Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 06:32 AM EST

PDB ID	:	3O4P
Title	:	DFPase at 0.85 Angstrom resolution (H atoms included)
Authors	:	Liebschner, D.; Elias, M.; Koepke, J.; Lecomte, C.; Guillot, B.; Jelsch, C.; Chabriere, E.
Deposited on	:	2010-07-27
Resolution	:	0.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

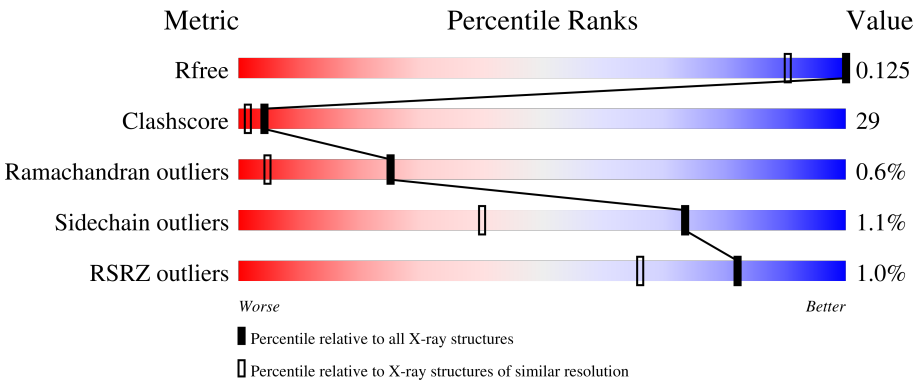
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 0.85 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	1071 (1.04-0.70)
Clashscore	141614	1143 (1.04-0.68)
Ramachandran outliers	138981	1065 (1.04-0.68)
Sidechain outliers	138945	1066 (1.04-0.68)
RSRZ outliers	127900	1038 (1.04-0.70)

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	% 74% 21%

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
2	GOL	A	401	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	A	411	-	-	X	-
3	MES	A	412	-	-	X	-
4	EDO	A	423	-	-	X	-
4	EDO	A	425	-	-	X	-
4	EDO	A	427	-	-	X	-
5	PGE	A	434	-	X	X	-
6	DXE	A	443	-	-	X	-
7	MXE	A	451	-	X	X	-
7	MXE	A	452	-	-	X	-
8	PEG	A	461	-	X	X	-
9	ME2	A	471	-	-	X	-

2 Entry composition (i)

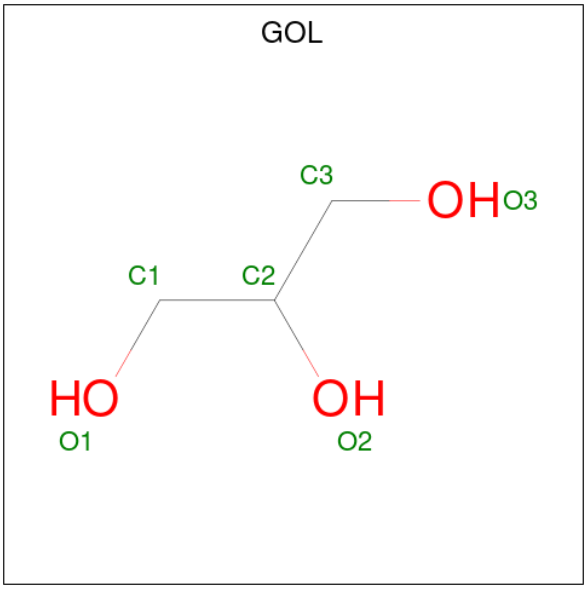
There are 11 unique types of molecules in this entry. The entry contains 5370 atoms, of which 2096 are hydrogens and 0 are deuteriums.

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 Diisopropyl-fluorophosphatase.

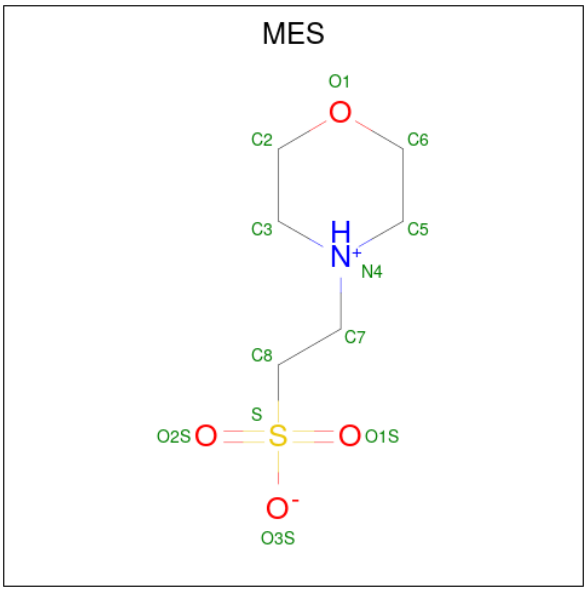
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	314	4722	1688	2065	456	495	18	0	46	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



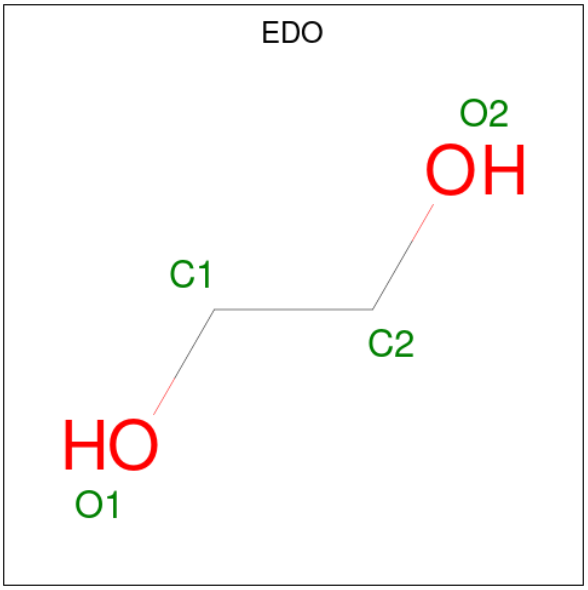
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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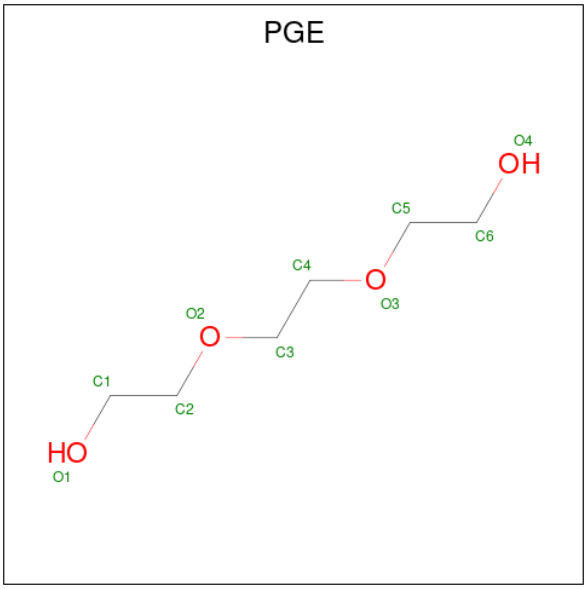
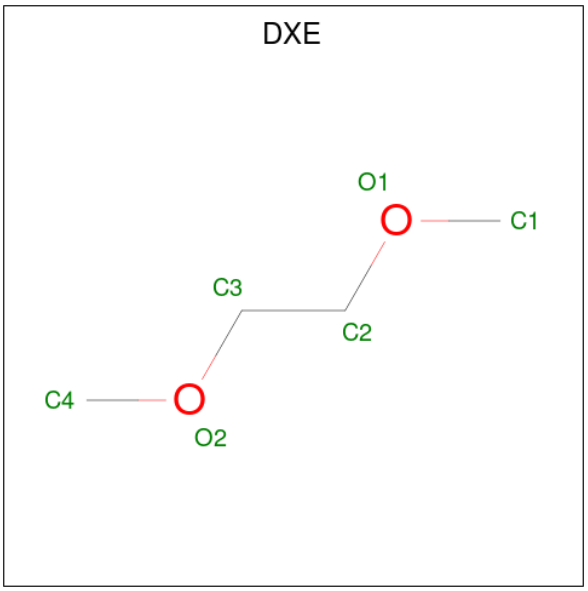
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



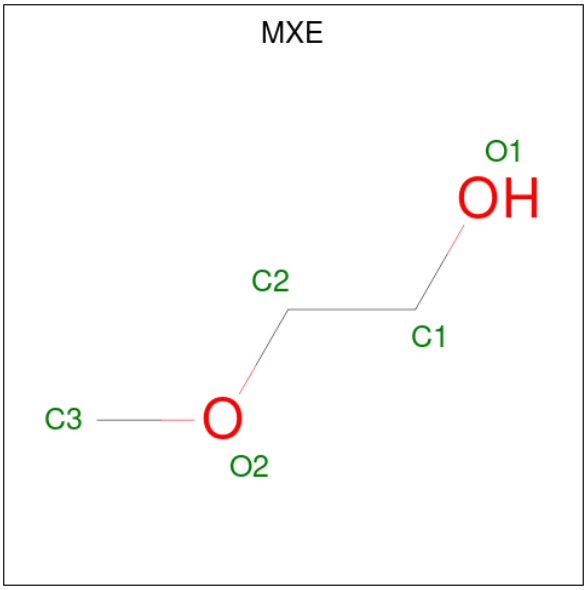
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	10	6	4		0	0
			Total	C	O			
5	A	1	10	6	4		0	0

- Molecule 6 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: $C_4H_{10}O_2$).



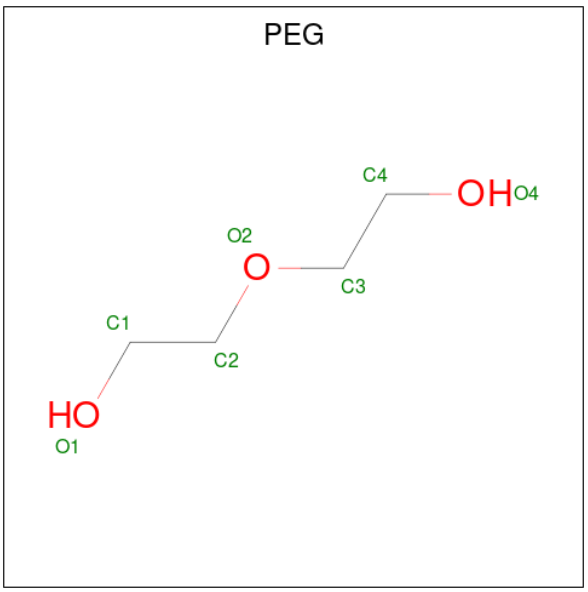
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	4	2	0	0
			Total	C	O		
6	A	1	6	4	2	0	0

- Molecule 7 is 2-METHOXYETHANOL (three-letter code: MXE) (formula: $C_3H_8O_2$).



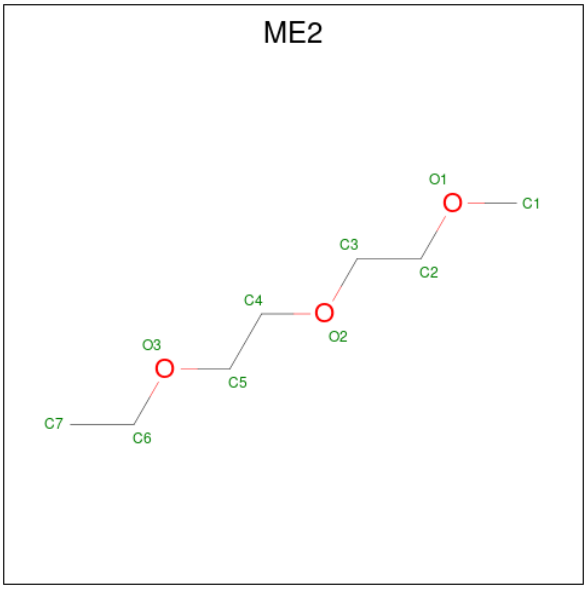
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	5	3	2	0	0
			Total	C	O		
7	A	1	5	3	2	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	7	4	3	0	0
			Total	C	O		
8	A	1	7	4	3	0	0

- Molecule 9 is 1-ETHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: ME2) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	10	7	3	0	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
10	A	2	2	2	0	0

- Molecule 11 is water.

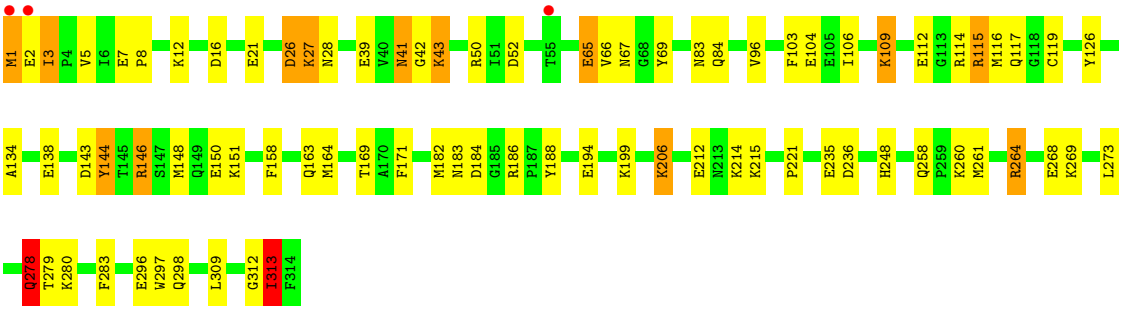
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
11	A	466	512	31	481	0	15

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: Diisopropyl-fluorophosphatase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	43.11Å 81.85Å 86.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.80 – 0.85 20.92 – 0.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.80-0.85) 86.3 (20.92-0.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 0.83Å)	Xtriage
Refinement program	MoPro	Depositor
R, R_{free}	0.103 , 0.121 0.110 , 0.125	Depositor DCC
R_{free} test set	2584 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	6.3	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 88.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	5370	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ME2, MES, CA, MXE, PGE, GOL, EDO, PEG, DXE

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	1.59	37/2949 (1.3%)	1.67	53/3975 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ARG	NE-CZ	-22.21	1.04	1.33
1	A	278	GLN	CD-OE1	19.77	1.67	1.24
1	A	39	GLU	CD-OE1	19.76	1.47	1.25
1	A	41	ASN	CB-CG	17.99	1.92	1.51
1	A	41	ASN	CG-OD1	17.60	1.62	1.24
1	A	112	GLU	CD-OE2	-16.37	1.07	1.25
1	A	150	GLU	CD-OE2	15.62	1.42	1.25
1	A	264	ARG	CZ-NH2	13.17	1.50	1.33
1	A	109	LYS	CD-CE	11.89	1.80	1.51
1	A	27	LYS	CE-NZ	-10.46	1.23	1.49
1	A	67	ASN	CG-OD1	10.46	1.47	1.24
1	A	65	GLU	CD-OE2	10.26	1.36	1.25
1	A	298	GLN	CD-OE1	-9.54	1.02	1.24
1	A	150	GLU	CG-CD	-9.16	1.38	1.51
1	A	28	ASN	CG-OD1	9.11	1.44	1.24
1	A	183	ASN	CG-ND2	8.39	1.53	1.32
1	A	41	ASN	CA-CB	8.23	1.74	1.53
1	A	264	ARG	CD-NE	7.65	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	LYS	CE-NZ	7.63	1.68	1.49
1	A	112	GLU	CB-CG	7.50	1.66	1.52
1	A	42	GLY	C-O	-7.09	1.12	1.23
1	A	104	GLU	CG-CD	-7.07	1.41	1.51
1	A	278	GLN	CG-CD	-6.94	1.35	1.51
1	A	235	GLU	CG-CD	6.60	1.61	1.51
1	A	183	ASN	CG-OD1	-6.56	1.09	1.24
1	A	39	GLU	CD-OE2	-6.52	1.18	1.25
1	A	109	LYS	CE-NZ	6.21	1.64	1.49
1	A	104	GLU	CD-OE1	5.95	1.32	1.25
1	A	199	LYS	CE-NZ	-5.92	1.34	1.49
1	A	52	ASP	CG-OD1	-5.88	1.11	1.25
1	A	28	ASN	CG-ND2	-5.72	1.18	1.32
1	A	183	ASN	CB-CG	5.65	1.64	1.51
1	A	67	ASN	CG-ND2	-5.61	1.18	1.32
1	A	112	GLU	CA-CB	5.39	1.65	1.53
1	A	16	ASP	CG-OD2	5.14	1.37	1.25
1	A	39	GLU	CG-CD	-5.08	1.44	1.51
1	A	12	LYS	CD-CE	-5.04	1.38	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	ARG	NE-CZ-NH1	24.49	132.54	120.30
1	A	186[A]	ARG	NE-CZ-NH2	18.20	129.40	120.30
1	A	186[B]	ARG	NE-CZ-NH2	18.20	129.40	120.30
1	A	43	LYS	CG-CD-CE	16.62	161.75	111.90
1	A	115[A]	ARG	CD-NE-CZ	15.70	145.57	123.60
1	A	115[B]	ARG	CD-NE-CZ	15.70	145.57	123.60
1	A	115[A]	ARG	NE-CZ-NH2	15.44	128.02	120.30
1	A	115[B]	ARG	NE-CZ-NH2	15.44	128.02	120.30
1	A	186[A]	ARG	CD-NE-CZ	14.30	143.62	123.60
1	A	186[B]	ARG	CD-NE-CZ	14.30	143.62	123.60
1	A	41	ASN	OD1-CG-ND2	11.83	149.11	121.90
1	A	43	LYS	CD-CE-NZ	11.40	137.91	111.70
1	A	112	GLU	CG-CD-OE1	-10.72	96.86	118.30
1	A	264	ARG	NH1-CZ-NH2	-10.64	107.70	119.40
1	A	114[A]	ARG	CD-NE-CZ	9.87	137.42	123.60
1	A	114[B]	ARG	CD-NE-CZ	9.87	137.42	123.60
1	A	186[A]	ARG	NE-CZ-NH1	-9.58	115.51	120.30
1	A	186[B]	ARG	NE-CZ-NH1	-9.58	115.51	120.30
1	A	41	ASN	CB-CG-ND2	-9.57	93.73	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143[A]	ASP	CB-CG-OD1	-8.65	110.52	118.30
1	A	143[B]	ASP	CB-CG-OD1	-8.65	110.52	118.30
1	A	1[A]	MET	C-N-CA	8.50	142.95	121.70
1	A	1[B]	MET	C-N-CA	8.50	142.95	121.70
1	A	169[A]	THR	CA-CB-CG2	-7.94	101.28	112.40
1	A	169[B]	THR	CA-CB-CG2	-7.94	101.28	112.40
1	A	182	MET	CG-SD-CE	-7.76	87.78	100.20
1	A	236	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	A	146[A]	ARG	CB-CA-C	-7.59	95.22	110.40
1	A	146[B]	ARG	CB-CA-C	-7.59	95.22	110.40
1	A	114[A]	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	114[B]	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	112	GLU	OE1-CD-OE2	6.72	131.37	123.30
1	A	126	TYR	CB-CG-CD2	6.61	124.97	121.00
1	A	150	GLU	CG-CD-OE1	6.57	131.44	118.30
1	A	115[A]	ARG	NH1-CZ-NH2	-6.54	112.20	119.40
1	A	115[B]	ARG	NH1-CZ-NH2	-6.54	112.20	119.40
1	A	235	GLU	OE1-CD-OE2	6.38	130.96	123.30
1	A	112	GLU	CG-CD-OE2	6.10	130.50	118.30
1	A	67	ASN	CB-CG-OD1	-5.99	109.62	121.60
1	A	309	LEU	CB-CG-CD2	5.93	121.07	111.00
1	A	184	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	188	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	150	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	A	114[A]	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	114[B]	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	52	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	188	TYR	CD1-CG-CD2	5.49	123.94	117.90
1	A	184	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	143[A]	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	143[B]	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	144	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	188	TYR	CG-CD2-CE2	-5.11	117.21	121.30
1	A	26	ASP	CB-CG-OD2	-5.08	113.73	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLN	Sidechain

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	2657	2065	2566	135	0
2	A	12	0	9	0	0
3	A	24	0	26	16	0
4	A	32	0	48	30	0
5	A	20	0	28	15	0
6	A	12	0	20	12	0
7	A	10	0	16	22	0
8	A	14	0	20	7	0
9	A	10	0	16	9	0
10	A	2	0	0	0	0
11	A	481	31	0	38	0
All	All	3274	2096	2749	166	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 29.

All (166) 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:109:LYS:CD	1:A:109:LYS:CE	1.81	1.58
1:A:41:ASN:CA	1:A:41:ASN:CB	1.74	1.57
1:A:43:LYS:CE	1:A:43:LYS:NZ	1.68	1.55
1:A:41:ASN:CB	1:A:41:ASN:CG	1.92	1.38
1:A:43:LYS:NZ	3:A:411:MES:H31	1.34	1.38
1:A:278:GLN:OE1	1:A:278:GLN:CD	1.67	1.32
1:A:50[C]:ARG:CZ	11:A:1039:HOH:O	1.78	1.27
1:A:146[B]:ARG:NH2	11:A:948:HOH:O	1.70	1.22
1:A:2[B]:GLU:CA	11:A:861:HOH:O	1.88	1.21
4:A:423:EDO:O1	11:A:959:HOH:O	1.57	1.20
1:A:115[B]:ARG:HD3	4:A:423:EDO:O2	1.40	1.17
1:A:96[A]:VAL:HG23	1:A:106[A]:ILE:HD11	1.16	1.16
1:A:260[B]:LYS:NZ	4:A:427:EDO:H22	1.60	1.15
1:A:2[B]:GLU:CA	1:A:3[B]:ILE:HB	1.81	1.11
1:A:151[B]:LYS:HE3	7:A:452:MXE:H32	1.31	1.09
1:A:215[C]:LYS:HE2	11:A:1046:HOH:O	0.92	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:443:DXE:H43	11:A:770:HOH:O	1.56	1.05
4:A:428:EDO:H12	11:A:1082:HOH:O	1.54	1.04
1:A:312[B]:GLY:C	1:A:313[B]:ILE:HG13	1.74	1.03
1:A:280[B]:LYS:HE2	5:A:434:PGE:O3	1.60	1.02
1:A:264:ARG:HH11	9:A:471:ME2:H51	1.20	1.01
4:A:425:EDO:H21	11:A:876:HOH:O	1.62	0.98
1:A:50[A]:ARG:NH2	11:A:1040:HOH:O	1.95	0.97
1:A:43:LYS:NZ	3:A:411:MES:C3	2.28	0.96
1:A:50[C]:ARG:NH2	11:A:1039:HOH:O	1.83	0.96
1:A:312[B]:GLY:O	1:A:313[B]:ILE:HG13	1.64	0.95
1:A:96[A]:VAL:CG2	1:A:106[A]:ILE:HD11	1.98	0.94
1:A:151[B]:LYS:HE3	7:A:452:MXE:C3	1.97	0.93
1:A:151[A]:LYS:HZ3	7:A:452:MXE:H31	1.33	0.93
1:A:43:LYS:HZ3	3:A:411:MES:H31	1.10	0.93
1:A:43:LYS:HZ2	3:A:411:MES:H31	1.16	0.90
1:A:151[A]:LYS:NZ	7:A:452:MXE:H31	1.86	0.90
1:A:50[A]:ARG:CZ	11:A:1040:HOH:O	2.19	0.90
1:A:296:GLU:HB2	6:A:443:DXE:H42	1.54	0.90
9:A:471:ME2:O2	9:A:471:ME2:H62	1.73	0.87
1:A:41:ASN:CB	1:A:41:ASN:ND2	2.38	0.85
1:A:260[B]:LYS:HZ3	4:A:427:EDO:H22	1.39	0.84
1:A:115[B]:ARG:CD	4:A:423:EDO:O2	2.22	0.84
1:A:43:LYS:HZ3	3:A:411:MES:C3	1.86	0.84
1:A:116[A]:MET:HE3	1:A:164:MET:HG2	1.60	0.83
1:A:260[B]:LYS:HZ2	4:A:427:EDO:H22	1.43	0.83
1:A:215[C]:LYS:CE	11:A:1046:HOH:O	1.65	0.82
1:A:171[B]:PHE:CD2	7:A:452:MXE:H21	2.15	0.82
1:A:151[B]:LYS:CE	7:A:452:MXE:C3	2.59	0.81
1:A:312[B]:GLY:O	1:A:313[B]:ILE:CG1	2.29	0.80
1:A:109:LYS:CE	1:A:109:LYS:CG	2.58	0.80
1:A:296:GLU:O	6:A:443:DXE:C4	2.29	0.80
1:A:65:GLU:O	3:A:412:MES:H61	1.81	0.79
5:A:434:PGE:C6	11:A:544:HOH:O	2.28	0.79
1:A:264:ARG:NH1	9:A:471:ME2:H51	1.96	0.79
1:A:296:GLU:O	6:A:443:DXE:H41	1.81	0.79
1:A:116[A]:MET:CE	1:A:164:MET:HG2	2.14	0.77
1:A:312[B]:GLY:C	1:A:313[B]:ILE:CG1	2.52	0.77
1:A:268[A]:GLU:OE1	11:A:1014:HOH:O	2.01	0.77
4:A:424:EDO:H11	5:A:433:PGE:H42	1.66	0.77
1:A:151[B]:LYS:HE2	7:A:452:MXE:H31	1.66	0.76
1:A:103:PHE:CZ	3:A:412:MES:H52	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163[B]:GLN:NE2	11:A:978:HOH:O	2.19	0.76
1:A:260[B]:LYS:NZ	4:A:427:EDO:C2	2.47	0.74
1:A:260[B]:LYS:CE	4:A:427:EDO:H22	2.20	0.72
1:A:43:LYS:HZ2	3:A:411:MES:C3	1.96	0.72
7:A:452:MXE:H33	11:A:531:HOH:O	1.89	0.72
1:A:50[A]:ARG:NE	11:A:1040:HOH:O	2.22	0.71
5:A:434:PGE:H62	11:A:544:HOH:O	1.90	0.71
1:A:151[B]:LYS:CE	7:A:452:MXE:H32	2.16	0.71
1:A:221:PRO:HA	4:A:425:EDO:H11	1.72	0.70
1:A:151[B]:LYS:CE	7:A:452:MXE:H31	2.20	0.70
1:A:103:PHE:CE1	3:A:412:MES:H52	2.26	0.69
1:A:260[A]:LYS:HE3	11:A:942:HOH:O	1.91	0.69
1:A:106[B]:ILE:HD12	8:A:461:PEG:C4	2.23	0.69
1:A:41:ASN:CB	1:A:41:ASN:C	2.59	0.68
1:A:214[A]:LYS:NZ	7:A:452:MXE:H11	2.08	0.68
4:A:421:EDO:H22	11:A:859:HOH:O	1.93	0.68
5:A:433:PGE:H5	11:A:644:HOH:O	1.92	0.68
1:A:26:ASP:HB2	1:A:83:ASN:HD21	1.59	0.67
1:A:171[B]:PHE:CD2	7:A:452:MXE:C2	2.77	0.67
1:A:248:HIS:NE2	9:A:471:ME2:H52	2.10	0.66
1:A:115[B]:ARG:HD2	1:A:138[B]:GLU:OE2	1.96	0.65
1:A:260[B]:LYS:HZ2	4:A:427:EDO:C2	2.07	0.65
1:A:258:GLN:NE2	4:A:425:EDO:O1	2.30	0.64
4:A:424:EDO:H11	5:A:433:PGE:C4	2.28	0.64
1:A:41:ASN:CB	1:A:41:ASN:N	2.59	0.63
1:A:69:TYR:CD1	3:A:411:MES:H81	2.33	0.63
1:A:215[C]:LYS:NZ	11:A:1046:HOH:O	2.08	0.63
4:A:426:EDO:H11	5:A:433:PGE:O4	1.99	0.62
1:A:258:GLN:H	4:A:427:EDO:H11	1.64	0.61
5:A:434:PGE:H42	11:A:735:HOH:O	1.99	0.61
1:A:65:GLU:HG3	8:A:462:PEG:H42	1.82	0.60
1:A:8:PRO:HB3	6:A:443:DXE:C4	2.32	0.60
1:A:279:THR:HB	5:A:434:PGE:H2	1.84	0.58
4:A:428:EDO:C1	11:A:1082:HOH:O	2.30	0.58
1:A:106[B]:ILE:CD1	8:A:461:PEG:C4	2.82	0.58
4:A:422:EDO:H21	11:A:517:HOH:O	2.04	0.58
4:A:425:EDO:C2	11:A:876:HOH:O	2.35	0.57
1:A:115[B]:ARG:HD3	4:A:423:EDO:C2	2.34	0.57
1:A:27:LYS:H	1:A:83:ASN:ND2	2.01	0.57
4:A:421:EDO:C2	11:A:859:HOH:O	2.51	0.55
1:A:264:ARG:HH11	9:A:471:ME2:C5	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2[B]:GLU:N	11:A:861:HOH:O	2.24	0.55
1:A:8:PRO:HB3	6:A:443:DXE:H41	1.90	0.54
1:A:84:GLN:HE22	8:A:461:PEG:H22	1.72	0.54
1:A:69:TYR:CE1	3:A:411:MES:H81	2.43	0.53
1:A:66:VAL:HG22	3:A:412:MES:H22	1.91	0.53
7:A:451:MXE:H33	11:A:859:HOH:O	2.09	0.53
1:A:258:GLN:N	4:A:427:EDO:H11	2.24	0.53
9:A:471:ME2:O2	9:A:471:ME2:C6	2.51	0.52
1:A:27:LYS:H	1:A:83:ASN:HD21	1.57	0.52
1:A:214[A]:LYS:HZ1	7:A:452:MXE:H11	1.75	0.52
1:A:248:HIS:NE2	9:A:471:ME2:C5	2.73	0.51
1:A:106[B]:ILE:HD12	8:A:461:PEG:H42	1.92	0.51
1:A:41:ASN:CB	1:A:41:ASN:HD22	2.23	0.51
1:A:7[B]:GLU:OE1	9:A:471:ME2:H21	2.12	0.49
7:A:451:MXE:C3	11:A:859:HOH:O	2.60	0.49
1:A:27:LYS:NZ	11:A:862[B]:HOH:O	2.45	0.49
1:A:151[A]:LYS:NZ	7:A:452:MXE:C3	2.68	0.49
1:A:258:GLN:HE22	4:A:425:EDO:C1	2.26	0.49
1:A:206[B]:LYS:HE3	1:A:212[B]:GLU:OE1	2.13	0.49
1:A:106[B]:ILE:CD1	8:A:461:PEG:H42	2.43	0.48
1:A:148[A]:MET:HG3	5:A:433:PGE:O4	2.13	0.48
5:A:434:PGE:H62	5:A:434:PGE:H4	1.69	0.47
1:A:116[A]:MET:HE2	1:A:116[A]:MET:HB2	1.73	0.46
1:A:116[A]:MET:HE1	1:A:164:MET:HG2	1.95	0.46
1:A:297:TRP:O	6:A:443:DXE:H13	2.16	0.46
4:A:422:EDO:C1	11:A:517:HOH:O	2.63	0.46
1:A:8:PRO:CB	6:A:443:DXE:C4	2.95	0.45
1:A:258:GLN:H	4:A:427:EDO:C1	2.27	0.45
1:A:5:VAL:O	9:A:471:ME2:H13	2.16	0.45
1:A:144:TYR:OH	1:A:146[A]:ARG:HD3	2.17	0.44
1:A:50[C]:ARG:NH1	11:A:1042:HOH:O	1.87	0.44
1:A:258:GLN:O	4:A:427:EDO:H21	2.18	0.44
6:A:443:DXE:H32	11:A:770:HOH:O	2.17	0.44
1:A:41:ASN:CB	1:A:41:ASN:O	2.66	0.43
1:A:158:PHE:CE2	4:A:422:EDO:H12	2.52	0.43
1:A:69:TYR:CE1	3:A:411:MES:H51	2.53	0.43
1:A:43:LYS:CE	3:A:411:MES:H71	2.48	0.43
1:A:65:GLU:HG3	8:A:462:PEG:C4	2.48	0.43
3:A:412:MES:O2S	11:A:1129:HOH:O	2.19	0.43
1:A:151[A]:LYS:HZ1	7:A:452:MXE:H31	1.76	0.42
1:A:8:PRO:CB	6:A:443:DXE:H41	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:OE1	7:A:452:MXE:C3	2.68	0.42
1:A:194:GLU:OE1	7:A:452:MXE:H32	2.19	0.42
1:A:296:GLU:OE2	5:A:434:PGE:H22	2.19	0.42
1:A:296:GLU:CB	6:A:443:DXE:H42	2.36	0.42
1:A:269:LYS:HZ3	6:A:442:DXE:C1	2.31	0.42
1:A:163[B]:GLN:CD	11:A:978:HOH:O	2.54	0.42
1:A:171[B]:PHE:CE2	7:A:452:MXE:C2	3.03	0.42
1:A:261[B]:MET:HB2	1:A:261[B]:MET:HE2	1.64	0.42
1:A:212[A]:GLU:HG3	11:A:997:HOH:O	2.20	0.41
3:A:412:MES:H51	3:A:412:MES:H81	1.33	0.41
1:A:260[B]:LYS:HD3	4:A:427:EDO:C2	2.50	0.41
1:A:212[A]:GLU:OE2	11:A:997:HOH:O	2.20	0.41
1:A:41:ASN:CA	1:A:41:ASN:HD22	2.33	0.41
1:A:116[A]:MET:HG3	1:A:117:GLN:N	2.36	0.40
1:A:119:CYS:HA	1:A:134:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

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	360/314 (115%)	343 (95%)	13 (4%)	4 (1%)	14 2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3[A]	ILE
1	A	3[B]	ILE
1	A	313[A]	ILE
1	A	313[B]	ILE

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	307/263 (117%)	302 (98%)	5 (2%)	62 27

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	206[A]	LYS
1	A	206[B]	LYS
1	A	313[A]	ILE
1	A	313[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	83	ASN
1	A	258	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
4	EDO	A	428	-	3,3,3	0.92	0	2,2,2	0.42	0
4	EDO	A	422	-	3,3,3	0.65	0	2,2,2	2.49	2 (100%)
4	EDO	A	426	-	3,3,3	1.21	0	2,2,2	0.60	0
4	EDO	A	423	-	3,3,3	0.89	0	2,2,2	1.88	1 (50%)
7	MXE	A	452	-	4,4,4	0.47	0	3,3,3	3.48	2 (66%)
4	EDO	A	421	-	3,3,3	0.56	0	2,2,2	0.60	0
5	PGE	A	433	-	9,9,9	0.99	0	8,8,8	1.77	3 (37%)
3	MES	A	411	-	12,12,12	2.35	5 (41%)	14,16,16	4.39	9 (64%)
4	EDO	A	425	-	3,3,3	0.76	0	2,2,2	0.77	0
6	DXE	A	442	-	5,5,5	0.56	0	4,4,4	2.96	3 (75%)
2	GOL	A	403	-	5,5,5	3.66	4 (80%)	5,5,5	1.09	1 (20%)
5	PGE	A	434	-	9,9,9	1.07	0	8,8,8	2.21	5 (62%)
4	EDO	A	424	-	3,3,3	0.95	0	2,2,2	0.07	0
6	DXE	A	443	-	5,5,5	0.68	0	4,4,4	1.75	1 (25%)
2	GOL	A	401	-	5,5,5	4.00	3 (60%)	5,5,5	2.47	2 (40%)
8	PEG	A	462	-	6,6,6	1.17	0	5,5,5	2.09	1 (20%)
8	PEG	A	461	-	6,6,6	0.70	0	5,5,5	3.34	4 (80%)
4	EDO	A	427	-	3,3,3	0.52	0	2,2,2	1.97	1 (50%)
3	MES	A	412	-	12,12,12	1.73	4 (33%)	14,16,16	2.55	7 (50%)
9	ME2	A	471	-	9,9,9	0.96	0	8,8,8	1.07	1 (12%)
7	MXE	A	451	-	4,4,4	0.90	0	3,3,3	4.75	2 (66%)

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
4	EDO	A	428	-	-	0/1/1/1	-
4	EDO	A	422	-	-	0/1/1/1	-
4	EDO	A	426	-	-	0/1/1/1	-
4	EDO	A	423	-	-	1/1/1/1	-
7	MXE	A	452	-	-	1/2/2/2	-
4	EDO	A	421	-	-	0/1/1/1	-
5	PGE	A	433	-	-	6/7/7/7	-
3	MES	A	411	-	-	0/6/14/14	0/1/1/1
4	EDO	A	425	-	-	1/1/1/1	-
6	DXE	A	442	-	-	1/3/3/3	-
2	GOL	A	403	-	-	0/4/4/4	-
5	PGE	A	434	-	-	7/7/7/7	-
4	EDO	A	424	-	-	0/1/1/1	-
6	DXE	A	443	-	-	2/3/3/3	-
2	GOL	A	401	-	-	2/4/4/4	-
8	PEG	A	462	-	-	3/4/4/4	-
8	PEG	A	461	-	-	2/4/4/4	-
4	EDO	A	427	-	-	1/1/1/1	-
3	MES	A	412	-	-	0/6/14/14	0/1/1/1
9	ME2	A	471	-	-	6/7/7/7	-
7	MXE	A	451	-	-	2/2/2/2	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GOL	C3-C2	-7.47	1.21	1.51
2	A	403	GOL	C3-C2	-6.45	1.25	1.51
3	A	411	MES	O2S-S	4.33	1.57	1.45
3	A	411	MES	C8-S	3.95	1.83	1.77
3	A	412	MES	C5-N4	3.61	1.56	1.46
2	A	403	GOL	O3-C3	3.58	1.57	1.42
3	A	412	MES	O1S-S	-3.29	1.35	1.45
2	A	401	GOL	O1-C1	3.25	1.56	1.42
3	A	411	MES	C7-N4	3.09	1.54	1.47
3	A	411	MES	O3S-S	-3.03	1.37	1.47
2	A	401	GOL	O3-C3	2.92	1.54	1.42
2	A	403	GOL	O1-C1	2.88	1.54	1.42
3	A	412	MES	C3-N4	2.24	1.53	1.46
3	A	412	MES	C7-N4	2.13	1.52	1.47
3	A	411	MES	C3-N4	2.07	1.52	1.46
2	A	403	GOL	C1-C2	-2.01	1.43	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	411	MES	O1S-S-C8	-8.88	96.23	106.92
3	A	411	MES	O3S-S-O1S	8.40	131.79	111.27
7	A	451	MXE	C3-O2-C2	6.69	154.61	112.96
3	A	411	MES	O3S-S-C8	-6.66	95.00	105.77
3	A	412	MES	C2-C3-N4	-5.55	101.69	110.10
8	A	461	PEG	O2-C2-C1	5.53	134.38	110.07
3	A	411	MES	O2S-S-C8	-5.45	100.35	106.92
7	A	452	MXE	C3-O2-C2	4.89	143.40	112.96
7	A	451	MXE	O1-C1-C2	4.44	137.56	111.81
8	A	462	PEG	O2-C3-C4	4.29	128.91	110.07
3	A	412	MES	C7-N4-C5	-4.05	100.89	111.23
3	A	411	MES	C2-C3-N4	-3.98	104.07	110.10
5	A	434	PGE	O2-C2-C1	3.91	127.27	110.07
2	A	401	GOL	O2-C2-C3	3.89	126.25	109.12
6	A	442	DXE	O1-C2-C3	3.74	139.62	111.07
6	A	442	DXE	C1-O1-C2	3.66	135.73	112.96
5	A	433	PGE	C5-O3-C4	3.49	128.39	113.29
7	A	452	MXE	O1-C1-C2	3.47	131.94	111.81
8	A	461	PEG	C3-O2-C2	3.18	127.06	113.29
2	A	401	GOL	O3-C3-C2	3.13	125.22	110.20
8	A	461	PEG	O2-C3-C4	3.04	123.42	110.07
3	A	411	MES	C7-N4-C5	-3.00	103.56	111.23
3	A	412	MES	O2S-S-C8	-2.87	103.46	106.92
3	A	411	MES	C7-N4-C3	-2.78	104.12	111.23
6	A	442	DXE	O2-C3-C2	2.71	131.75	111.07
4	A	422	EDO	O1-C1-C2	2.70	131.34	111.91
3	A	412	MES	C5-N4-C3	-2.67	102.81	108.83
6	A	443	DXE	O1-C2-C3	2.67	131.42	111.07
5	A	434	PGE	O3-C4-C3	2.58	122.01	110.39
3	A	411	MES	C6-C5-N4	2.53	113.93	110.10
3	A	412	MES	O3S-S-C8	2.45	109.74	105.77
9	A	471	ME2	O1-C2-C3	2.42	129.49	111.07
4	A	423	EDO	O1-C1-C2	2.38	129.01	111.91
3	A	412	MES	O1S-S-C8	2.37	109.77	106.92
5	A	434	PGE	O1-C1-C2	2.33	125.35	111.81
4	A	427	EDO	O1-C1-C2	2.33	128.68	111.91
5	A	433	PGE	O2-C2-C1	2.31	120.24	110.07
3	A	411	MES	O3S-S-O2S	-2.30	105.65	111.27
4	A	422	EDO	O2-C2-C1	2.26	128.17	111.91
5	A	434	PGE	O3-C5-C6	2.25	119.95	110.07
5	A	433	PGE	O3-C5-C6	2.20	119.74	110.07
5	A	434	PGE	O2-C3-C4	2.16	120.14	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	403	GOL	O2-C2-C3	2.13	118.50	109.12
8	A	461	PEG	O1-C1-C2	2.09	123.91	111.81
3	A	412	MES	O1-C6-C5	-2.00	107.39	111.80

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
8	A	462	PEG	C1-C2-O2-C3
9	A	471	ME2	C2-C3-O2-C4
5	A	434	PGE	C6-C5-O3-C4
6	A	442	DXE	O1-C2-C3-O2
5	A	433	PGE	O2-C3-C4-O3
2	A	401	GOL	O2-C2-C3-O3
5	A	434	PGE	C1-C2-O2-C3
5	A	433	PGE	O1-C1-C2-O2
7	A	452	MXE	O1-C1-C2-O2
5	A	434	PGE	O3-C5-C6-O4
5	A	434	PGE	O2-C3-C4-O3
8	A	461	PEG	O2-C3-C4-O4
4	A	423	EDO	O1-C1-C2-O2
4	A	427	EDO	O1-C1-C2-O2
9	A	471	ME2	O2-C4-C5-O3
6	A	443	DXE	O1-C2-C3-O2
5	A	434	PGE	O1-C1-C2-O2
6	A	443	DXE	C2-C3-O2-C4
8	A	462	PEG	O1-C1-C2-O2
5	A	434	PGE	C4-C3-O2-C2
5	A	433	PGE	C4-C3-O2-C2
5	A	434	PGE	C3-C4-O3-C5
8	A	461	PEG	O1-C1-C2-O2
9	A	471	ME2	C3-C2-O1-C1
8	A	462	PEG	O2-C3-C4-O4
5	A	433	PGE	C3-C4-O3-C5
5	A	433	PGE	C6-C5-O3-C4
9	A	471	ME2	C4-C5-O3-C6
4	A	425	EDO	O1-C1-C2-O2
9	A	471	ME2	O1-C2-C3-O2
7	A	451	MXE	C1-C2-O2-C3
9	A	471	ME2	C7-C6-O3-C5
7	A	451	MXE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	433	PGE	C1-C2-O2-C3

There are no ring outliers.

19 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	428	EDO	2	0
4	A	422	EDO	3	0
4	A	426	EDO	1	0
4	A	423	EDO	4	0
7	A	452	MXE	18	0
4	A	421	EDO	2	0
5	A	433	PGE	5	0
3	A	411	MES	10	0
4	A	425	EDO	5	0
6	A	442	DXE	1	0
5	A	434	PGE	10	0
4	A	424	EDO	2	0
6	A	443	DXE	11	0
8	A	462	PEG	2	0
8	A	461	PEG	5	0
4	A	427	EDO	11	0
3	A	412	MES	6	0
9	A	471	ME2	9	0
7	A	451	MXE	4	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 (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	314/314 (100%)	-0.18	3 (0%)	82	66	4, 8, 18, 41	21 (6%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1[A]	MET	7.9
1	A	2[A]	GLU	4.5
1	A	55	THR	2.3

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(Å^2)	Q<0.9
8	PEG	A	462	7/7	0.54	0.31	37,40,48,52	7
6	DXE	A	442	6/6	0.64	0.25	15,30,31,34	6
4	EDO	A	428	4/4	0.69	0.22	55,65,74,77	0
4	EDO	A	423	4/4	0.75	0.18	18,30,30,43	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PEG	A	461	7/7	0.76	0.21	24,37,52,52	7
4	EDO	A	426	4/4	0.81	0.17	22,22,29,54	4
5	PGE	A	433	10/10	0.82	0.20	16,25,30,30	10
3	MES	A	411	12/12	0.82	0.21	10,24,31,32	12
9	ME2	A	471	10/10	0.83	0.24	22,33,40,41	10
3	MES	A	412	12/12	0.84	0.23	16,33,43,44	12
4	EDO	A	421	4/4	0.84	0.12	24,26,32,34	4
7	MXE	A	451	5/5	0.86	0.15	13,15,24,24	5
6	DXE	A	443	6/6	0.86	0.26	22,40,44,49	5
4	EDO	A	425	4/4	0.88	0.13	22,24,29,39	4
2	GOL	A	403	6/6	0.89	0.14	10,13,16,19	6
5	PGE	A	434	10/10	0.89	0.21	12,22,34,35	10
4	EDO	A	427	4/4	0.92	0.15	22,27,32,36	4
7	MXE	A	452	5/5	0.93	0.13	13,16,22,27	5
4	EDO	A	422	4/4	0.94	0.15	8,11,16,23	4
2	GOL	A	401	6/6	0.95	0.07	12,18,22,24	0
4	EDO	A	424	4/4	0.96	0.10	14,16,22,24	0
10	CA	A	491	1/1	1.00	0.07	4,4,4,4	0
10	CA	A	492	1/1	1.00	0.07	4,4,4,4	0

6.5 Other polymers (i)

There are no such residues in this entry.