D:972:HOH:O	1.87	0.73
1:B:42:HIS:HB3	13:B:3002:HOH:O	1.88	0.72
1:A:257:ARG:HH12	3:A:404:6NA:HBC1	1.55	0.71
1:D:140:ARG:HH11	6:D:805:DMS:H21	1.57	0.70
1:B:258:ASP:CG	8:B:2713:GOL:H12	2.12	0.70
1:C:76:GLU:N	6:C:406:DMS:H22	2.03	0.70
1:D:180:ALA:HA	6:D:805:DMS:C2	2.21	0.69
1:C:265:LYS:HE3	10:C:411:PGE:H6	1.75	0.69
3:A:412:6NA:OXT	3:A:412:6NA:HGC1	1.91	0.68
1:A:133:GLU:OE2	13:A:501:HOH:O	2.11	0.68
1:D:261:ARG:HH22	6:D:806:DMS:C2	2.07	0.67
1:B:162:ALA:HB1	5:B:2703:EDO:C1	2.22	0.67
1:C:12:LYS:NZ	13:C:503:HOH:O	2.26	0.67
1:D:261:ARG:HH12	6:D:806:DMS:C1	2.08	0.67
6:C:415:DMS:C2	1:D:280:GLU:HG3	2.24	0.66
10:C:411:PGE:H2	1:D:265:LYS:NZ	2.10	0.66
6:C:406:DMS:O	13:C:501:HOH:O	2.14	0.66
1:D:90:GLY:N	5:D:804:EDO:H11	2.09	0.66
1:D:280:GLU:OE1	13:D:902:HOH:O	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:HH11	6:B:2707:DMS:C2	2.09	0.66
1:A:269:GLU:OE2	8:B:2713:GOL:H31	1.95	0.66
1:C:280:GLU:OE1	13:C:502:HOH:O	2.14	0.66
1:A:257:ARG:HH22	3:A:404:6NA:HBC1	1.61	0.65
1:C:261:ARG:HH22	8:C:412:GOL:C1	2.09	0.65
1:B:140:ARG:HD3	6:B:2707:DMS:H22	1.79	0.64
3:B:2705:6NA:HGC2	13:B:3082:HOH:O	1.98	0.64
1:B:180:ALA:HA	6:B:2707:DMS:C2	2.28	0.64
1:A:140:ARG:HH11	6:A:407:DMS:C1	2.09	0.64
1:A:280:GLU:OE2	13:A:502:HOH:O	2.16	0.63
10:C:411:PGE:C2	1:D:265:LYS:HZ1	2.10	0.63
1:A:140:ARG:NH1	6:A:407:DMS:H12	2.14	0.62
1:A:76:GLU:O	8:A:415:GOL:O2	2.17	0.62
1:A:257:ARG:HH12	3:A:404:6NA:CB	2.12	0.62
1:C:269:GLU:OE1	1:D:265:LYS:NZ	2.30	0.62
1:C:151:ARG:NH2	8:C:410:GOL:H2	2.09	0.61
1:C:309:MET:CE	1:D:309:MET:HE3	2.31	0.61
1:A:180:ALA:HA	6:A:407:DMS:C1	2.30	0.60
3:A:412:6NA:H6C2	13:A:819:HOH:O	2.01	0.60
1:D:261:ARG:HH22	6:D:806:DMS:H22	1.66	0.60
1:A:56:ARG:NH1	8:A:415:GOL:H11	2.17	0.59
1:C:119:ASP:OD1	8:C:407:GOL:H11	2.03	0.59
1:D:76:GLU:H	6:D:810:DMS:C1	2.16	0.59
1:A:56:ARG:HH11	8:A:415:GOL:H11	1.68	0.58
5:B:2703:EDO:O2	13:B:2803:HOH:O	2.17	0.58
1:A:30:THR:HA	8:A:416:GOL:H31	1.86	0.57
1:A:56:ARG:HH11	8:A:415:GOL:C1	2.17	0.57
1:C:77:SER:H	6:C:406:DMS:H11	1.69	0.57
1:B:162:ALA:CB	5:B:2703:EDO:H11	2.28	0.57
1:B:42:HIS:NE2	1:B:288:ASN:OD1	2.38	0.57
6:C:415:DMS:H22	1:D:280:GLU:HG3	1.85	0.57
1:D:162:ALA:HB3	5:D:804:EDO:H12	1.87	0.57
1:D:76:GLU:H	6:D:810:DMS:H13	1.69	0.56
6:C:415:DMS:H21	1:D:280:GLU:HG3	1.87	0.56
1:D:140:ARG:CD	6:D:805:DMS:H22	2.35	0.56
1:C:309:MET:HE3	1:D:309:MET:HE3	1.88	0.56
1:A:23:GLY:HA2	13:A:677:HOH:O	2.06	0.55
1:B:140:ARG:HH11	6:B:2707:DMS:H22	1.71	0.55
1:D:123:ALA:HB1	1:D:124:PRO:HA	1.88	0.55
1:A:257:ARG:NH1	3:A:404:6NA:HBC1	2.22	0.55
6:C:408:DMS:H11	13:C:562:HOH:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ALA:O	1:B:165:GLY:N	2.39	0.55
1:B:180:ALA:HA	6:B:2707:DMS:H21	1.88	0.54
1:A:269:GLU:CD	8:B:2713:GOL:H31	2.27	0.54
1:C:261:ARG:NH2	8:C:412:GOL:H12	2.20	0.54
1:C:309:MET:HE3	1:D:309:MET:CE	2.39	0.53
1:C:76:GLU:H	6:C:406:DMS:C2	2.09	0.52
1:C:265:LYS:CE	10:C:411:PGE:H6	2.39	0.52
1:B:42:HIS:CE1	1:B:288:ASN:OD1	2.63	0.52
1:D:261:ARG:HH22	6:D:806:DMS:H23	1.75	0.52
1:A:269:GLU:OE1	8:B:2713:GOL:H31	2.11	0.51
8:C:412:GOL:H11	13:D:978:HOH:O	2.09	0.51
1:B:140:ARG:HH11	6:B:2707:DMS:H21	1.73	0.51
1:C:261:ARG:HH12	8:C:412:GOL:H12	1.76	0.51
1:B:180:ALA:HA	6:B:2707:DMS:H23	1.91	0.51
1:B:221:ASP:CG	1:B:228:ARG:HH22	2.14	0.51
1:C:55:ILE:HD12	5:C:404:EDO:H22	1.93	0.51
1:C:309:MET:CE	1:D:309:MET:CE	2.89	0.51
1:A:257:ARG:NH2	3:A:404:6NA:HBC1	2.26	0.50
1:D:4:THR:HG23	1:D:5:PRO:CD	2.41	0.50
1:D:217:ILE:HG23	2:D:801:NPO:C4	2.42	0.50
1:B:257:ARG:NH1	3:B:2705:6NA:HGC1	2.22	0.50
1:C:76:GLU:HB2	6:C:406:DMS:H13	1.94	0.49
1:A:269:GLU:OE1	8:B:2713:GOL:C3	2.60	0.49
1:B:302:ARG:NE	5:B:2708:EDO:H21	2.27	0.49
1:D:140:ARG:CG	6:D:805:DMS:H22	2.41	0.49
1:D:140:ARG:NH1	6:D:805:DMS:H21	2.26	0.49
1:C:152:THR:OG1	7:C:409:DIO:H1'2	2.12	0.49
1:D:77:SER:H	6:D:810:DMS:C2	2.25	0.49
1:B:30:THR:HG22	1:B:33:GLU:CD	2.33	0.49
1:C:149:LEU:HD23	13:C:533:HOH:O	2.13	0.49
1:B:30:THR:HG22	1:B:33:GLU:OE1	2.13	0.48
1:A:309:MET:CE	1:B:309:MET:HE3	2.43	0.48
1:A:309:MET:CE	1:B:309:MET:CE	2.92	0.48
1:C:80:ALA:HB2	7:C:409:DIO:H2'1	1.94	0.48
1:B:30:THR:HG21	13:B:3021:HOH:O	2.13	0.48
1:A:309:MET:HE3	1:B:309:MET:CE	2.44	0.47
1:D:140:ARG:HH11	6:D:805:DMS:H22	1.77	0.47
1:C:205:ALA:CB	5:C:413:EDO:H22	2.43	0.47
1:C:151:ARG:HH22	8:C:410:GOL:C2	2.13	0.47
1:B:123:ALA:HB1	1:B:124:PRO:HA	1.96	0.47
1:C:309:MET:HE2	1:D:309:MET:HE3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HG2	5:A:406:EDO:H11	1.98	0.46
1:D:90:GLY:CA	5:D:804:EDO:H11	2.46	0.46
1:A:96:ASP:HB2	3:A:412:6NA:H6C1	1.98	0.46
1:C:123:ALA:HB1	1:C:124:PRO:HA	1.97	0.46
1:D:4:THR:HG23	1:D:5:PRO:HD3	1.96	0.46
1:D:14:PHE:CE2	1:D:18:ILE:HD11	2.51	0.46
1:D:180:ALA:HA	6:D:805:DMS:H23	1.99	0.45
1:C:77:SER:H	6:C:406:DMS:C1	2.30	0.45
1:B:44:MET:HE3	1:B:44:MET:HB2	1.82	0.45
1:B:140:ARG:CD	6:B:2707:DMS:H22	2.46	0.45
1:A:257:ARG:HH22	3:A:404:6NA:HDC1	1.82	0.45
2:B:2702:NPO:N1	5:B:2703:EDO:H12	2.31	0.44
1:D:91:GLY:H	5:D:804:EDO:C1	2.29	0.44
1:B:261:ARG:HD2	8:B:2713:GOL:H11	1.98	0.44
1:B:131:ALA:HB2	13:B:2860:HOH:O	2.18	0.44
1:A:58:LEU:HD23	1:A:58:LEU:N	2.33	0.43
1:B:189:PRO:HD2	1:B:247:ILE:O	2.19	0.43
1:A:161:ASP:HB2	1:A:191:PHE:CE1	2.54	0.43
1:A:217:ILE:HG23	2:A:401:NPO:C4	2.49	0.43
1:A:119:ASP:OD1	3:A:412:6NA:H6C3	2.18	0.43
1:A:228:ARG:HA	1:A:234:PHE:CE1	2.54	0.43
1:D:25:THR:O	1:D:29:MET:HG3	2.19	0.43
1:C:265:LYS:NZ	10:C:411:PGE:H6	2.34	0.42
1:A:23:GLY:CA	13:A:677:HOH:O	2.66	0.42
1:D:78:ARG:HD2	1:D:114:PRO:HG3	2.00	0.42
1:A:123:ALA:HB1	1:A:124:PRO:HA	2.02	0.42
1:C:180:ALA:HA	6:C:405:DMS:O	2.20	0.42
1:D:140:ARG:HB3	6:D:805:DMS:H22	2.02	0.42
1:B:257:ARG:HH22	3:B:2705:6NA:H6C3	1.84	0.42
1:B:302:ARG:HG2	5:B:2708:EDO:H22	2.02	0.42
1:D:162:ALA:CB	5:D:804:EDO:H12	2.50	0.42
1:A:96:ASP:CB	3:A:412:6NA:H6C1	2.50	0.41
1:B:38:TYR:HE1	7:B:2714:DIO:H21	1.85	0.41
1:D:228:ARG:HA	1:D:234:PHE:CE1	2.55	0.41
1:B:162:ALA:O	1:B:163:ALA:C	2.59	0.41
6:A:407:DMS:H11	13:A:601:HOH:O	2.20	0.41
1:D:77:SER:H	6:D:810:DMS:H21	1.86	0.41
1:B:4:THR:N	13:B:2817:HOH:O	2.53	0.41
1:C:162:ALA:HB2	1:C:284:HIS:CE1	2.55	0.41
1:A:101:HIS:O	1:A:105:THR:HG23	2.21	0.40
1:A:172:SER:HB2	13:A:624:HOH:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2709:EDO:H12	5:B:2711:EDO:H11	2.03	0.40
6:C:415:DMS:H23	13:D:1081:HOH:O	2.22	0.40
6:D:808:DMS:H21	13:D:1087:HOH:O	2.21	0.40
1:B:257:ARG:HH22	3:B:2705:6NA:HGC1	1.87	0.40

All (2) 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)
13:B:2807:HOH:O	13:D:932:HOH:O[3_554]	1.97	0.23
13:A:721:HOH:O	13:C:801:HOH:O[3_544]	2.11	0.09

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	307/314 (98%)	297 (97%)	10 (3%)	0	100	100
1	B	307/314 (98%)	297 (97%)	10 (3%)	0	100	100
1	C	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
1	D	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
All	All	1228/1256 (98%)	1192 (97%)	36 (3%)	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	231/239 (97%)	230 (100%)	1 (0%)	91	87
1	B	233/239 (98%)	229 (98%)	4 (2%)	60	46
1	C	232/239 (97%)	231 (100%)	1 (0%)	91	87
1	D	235/239 (98%)	232 (99%)	3 (1%)	69	56
All	All	931/956 (97%)	922 (99%)	9 (1%)	76	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ARG
1	B	42	HIS
1	B	87	TYR
1	B	151	ARG
1	B	288	ASN
1	C	87	TYR
1	D	4	THR
1	D	87	TYR
1	D	151	ARG

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 64 ligands modelled in this entry, 1 is monoatomic - leaving 63 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	$\#\|Z\| > 2$
8	GOL	D	811	-	5,5,5	0.84	0	5,5,5	1.00	0
9	SO4	D	813	-	4,4,4	0.14	0	6,6,6	0.05	0
5	EDO	B	2708	-	3,3,3	0.49	0	2,2,2	0.30	0
2	NPO	D	812	-	9,10,10	1.67	2 (22%)	11,13,13	2.39	5 (45%)
6	DMS	A	408	-	3,3,3	0.64	0	3,3,3	0.79	0
6	DMS	C	406	-	3,3,3	0.65	0	3,3,3	0.66	0
7	DIO	A	411	-	6,6,6	0.65	0	6,6,6	0.77	0
7	DIO	A	409	-	6,6,6	0.65	0	6,6,6	0.55	0
5	EDO	A	406	-	3,3,3	0.54	0	2,2,2	0.17	0
6	DMS	D	810	-	3,3,3	0.64	0	3,3,3	0.85	0
2	NPO	C	402	-	9,10,10	1.52	2 (22%)	11,13,13	0.82	0
4	PEG	A	405	-	6,6,6	0.46	0	5,5,5	0.19	0
8	GOL	B	2713	-	5,5,5	1.29	1 (20%)	5,5,5	1.31	1 (20%)
8	GOL	C	410	-	5,5,5	0.99	0	5,5,5	0.93	0
8	GOL	C	412	-	5,5,5	0.91	0	5,5,5	1.07	1 (20%)
8	GOL	A	415	-	5,5,5	0.87	0	5,5,5	0.94	0
8	GOL	A	414	-	5,5,5	0.76	0	5,5,5	1.15	0
7	DIO	C	409	-	6,6,6	0.68	0	6,6,6	0.49	0
8	GOL	A	416	-	5,5,5	1.02	0	5,5,5	0.88	0
7	DIO	A	413	-	6,6,6	0.67	0	6,6,6	1.34	1 (16%)
12	MES	D	807	-	12,12,12	2.05	1 (8%)	14,16,16	2.21	5 (35%)
2	NPO	C	401	-	9,10,10	1.47	2 (22%)	11,13,13	0.61	0
5	EDO	D	804	-	3,3,3	0.38	0	2,2,2	0.55	0
6	DMS	C	415	-	3,3,3	0.67	0	3,3,3	0.53	0
3	6NA	B	2705	-	7,7,7	0.76	0	7,7,7	1.28	1 (14%)
5	EDO	C	404	-	3,3,3	0.50	0	2,2,2	0.20	0
5	EDO	A	410	-	3,3,3	0.50	0	2,2,2	0.29	0
3	6NA	A	412	-	7,7,7	1.35	1 (14%)	7,7,7	1.82	2 (28%)
9	SO4	C	416	-	4,4,4	0.13	0	6,6,6	0.10	0
10	PGE	C	411	-	9,9,9	0.50	0	8,8,8	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NPO	B	2702	-	9,10,10	1.47	2 (22%)	11,13,13	0.85	0
5	EDO	B	2712	-	3,3,3	0.46	0	2,2,2	0.20	0
2	NPO	D	802	-	9,10,10	1.58	2 (22%)	11,13,13	0.61	0
6	DMS	D	806	-	3,3,3	0.67	0	3,3,3	0.82	0
6	DMS	D	805	-	3,3,3	0.61	0	3,3,3	0.37	0
7	DIO	C	414	-	6,6,6	0.49	0	6,6,6	0.51	0
8	GOL	C	407	-	5,5,5	1.09	1 (20%)	5,5,5	1.30	1 (20%)
2	NPO	C	403	-	9,10,10	1.45	2 (22%)	11,13,13	0.59	0
2	NPO	D	801	-	9,10,10	1.54	2 (22%)	11,13,13	0.46	0
9	SO4	A	418	-	4,4,4	0.13	0	6,6,6	0.11	0
2	NPO	A	401	-	9,10,10	1.44	2 (22%)	11,13,13	0.67	0
2	NPO	B	2704	-	9,10,10	1.50	2 (22%)	11,13,13	0.80	1 (9%)
9	SO4	B	2715	-	4,4,4	0.13	0	6,6,6	0.09	0
9	SO4	B	2716	-	4,4,4	0.15	0	6,6,6	0.20	0
6	DMS	D	809	-	3,3,3	0.68	0	3,3,3	0.53	0
5	EDO	B	2703	-	3,3,3	0.42	0	2,2,2	0.16	0
5	EDO	B	2711	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	C	413	-	3,3,3	0.46	0	2,2,2	0.31	0
6	DMS	B	2710	-	3,3,3	0.64	0	3,3,3	0.57	0
7	DIO	B	2714	-	6,6,6	0.51	0	6,6,6	0.96	1 (16%)
5	EDO	B	2709	-	3,3,3	0.47	0	2,2,2	0.32	0
6	DMS	B	2707	-	3,3,3	0.59	0	3,3,3	0.37	0
6	DMS	D	808	-	3,3,3	0.70	0	3,3,3	0.77	0
8	GOL	A	417	-	5,5,5	0.89	0	5,5,5	0.93	0
10	PGE	B	2701	-	9,9,9	0.54	0	8,8,8	0.32	0
6	DMS	A	407	-	3,3,3	0.60	0	3,3,3	0.51	0
6	DMS	C	408	-	3,3,3	0.64	0	3,3,3	0.64	0
2	NPO	A	403	-	9,10,10	2.30	5 (55%)	11,13,13	0.99	1 (9%)
3	6NA	A	404	-	7,7,7	0.85	0	7,7,7	1.15	0
4	PEG	D	803	-	6,6,6	0.49	0	5,5,5	0.38	0
6	DMS	B	2706	-	3,3,3	0.67	0	3,3,3	0.59	0
6	DMS	C	405	-	3,3,3	1.21	0	3,3,3	0.81	0
2	NPO	A	402	-	9,10,10	2.31	4 (44%)	11,13,13	1.38	1 (9%)

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
8	GOL	D	811	-	-	2/4/4/4	-
5	EDO	B	2708	-	-	0/1/1/1	-
2	NPO	D	812	-	-	0/2/4/4	0/1/1/1
7	DIO	A	411	-	-	-	0/1/1/1
7	DIO	A	409	-	-	-	0/1/1/1
5	EDO	A	406	-	-	0/1/1/1	-
2	NPO	C	402	-	-	0/2/4/4	0/1/1/1
4	PEG	A	405	-	-	4/4/4/4	-
8	GOL	B	2713	-	-	4/4/4/4	-
8	GOL	C	410	-	-	0/4/4/4	-
8	GOL	C	412	-	-	3/4/4/4	-
8	GOL	A	415	-	-	2/4/4/4	-
8	GOL	A	414	-	-	4/4/4/4	-
7	DIO	C	409	-	-	-	0/1/1/1
8	GOL	A	416	-	-	3/4/4/4	-
7	DIO	A	413	-	-	-	0/1/1/1
12	MES	D	807	-	-	1/6/14/14	0/1/1/1
2	NPO	C	401	-	-	0/2/4/4	0/1/1/1
5	EDO	D	804	-	-	0/1/1/1	-
3	6NA	B	2705	-	-	4/5/5/5	-
5	EDO	C	404	-	-	1/1/1/1	-
5	EDO	A	410	-	-	1/1/1/1	-
3	6NA	A	412	-	-	3/5/5/5	-
10	PGE	C	411	-	-	2/7/7/7	-
2	NPO	B	2702	-	-	0/2/4/4	0/1/1/1
5	EDO	B	2712	-	-	1/1/1/1	-
2	NPO	D	802	-	-	0/2/4/4	0/1/1/1
7	DIO	C	414	-	-	-	0/1/1/1
8	GOL	C	407	-	-	4/4/4/4	-
2	NPO	C	403	-	-	0/2/4/4	0/1/1/1
2	NPO	D	801	-	-	0/2/4/4	0/1/1/1
2	NPO	A	401	-	-	0/2/4/4	0/1/1/1
2	NPO	B	2704	-	-	0/2/4/4	0/1/1/1
5	EDO	B	2703	-	-	0/1/1/1	-
5	EDO	B	2711	-	-	0/1/1/1	-
5	EDO	C	413	-	-	1/1/1/1	-
10	PGE	B	2701	-	-	4/7/7/7	-
7	DIO	B	2714	-	-	-	0/1/1/1
5	EDO	B	2709	-	-	0/1/1/1	-
8	GOL	A	417	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NPO	A	403	-	-	0/2/4/4	0/1/1/1
3	6NA	A	404	-	-	5/5/5/5	-
4	PEG	D	803	-	-	3/4/4/4	-
2	NPO	A	402	-	-	0/2/4/4	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	807	MES	C8-S	-6.79	1.67	1.77
2	A	402	NPO	O3-N1	-4.63	1.14	1.22
2	A	403	NPO	C1-N1	-4.37	1.34	1.45
2	D	812	NPO	C1-N1	-3.47	1.36	1.45
2	A	402	NPO	C1-N1	-2.94	1.38	1.45
2	B	2704	NPO	C5-C4	2.92	1.44	1.38
2	D	812	NPO	O3-N1	-2.90	1.17	1.22
2	D	801	NPO	C5-C4	2.88	1.44	1.38
2	C	402	NPO	C5-C4	2.87	1.44	1.38
3	A	412	6NA	OXT-C	-2.87	1.21	1.30
2	B	2702	NPO	C5-C4	2.85	1.44	1.38
2	A	401	NPO	C5-C4	2.84	1.44	1.38
2	D	802	NPO	C5-C4	2.82	1.44	1.38
2	C	401	NPO	C5-C4	2.76	1.44	1.38
2	A	403	NPO	C5-C4	-2.70	1.33	1.38
8	B	2713	GOL	O2-C2	-2.62	1.35	1.43
2	D	802	NPO	C2-C1	2.62	1.43	1.38
2	C	403	NPO	C5-C4	2.61	1.43	1.38
2	D	801	NPO	C2-C1	2.44	1.43	1.38
2	C	401	NPO	C2-C1	2.44	1.43	1.38
2	A	401	NPO	C2-C1	2.43	1.43	1.38
2	A	403	NPO	O3-N1	-2.37	1.18	1.22
2	C	402	NPO	C2-C1	2.33	1.43	1.38
2	B	2704	NPO	C2-C1	2.29	1.43	1.38
2	A	402	NPO	C5-C4	-2.27	1.34	1.38
2	C	403	NPO	C2-C1	2.27	1.43	1.38
2	B	2702	NPO	C2-C1	2.26	1.43	1.38
8	C	407	GOL	O1-C1	-2.25	1.32	1.42
2	A	403	NPO	C6-C5	-2.19	1.34	1.38
2	A	402	NPO	OH-C4	-2.11	1.32	1.37
2	A	403	NPO	OH-C4	-2.02	1.32	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	807	MES	C5-N4-C3	4.88	119.82	108.83
2	D	812	NPO	C6-C1-N1	-4.82	115.75	119.38
3	A	412	6NA	OXT-C-O	-3.55	114.44	123.30
12	D	807	MES	C7-N4-C3	3.38	119.87	111.23
12	D	807	MES	O1S-S-C8	3.19	110.76	106.92
2	D	812	NPO	C6-C1-C2	3.08	124.95	119.86
2	D	812	NPO	C5-C4-C3	2.75	124.41	119.77
7	A	413	DIO	C2-O1-C1	2.70	118.91	109.89
2	D	812	NPO	O3-N1-C1	2.62	122.50	118.80
2	D	812	NPO	C3-C2-C1	-2.60	116.46	120.08
12	D	807	MES	C7-N4-C5	2.52	117.68	111.23
3	A	412	6NA	CB-CA-C	-2.37	108.50	114.47
2	A	402	NPO	C2-C1-N1	2.32	121.12	119.38
8	B	2713	GOL	O2-C2-C1	-2.29	99.04	109.12
2	A	403	NPO	C3-C2-C1	-2.23	116.98	120.08
7	B	2714	DIO	C2-O1-C1	2.19	117.22	109.89
3	B	2705	6NA	OXT-C-CA	2.16	120.95	114.03
2	B	2704	NPO	C6-C1-N1	2.15	121.00	119.38
12	D	807	MES	O2S-S-C8	2.12	109.47	106.92
8	C	407	GOL	C3-C2-C1	-2.11	103.51	111.70
8	C	412	GOL	C3-C2-C1	-2.07	103.64	111.70

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	404	EDO	O1-C1-C2-O2
8	A	414	GOL	O1-C1-C2-C3
8	A	414	GOL	C1-C2-C3-O3
8	A	415	GOL	O1-C1-C2-C3
8	B	2713	GOL	O1-C1-C2-O2
8	B	2713	GOL	O1-C1-C2-C3
8	C	407	GOL	O1-C1-C2-C3
8	C	407	GOL	C1-C2-C3-O3
8	D	811	GOL	C1-C2-C3-O3
12	D	807	MES	C8-C7-N4-C3
4	A	405	PEG	O2-C3-C4-O4
3	A	404	6NA	CA-CB-CG-CD
8	A	416	GOL	C1-C2-C3-O3
8	B	2713	GOL	C1-C2-C3-O3
8	C	412	GOL	C1-C2-C3-O3
4	A	405	PEG	O1-C1-C2-O2
10	B	2701	PGE	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	414	GOL	O1-C1-C2-O2
8	A	414	GOL	O2-C2-C3-O3
8	A	415	GOL	O1-C1-C2-O2
8	C	407	GOL	O1-C1-C2-O2
4	D	803	PEG	O1-C1-C2-O2
3	A	404	6NA	C-CA-CB-CG
8	C	407	GOL	O2-C2-C3-O3
8	D	811	GOL	O2-C2-C3-O3
3	A	404	6NA	C6-CD-CG-CB
3	A	412	6NA	C6-CD-CG-CB
4	D	803	PEG	O2-C3-C4-O4
5	A	410	EDO	O1-C1-C2-O2
3	B	2705	6NA	C6-CD-CG-CB
8	A	416	GOL	O2-C2-C3-O3
8	B	2713	GOL	O2-C2-C3-O3
10	C	411	PGE	O2-C3-C4-O3
5	C	413	EDO	O1-C1-C2-O2
10	B	2701	PGE	O2-C3-C4-O3
4	D	803	PEG	C4-C3-O2-C2
4	A	405	PEG	C4-C3-O2-C2
10	B	2701	PGE	C6-C5-O3-C4
4	A	405	PEG	C1-C2-O2-C3
3	B	2705	6NA	C-CA-CB-CG
5	B	2712	EDO	O1-C1-C2-O2
3	B	2705	6NA	O-C-CA-CB
3	A	412	6NA	OXT-C-CA-CB
3	A	404	6NA	OXT-C-CA-CB
3	A	412	6NA	O-C-CA-CB
3	A	404	6NA	O-C-CA-CB
8	A	416	GOL	O1-C1-C2-O2
3	B	2705	6NA	OXT-C-CA-CB
8	C	412	GOL	O1-C1-C2-O2
10	B	2701	PGE	C3-C4-O3-C5
8	A	417	GOL	O1-C1-C2-C3
10	C	411	PGE	O1-C1-C2-O2
8	C	412	GOL	O2-C2-C3-O3

There are no ring outliers.

33 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2708	EDO	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	406	DMS	7	0
5	A	406	EDO	1	0
6	D	810	DMS	4	0
8	B	2713	GOL	6	0
8	C	410	GOL	3	0
8	C	412	GOL	6	0
8	A	415	GOL	4	0
7	C	409	DIO	2	0
8	A	416	GOL	1	0
5	D	804	EDO	7	0
6	C	415	DMS	4	0
3	B	2705	6NA	5	0
5	C	404	EDO	1	0
3	A	412	6NA	5	0
10	C	411	PGE	6	0
2	B	2702	NPO	2	0
6	D	806	DMS	6	0
6	D	805	DMS	11	0
8	C	407	GOL	1	0
2	D	801	NPO	1	0
2	A	401	NPO	1	0
5	B	2703	EDO	6	0
5	B	2711	EDO	1	0
5	C	413	EDO	1	0
7	B	2714	DIO	2	0
5	B	2709	EDO	1	0
6	B	2707	DMS	8	0
6	D	808	DMS	1	0
6	A	407	DMS	6	0
6	C	408	DMS	3	0
3	A	404	6NA	6	0
6	C	405	DMS	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	309/314 (98%)	0.15	9 (2%)	51	56	22, 27, 42, 52	0
1	B	309/314 (98%)	0.18	10 (3%)	47	52	24, 31, 47, 118	0
1	C	309/314 (98%)	0.19	8 (2%)	56	60	21, 28, 42, 55	0
1	D	309/314 (98%)	0.41	21 (6%)	17	19	24, 32, 50, 64	0
All	All	1236/1256 (98%)	0.23	48 (3%)	39	44	21, 29, 47, 118	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	PHE	8.6
1	B	17	ALA	6.1
1	D	26	LEU	5.2
1	D	27	ALA	5.1
1	B	4	THR	4.4
1	D	4	THR	4.3
1	A	77	SER	4.3
1	B	27	ALA	4.0
1	C	77	SER	3.9
1	C	135	CYS	3.8
1	D	30	THR	3.7
1	D	219	PHE	3.6
1	D	24	PRO	3.6
1	D	31	LEU	3.5
1	A	147	SER	3.4
1	D	275	VAL	3.2
1	D	25	THR	3.2
1	B	30	THR	3.1
1	D	28	GLU	3.0
1	A	80	ALA	2.9
1	C	76	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	79	GLU	2.8
1	C	274	VAL	2.8
1	D	247	ILE	2.8
1	A	79	GLU	2.7
1	D	225	LYS	2.7
1	A	58	LEU	2.7
1	B	63	PRO	2.6
1	D	64	ALA	2.6
1	D	215	ALA	2.5
1	B	18	ILE	2.5
1	A	149	LEU	2.5
1	D	23	GLY	2.4
1	D	22	ALA	2.4
1	B	31	LEU	2.4
1	B	178	LYS	2.3
1	D	248	VAL	2.3
1	B	26	LEU	2.3
1	A	152	THR	2.3
1	D	34	ALA	2.2
1	D	276	TYR	2.1
1	A	56	ARG	2.1
1	C	149	LEU	2.1
1	A	146	PRO	2.1
1	D	178	LYS	2.1
1	C	4	THR	2.1
1	D	198	VAL	2.1
1	C	306	ALA	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 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
5	EDO	B	2711	4/4	0.30	1.00	62,87,97,106	0
2	NPO	D	812	10/10	0.50	0.28	73,85,103,104	15
10	PGE	C	411	10/10	0.59	0.31	41,57,68,72	0
8	GOL	C	410	6/6	0.63	0.38	52,62,75,75	0
10	PGE	B	2701	10/10	0.69	0.17	31,48,64,65	23
3	6NA	A	412	8/8	0.69	0.23	25,33,44,54	19
5	EDO	A	410	4/4	0.72	0.26	44,53,59,64	0
8	GOL	D	811	6/6	0.72	0.12	46,55,65,70	0
7	DIO	B	2714	6/6	0.73	0.18	46,58,70,70	0
7	DIO	C	409	6/6	0.73	0.44	56,68,78,78	0
5	EDO	B	2709	4/4	0.74	0.13	51,62,76,76	0
6	DMS	D	806	4/4	0.74	0.19	32,39,61,63	0
7	DIO	A	409	6/6	0.75	0.42	58,69,74,74	0
4	PEG	A	405	7/7	0.76	0.25	35,44,53,58	17
7	DIO	A	411	6/6	0.76	0.28	61,74,81,81	0
7	DIO	C	414	6/6	0.76	0.21	44,54,60,60	14
8	GOL	A	415	6/6	0.76	0.39	55,61,69,73	0
8	GOL	A	417	6/6	0.77	0.23	50,61,71,72	0
8	GOL	C	407	6/6	0.78	0.16	33,40,48,50	13
3	6NA	B	2705	8/8	0.79	0.20	35,44,58,58	0
8	GOL	A	416	6/6	0.79	0.34	40,55,65,67	0
5	EDO	A	406	4/4	0.80	0.17	44,53,57,68	0
7	DIO	A	413	6/6	0.81	0.37	51,73,88,88	0
3	6NA	A	404	8/8	0.82	0.18	34,46,57,57	0
6	DMS	C	408	4/4	0.83	0.22	40,53,69,72	0
9	SO4	C	416	5/5	0.85	0.40	61,64,77,79	5
6	DMS	D	805	4/4	0.85	0.28	38,46,64,65	0
5	EDO	D	804	4/4	0.85	0.22	39,47,50,53	0
9	SO4	B	2715	5/5	0.86	0.31	70,75,86,90	0
6	DMS	B	2707	4/4	0.86	0.25	31,37,52,60	10
4	PEG	D	803	7/7	0.86	0.18	31,44,58,58	0
6	DMS	D	809	4/4	0.86	0.36	65,78,87,87	0
5	EDO	C	413	4/4	0.87	0.23	46,56,62,63	0
8	GOL	B	2713	6/6	0.87	0.20	29,44,56,56	12
8	GOL	A	414	6/6	0.87	0.17	43,51,61,61	0
2	NPO	D	802	10/10	0.88	0.17	45,48,57,64	0
6	DMS	C	405	4/4	0.88	0.14	32,38,47,56	8
9	SO4	D	813	5/5	0.88	0.38	81,82,89,92	0
6	DMS	A	407	4/4	0.88	0.19	30,36,50,59	10
6	DMS	A	408	4/4	0.88	0.23	54,67,74,74	1
5	EDO	B	2712	4/4	0.89	0.29	38,48,57,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DMS	D	808	4/4	0.89	0.15	29,52,53,56	10
6	DMS	C	406	4/4	0.89	0.24	44,52,61,66	0
9	SO4	B	2716	5/5	0.89	0.14	31,31,41,43	5
2	NPO	D	801	10/10	0.90	0.19	42,47,58,59	0
2	NPO	C	401	10/10	0.91	0.13	30,34,41,44	0
2	NPO	A	403	10/10	0.91	0.16	42,51,61,70	0
8	GOL	C	412	6/6	0.92	0.27	33,47,58,60	0
2	NPO	C	403	10/10	0.92	0.16	41,49,59,70	0
5	EDO	C	404	4/4	0.92	0.29	37,53,56,66	0
5	EDO	B	2708	4/4	0.92	0.20	43,51,57,68	0
12	MES	D	807	12/12	0.92	0.15	30,44,53,55	0
2	NPO	B	2704	10/10	0.93	0.12	38,42,52,52	0
6	DMS	D	810	4/4	0.93	0.14	30,37,62,68	0
2	NPO	A	401	10/10	0.93	0.14	31,35,40,42	1
2	NPO	C	402	10/10	0.93	0.14	30,35,45,48	0
2	NPO	B	2702	10/10	0.94	0.11	34,41,47,48	0
5	EDO	B	2703	4/4	0.94	0.23	36,46,52,58	0
11	NA	B	2717	1/1	0.94	0.31	53,53,53,53	0
6	DMS	B	2710	4/4	0.94	0.29	62,75,78,78	0
6	DMS	C	415	4/4	0.95	0.14	46,62,67,67	10
2	NPO	A	402	10/10	0.96	0.10	25,31,37,44	15
6	DMS	B	2706	4/4	0.96	0.36	46,75,80,80	0
9	SO4	A	418	5/5	0.97	0.07	52,54,60,61	5

6.5 Other polymers (i)

There are no such residues in this entry.