



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:08 am BST

PDB ID : 6M9U
Title : Structure of the apo-form of 20beta-Hydroxysteroid Dehydrogenase from Bifidobacterium adolescentis strain L2-32
Authors : Mythen, S.M.; Pollet, R.M.; Koropatkin, N.M.; Ridlon, J.M.
Deposited on : 2018-08-24
Resolution : 2.20 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 ⓘ 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 : 2.11
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) : 2.11

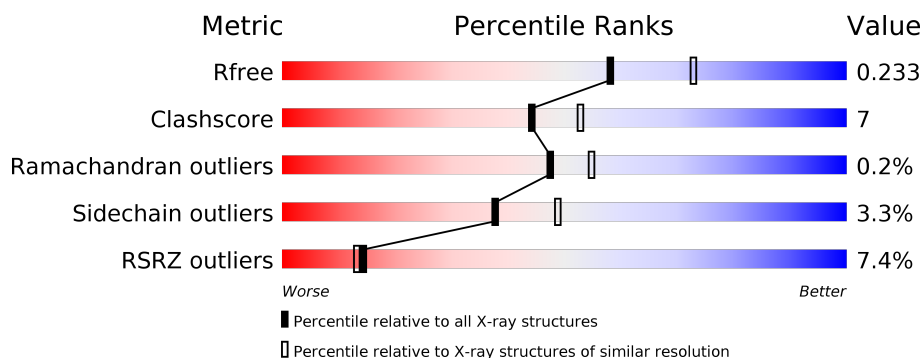
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	283	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>11%</div> </div> </div>
1	B	283	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>12%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	312	-	-	-	X
4	EDO	A	313	-	-	X	X
6	PEG	A	318	-	-	-	X

2 Entry composition [i](#)

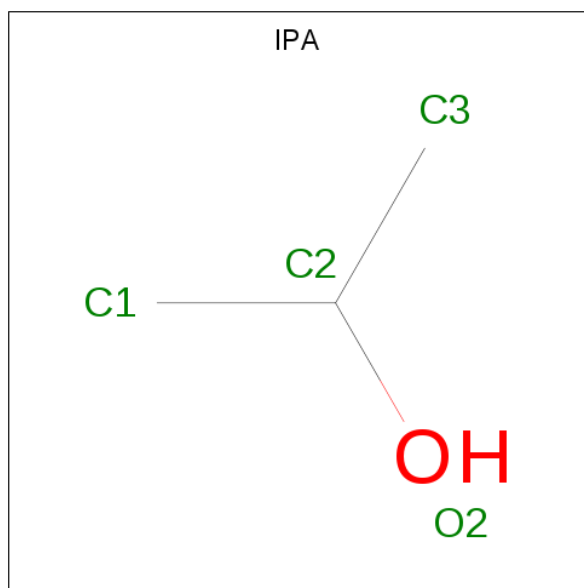
There are 10 unique types of molecules in this entry. The entry contains 8205 atoms, of which 4013 are hydrogens and 0 are deuteriums.

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 Oxidoreductase, short chain dehydrogenase/reductase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	251	Total	C	H	N	O	S	0	1	0
			3768	1196	1857	332	375	8			
1	B	250	Total	C	H	N	O	S	0	5	0
			3841	1219	1899	338	378	7			

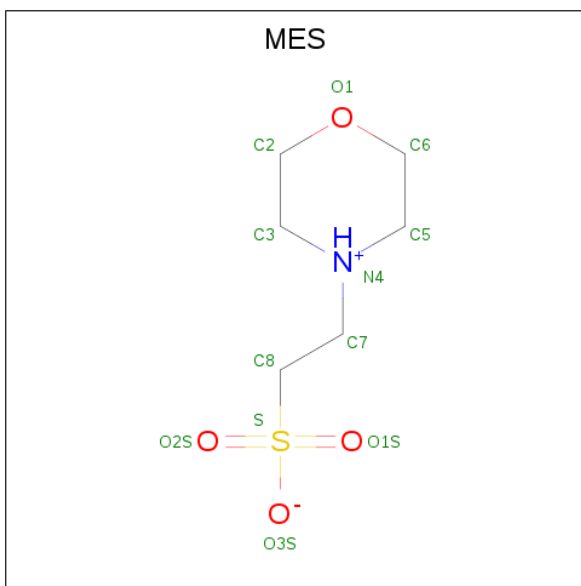
- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			12	3	8	1		
2	A	1	Total	C	H	O	0	0
			12	3	8	1		
2	B	1	Total	C	H	O	0	0
			12	3	8	1		

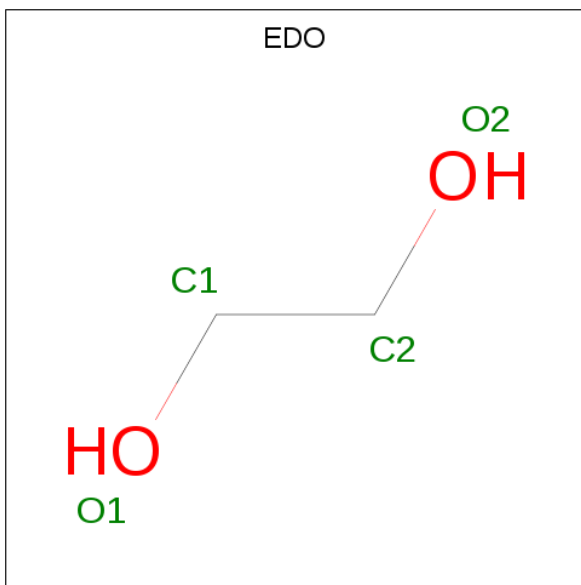
- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			24	6	14	4		
5	B	1	Total	C	H	O	0	0
			24	6	14	4		

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



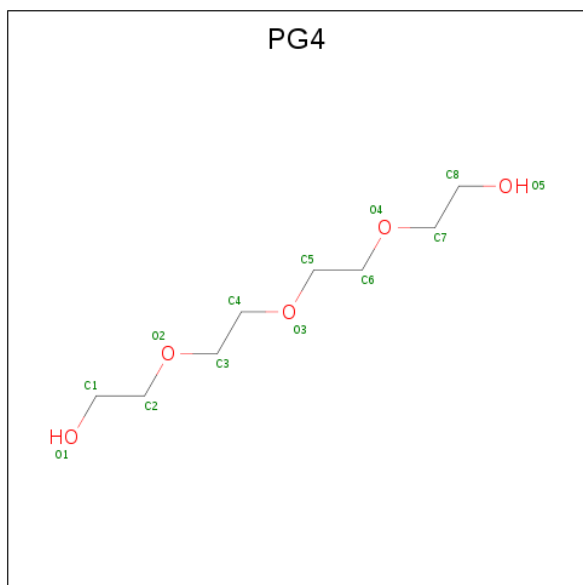
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	A	1	Total	C	H	O	0	0
			17	4	10	3		

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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

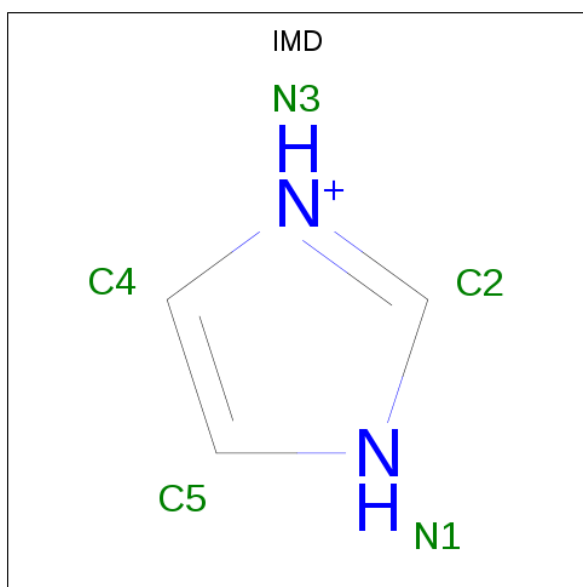


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		

- Molecule 9 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	N	0	0
			10	3	5	2		
9	B	1	Total	C	H	N	0	0
			10	3	5	2		

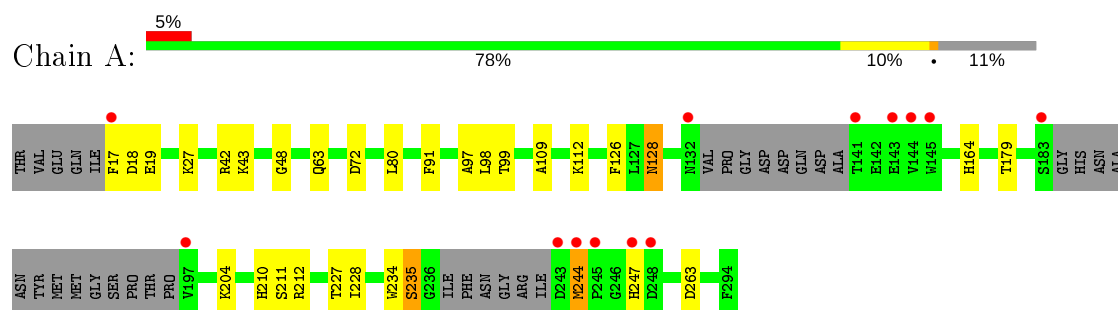
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	77	Total	O	0	0
			77	77		
10	B	83	Total	O	0	0
			83	83		

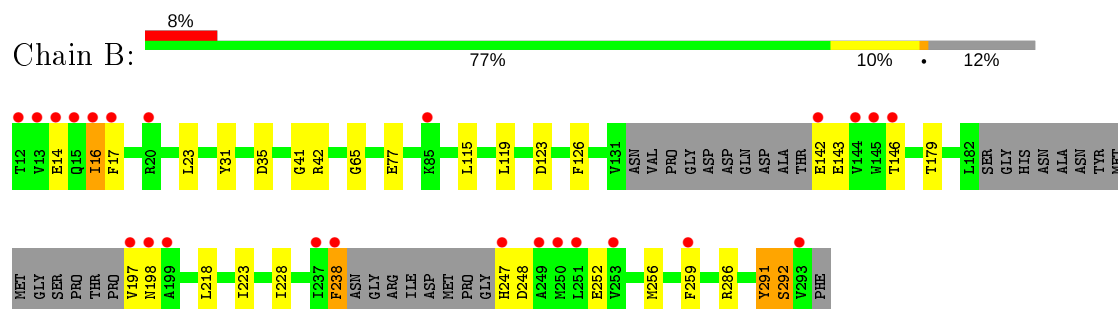
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Oxidoreductase, short chain dehydrogenase/reductase family protein



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.37Å 168.37Å 126.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.69 – 2.20 50.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.69-2.20) 84.9 (50.69-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.196 , 0.231 0.197 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8205	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, IMD, CL, EDO, PG4, PGE, MES, PEG

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	0.57	1/1946 (0.1%)	0.70	1/2632 (0.0%)
1	B	0.53	0/1989	0.67	0/2691
All	All	0.55	1/3935 (0.0%)	0.69	1/5323 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	ASN	CA-CB	6.36	1.69	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	PHE	O-C-N	5.92	132.17	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1911	1857	1858	30	0
1	B	1942	1899	1890	24	0
2	A	8	16	16	5	0
2	B	4	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	13	13	0	0
4	A	40	60	60	7	0
4	B	36	54	54	4	0
5	A	10	14	14	2	0
5	B	10	14	14	3	0
6	A	28	40	40	4	0
6	B	7	10	10	0	0
7	B	13	18	18	3	0
8	B	1	0	0	0	0
9	B	10	10	10	0	0
10	A	77	0	0	5	0
10	B	83	0	0	1	0
All	All	4192	4013	4005	53	0

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 7.

All (53) 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:A:164:HIS:HE2	4:A:313:EDO:HO1	1.27	0.82
1:A:263:ASP:OD2	2:A:301:IPA:H13	1.86	0.76
1:A:63:GLN:HE21	7:B:311:PG4:H51	1.55	0.72
1:B:286[A]:ARG:CZ	1:B:292:SER:OG	2.45	0.64
1:A:128:ASN:ND2	10:A:402:HOH:O	2.31	0.63
2:A:301:IPA:H11	1:B:31:TYR:OH	2.01	0.61
1:A:126:PHE:HE1	1:A:179:THR:HG23	1.66	0.60
1:A:244:MET:O	1:A:247:HIS:HB3	2.02	0.59
1:B:65:GLY:O	5:B:312:PGE:H5	2.03	0.58
1:A:211:SER:HB3	4:A:304:EDO:H11	1.86	0.58
1:B:286[A]:ARG:NH2	1:B:292:SER:OG	2.39	0.55
1:A:204:LYS:HA	2:A:302:IPA:H12	1.87	0.55
1:A:91:PHE:HA	7:B:311:PG4:H72	1.89	0.54
1:A:109:ALA:HB1	6:A:318:PEG:H12	1.91	0.53
1:A:42:ARG:NH1	10:A:406:HOH:O	2.41	0.51
1:B:126:PHE:HE1	1:B:179:THR:HG23	1.78	0.49
1:B:77:GLU:OE2	4:B:309:EDO:O1	2.23	0.49
1:B:291[A]:TYR:CD1	1:B:292:SER:N	2.81	0.48
1:A:179:THR:HG22	1:A:228:ILE:HB	1.96	0.48
1:A:48:GLY:HA2	6:A:317:PEG:H32	1.95	0.48
1:B:42:ARG:HE	1:B:123:ASP:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HD3	6:A:318:PEG:H22	1.96	0.48
1:A:99:THR:OG1	5:A:314:PGE:H22	2.13	0.47
1:A:234:TRP:CZ2	1:B:17:PHE:HB3	2.49	0.47
1:B:42:ARG:HD3	10:B:417:HOH:O	2.14	0.46
1:A:179:THR:CG2	1:A:228:ILE:HB	2.45	0.46
1:A:204:LYS:HA	2:A:302:IPA:C1	2.45	0.46
1:B:218:LEU:HB3	1:B:223:ILE:HB	1.97	0.45
1:B:197:VAL:HG13	1:B:198:ASN:H	1.80	0.45
1:B:35[A]:ASP:O	4:B:306:EDO:H11	2.17	0.45
1:A:227:THR:HG23	4:A:304:EDO:H11	1.98	0.45
1:A:227:THR:HB	2:A:302:IPA:C3	2.47	0.45
1:B:179:THR:CG2	1:B:228:ILE:HB	2.47	0.45
4:A:310:EDO:H12	4:A:313:EDO:H22	1.99	0.45
1:A:212:ARG:HG3	4:A:304:EDO:H21	2.00	0.44
1:B:179:THR:HA	4:B:305:EDO:C1	2.46	0.44
1:A:235:SER:HA	1:B:23:LEU:HD22	1.98	0.44
1:B:35[B]:ASP:O	4:B:306:EDO:H11	2.17	0.44
1:A:235:SER:HB2	10:A:424:HOH:O	2.18	0.43
10:A:437:HOH:O	1:B:256:MET:HE1	2.17	0.43
1:A:80:LEU:HB3	1:A:97:ALA:HB1	2.01	0.43
1:A:98:LEU:HA	5:A:314:PGE:H1	2.01	0.43
1:A:63:GLN:NE2	7:B:311:PG4:H51	2.29	0.42
1:B:115:LEU:O	1:B:119:LEU:HB2	2.20	0.41
1:A:210:HIS:CE1	4:A:313:EDO:H12	2.56	0.41
1:B:238:PHE:CD1	1:B:238:PHE:C	2.94	0.41
1:B:41:GLY:H	5:B:312:PGE:C4	2.34	0.41
1:A:27:LYS:NZ	10:A:410:HOH:O	2.54	0.41
1:B:247:HIS:CD2	1:B:259:PHE:HE1	2.38	0.41
1:B:41:GLY:CA	5:B:312:PGE:H6	2.51	0.41
1:A:72:ASP:OD2	6:A:317:PEG:H41	2.20	0.40
1:A:164:HIS:NE2	4:A:313:EDO:O1	2.24	0.40
1:B:143:GLU:O	1:B:146:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

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	244/283 (86%)	234 (96%)	10 (4%)	0	100	100
1	B	247/283 (87%)	241 (98%)	5 (2%)	1 (0%)	34	37
All	All	491/566 (87%)	475 (97%)	15 (3%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	16	ILE

5.3.2 Protein sidechains ⓘ

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	199/224 (89%)	194 (98%)	5 (2%)	47	60
1	B	203/224 (91%)	194 (96%)	9 (4%)	28	35
All	All	402/448 (90%)	388 (96%)	14 (4%)	38	46

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

Mol	Chain	Res	Type
1	A	18	ASP
1	A	19	GLU
1	A	43	LYS
1	A	235	SER
1	A	244	MET
1	B	14	GLU
1	B	16	ILE
1	B	142	GLU
1	B	238	PHE
1	B	248	ASP
1	B	252	GLU

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Mol	Chain	Res	Type
1	B	291[A]	TYR
1	B	291[B]	TYR
1	B	292	SER

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PEG	A	317	-	6,6,6	0.44	0	5,5,5	0.69	0
9	IMD	B	315	-	3,5,5	0.55	0	4,5,5	0.49	0
4	EDO	A	311	-	3,3,3	0.48	0	2,2,2	0.17	0
4	EDO	A	309	-	3,3,3	0.49	0	2,2,2	0.37	0
4	EDO	B	308	-	3,3,3	0.49	0	2,2,2	0.09	0
5	PGE	A	314	-	9,9,9	0.67	0	8,8,8	0.32	0
4	EDO	A	313	-	3,3,3	0.41	0	2,2,2	0.87	0
6	PEG	A	318	-	6,6,6	0.47	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IPA	A	302	-	3,3,3	0.29	0	3,3,3	0.76	0
4	EDO	A	305	-	3,3,3	0.62	0	2,2,2	0.17	0
4	EDO	A	308	-	3,3,3	0.51	0	2,2,2	0.68	0
4	EDO	A	312	-	3,3,3	0.45	0	2,2,2	0.16	0
4	EDO	A	307	-	3,3,3	0.42	0	2,2,2	0.67	0
4	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.12	0
4	EDO	A	304	-	3,3,3	0.45	0	2,2,2	0.62	0
2	IPA	A	301	-	3,3,3	0.49	0	3,3,3	0.90	0
7	PG4	B	311	-	12,12,12	0.76	0	11,11,11	0.58	0
6	PEG	A	316	-	6,6,6	0.45	0	5,5,5	0.57	0
4	EDO	A	306	-	3,3,3	0.43	0	2,2,2	0.13	0
6	PEG	A	315	-	6,6,6	0.39	0	5,5,5	0.83	0
4	EDO	B	309	-	3,3,3	0.34	0	2,2,2	0.30	0
4	EDO	A	310	-	3,3,3	0.80	0	2,2,2	2.49	1 (50%)
3	MES	A	303	-	12,12,12	1.27	2 (16%)	14,16,16	2.03	6 (42%)
6	PEG	B	313	-	6,6,6	0.51	0	5,5,5	0.77	0
4	EDO	B	307	-	3,3,3	0.41	0	2,2,2	0.21	0
4	EDO	B	310	-	3,3,3	0.39	0	2,2,2	0.16	0
9	IMD	B	316	-	3,5,5	0.57	0	4,5,5	0.48	0
4	EDO	B	306	-	3,3,3	0.60	0	2,2,2	0.22	0
5	PGE	B	312	-	9,9,9	0.71	0	8,8,8	0.57	0
4	EDO	B	305	-	3,3,3	0.36	0	2,2,2	0.30	0
4	EDO	B	303	-	3,3,3	0.43	0	2,2,2	0.08	0
2	IPA	B	301	-	3,3,3	0.48	0	3,3,3	0.53	0
4	EDO	B	302	-	3,3,3	0.56	0	2,2,2	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	317	-	-	1/4/4/4	-
9	IMD	B	315	-	-	-	0/1/1/1
4	EDO	A	311	-	-	1/1/1/1	-
4	EDO	A	309	-	-	0/1/1/1	-
4	EDO	B	308	-	-	1/1/1/1	-
5	PGE	A	314	-	-	3/7/7/7	-
4	EDO	A	313	-	-	0/1/1/1	-
6	PEG	A	318	-	-	4/4/4/4	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	A	308	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	312	-	-	1/1/1/1	-
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	A	304	-	-	1/1/1/1	-
6	PEG	A	316	-	-	2/4/4/4	-
4	EDO	A	306	-	-	0/1/1/1	-
6	PEG	A	315	-	-	2/4/4/4	-
4	EDO	B	309	-	-	1/1/1/1	-
4	EDO	A	310	-	-	1/1/1/1	-
3	MES	A	303	-	-	1/6/14/14	0/1/1/1
6	PEG	B	313	-	-	2/4/4/4	-
4	EDO	B	307	-	-	0/1/1/1	-
4	EDO	B	310	-	-	1/1/1/1	-
9	IMD	B	316	-	-	-	0/1/1/1
4	EDO	B	306	-	-	1/1/1/1	-
7	PG4	B	311	-	-	5/10/10/10	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
5	PGE	B	312	-	-	2/7/7/7	-
4	EDO	B	302	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	MES	C8-S	2.70	1.81	1.77
3	A	303	MES	O2S-S	2.12	1.51	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	MES	O3S-S-O1S	-3.99	101.52	111.27
4	A	310	EDO	O1-C1-C2	-3.53	86.55	111.91
3	A	303	MES	C5-N4-C3	3.15	115.92	108.83
3	A	303	MES	O3S-S-C8	3.11	110.80	105.77
3	A	303	MES	O2S-S-C8	2.40	109.81	106.92
3	A	303	MES	C7-N4-C3	-2.35	105.23	111.23
3	A	303	MES	O1S-S-C8	2.31	109.70	106.92

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	MES	N4-C7-C8-S
7	B	311	PG4	C4-C3-O2-C2
5	A	314	PGE	O2-C3-C4-O3
6	A	317	PEG	O1-C1-C2-O2
6	A	316	PEG	O2-C3-C4-O4
5	B	312	PGE	O1-C1-C2-O2
5	A	314	PGE	O3-C5-C6-O4
4	B	308	EDO	O1-C1-C2-O2
4	A	312	EDO	O1-C1-C2-O2
4	B	309	EDO	O1-C1-C2-O2
4	B	310	EDO	O1-C1-C2-O2
7	B	311	PG4	O1-C1-C2-O2
6	A	316	PEG	O1-C1-C2-O2
4	B	306	EDO	O1-C1-C2-O2
7	B	311	PG4	O3-C5-C6-O4
6	A	318	PEG	O1-C1-C2-O2
6	B	313	PEG	O1-C1-C2-O2
6	A	318	PEG	C1-C2-O2-C3
6	A	318	PEG	C4-C3-O2-C2
5	B	312	PGE	C3-C4-O3-C5
5	A	314	PGE	C6-C5-O3-C4
7	B	311	PG4	C3-C4-O3-C5
6	A	318	PEG	O2-C3-C4-O4
4	A	304	EDO	O1-C1-C2-O2
6	B	313	PEG	C1-C2-O2-C3
7	B	311	PG4	O2-C3-C4-O3
6	A	315	PEG	O2-C3-C4-O4
6	A	315	PEG	C1-C2-O2-C3
4	B	304	EDO	O1-C1-C2-O2
4	A	311	EDO	O1-C1-C2-O2
4	A	310	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	317	PEG	2	0
5	A	314	PGE	2	0
4	A	313	EDO	4	0
6	A	318	PEG	2	0
2	A	302	IPA	3	0
4	A	304	EDO	3	0
2	A	301	IPA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	311	PG4	3	0
4	B	309	EDO	1	0
4	A	310	EDO	1	0
4	B	306	EDO	2	0
5	B	312	PGE	3	0
4	B	305	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	251/283 (88%)	0.10	13 (5%) 27 26	34, 50, 110, 175	0
1	B	250/283 (88%)	0.33	24 (9%) 8 6	35, 47, 113, 153	0
All	All	501/566 (88%)	0.22	37 (7%) 14 13	34, 49, 113, 175	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	MET	8.0
1	B	17	PHE	8.0
1	B	12	THR	7.1
1	B	197	VAL	6.5
1	A	245	PRO	6.0
1	B	249	ALA	5.6
1	B	13	VAL	5.5
1	B	16	ILE	5.3
1	B	293	VAL	4.8
1	B	15	GLN	4.8
1	B	145	TRP	4.7
1	B	250	MET	4.6
1	B	238	PHE	4.3
1	A	17	PHE	4.1
1	B	144	VAL	3.8
1	B	247	HIS	3.8
1	A	248	ASP	3.6
1	A	145	TRP	3.4
1	B	14	GLU	3.3
1	B	142	GLU	3.2
1	A	143	GLU	3.2
1	B	237	ILE	3.0
1	A	243	ASP	3.0
1	A	197	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	183	SER	2.7
1	A	141	THR	2.7
1	B	199	ALA	2.7
1	B	198	ASN	2.6
1	A	247	HIS	2.4
1	B	20	ARG	2.3
1	B	251	LEU	2.3
1	A	144	VAL	2.3
1	B	146	THR	2.2
1	B	85	LYS	2.1
1	A	132	ASN	2.1
1	B	259	PHE	2.1
1	B	253	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
6	PEG	A	318	7/7	0.41	0.57	85,107,129,129	0
6	PEG	A	315	7/7	0.59	0.31	96,134,162,166	0
4	EDO	A	312	4/4	0.62	0.72	71,99,121,121	0
6	PEG	B	313	7/7	0.62	0.33	81,104,141,141	0
4	EDO	B	306	4/4	0.67	0.24	75,90,104,104	0
5	PGE	B	312	10/10	0.69	0.36	68,112,143,144	0
7	PG4	B	311	13/13	0.70	0.37	70,90,121,135	0
6	PEG	A	317	7/7	0.71	0.30	70,103,170,170	0
4	EDO	B	310	4/4	0.76	0.39	77,100,121,126	0
4	EDO	B	303	4/4	0.76	0.36	76,92,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	313	4/4	0.77	0.55	94,136,167,167	0
4	EDO	A	310	4/4	0.80	0.28	74,97,122,133	0
6	PEG	A	316	7/7	0.82	0.28	66,89,147,147	0
5	PGE	A	314	10/10	0.83	0.40	76,99,113,119	0
4	EDO	A	305	4/4	0.83	0.26	56,67,81,81	0
4	EDO	A	311	4/4	0.84	0.26	69,88,94,106	0
2	IPA	B	301	4/4	0.84	0.14	46,58,80,86	0
4	EDO	B	304	4/4	0.85	0.15	63,79,96,96	0
9	IMD	B	315	5/5	0.87	0.30	86,98,113,118	10
4	EDO	A	306	4/4	0.89	0.19	63,85,87,104	0
9	IMD	B	316	5/5	0.89	0.45	107,114,137,137	10
4	EDO	B	308	4/4	0.89	0.35	61,74,87,87	0
3	MES	A	303	12/12	0.90	0.26	68,91,110,112	0
4	EDO	A	308	4/4	0.90	0.44	60,72,82,82	0
4	EDO	A	309	4/4	0.90	0.22	52,75,93,93	0
4	EDO	A	307	4/4	0.90	0.17	57,79,96,97	0
4	EDO	A	304	4/4	0.91	0.18	43,68,72,82	0
2	IPA	A	301	4/4	0.91	0.20	39,49,67,81	0
2	IPA	A	302	4/4	0.91	0.28	58,70,96,96	0
4	EDO	B	309	4/4	0.92	0.21	58,86,98,118	0
8	CL	B	314	1/1	0.93	0.39	81,81,81,81	0
4	EDO	B	305	4/4	0.94	0.12	60,73,89,107	0
4	EDO	B	307	4/4	0.97	0.09	51,62,64,68	0
4	EDO	B	302	4/4	0.97	0.12	42,51,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.