



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:50 pm GMT

PDB ID : 4H2P  
Title : Tetrameric form of 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase (MHPCO)  
Authors : Kobayashi, J.; Yoshida, H.; Mikami, B.; Hayashi, H.; Kamitori, S.; Yagi, T.  
Deposited on : 2012-09-13  
Resolution : 1.98 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

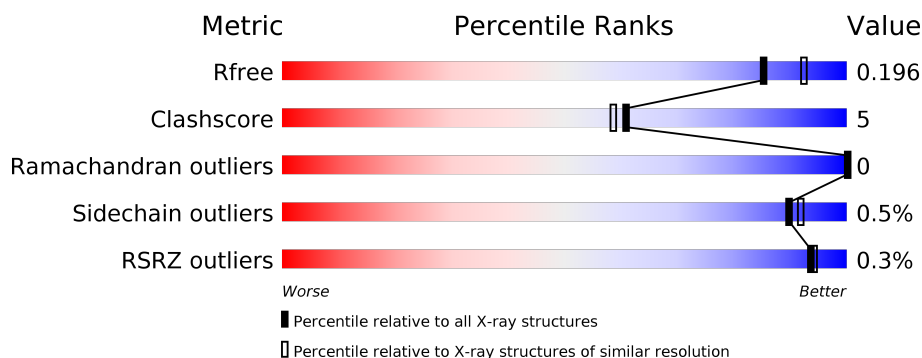
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	111664	10189 (2.00-1.96)
Clashscore	122126	11405 (2.00-1.96)
Ramachandran outliers	120053	11281 (2.00-1.96)
Sidechain outliers	120020	11280 (2.00-1.96)
RSRZ outliers	108989	9953 (2.00-1.96)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	379	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	379	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	379	<div> <div></div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	379	<div> <div></div> <div> <div></div> <div>89%</div> <div>9%</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
5	EDO	A	405	-	-	X	-

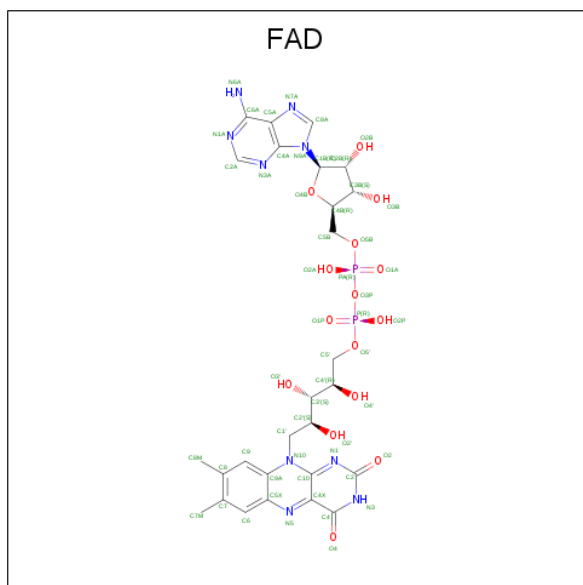


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total 2914	C 1842	N 515	O 542	S 15	0	9	0
1	B	371	Total 2917	C 1844	N 515	O 543	S 15	0	9	0
1	C	370	Total 2915	C 1841	N 517	O 542	S 15	0	9	0
1	D	369	Total 2911	C 1837	N 515	O 544	S 15	0	10	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



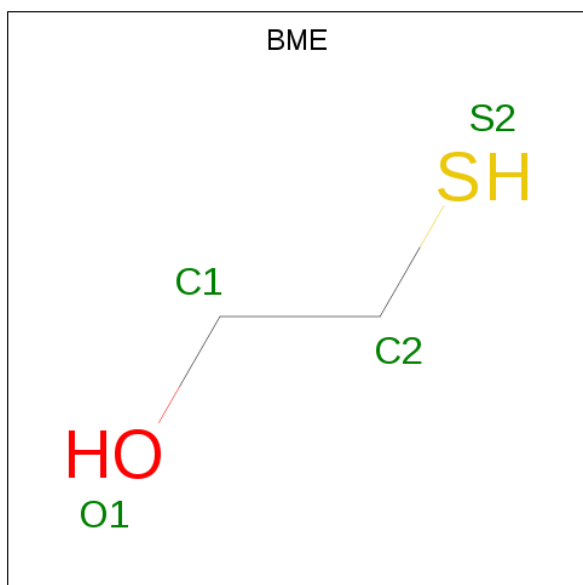
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

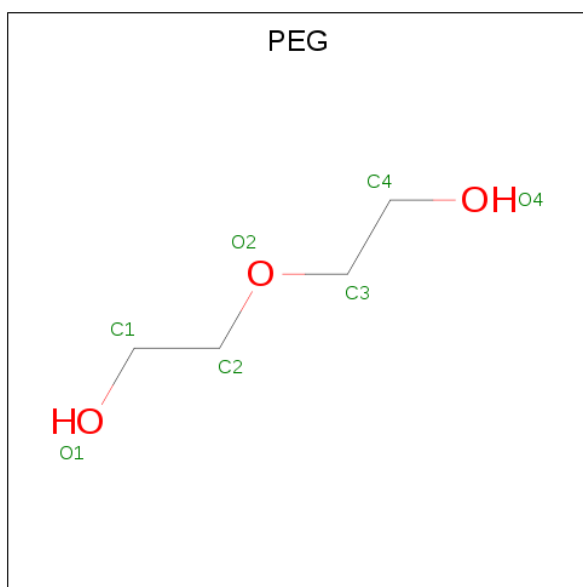
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



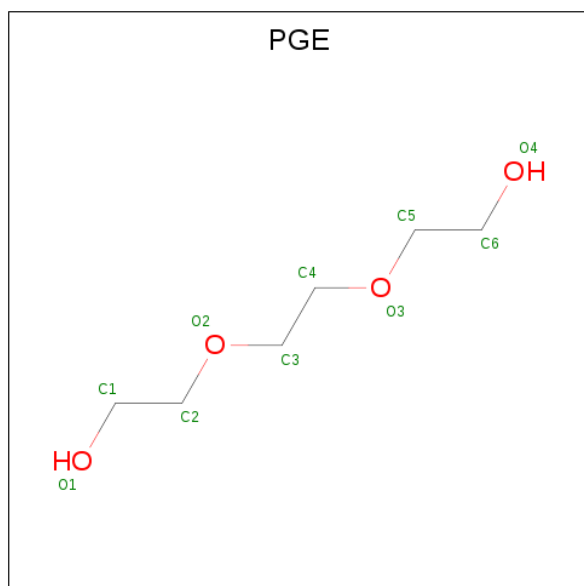
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	1
			14	8	6		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	1
			14	8	6		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 14 8 6	0	1
6	D	1	Total C O 7 4 3	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		
8	C	1	Total	C	O	0	0
			13	8	5		
8	D	1	Total	C	O	0	0
			13	8	5		

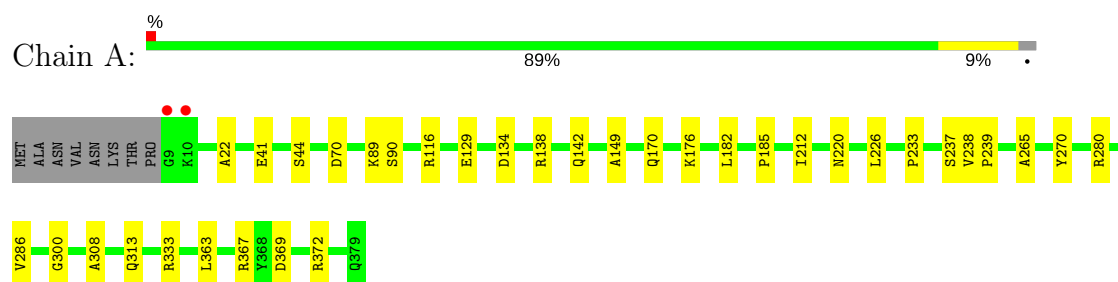
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	379	Total	O	0	0
			379	379		
9	B	372	Total	O	0	0
			372	372		
9	C	316	Total	O	0	0
			316	316		
9	D	311	Total	O	0	0
			311	311		

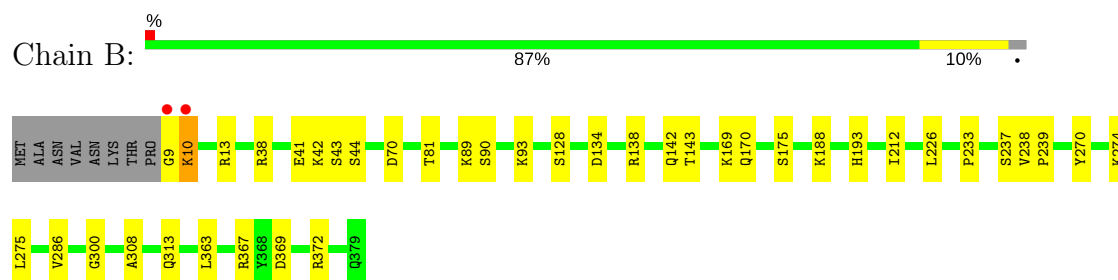
### 3 Residue-property plots

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.

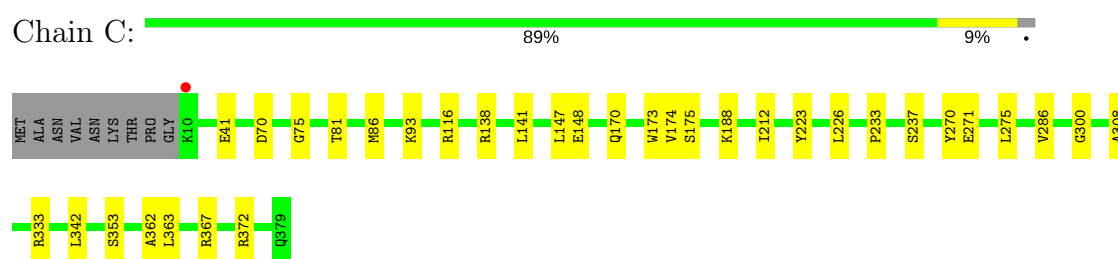
- Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase



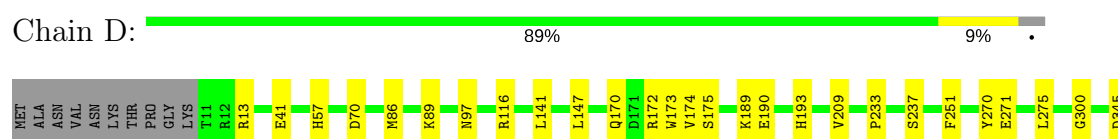
- Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase



- Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase



- Molecule 1: 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase



N349	S353	L363	R367	R372	W377	R378	R379
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.84Å 103.84Å 452.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.91 – 1.98 49.10 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.91-1.98) 97.5 (49.10-1.98)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.68 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.172 , 0.200 0.168 , 0.196	Depositor DCC
$R_{free}$ test set	9859 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGE, BME, EDO, PG4, SO4, PEG, FAD

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	0.37	0/3011	0.55	0/4087
1	B	0.37	0/3010	0.55	0/4085
1	C	0.34	0/3008	0.53	0/4082
1	D	0.34	0/3011	0.53	0/4087
All	All	0.36	0/12040	0.54	0/16341

There are no bond length outliers.

There are no bond angle outliers.

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	2914	0	2896	31	0
1	B	2917	0	2900	36	0
1	C	2915	0	2897	22	0
1	D	2911	0	2887	31	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	A	4	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	5	2	0
3	C	4	0	5	1	0
3	D	4	0	5	1	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	20	0	0	0	0
5	A	32	0	48	7	0
5	B	60	0	90	13	0
5	C	52	0	78	2	0
5	D	60	0	90	9	0
6	A	56	0	80	6	0
6	B	63	0	90	8	0
6	C	35	0	50	6	0
6	D	28	0	40	4	0
7	A	10	0	14	0	0
7	B	10	0	14	0	0
8	B	13	0	18	2	0
8	C	13	0	18	0	0
8	D	13	0	18	0	0
9	A	379	0	0	1	0
9	B	372	0	0	1	0
9	C	316	0	0	0	0
9	D	311	0	0	0	0
All	All	13768	0	12372	121	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 5.

All (121) 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:129:GLU:H	5:A:405:EDO:H11	1.32	0.93
1:B:313:GLN:HE21	6:B:425:PEG:H12	1.32	0.90
1:C:188:LYS:H	5:C:418:EDO:H12	1.42	0.85
1:B:188:LYS:H	5:B:409:EDO:H22	1.48	0.79
1:C:116:ARG:HH22	5:C:406:EDO:H12	1.48	0.78
1:B:143:THR:HG23	5:B:412:EDO:H11	1.66	0.77
1:A:89:LYS:HD2	6:C:420:PEG:H41	1.70	0.74
1:C:70:ASP:OD2	1:D:372:ARG:NH2	2.21	0.74
1:A:44:SER:H	5:A:409:EDO:H21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HH22	5:D:407:EDO:H21	1.57	0.69
1:A:233:PRO:O	1:A:237[A]:SER:OG	2.10	0.69
1:C:75:GLY:H	6:C:421:PEG:H12	1.56	0.69
1:C:233:PRO:O	1:C:237[A]:SER:OG	2.10	0.68
1:B:89:LYS:HD2	6:B:427:PEG:H12	1.75	0.68
1:A:142:GLN:HB3	5:A:405:EDO:H12	1.75	0.68
1:B:212:ILE:HG12	1:B:226:LEU:HD22	1.76	0.67
1:D:193:HIS:H	6:D:424:PEG:H32	1.59	0.67
1:B:367:ARG:HH22	8:B:430:PG4:H42	1.61	0.65
1:C:81[A]:THR:HG21	1:C:93:LYS:HB3	1.78	0.65
1:D:189:LYS:H	5:D:421:EDO:H22	1.61	0.65
1:B:13:ARG:HH12	6:B:422:PEG:H21	1.61	0.64
1:D:300:GLY:HA3	2:D:401:FAD:H1'2	1.78	0.63
1:B:233:PRO:O	1:B:237[A]:SER:OG	2.17	0.63
1:B:142:GLN:HB3	5:B:412:EDO:H22	1.81	0.62
1:A:372:ARG:NH2	1:B:70:ASP:OD2	2.29	0.62
1:B:286[B]:VAL:HG11	1:B:308:ALA:HB2	1.82	0.62
1:C:372:ARG:NH2	1:D:70:ASP:OD2	2.32	0.62
1:D:233:PRO:O	1:D:237[A]:SER:OG	2.17	0.62
1:D:345[B]:ASP:OD1	1:D:349:ASN:ND2	2.33	0.61
1:B:367:ARG:HH12	8:B:430:PG4:H52	1.66	0.61
1:A:313:GLN:HE21	6:A:417:PEG:H31	1.66	0.60
1:D:116:ARG:HH22	5:D:409:EDO:H21	1.65	0.60
1:D:377:TRP:HE1	6:D:423[A]:PEG:H21	1.65	0.60
1:D:209:VAL:HG21	5:D:414:EDO:H12	1.84	0.59
1:A:212:ILE:HG12	1:A:226:LEU:HD22	1.84	0.59
1:C:174:VAL:HG22	1:C:271:GLU:HG2	1.83	0.58
3:B:402:BME:H11	6:B:423:PEG:H41	1.85	0.58
1:C:300:GLY:HA3	2:C:401:FAD:H1'2	1.86	0.57
1:C:75:GLY:N	6:C:421:PEG:H12	2.19	0.57
1:A:129:GLU:H	5:A:405:EDO:C1	2.10	0.57
5:B:411:EDO:H21	1:D:89:LYS:HE2	1.87	0.56
1:A:116:ARG:HH22	5:A:412:EDO:H11	1.71	0.55
1:A:70:ASP:OD2	1:B:372:ARG:NH2	2.37	0.55
1:B:193:HIS:H	6:B:426:PEG:H41	1.71	0.55
1:B:38:ARG:HH12	6:B:422:PEG:H41	1.73	0.54
1:A:90:SER:H	6:C:420:PEG:C4	2.21	0.54
1:B:128:SER:HA	5:B:412:EDO:H12	1.90	0.54
1:A:286[B]:VAL:HG11	1:A:308:ALA:HB2	1.89	0.53
1:B:81[B]:THR:HG21	1:B:93:LYS:HB3	1.91	0.53
1:D:174:VAL:HG22	1:D:271:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:PHE:CE1	5:D:411:EDO:H11	2.44	0.52
1:A:300:GLY:HA3	2:A:401:FAD:H1'2	1.91	0.52
1:B:44:SER:H	5:B:418:EDO:H22	1.75	0.51
1:D:41:GLU:OE2	2:D:401:FAD:O3B	2.23	0.51
1:A:134:ASP:HB3	1:A:138:ARG:HB2	1.92	0.51
1:B:270:TYR:CG	3:B:402:BME:H22	2.46	0.50
1:B:188:LYS:N	5:B:409:EDO:H22	2.23	0.50
1:A:270:TYR:CG	3:A:402:BME:H22	2.46	0.50
1:B:300:GLY:HA3	2:B:401:FAD:H1'2	1.93	0.50
1:D:270:TYR:CG	3:D:402:BME:H22	2.47	0.50
1:A:41:GLU:OE2	2:A:401:FAD:O3B	2.28	0.50
1:C:286[B]:VAL:HG11	1:C:308:ALA:HB2	1.93	0.50
1:C:363:LEU:O	1:C:367:ARG:HG3	2.11	0.50
1:C:41:GLU:OE2	2:C:401:FAD:O3B	2.22	0.50
1:A:369:ASP:OD2	1:A:372:ARG:HD3	2.13	0.49
1:D:367:ARG:HH12	5:D:416:EDO:H22	1.77	0.49
1:A:313:GLN:HG2	6:A:417:PEG:H22	1.95	0.49
1:A:185:PRO:HD3	6:A:415:PEG:H42	1.95	0.48
1:A:372:ARG:HH21	5:B:413:EDO:H11	1.78	0.48
1:D:363:LEU:O	1:D:367:ARG:HG3	2.14	0.48
1:A:170:GLN:HG2	9:A:716:HOH:O	2.13	0.48
2:D:401:FAD:H1'1	2:D:401:FAD:H9	1.60	0.47
1:A:182:LEU:HD21	1:A:265:ALA:HB2	1.96	0.47
1:A:149:ALA:N	6:A:418[A]:PEG:H21	2.28	0.47
1:B:188:LYS:HB3	5:B:409:EDO:H11	1.97	0.47
1:A:313:GLN:HE21	6:A:417:PEG:C3	2.28	0.46
1:A:129:GLU:N	5:A:405:EDO:H11	2.14	0.46
1:B:274:LYS:HG2	5:B:408:EDO:H22	1.98	0.46
1:C:141:LEU:HD11	1:C:147:LEU:HD11	1.98	0.46
1:B:41:GLU:OE2	2:B:401:FAD:O3B	2.26	0.46
1:D:57:HIS:CD2	6:D:423[B]:PEG:H21	2.51	0.46
1:B:363:LEU:O	1:B:367:ARG:HG3	2.15	0.45
1:C:170:GLN:HB3	1:C:275:LEU:HD22	1.97	0.45
1:C:86:MET:CE	1:C:353:SER:HB2	2.45	0.45
1:B:169:LYS:HG3	5:B:416:EDO:H12	1.98	0.45
1:B:175:SER:HB3	1:B:270:TYR:HB2	1.98	0.45
1:B:170:GLN:HG2	9:B:639:HOH:O	2.15	0.45
1:C:86:MET:HE1	1:C:353:SER:HB2	1.97	0.45
1:A:220:ASN:HB2	6:A:413:PEG:H31	1.97	0.45
1:B:9:GLY:HA2	1:B:10:LYS:HA	1.57	0.45
1:D:190:GLU:N	1:D:190:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ALA:HB1	1:A:286[B]:VAL:HG12	1.99	0.45
1:D:141:LEU:HD11	1:D:147:LEU:HD11	1.99	0.45
1:D:173:TRP:CH2	1:D:175[B]:SER:HB3	2.52	0.45
1:D:173:TRP:CH2	1:D:175[A]:SER:HB2	2.52	0.45
1:D:86:MET:HE1	1:D:353:SER:HB2	1.99	0.45
1:D:172:ARG:HH22	5:D:420:EDO:H11	1.81	0.44
1:D:170:GLN:HB3	1:D:275:LEU:HD22	1.99	0.44
1:D:251:PHE:CD1	5:D:411:EDO:H11	2.52	0.44
1:B:43:SER:HB2	5:B:418:EDO:H22	1.99	0.44
1:A:238:VAL:HA	1:A:239:PRO:C	2.39	0.43
1:B:369:ASP:OD2	1:B:372:ARG:HD3	2.19	0.43
1:C:173:TRP:CH2	1:C:175[A]:SER:HB2	2.53	0.43
1:B:170:GLN:HB3	1:B:275:LEU:HD22	2.01	0.43
1:A:142:GLN:CB	5:A:405:EDO:H12	2.44	0.43
6:B:425:PEG:H42	6:B:425:PEG:H22	1.78	0.43
1:C:212:ILE:HG12	1:C:226:LEU:HD22	2.00	0.43
1:C:342:LEU:HD23	1:C:362:ALA:HA	2.00	0.42
1:B:134:ASP:HB3	1:B:138:ARG:HB2	2.01	0.42
1:D:377:TRP:HE1	6:D:423[B]:PEG:H21	1.82	0.42
2:B:401:FAD:H9	2:B:401:FAD:H1'1	1.60	0.42
1:D:86:MET:CE	1:D:353:SER:HB2	2.49	0.42
1:C:270:TYR:CG	3:C:402:BME:H22	2.55	0.42
1:A:363:LEU:O	1:A:367:ARG:HG3	2.20	0.41
1:C:138:ARG:HG2	1:C:148:GLU:HG2	2.02	0.41
6:C:420:PEG:H11	6:C:420:PEG:H31	1.76	0.41
1:B:42:LYS:HZ1	5:B:420:EDO:C2	2.34	0.41
1:B:90:SER:H	6:B:427:PEG:C1	2.34	0.41
6:C:421:PEG:O4	1:D:97:ASN:HB3	2.21	0.41
1:B:238:VAL:HA	1:B:239:PRO:C	2.42	0.40
1:D:13:ARG:HH12	5:D:407:EDO:H12	1.85	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	378/379 (100%)	367 (97%)	11 (3%)	0	100	100
1	B	378/379 (100%)	366 (97%)	12 (3%)	0	100	100
1	C	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
1	D	377/379 (100%)	367 (97%)	10 (3%)	0	100	100
All	All	1510/1516 (100%)	1465 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	307/305 (101%)	304 (99%)	3 (1%)	78	81
1	B	307/305 (101%)	306 (100%)	1 (0%)	93	95
1	C	307/305 (101%)	305 (99%)	2 (1%)	85	88
1	D	307/305 (101%)	307 (100%)	0	100	100
All	All	1228/1220 (101%)	1222 (100%)	6 (0%)	90	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	280	ARG
1	A	333	ARG
1	B	10	LYS
1	C	223	TYR
1	C	333	ARG

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

Mol	Chain	Res	Type
1	B	220	ASN
1	B	313	GLN
1	D	349	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

102 ligands are modelled in this entry.

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	$\# Z  > 2$
2	FAD	A	401	-	51,58,58	2.02	10 (19%)	57,89,89	2.77	14 (24%)
3	BME	A	402	-	3,3,3	0.21	0	1,2,2	0.62	0
4	SO4	A	403	-	4,4,4	0.26	0	6,6,6	0.23	0
4	SO4	A	404	-	4,4,4	0.22	0	6,6,6	0.11	0
5	EDO	A	405	-	3,3,3	0.36	0	2,2,2	0.53	0
5	EDO	A	406	-	3,3,3	0.50	0	2,2,2	0.39	0
5	EDO	A	407	-	3,3,3	0.50	0	2,2,2	0.38	0
5	EDO	A	408	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	A	409	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	A	410	-	3,3,3	0.43	0	2,2,2	0.64	0
5	EDO	A	411	-	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	A	412	-	3,3,3	0.47	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PEG	A	413	-	6,6,6	0.48	0	5,5,5	0.26	0
6	PEG	A	414	-	6,6,6	0.47	0	5,5,5	0.37	0
6	PEG	A	415	-	6,6,6	0.45	0	5,5,5	0.33	0
6	PEG	A	416[A]	-	6,6,6	0.47	0	5,5,5	0.16	0
6	PEG	A	416[B]	-	6,6,6	0.48	0	5,5,5	0.19	0
6	PEG	A	417	-	6,6,6	0.52	0	5,5,5	0.22	0
6	PEG	A	418[A]	-	6,6,6	0.50	0	5,5,5	0.48	0
6	PEG	A	418[B]	-	6,6,6	0.46	0	5,5,5	0.32	0
7	PGE	A	419	-	9,9,9	0.48	0	8,8,8	0.28	0
2	FAD	B	401	-	51,58,58	2.01	12 (23%)	57,89,89	2.86	14 (24%)
3	BME	B	402	-	3,3,3	0.26	0	1,2,2	0.25	0
4	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.18	0
4	SO4	B	404	-	4,4,4	0.22	0	6,6,6	0.06	0
4	SO4	B	405	-	4,4,4	0.22	0	6,6,6	0.11	0
5	EDO	B	406	-	3,3,3	0.53	0	2,2,2	0.29	0
5	EDO	B	407	-	3,3,3	0.51	0	2,2,2	0.22	0
5	EDO	B	408	-	3,3,3	0.51	0	2,2,2	0.29	0
5	EDO	B	409	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	B	410	-	3,3,3	0.49	0	2,2,2	0.34	0
5	EDO	B	411	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	B	412	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	B	413	-	3,3,3	0.51	0	2,2,2	0.36	0
5	EDO	B	414	-	3,3,3	0.50	0	2,2,2	0.35	0
5	EDO	B	415	-	3,3,3	0.49	0	2,2,2	0.33	0
5	EDO	B	416	-	3,3,3	0.32	0	2,2,2	0.55	0
5	EDO	B	417	-	3,3,3	0.51	0	2,2,2	0.31	0
5	EDO	B	418	-	3,3,3	0.44	0	2,2,2	0.38	0
5	EDO	B	419	-	3,3,3	0.45	0	2,2,2	0.50	0
5	EDO	B	420	-	3,3,3	0.46	0	2,2,2	0.33	0
6	PEG	B	421	-	6,6,6	0.51	0	5,5,5	0.55	0
6	PEG	B	422	-	6,6,6	0.47	0	5,5,5	0.40	0
6	PEG	B	423	-	6,6,6	0.44	0	5,5,5	0.48	0
6	PEG	B	424[A]	-	6,6,6	0.51	0	5,5,5	0.23	0
6	PEG	B	424[B]	-	6,6,6	0.45	0	5,5,5	0.20	0
6	PEG	B	425	-	6,6,6	0.54	0	5,5,5	0.55	0
6	PEG	B	426	-	6,6,6	0.53	0	5,5,5	0.20	0
6	PEG	B	427	-	6,6,6	0.31	0	5,5,5	0.63	0
6	PEG	B	428	-	6,6,6	0.52	0	5,5,5	0.21	0
7	PGE	B	429	-	9,9,9	0.52	0	8,8,8	0.22	0
8	PG4	B	430	-	12,12,12	0.48	0	11,11,11	0.48	0
2	FAD	C	401	-	51,58,58	2.05	11 (21%)	57,89,89	2.89	16 (28%)
3	BME	C	402	-	3,3,3	0.30	0	1,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.28	0
4	SO4	C	404	-	4,4,4	0.20	0	6,6,6	0.09	0
4	SO4	C	405	-	4,4,4	0.20	0	6,6,6	0.17	0
5	EDO	C	406	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	C	407	-	3,3,3	0.48	0	2,2,2	0.35	0
5	EDO	C	408	-	3,3,3	0.52	0	2,2,2	0.23	0
5	EDO	C	409	-	3,3,3	0.56	0	2,2,2	0.19	0
5	EDO	C	410	-	3,3,3	0.50	0	2,2,2	0.18	0
5	EDO	C	411	-	3,3,3	0.47	0	2,2,2	0.43	0
5	EDO	C	412	-	3,3,3	0.51	0	2,2,2	0.28	0
5	EDO	C	413	-	3,3,3	0.50	0	2,2,2	0.25	0
5	EDO	C	414	-	3,3,3	0.50	0	2,2,2	0.35	0
5	EDO	C	415	-	3,3,3	0.46	0	2,2,2	0.43	0
5	EDO	C	416	-	3,3,3	0.51	0	2,2,2	0.34	0
5	EDO	C	417	-	3,3,3	0.36	0	2,2,2	0.68	0
5	EDO	C	418	-	3,3,3	0.55	0	2,2,2	0.15	0
6	PEG	C	419	-	6,6,6	0.46	0	5,5,5	0.45	0
6	PEG	C	420	-	6,6,6	0.30	0	5,5,5	0.68	0
6	PEG	C	421	-	6,6,6	0.42	0	5,5,5	0.69	0
6	PEG	C	422	-	6,6,6	0.47	0	5,5,5	0.23	0
6	PEG	C	423	-	6,6,6	0.53	0	5,5,5	0.18	0
8	PG4	C	424	-	12,12,12	0.53	0	11,11,11	0.14	0
2	FAD	D	401	-	51,58,58	2.04	12 (23%)	57,89,89	2.91	13 (22%)
3	BME	D	402	-	3,3,3	0.22	0	1,2,2	0.59	0
4	SO4	D	403	-	4,4,4	0.18	0	6,6,6	0.25	0
4	SO4	D	404	-	4,4,4	0.20	0	6,6,6	0.11	0
4	SO4	D	405	-	4,4,4	0.20	0	6,6,6	0.09	0
4	SO4	D	406	-	4,4,4	0.21	0	6,6,6	0.15	0
5	EDO	D	407	-	3,3,3	0.50	0	2,2,2	0.30	0
5	EDO	D	408	-	3,3,3	0.52	0	2,2,2	0.29	0
5	EDO	D	409	-	3,3,3	0.45	0	2,2,2	0.43	0
5	EDO	D	410	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	D	411	-	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	D	412	-	3,3,3	0.49	0	2,2,2	0.36	0
5	EDO	D	413	-	3,3,3	0.53	0	2,2,2	0.23	0
5	EDO	D	414	-	3,3,3	0.52	0	2,2,2	0.22	0
5	EDO	D	415	-	3,3,3	0.49	0	2,2,2	0.29	0
5	EDO	D	416	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	D	417	-	3,3,3	0.51	0	2,2,2	0.36	0
5	EDO	D	418	-	3,3,3	0.50	0	2,2,2	0.34	0
5	EDO	D	419	-	3,3,3	0.48	0	2,2,2	0.44	0
5	EDO	D	420	-	3,3,3	0.48	0	2,2,2	0.38	0
5	EDO	D	421	-	3,3,3	0.47	0	2,2,2	0.30	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PEG	D	422	-	6,6,6	0.58	0	5,5,5	0.23	0
6	PEG	D	423[A]	-	6,6,6	0.51	0	5,5,5	0.20	0
6	PEG	D	423[B]	-	6,6,6	0.44	0	5,5,5	0.52	0
6	PEG	D	424	-	6,6,6	0.50	0	5,5,5	0.38	0
8	PG4	D	425	-	12,12,12	0.51	0	11,11,11	0.36	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
2	FAD	A	401	-	-	0/28/50/50	0/6/6/6
3	BME	A	402	-	-	0/1/1/1	0/0/0/0
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
4	SO4	A	404	-	-	0/0/0/0	0/0/0/0
5	EDO	A	405	-	-	0/1/1/1	0/0/0/0
5	EDO	A	406	-	-	0/1/1/1	0/0/0/0
5	EDO	A	407	-	-	0/1/1/1	0/0/0/0
5	EDO	A	408	-	-	0/1/1/1	0/0/0/0
5	EDO	A	409	-	-	0/1/1/1	0/0/0/0
5	EDO	A	410	-	-	0/1/1/1	0/0/0/0
5	EDO	A	411	-	-	0/1/1/1	0/0/0/0
5	EDO	A	412	-	-	0/1/1/1	0/0/0/0
6	PEG	A	413	-	-	0/4/4/4	0/0/0/0
6	PEG	A	414	-	-	0/4/4/4	0/0/0/0
6	PEG	A	415	-	-	0/4/4/4	0/0/0/0
6	PEG	A	416[A]	-	-	0/4/4/4	0/0/0/0
6	PEG	A	416[B]	-	-	0/4/4/4	0/0/0/0
6	PEG	A	417	-	-	0/4/4/4	0/0/0/0
6	PEG	A	418[A]	-	-	0/4/4/4	0/0/0/0
6	PEG	A	418[B]	-	-	0/4/4/4	0/0/0/0
7	PGE	A	419	-	-	0/7/7/7	0/0/0/0
2	FAD	B	401	-	-	0/28/50/50	0/6/6/6
3	BME	B	402	-	-	0/1/1/1	0/0/0/0
4	SO4	B	403	-	-	0/0/0/0	0/0/0/0
4	SO4	B	404	-	-	0/0/0/0	0/0/0/0
4	SO4	B	405	-	-	0/0/0/0	0/0/0/0
5	EDO	B	406	-	-	0/1/1/1	0/0/0/0
5	EDO	B	407	-	-	0/1/1/1	0/0/0/0
5	EDO	B	408	-	-	0/1/1/1	0/0/0/0
5	EDO	B	409	-	-	0/1/1/1	0/0/0/0
5	EDO	B	410	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	411	-	-	0/1/1/1	0/0/0/0
5	EDO	B	412	-	-	0/1/1/1	0/0/0/0
5	EDO	B	413	-	-	0/1/1/1	0/0/0/0
5	EDO	B	414	-	-	0/1/1/1	0/0/0/0
5	EDO	B	415	-	-	0/1/1/1	0/0/0/0
5	EDO	B	416	-	-	0/1/1/1	0/0/0/0
5	EDO	B	417	-	-	0/1/1/1	0/0/0/0
5	EDO	B	418	-	-	0/1/1/1	0/0/0/0
5	EDO	B	419	-	-	0/1/1/1	0/0/0/0
5	EDO	B	420	-	-	0/1/1/1	0/0/0/0
6	PEG	B	421	-	-	0/4/4/4	0/0/0/0
6	PEG	B	422	-	-	0/4/4/4	0/0/0/0
6	PEG	B	423	-	-	0/4/4/4	0/0/0/0
6	PEG	B	424[A]	-	-	0/4/4/4	0/0/0/0
6	PEG	B	424[B]	-	-	0/4/4/4	0/0/0/0
6	PEG	B	425	-	-	0/4/4/4	0/0/0/0
6	PEG	B	426	-	-	0/4/4/4	0/0/0/0
6	PEG	B	427	-	-	0/4/4/4	0/0/0/0
6	PEG	B	428	-	-	0/4/4/4	0/0/0/0
7	PGE	B	429	-	-	0/7/7/7	0/0/0/0
8	PG4	B	430	-	-	0/10/10/10	0/0/0/0
2	FAD	C	401	-	-	0/28/50/50	0/6/6/6
3	BME	C	402	-	-	0/1/1/1	0/0/0/0
4	SO4	C	403	-	-	0/0/0/0	0/0/0/0
4	SO4	C	404	-	-	0/0/0/0	0/0/0/0
4	SO4	C	405	-	-	0/0/0/0	0/0/0/0
5	EDO	C	406	-	-	0/1/1/1	0/0/0/0
5	EDO	C	407	-	-	0/1/1/1	0/0/0/0
5	EDO	C	408	-	-	0/1/1/1	0/0/0/0
5	EDO	C	409	-	-	0/1/1/1	0/0/0/0
5	EDO	C	410	-	-	0/1/1/1	0/0/0/0
5	EDO	C	411	-	-	0/1/1/1	0/0/0/0
5	EDO	C	412	-	-	0/1/1/1	0/0/0/0
5	EDO	C	413	-	-	0/1/1/1	0/0/0/0
5	EDO	C	414	-	-	0/1/1/1	0/0/0/0
5	EDO	C	415	-	-	0/1/1/1	0/0/0/0
5	EDO	C	416	-	-	0/1/1/1	0/0/0/0
5	EDO	C	417	-	-	0/1/1/1	0/0/0/0
5	EDO	C	418	-	-	0/1/1/1	0/0/0/0
6	PEG	C	419	-	-	0/4/4/4	0/0/0/0
6	PEG	C	420	-	-	0/4/4/4	0/0/0/0
6	PEG	C	421	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	C	422	-	-	0/4/4/4	0/0/0/0
6	PEG	C	423	-	-	0/4/4/4	0/0/0/0
8	PG4	C	424	-	-	0/10/10/10	0/0/0/0
2	FAD	D	401	-	-	0/28/50/50	0/6/6/6
3	BME	D	402	-	-	0/1/1/1	0/0/0/0
4	SO4	D	403	-	-	0/0/0/0	0/0/0/0
4	SO4	D	404	-	-	0/0/0/0	0/0/0/0
4	SO4	D	405	-	-	0/0/0/0	0/0/0/0
4	SO4	D	406	-	-	0/0/0/0	0/0/0/0
5	EDO	D	407	-	-	0/1/1/1	0/0/0/0
5	EDO	D	408	-	-	0/1/1/1	0/0/0/0
5	EDO	D	409	-	-	0/1/1/1	0/0/0/0
5	EDO	D	410	-	-	0/1/1/1	0/0/0/0
5	EDO	D	411	-	-	0/1/1/1	0/0/0/0
5	EDO	D	412	-	-	0/1/1/1	0/0/0/0
5	EDO	D	413	-	-	0/1/1/1	0/0/0/0
5	EDO	D	414	-	-	0/1/1/1	0/0/0/0
5	EDO	D	415	-	-	0/1/1/1	0/0/0/0
5	EDO	D	416	-	-	0/1/1/1	0/0/0/0
5	EDO	D	417	-	-	0/1/1/1	0/0/0/0
5	EDO	D	418	-	-	0/1/1/1	0/0/0/0
5	EDO	D	419	-	-	0/1/1/1	0/0/0/0
5	EDO	D	420	-	-	0/1/1/1	0/0/0/0
5	EDO	D	421	-	-	0/1/1/1	0/0/0/0
6	PEG	D	422	-	-	0/4/4/4	0/0/0/0
6	PEG	D	423[A]	-	-	0/4/4/4	0/0/0/0
6	PEG	D	423[B]	-	-	0/4/4/4	0/0/0/0
6	PEG	D	424	-	-	0/4/4/4	0/0/0/0
8	PG4	D	425	-	-	0/10/10/10	0/0/0/0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	C8M-C8	-5.40	1.40	1.51
2	B	401	FAD	C7M-C7	-5.33	1.40	1.51
2	C	401	FAD	C8M-C8	-5.18	1.40	1.51
2	D	401	FAD	C7M-C7	-5.16	1.40	1.51
2	A	401	FAD	C7M-C7	-5.05	1.41	1.51
2	A	401	FAD	C8M-C8	-4.95	1.41	1.51
2	B	401	FAD	C8M-C8	-4.95	1.41	1.51
2	C	401	FAD	C7M-C7	-4.80	1.41	1.51
2	D	401	FAD	C9A-N10	-2.75	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FAD	C5A-C4A	-2.64	1.34	1.40
2	C	401	FAD	C5A-C4A	-2.62	1.34	1.40
2	B	401	FAD	C9A-N10	-2.58	1.35	1.38
2	D	401	FAD	C5A-C4A	-2.57	1.34	1.40
2	B	401	FAD	C5A-C4A	-2.50	1.34	1.40
2	C	401	FAD	C9A-N10	-2.49	1.35	1.38
2	A	401	FAD	C9A-N10	-2.48	1.35	1.38
2	B	401	FAD	C8A-N9A	-2.00	1.34	1.36
2	D	401	FAD	C5'-C4'	2.41	1.55	1.51
2	D	401	FAD	O4B-C4B	2.55	1.50	1.45
2	A	401	FAD	C2A-N1A	2.59	1.38	1.33
2	B	401	FAD	C2A-N1A	2.61	1.38	1.33
2	C	401	FAD	C2A-N1A	2.64	1.38	1.33
2	B	401	FAD	O4B-C4B	2.65	1.50	1.45
2	C	401	FAD	O4B-C4B	2.66	1.50	1.45
2	D	401	FAD	C2A-N1A	2.91	1.39	1.33
2	D	401	FAD	C5X-N5	3.09	1.40	1.35
2	A	401	FAD	C5X-N5	3.12	1.40	1.35
2	C	401	FAD	C4-N3	3.45	1.39	1.33
2	B	401	FAD	C5X-N5	3.50	1.40	1.35
2	C	401	FAD	C5X-N5	3.54	1.40	1.35
2	A	401	FAD	C4-N3	3.68	1.39	1.33
2	D	401	FAD	C4-N3	3.72	1.39	1.33
2	B	401	FAD	C4-N3	3.74	1.39	1.33
2	B	401	FAD	C2A-N3A	4.00	1.38	1.32
2	D	401	FAD	C10-N1	4.32	1.39	1.33
2	A	401	FAD	C2A-N3A	4.40	1.39	1.32
2	D	401	FAD	C4X-N5	4.52	1.39	1.33
2	C	401	FAD	C10-N1	4.58	1.39	1.33
2	B	401	FAD	C10-N1	4.76	1.39	1.33
2	D	401	FAD	C2A-N3A	4.88	1.40	1.32
2	C	401	FAD	C4X-N5	4.98	1.40	1.33
2	C	401	FAD	C2A-N3A	5.15	1.40	1.32
2	B	401	FAD	C4X-N5	5.23	1.40	1.33
2	A	401	FAD	C10-N1	5.25	1.40	1.33
2	A	401	FAD	C4X-N5	5.31	1.41	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	N3A-C2A-N1A	-13.01	117.73	128.86
2	D	401	FAD	N3A-C2A-N1A	-12.84	117.87	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FAD	N3A-C2A-N1A	-12.71	117.98	128.86
2	A	401	FAD	N3A-C2A-N1A	-12.32	118.32	128.86
2	B	401	FAD	O4B-C4B-C5B	-9.49	77.78	109.39
2	D	401	FAD	O4B-C4B-C5B	-9.35	78.23	109.39
2	C	401	FAD	O4B-C4B-C5B	-9.29	78.46	109.39
2	A	401	FAD	O4B-C4B-C5B	-8.82	80.02	109.39
2	B	401	FAD	O4B-C4B-C3B	-7.11	91.08	105.15
2	D	401	FAD	O4B-C4B-C3B	-6.93	91.45	105.15
2	C	401	FAD	O4B-C4B-C3B	-6.87	91.57	105.15
2	A	401	FAD	O4B-C4B-C3B	-6.52	92.25	105.15
2	D	401	FAD	C2B-C3B-C4B	-3.13	96.61	102.62
2	D	401	FAD	O5B-C5B-C4B	-3.09	98.25	109.00
2	C	401	FAD	O5B-C5B-C4B	-3.04	98.44	109.00
2	C	401	FAD	C2B-C3B-C4B	-3.02	96.81	102.62
2	D	401	FAD	O2B-C2B-C3B	-2.96	102.34	111.83
2	C	401	FAD	O2B-C2B-C3B	-2.92	102.46	111.83
2	A	401	FAD	C2B-C3B-C4B	-2.83	97.19	102.62
2	B	401	FAD	O5B-C5B-C4B	-2.82	99.18	109.00
2	B	401	FAD	O2B-C2B-C3B	-2.73	103.08	111.83
2	A	401	FAD	O5B-C5B-C4B	-2.72	99.52	109.00
2	A	401	FAD	O2B-C2B-C3B	-2.65	103.35	111.83
2	B	401	FAD	C4X-C4-N3	-2.53	119.87	123.47
2	A	401	FAD	C4X-C4-N3	-2.37	120.10	123.47
2	D	401	FAD	C4X-C4-N3	-2.36	120.12	123.47
2	C	401	FAD	C4X-C4-N3	-2.29	120.21	123.47
2	A	401	FAD	C9A-C5X-N5	-2.25	119.12	122.32
2	B	401	FAD	C9A-C5X-N5	-2.25	119.13	122.32
2	B	401	FAD	C2B-C3B-C4B	-2.22	98.36	102.62
2	D	401	FAD	C9A-C5X-N5	-2.20	119.19	122.32
2	C	401	FAD	C9A-C5X-N5	-2.12	119.31	122.32
2	C	401	FAD	C4A-C5A-N7A	-2.11	107.37	109.41
2	C	401	FAD	O3'-C3'-C2'	2.05	113.86	108.82
2	A	401	FAD	PA-O5B-C5B	2.07	133.81	121.68
2	C	401	FAD	PA-O5B-C5B	2.10	133.99	121.68
2	B	401	FAD	O4'-C4'-C3'	2.20	114.54	109.10
2	A	401	FAD	O3B-C3B-C2B	2.32	119.27	111.83
2	A	401	FAD	C1'-N10-C10	2.54	121.00	118.46
2	C	401	FAD	C1'-N10-C10	2.89	121.35	118.46
2	B	401	FAD	O3B-C3B-C2B	3.07	121.65	111.83
2	C	401	FAD	O3B-C3B-C2B	3.11	121.80	111.83
2	B	401	FAD	C1'-N10-C10	3.16	121.62	118.46
2	D	401	FAD	O3B-C3B-C2B	3.48	122.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FAD	C1'-N10-C10	3.61	122.06	118.46
2	D	401	FAD	C5X-C9A-N10	4.13	120.86	117.71
2	C	401	FAD	C5X-C9A-N10	4.13	120.87	117.71
2	A	401	FAD	C5X-C9A-N10	4.16	120.89	117.71
2	B	401	FAD	C5X-C9A-N10	4.22	120.93	117.71
2	B	401	FAD	C5B-C4B-C3B	5.00	134.09	115.29
2	C	401	FAD	C5B-C4B-C3B	5.03	134.22	115.29
2	B	401	FAD	C4-N3-C2	5.08	119.47	115.14
2	A	401	FAD	C5B-C4B-C3B	5.15	134.66	115.29
2	D	401	FAD	C5B-C4B-C3B	5.36	135.46	115.29
2	D	401	FAD	C4-N3-C2	5.70	120.00	115.14
2	C	401	FAD	C4-N3-C2	5.82	120.10	115.14
2	A	401	FAD	C4-N3-C2	5.95	120.20	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

43 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FAD	2	0
3	A	402	BME	1	0
5	A	405	EDO	5	0
5	A	409	EDO	1	0
5	A	412	EDO	1	0
6	A	413	PEG	1	0
6	A	415	PEG	1	0
6	A	417	PEG	3	0
6	A	418[A]	PEG	1	0
2	B	401	FAD	3	0
3	B	402	BME	2	0
5	B	408	EDO	1	0
5	B	409	EDO	3	0
5	B	411	EDO	1	0
5	B	412	EDO	3	0
5	B	413	EDO	1	0
5	B	416	EDO	1	0
5	B	418	EDO	2	0
5	B	420	EDO	1	0
6	B	422	PEG	2	0
6	B	423	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	425	PEG	2	0
6	B	426	PEG	1	0
6	B	427	PEG	2	0
8	B	430	PG4	2	0
2	C	401	FAD	2	0
3	C	402	BME	1	0
5	C	406	EDO	1	0
5	C	418	EDO	1	0
6	C	420	PEG	3	0
6	C	421	PEG	3	0
2	D	401	FAD	3	0
3	D	402	BME	1	0
5	D	407	EDO	2	0
5	D	409	EDO	1	0
5	D	411	EDO	2	0
5	D	414	EDO	1	0
5	D	416	EDO	1	0
5	D	420	EDO	1	0
5	D	421	EDO	1	0
6	D	423[A]	PEG	1	0
6	D	423[B]	PEG	2	0
6	D	424	PEG	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	371/379 (97%)	-0.04	2 (0%) 90 92	12, 19, 34, 84	0
1	B	371/379 (97%)	-0.04	2 (0%) 90 92	12, 19, 34, 81	0
1	C	370/379 (97%)	-0.02	1 (0%) 93 94	14, 23, 39, 78	0
1	D	369/379 (97%)	-0.04	0 100 100	15, 23, 38, 52	0
All	All	1481/1516 (97%)	-0.03	5 (0%) 93 94	12, 21, 37, 84	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	LYS	5.4
1	A	10	LYS	3.3
1	A	9	GLY	2.3
1	B	9	GLY	2.2
1	C	10	LYS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	PEG	D	424	7/7	0.68	0.21	44,49,58,61	0
6	PEG	D	422	7/7	0.68	0.20	43,46,50,51	0
5	EDO	D	413	4/4	0.70	0.19	44,47,53,57	0
7	PGE	B	429	10/10	0.71	0.21	43,54,63,65	0
6	PEG	B	422	7/7	0.71	0.21	60,62,73,78	0
8	PG4	B	430	13/13	0.72	0.28	33,49,59,62	0
5	EDO	B	413	4/4	0.72	0.38	45,47,57,57	0
5	EDO	D	407	4/4	0.73	0.25	61,70,71,75	0
6	PEG	C	423	7/7	0.75	0.16	45,47,55,58	0
5	EDO	C	409	4/4	0.76	0.31	44,44,47,56	0
6	PEG	B	424[A]	7/7	0.76	0.23	37,41,46,50	7
5	EDO	D	415	4/4	0.76	0.18	40,43,50,50	0
6	PEG	A	418[B]	7/7	0.76	0.26	32,38,41,43	7
6	PEG	A	418[A]	7/7	0.76	0.26	37,39,43,43	7
6	PEG	B	424[B]	7/7	0.76	0.23	35,41,46,50	7
5	EDO	B	420	4/4	0.76	0.17	50,52,58,66	0
5	EDO	B	407	4/4	0.76	0.22	47,54,55,59	0
5	EDO	B	415	4/4	0.78	0.17	40,50,51,53	0
6	PEG	B	428	7/7	0.78	0.24	42,50,53,54	0
6	PEG	D	423[B]	7/7	0.79	0.27	25,32,41,42	7
6	PEG	D	423[A]	7/7	0.79	0.27	24,33,40,44	7
5	EDO	D	408	4/4	0.80	0.29	50,53,53,57	0
6	PEG	A	417	7/7	0.80	0.35	31,42,50,51	0
6	PEG	B	423	7/7	0.80	0.33	41,50,57,64	0
5	EDO	B	408	4/4	0.80	0.29	37,45,48,51	0
3	BME	B	402	4/4	0.80	0.18	30,32,44,47	0
5	EDO	C	406	4/4	0.80	0.23	47,53,53,54	0
6	PEG	A	414	7/7	0.81	0.13	48,53,57,61	0
6	PEG	C	419	7/7	0.81	0.24	40,56,61,64	0
5	EDO	C	410	4/4	0.81	0.15	45,46,47,55	0
6	PEG	B	425	7/7	0.81	0.27	27,46,52,52	0
5	EDO	C	407	4/4	0.82	0.22	53,60,61,61	0
5	EDO	D	410	4/4	0.82	0.18	52,53,56,58	0
3	BME	C	402	4/4	0.82	0.28	33,34,50,51	0
5	EDO	D	418	4/4	0.82	0.11	53,58,62,64	0
5	EDO	B	417	4/4	0.82	0.28	48,50,52,63	0
3	BME	D	402	4/4	0.82	0.24	36,37,47,53	0
5	EDO	A	408	4/4	0.82	0.17	45,51,55,56	0
5	EDO	C	414	4/4	0.83	0.10	45,50,56,59	0
5	EDO	A	411	4/4	0.83	0.13	44,47,55,60	0
6	PEG	C	420	7/7	0.84	0.16	27,31,41,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	C	422	7/7	0.84	0.15	51,58,65,68	0
6	PEG	A	413	7/7	0.84	0.23	43,47,55,58	0
6	PEG	B	426	7/7	0.84	0.23	45,47,53,62	0
5	EDO	C	411	4/4	0.84	0.18	42,50,55,65	0
8	PG4	D	425	13/13	0.84	0.20	34,45,55,56	0
6	PEG	A	415	7/7	0.85	0.20	36,44,50,50	0
5	EDO	C	413	4/4	0.85	0.11	48,48,52,57	0
5	EDO	A	406	4/4	0.85	0.10	44,48,48,52	0
6	PEG	B	421	7/7	0.85	0.30	38,49,54,55	0
5	EDO	D	419	4/4	0.85	0.10	42,52,53,58	0
6	PEG	C	421	7/7	0.85	0.24	34,38,46,53	0
8	PG4	C	424	13/13	0.85	0.22	34,45,52,53	0
5	EDO	C	415	4/4	0.85	0.20	45,47,53,65	0
4	SO4	B	404	5/5	0.86	0.23	45,53,72,75	0
7	PGE	A	419	10/10	0.86	0.14	44,47,58,59	0
5	EDO	B	411	4/4	0.86	0.30	38,42,42,65	0
5	EDO	A	407	4/4	0.86	0.15	47,47,48,50	0
5	EDO	D	420	4/4	0.86	0.29	45,45,52,58	0
4	SO4	C	405	5/5	0.87	0.30	54,72,89,91	0
6	PEG	B	427	7/7	0.87	0.17	28,31,40,53	0
5	EDO	D	412	4/4	0.87	0.23	54,55,56,56	0
4	SO4	D	406	5/5	0.87	0.27	68,71,87,92	0
6	PEG	A	416[B]	7/7	0.87	0.20	38,40,44,51	7
6	PEG	A	416[A]	7/7	0.87	0.20	32,40,44,51	7
5	EDO	B	414	4/4	0.88	0.44	41,41,43,45	0
5	EDO	B	406	4/4	0.88	0.18	36,40,41,43	0
5	EDO	C	416	4/4	0.88	0.11	46,51,53,57	0
5	EDO	D	414	4/4	0.88	0.24	44,52,53,53	0
4	SO4	B	405	5/5	0.89	0.26	49,65,90,90	0
5	EDO	C	408	4/4	0.89	0.26	40,41,45,45	0
5	EDO	A	410	4/4	0.89	0.17	29,29,39,51	0
5	EDO	B	418	4/4	0.89	0.20	24,43,47,47	0
5	EDO	B	409	4/4	0.89	0.17	29,34,47,49	0
5	EDO	C	418	4/4	0.90	0.16	22,40,42,49	0
5	EDO	D	417	4/4	0.90	0.26	46,49,50,57	0
5	EDO	C	412	4/4	0.90	0.11	47,50,54,55	0
5	EDO	B	410	4/4	0.90	0.20	49,53,55,55	0
5	EDO	B	419	4/4	0.90	0.08	42,42,45,50	0
5	EDO	D	411	4/4	0.90	0.29	33,40,40,48	0
4	SO4	C	404	5/5	0.91	0.21	60,65,74,81	0
5	EDO	D	409	4/4	0.91	0.10	50,51,51,55	0
5	EDO	B	416	4/4	0.91	0.16	26,32,37,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	412	4/4	0.92	0.12	42,42,45,51	0
5	EDO	D	416	4/4	0.92	0.11	50,51,55,55	0
3	BME	A	402	4/4	0.92	0.15	33,36,46,48	0
5	EDO	C	417	4/4	0.93	0.14	29,33,44,58	0
4	SO4	D	405	5/5	0.93	0.23	57,60,73,78	0
5	EDO	D	421	4/4	0.93	0.16	31,39,41,49	0
5	EDO	B	412	4/4	0.93	0.38	26,33,35,45	0
5	EDO	A	409	4/4	0.93	0.12	23,39,47,47	0
5	EDO	A	405	4/4	0.94	0.22	24,36,37,45	0
2	FAD	D	401	53/53	0.94	0.12	14,19,24,26	0
2	FAD	C	401	53/53	0.95	0.12	14,19,25,27	0
2	FAD	B	401	53/53	0.95	0.11	10,16,21,23	0
2	FAD	A	401	53/53	0.95	0.12	10,16,22,22	0
4	SO4	A	404	5/5	0.96	0.18	51,56,67,69	0
4	SO4	C	403	5/5	0.97	0.11	28,32,44,49	0
4	SO4	B	403	5/5	0.97	0.14	26,33,44,46	0
4	SO4	D	404	5/5	0.98	0.19	51,59,63,70	0
4	SO4	D	403	5/5	0.98	0.10	26,32,45,45	0
4	SO4	A	403	5/5	0.99	0.09	24,31,45,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.