



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2022 – 02:19 PM 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 wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.26
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)	:	2.26

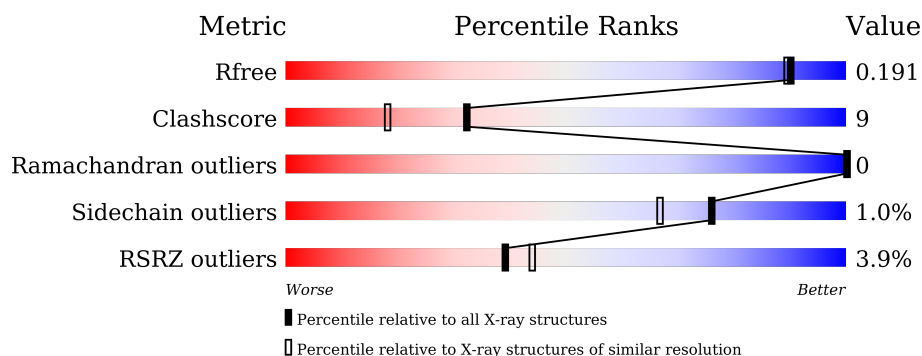
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> <div>.</div> </div>
1	B	314	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> <div>..</div> </div>
1	C	314	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> <div>.</div> </div>
1	D	314	<div> <div>7%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit 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

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.

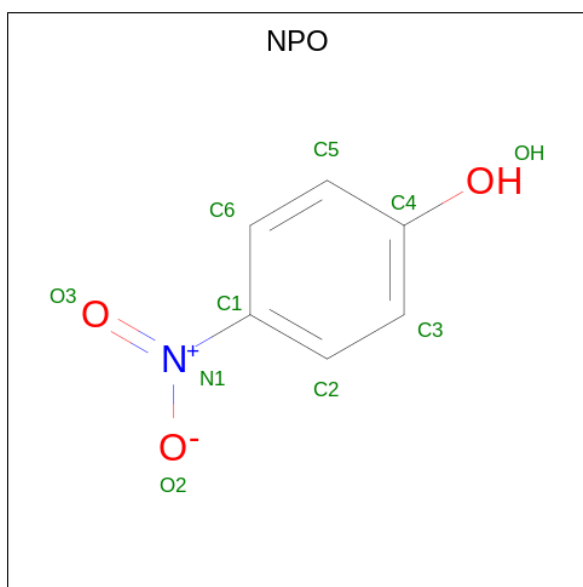
- Molecule 1 is a protein called Lipase.

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:

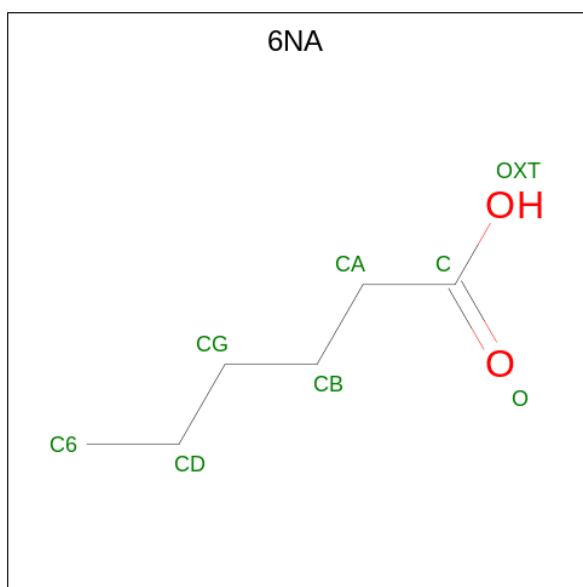
Chain	Residue	Modelled	Actual	Comment	Reference
A	162	ALA	SER	engineered mutation	UNP A0A074MDU6
B	162	ALA	SER	engineered mutation	UNP A0A074MDU6
C	162	ALA	SER	engineered mutation	UNP A0A074MDU6
D	162	ALA	SER	engineered mutation	UNP A0A074MDU6

- Molecule 2 is P-NITROPHENOL (three-letter code: NPO) (formula: C₆H₅NO₃).



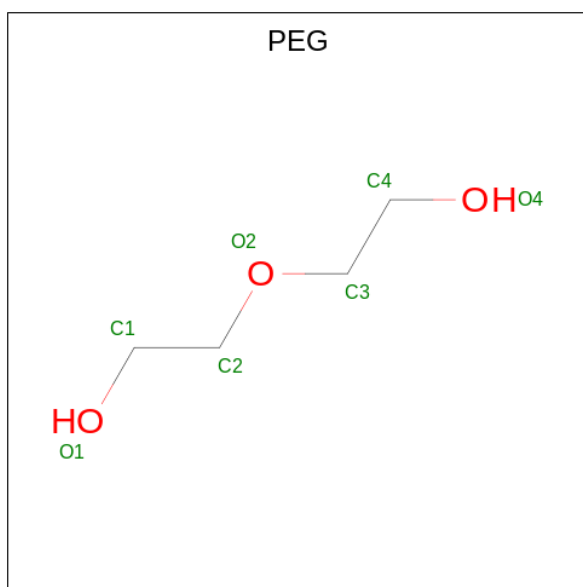
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	A	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	A	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	B	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	B	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	C	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
2	C	1	Total	C	H	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: C₆H₁₂O₂).



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: $C_4H_{10}O_3$).



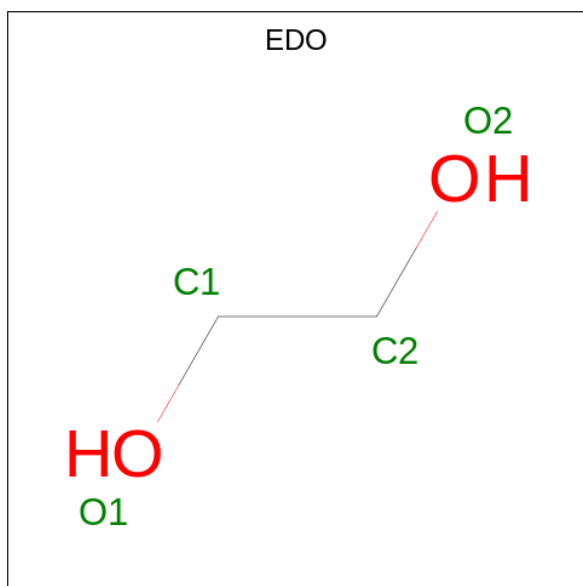
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

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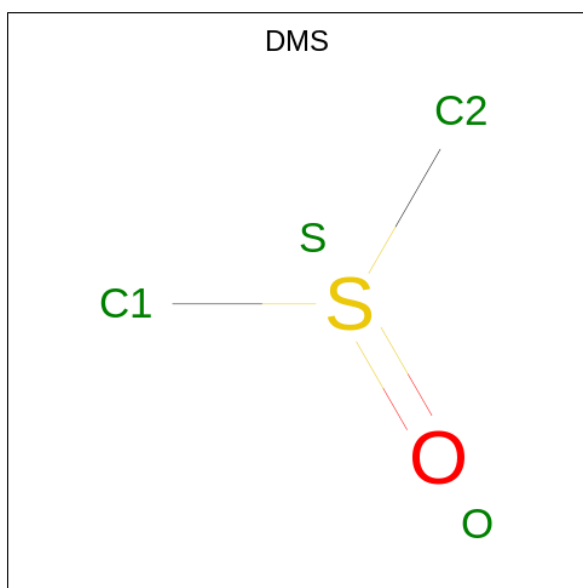
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			17	4	10	3		

- 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	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).



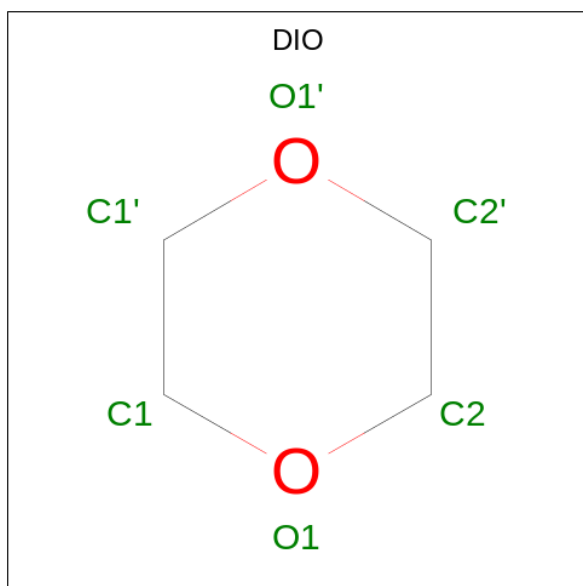
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			8	2	4	1	1		
6	C	1	Total	C	H	O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

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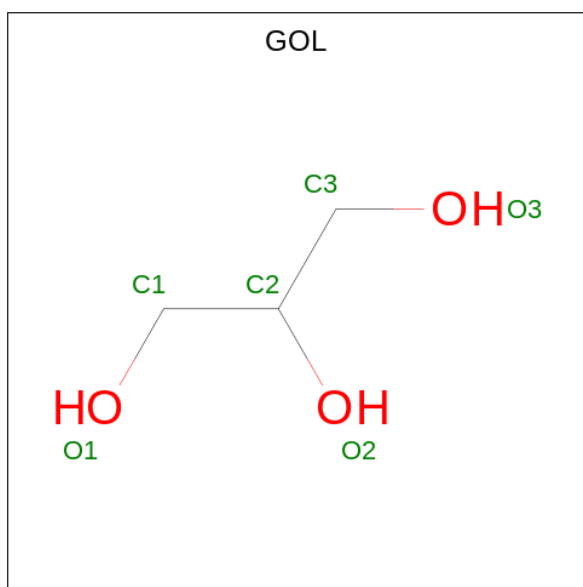
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



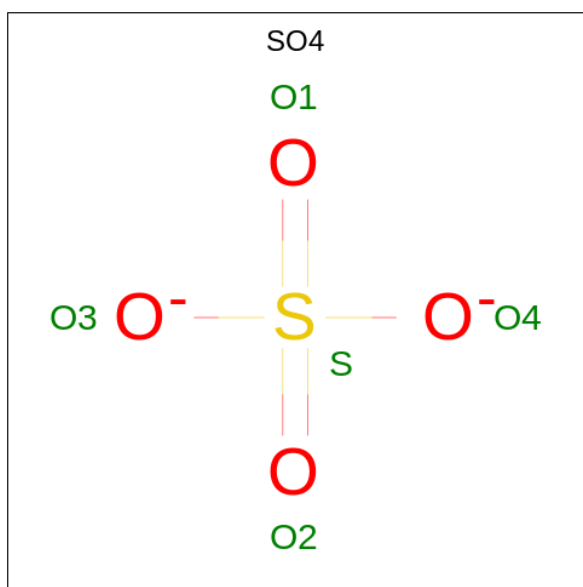
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	O		0	0
			14	4	8	2			
7	A	1	Total	C	H	O		0	0
			14	4	8	2			
7	A	1	Total	C	H	O		0	0
			14	4	8	2			
7	B	1	Total	C	H	O		0	0
			14	4	8	2			
7	C	1	Total	C	H	O		0	0
			14	4	8	2			
7	C	1	Total	C	H	O		0	0
			14	4	8	2			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



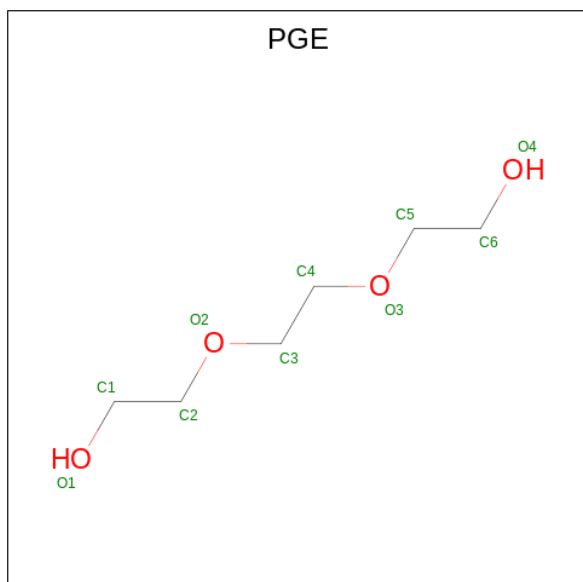
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			12	3	6	3		
8	A	1	Total	C	H	O	0	0
			13	3	7	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	B	1	Total	C	H	O	0	0
			12	3	6	3		
8	C	1	Total	C	H	O	0	0
			13	3	7	3		
8	C	1	Total	C	H	O	0	0
			14	3	8	3		
8	C	1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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).

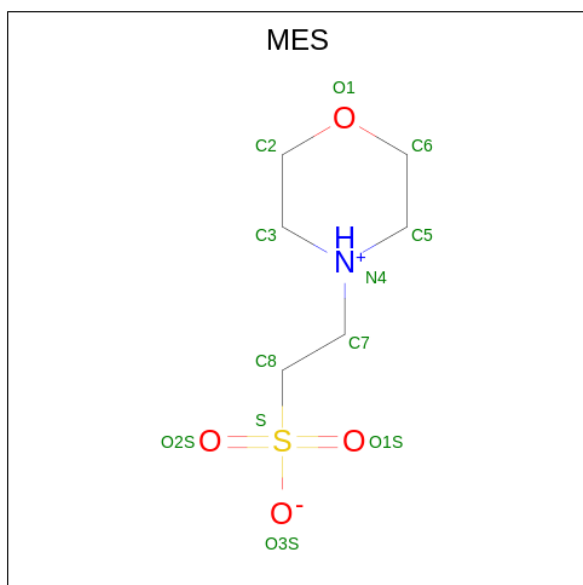


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			23	6	13	4		
10	C	1	Total	C	H	O	0	0
			22	6	12	4		

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

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

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 13 is water.

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

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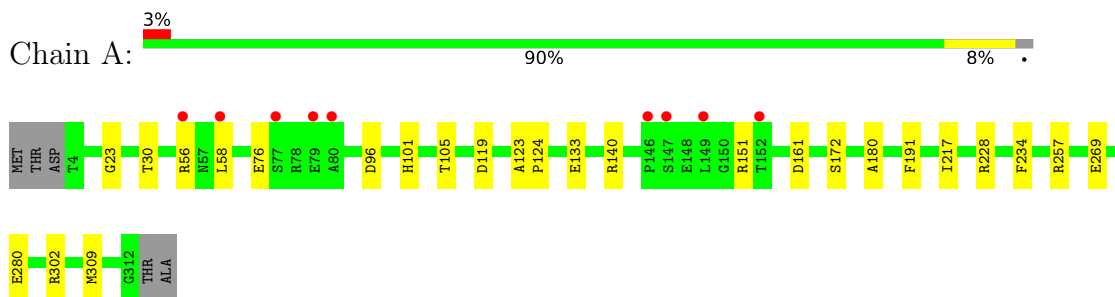
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	305	Total 305	O 305	0	0

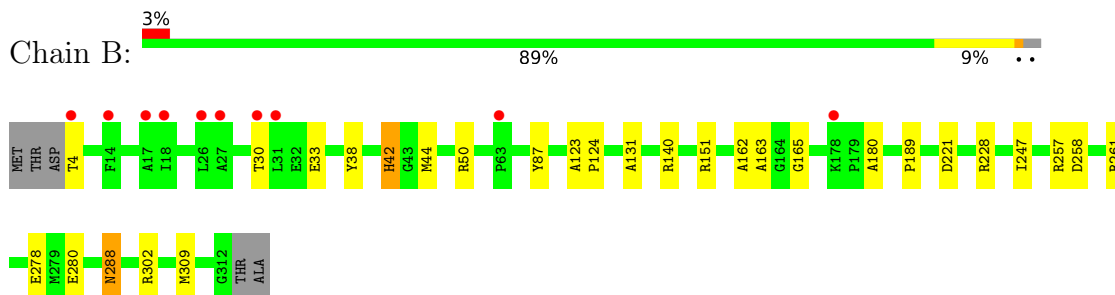
3 Residue-property plots [i](#)

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.

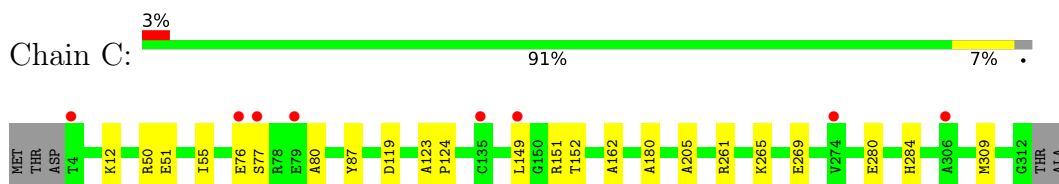
- Molecule 1: Lipase



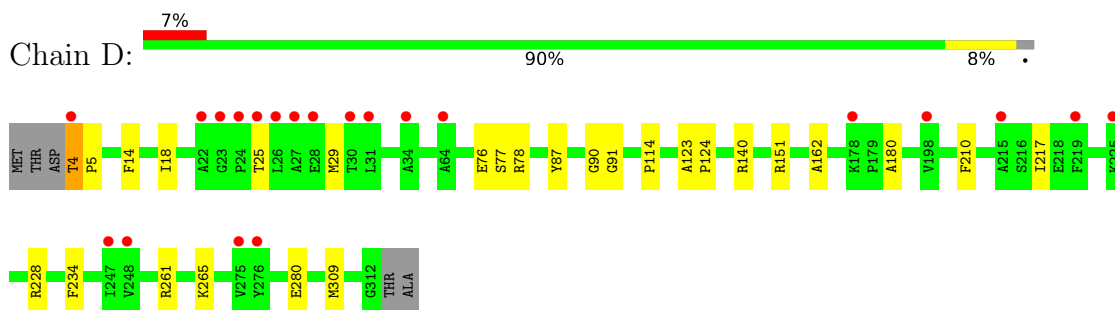
- Molecule 1: Lipase



- Molecule 1: Lipase



- Molecule 1: Lipase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NPO, PEG, MES, NA, EDO, DIO, SO4, GOL, DMS, PGE, 6NA

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(°)	Ideal(°)
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.

The worst 5 of 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

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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	87	TYR
1	D	151	ARG
1	B	151	ARG
1	B	288	ASN
1	C	87	TYR

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

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
5	EDO	B	2703	-	3,3,3	0.42	0	2,2,2	0.16	0
9	SO4	B	2716	-	4,4,4	0.15	0	6,6,6	0.20	0
5	EDO	B	2712	-	3,3,3	0.46	0	2,2,2	0.20	0
2	NPO	B	2702	-	9,10,10	1.47	2 (22%)	11,13,13	0.85	0
8	GOL	D	811	-	5,5,5	0.84	0	5,5,5	1.00	0
3	6NA	A	412	-	4,7,7	0.18	0	3,7,7	0.77	0
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	C	415	-	3,3,3	0.67	0	3,3,3	0.53	0
8	GOL	C	410	-	5,5,5	0.99	0	5,5,5	0.93	0
7	DIO	A	413	-	6,6,6	0.67	0	6,6,6	1.34	1 (16%)
5	EDO	D	804	-	3,3,3	0.38	0	2,2,2	0.55	0
6	DMS	D	808	-	3,3,3	0.70	0	3,3,3	0.77	0
6	DMS	B	2710	-	3,3,3	0.64	0	3,3,3	0.57	0
7	DIO	A	411	-	6,6,6	0.65	0	6,6,6	0.77	0
8	GOL	A	414	-	5,5,5	0.76	0	5,5,5	1.15	0
2	NPO	A	403	-	9,10,10	2.30	5 (55%)	11,13,13	0.99	1 (9%)
7	DIO	A	409	-	6,6,6	0.65	0	6,6,6	0.55	0
7	DIO	B	2714	-	6,6,6	0.51	0	6,6,6	0.96	1 (16%)
9	SO4	A	418	-	4,4,4	0.13	0	6,6,6	0.11	0
10	PGE	B	2701	-	9,9,9	0.54	0	8,8,8	0.32	0
6	DMS	D	809	-	3,3,3	0.68	0	3,3,3	0.53	0
5	EDO	B	2711	-	3,3,3	0.47	0	2,2,2	0.31	0
10	PGE	C	411	-	9,9,9	0.50	0	8,8,8	0.19	0
2	NPO	B	2704	-	9,10,10	1.50	2 (22%)	11,13,13	0.80	1 (9%)
3	6NA	B	2705	-	4,7,7	0.31	0	3,7,7	0.67	0
5	EDO	C	404	-	3,3,3	0.50	0	2,2,2	0.20	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%)
5	EDO	A	406	-	3,3,3	0.54	0	2,2,2	0.17	0
8	GOL	A	415	-	5,5,5	0.87	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	416	-	5,5,5	1.02	0	5,5,5	0.88	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
6	DMS	D	806	-	3,3,3	0.67	0	3,3,3	0.82	0
2	NPO	D	801	-	9,10,10	1.54	2 (22%)	11,13,13	0.46	0
2	NPO	D	802	-	9,10,10	1.58	2 (22%)	11,13,13	0.61	0
6	DMS	A	407	-	3,3,3	0.60	0	3,3,3	0.51	0
7	DIO	C	414	-	6,6,6	0.49	0	6,6,6	0.51	0
9	SO4	D	813	-	4,4,4	0.14	0	6,6,6	0.05	0
6	DMS	C	406	-	3,3,3	0.65	0	3,3,3	0.66	0
5	EDO	A	410	-	3,3,3	0.50	0	2,2,2	0.29	0
3	6NA	A	404	-	4,7,7	0.35	0	3,7,7	0.61	0
6	DMS	D	810	-	3,3,3	0.64	0	3,3,3	0.85	0
2	NPO	C	401	-	9,10,10	1.47	2 (22%)	11,13,13	0.61	0
8	GOL	C	407	-	5,5,5	1.09	1 (20%)	5,5,5	1.30	1 (20%)
2	NPO	A	402	-	9,10,10	2.31	4 (44%)	11,13,13	1.38	1 (9%)
7	DIO	C	409	-	6,6,6	0.68	0	6,6,6	0.49	0
4	PEG	D	803	-	6,6,6	0.49	0	5,5,5	0.38	0
8	GOL	C	412	-	5,5,5	0.91	0	5,5,5	1.07	1 (20%)
2	NPO	A	401	-	9,10,10	1.44	2 (22%)	11,13,13	0.67	0
6	DMS	A	408	-	3,3,3	0.64	0	3,3,3	0.79	0
9	SO4	B	2715	-	4,4,4	0.13	0	6,6,6	0.09	0
8	GOL	A	417	-	5,5,5	0.89	0	5,5,5	0.93	0
2	NPO	C	402	-	9,10,10	1.52	2 (22%)	11,13,13	0.82	0
2	NPO	C	403	-	9,10,10	1.45	2 (22%)	11,13,13	0.59	0
5	EDO	C	413	-	3,3,3	0.46	0	2,2,2	0.31	0
9	SO4	C	416	-	4,4,4	0.13	0	6,6,6	0.10	0
6	DMS	D	805	-	3,3,3	0.61	0	3,3,3	0.37	0
6	DMS	C	408	-	3,3,3	0.64	0	3,3,3	0.64	0
8	GOL	B	2713	-	5,5,5	1.29	1 (20%)	5,5,5	1.31	1 (20%)
4	PEG	A	405	-	6,6,6	0.46	0	5,5,5	0.19	0
12	MES	D	807	-	12,12,12	2.05	1 (8%)	14,16,16	2.21	5 (35%)

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
5	EDO	B	2703	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	2712	-	-	1/1/1/1	-
2	NPO	B	2702	-	-	0/2/4/4	0/1/1/1
8	GOL	D	811	-	-	2/4/4/4	-
3	6NA	A	412	-	-	1/3/5/5	-
5	EDO	B	2709	-	-	0/1/1/1	-
8	GOL	C	410	-	-	0/4/4/4	-
7	DIO	A	413	-	-	-	0/1/1/1
5	EDO	D	804	-	-	0/1/1/1	-
7	DIO	A	411	-	-	-	0/1/1/1
8	GOL	A	414	-	-	4/4/4/4	-
2	NPO	A	403	-	-	0/2/4/4	0/1/1/1
7	DIO	A	409	-	-	-	0/1/1/1
7	DIO	B	2714	-	-	-	0/1/1/1
10	PGE	B	2701	-	-	4/7/7/7	-
5	EDO	B	2711	-	-	0/1/1/1	-
10	PGE	C	411	-	-	2/7/7/7	-
2	NPO	B	2704	-	-	0/2/4/4	0/1/1/1
3	6NA	B	2705	-	-	2/3/5/5	-
5	EDO	C	404	-	-	1/1/1/1	-
5	EDO	B	2708	-	-	0/1/1/1	-
2	NPO	D	812	-	-	0/2/4/4	0/1/1/1
5	EDO	A	406	-	-	0/1/1/1	-
8	GOL	A	415	-	-	2/4/4/4	-
8	GOL	A	416	-	-	3/4/4/4	-
2	NPO	D	801	-	-	0/2/4/4	0/1/1/1
2	NPO	D	802	-	-	0/2/4/4	0/1/1/1
7	DIO	C	414	-	-	-	0/1/1/1
5	EDO	A	410	-	-	1/1/1/1	-
3	6NA	A	404	-	-	3/3/5/5	-
2	NPO	C	401	-	-	0/2/4/4	0/1/1/1
8	GOL	C	407	-	-	4/4/4/4	-
2	NPO	A	402	-	-	0/2/4/4	0/1/1/1
7	DIO	C	409	-	-	-	0/1/1/1
4	PEG	D	803	-	-	3/4/4/4	-
8	GOL	C	412	-	-	3/4/4/4	-
2	NPO	A	401	-	-	0/2/4/4	0/1/1/1
8	GOL	A	417	-	-	1/4/4/4	-
2	NPO	C	402	-	-	0/2/4/4	0/1/1/1
2	NPO	C	403	-	-	0/2/4/4	0/1/1/1
5	EDO	C	413	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	2713	-	-	4/4/4/4	-
4	PEG	A	405	-	-	4/4/4/4	-
12	MES	D	807	-	-	1/6/14/14	0/1/1/1

The worst 5 of 30 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

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	6NA	C-CA-CB-CG
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

There are no ring outliers.

33 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2703	EDO	6	0
2	B	2702	NPO	2	0
3	A	412	6NA	5	0
5	B	2709	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2707	DMS	8	0
6	C	415	DMS	4	0
8	C	410	GOL	3	0
5	D	804	EDO	7	0
6	D	808	DMS	1	0
7	B	2714	DIO	2	0
5	B	2711	EDO	1	0
10	C	411	PGE	6	0
3	B	2705	6NA	5	0
5	C	404	EDO	1	0
5	B	2708	EDO	2	0
5	A	406	EDO	1	0
8	A	415	GOL	4	0
8	A	416	GOL	1	0
6	C	405	DMS	1	0
6	D	806	DMS	6	0
2	D	801	NPO	1	0
6	A	407	DMS	6	0
6	C	406	DMS	7	0
3	A	404	6NA	6	0
6	D	810	DMS	4	0
8	C	407	GOL	1	0
7	C	409	DIO	2	0
8	C	412	GOL	6	0
2	A	401	NPO	1	0
5	C	413	EDO	1	0
6	D	805	DMS	11	0
6	C	408	DMS	3	0
8	B	2713	GOL	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

The worst 5 of 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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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.