



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:25 am GMT

PDB ID : 4I42  
Title : E.coli. 1,4-dihydroxy-2-naphthoyl coenzyme A synthase (ecMenB) in complex with 1-hydroxy-2-naphthoyl-CoA  
Authors : Sun, Y.; Song, H.; Li, J.; Li, Y.; Jiang, M.; Zhou, J.; Guo, Z.  
Deposited on : 2012-11-27  
Resolution : 1.85 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

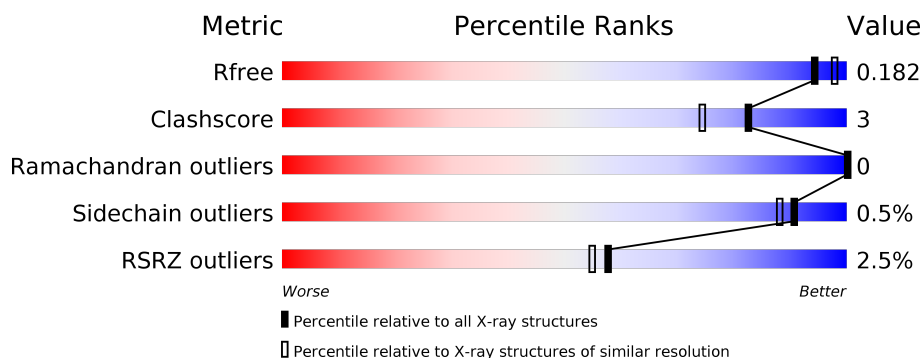
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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.



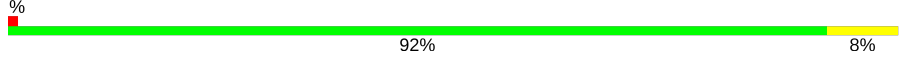
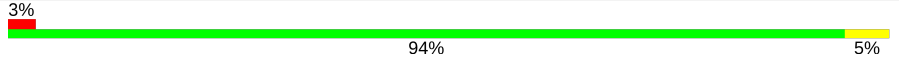
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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	285	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	285	<div> <div>2%</div> <div> <div></div> <div>97%</div> <div>•</div> </div> </div>
1	C	285	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5% •</div> </div> </div>
1	D	285	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>5% 6%</div> </div> </div>
1	E	285	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	F	285	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	285	
1	H	285	
1	I	285	
1	J	285	
1	K	285	
1	L	285	

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
3	EDO	B	304	-	-	-	X
3	EDO	C	305	-	-	-	X
3	EDO	C	306	-	-	-	X
3	EDO	D	306	-	-	-	X
3	EDO	E	305	-	-	X	-
3	EDO	G	306	-	-	-	X
3	EDO	H	305	-	-	-	X
3	EDO	H	306	-	-	-	X
4	SO4	D	307	-	-	-	X
4	SO4	E	309	-	-	-	X
4	SO4	H	308	-	-	-	X
5	CL	A	306	-	-	-	X
5	CL	J	307	-	-	-	X
6	BCT	D	308	-	-	-	X
6	BCT	F	309	-	-	-	X
7	GOL	B	302	-	-	-	X
7	GOL	C	302	-	-	-	X
7	GOL	C	303	-	-	-	X
7	GOL	D	301	-	-	-	X
7	GOL	D	302	-	-	-	X
7	GOL	E	303	-	-	-	X
7	GOL	F	302	-	-	-	X
7	GOL	G	302	-	-	X	X
7	GOL	G	303	-	-	-	X
7	GOL	H	302	-	-	-	X
7	GOL	H	303	-	-	-	X
7	GOL	I	302	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	I	303	-	-	-	X
7	GOL	J	302	-	-	-	X
7	GOL	J	303	-	-	-	X
7	GOL	J	304	-	-	-	X
7	GOL	L	302	-	-	-	X
8	PEG	C	304	-	-	-	X
8	PEG	E	304	-	-	-	X
8	PEG	H	304	-	-	-	X
8	PEG	K	303	-	-	-	X
9	BTB	C	310	-	-	-	X
9	BTB	F	308	-	-	-	X
9	BTB	I	309	-	-	-	X

## 2 Entry composition [i](#)

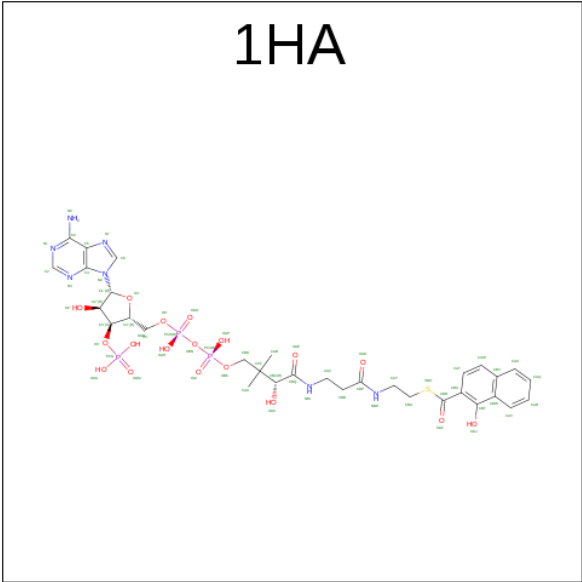
There are 10 unique types of molecules in this entry. The entry contains 30129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,4-Dihydroxy-2-naphthoyl-CoA synthase.

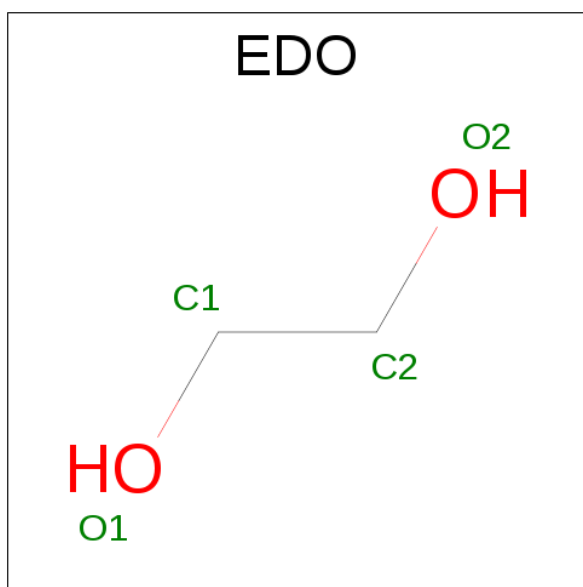
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	2	0
			2225	1391	398	416	20			
1	B	284	Total	C	N	O	S	0	2	0
			2213	1384	396	414	19			
1	C	282	Total	C	N	O	S	0	1	0
			2195	1372	393	411	19			
1	D	268	Total	C	N	O	S	0	1	0
			2087	1310	370	388	19			
1	E	285	Total	C	N	O	S	0	2	0
			2232	1397	396	418	21			
1	F	285	Total	C	N	O	S	0	3	0
			2242	1403	399	420	20			
1	G	285	Total	C	N	O	S	0	3	0
			2235	1401	399	415	20			
1	H	284	Total	C	N	O	S	0	2	0
			2219	1390	396	414	19			
1	I	285	Total	C	N	O	S	0	2	0
			2232	1397	398	417	20			
1	J	285	Total	C	N	O	S	0	2	0
			2230	1397	397	416	20			
1	K	285	Total	C	N	O	S	0	1	0
			2223	1392	396	415	20			
1	L	285	Total	C	N	O	S	0	2	0
			2227	1395	399	413	20			

- Molecule 2 is 1-HYDROXY-2-NAPHTHOYL-COA (three-letter code: 1HA) (formula:  $C_{32}H_{42}N_7O_{18}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



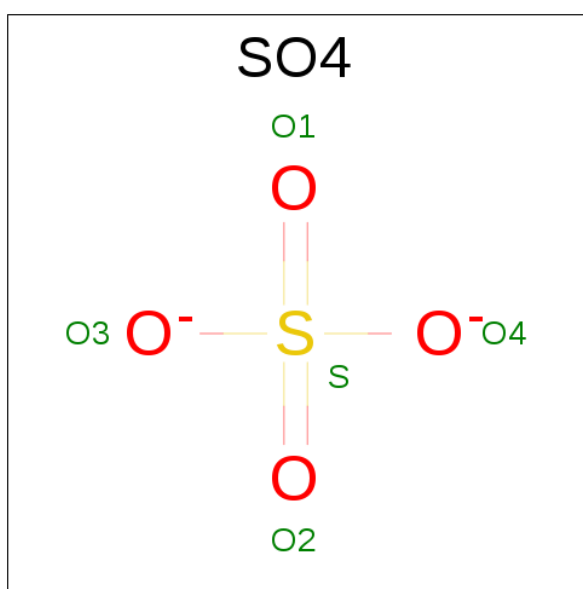
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

- 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	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	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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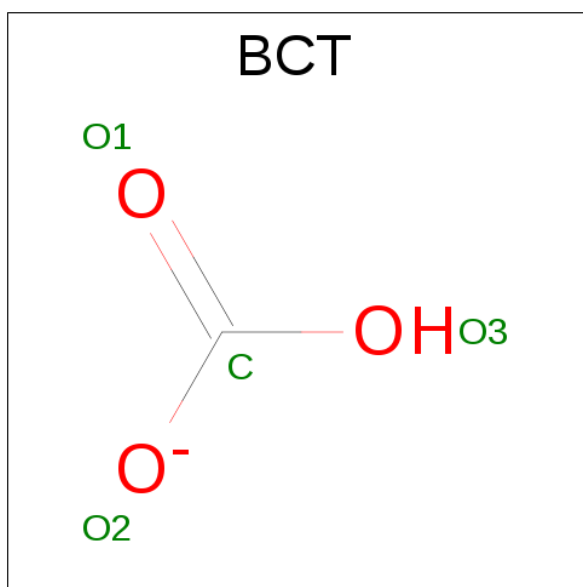
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

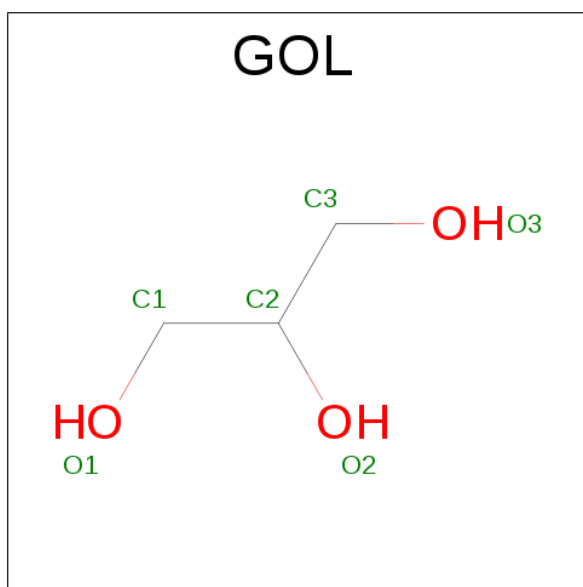
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cl	0	0
			1	1		
5	J	3	Total	Cl	0	0
			3	3		
5	K	2	Total	Cl	0	0
			2	2		
5	E	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	I	2	Total	Cl	0	0
			2	2		
5	C	1	Total	Cl	0	0
			1	1		
5	A	3	Total	Cl	0	0
			3	3		
5	L	2	Total	Cl	0	0
			2	2		
5	F	2	Total	Cl	0	0
			2	2		

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		
6	F	1	Total	C	O	0	0
			4	1	3		
6	I	1	Total	C	O	0	0
			4	1	3		
6	J	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



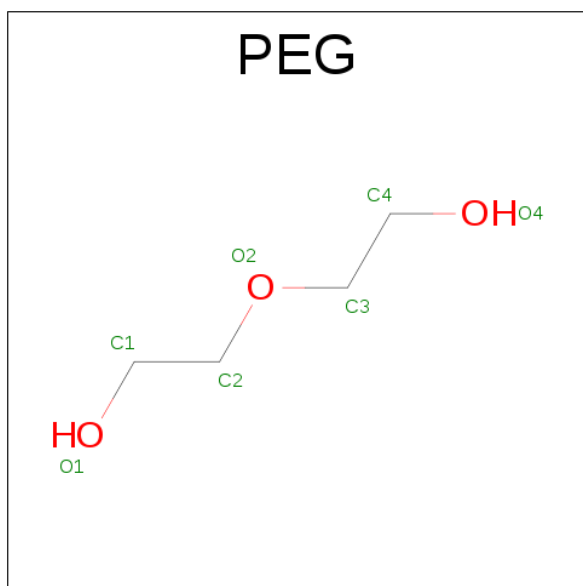
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	I	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	K	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



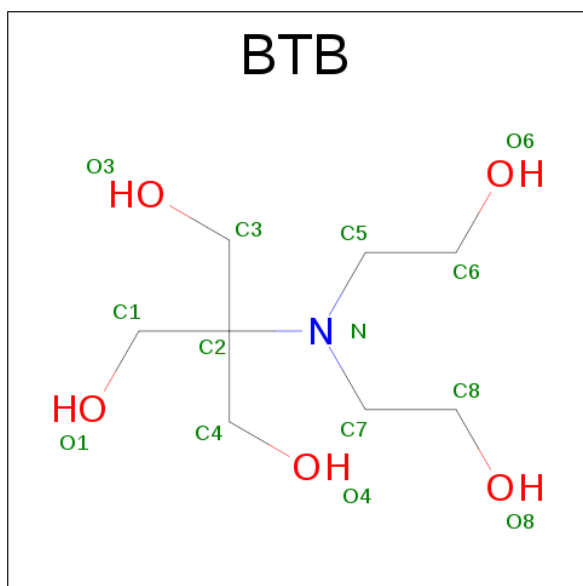
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		
8	C	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		
8	E	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			7	4	3		
8	F	1	Total	C	O	0	0
			7	4	3		
8	H	1	Total	C	O	0	0
			7	4	3		
8	I	1	Total	C	O	0	0
			7	4	3		
8	K	1	Total	C	O	0	0
			7	4	3		
8	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	F	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		

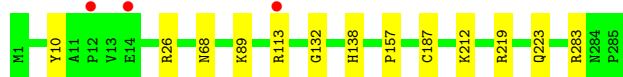
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	209	Total 209	O 209	0	0
10	B	183	Total 183	O 183	0	0
10	C	260	Total 260	O 260	0	0
10	D	179	Total 179	O 179	0	0
10	E	225	Total 225	O 225	0	0
10	F	212	Total 212	O 212	0	0
10	G	212	Total 212	O 212	0	0
10	H	195	Total 195	O 195	0	0
10	I	189	Total 189	O 189	0	0
10	J	204	Total 204	O 204	0	0
10	K	196	Total 196	O 196	0	0
10	L	212	Total 212	O 212	0	0

### 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: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



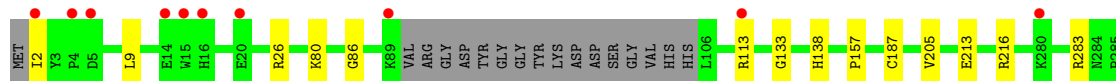
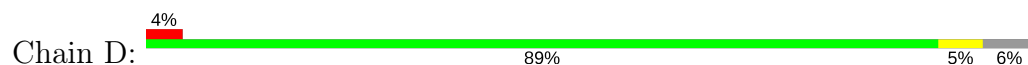
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



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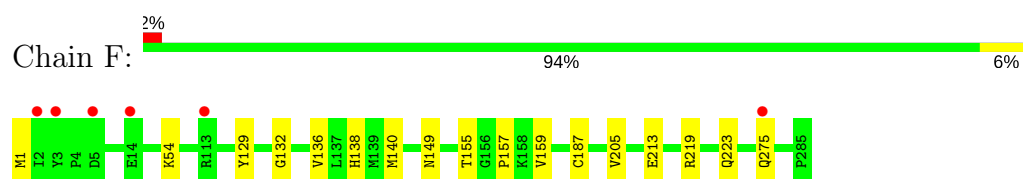
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



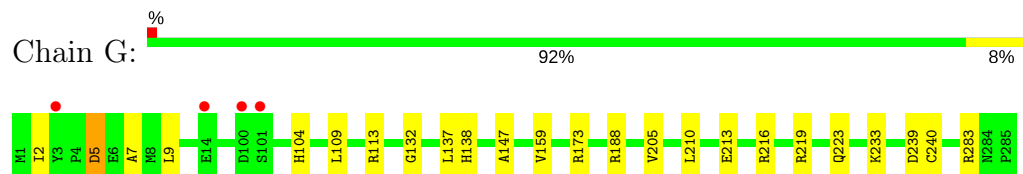
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



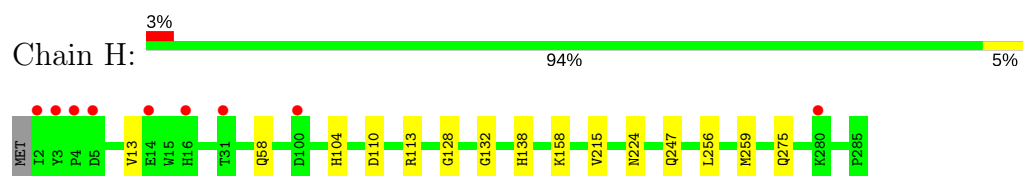
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



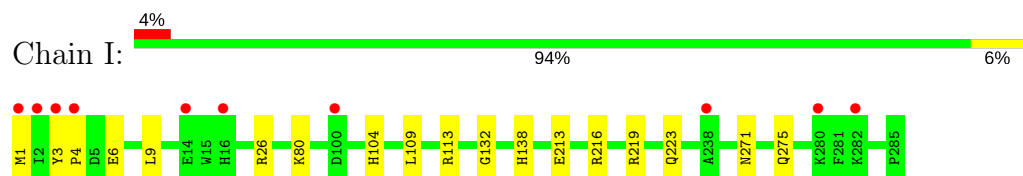
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



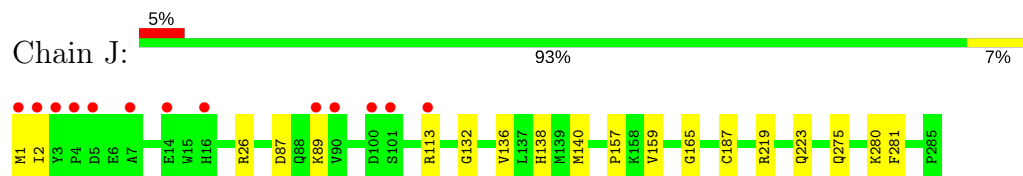
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



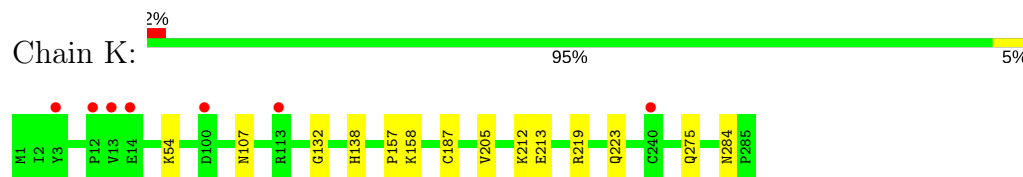
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



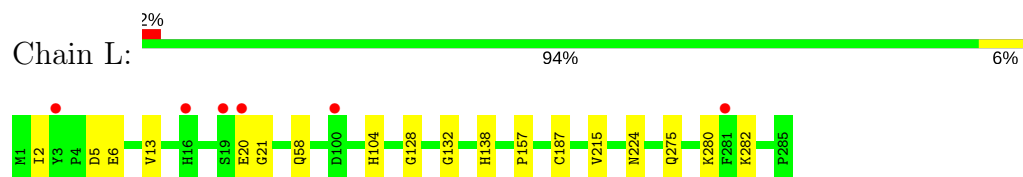
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.65Å 141.66Å 288.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.87 – 1.85 44.87 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.87-1.85) 91.2 (44.87-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.154 , 0.182 0.154 , 0.182	Depositor DCC
$R_{free}$ test set	2004 reflections (0.70%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.931	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	30129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: GOL, CL, EDO, 1HA, SO4, BTB, BCT, 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	0.36	0/2271	0.53	0/3060
1	B	0.33	0/2258	0.52	0/3043
1	C	0.39	0/2241	0.54	0/3019
1	D	0.35	0/2129	0.52	0/2869
1	E	0.37	0/2276	0.52	0/3067
1	F	0.35	0/2286	0.52	0/3081
1	G	0.35	0/2282	0.51	0/3074
1	H	0.33	0/2263	0.50	0/3052
1	I	0.35	0/2279	0.52	0/3071
1	J	0.34	0/2277	0.51	0/3069
1	K	0.35	0/2270	0.51	0/3059
1	L	0.36	0/2271	0.52	0/3060
All	All	0.35	0/27103	0.52	0/36524

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	2225	0	2181	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2213	0	2164	5	0
1	C	2195	0	2150	11	0
1	D	2087	0	2057	12	0
1	E	2232	0	2183	11	0
1	F	2242	0	2193	14	0
1	G	2235	0	2194	19	0
1	H	2219	0	2165	12	0
1	I	2232	0	2188	17	0
1	J	2230	0	2189	17	0
1	K	2223	0	2181	12	0
1	L	2227	0	2184	18	0
2	A	61	0	37	2	0
2	B	61	0	37	0	0
2	C	61	0	37	0	0
2	E	61	0	37	0	0
2	F	61	0	38	0	0
2	G	61	0	37	0	0
2	H	61	0	38	0	0
2	I	61	0	37	0	0
2	J	61	0	37	0	0
2	K	61	0	37	0	0
2	L	61	0	37	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	12	0	18	1	0
3	D	4	0	6	3	0
3	E	12	0	18	5	0
3	G	12	0	18	1	0
3	H	8	0	12	1	0
3	I	4	0	6	0	0
3	L	12	0	18	1	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	1	0
4	H	10	0	0	1	0
4	I	5	0	0	1	0
4	L	5	0	0	1	0
5	A	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	E	1	0	0	1	0
5	F	2	0	0	2	0
5	G	1	0	0	1	0
5	H	1	0	0	1	0
5	I	2	0	0	1	0
5	J	3	0	0	1	0
5	K	2	0	0	1	0
5	L	2	0	0	2	0
6	A	4	0	0	0	0
6	D	12	0	2	1	0
6	F	4	0	1	0	0
6	I	4	0	1	1	0
6	J	4	0	1	1	0
7	B	6	0	8	1	0
7	C	12	0	16	1	0
7	D	24	0	32	2	0
7	E	12	0	16	1	0
7	F	6	0	8	2	0
7	G	12	0	16	6	0
7	H	12	0	16	0	0
7	I	12	0	16	1	0
7	J	18	0	24	3	0
7	K	6	0	8	0	0
7	L	6	0	8	0	0
8	B	7	0	10	0	0
8	C	7	0	10	1	0
8	D	7	0	10	1	0
8	E	7	0	10	0	0
8	F	14	0	20	2	0
8	H	7	0	10	0	0
8	I	7	0	10	0	0
8	K	7	0	10	1	0
8	L	7	0	10	0	0
9	C	14	0	19	1	0
9	F	14	0	19	0	0
9	I	14	0	19	1	0
10	A	209	0	0	7	0
10	B	183	0	0	0	1
10	C	260	0	0	1	1
10	D	179	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	225	0	0	0	1
10	F	212	0	0	3	0
10	G	212	0	0	3	0
10	H	195	0	0	3	1
10	I	189	0	0	4	0
10	J	204	0	0	4	0
10	K	196	0	0	5	0
10	L	212	0	0	5	0
All	All	30129	0	26876	160	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (160) 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:I:275:GLN:NE2	10:I:561:HOH:O	1.87	1.06
1:A:212:LYS:NZ	10:A:567:HOH:O	1.92	1.00
2:A:301:1HA:OAM	10:A:574:HOH:O	1.81	0.98
1:J:113[A]:ARG:NH2	10:J:543:HOH:O	1.97	0.94
10:H:472:HOH:O	5:L:309:CL:CL	2.22	0.94
1:I:213:GLU:OE2	10:I:439:HOH:O	1.85	0.94
1:H:58:GLN:OE1	10:H:577:HOH:O	1.82	0.94
1:I:4:PRO:HB3	1:I:223[A]:GLN:HE22	1.31	0.94
1:C:113[A]:ARG:NH2	10:C:590:HOH:O	2.01	0.93
1:A:212:LYS:NZ	10:A:571:HOH:O	2.08	0.87
5:F:307:CL:CL	10:F:575:HOH:O	2.29	0.87
1:K:275:GLN:OE1	10:K:553:HOH:O	1.93	0.84
8:D:305:PEG:O4	10:D:551:HOH:O	1.96	0.83
1:J:280:LYS:HG2	10:J:489:HOH:O	1.81	0.80
1:L:20:GLU:HG3	1:L:21:GLY:H	1.49	0.78
1:K:284:ASN:O	10:K:544:HOH:O	2.02	0.78
1:I:4:PRO:HB3	1:I:223[A]:GLN:NE2	2.00	0.76
1:H:113[B]:ARG:NH1	10:H:487:HOH:O	2.20	0.74
1:K:205:VAL:HG11	1:K:213:GLU:HG3	1.69	0.74
1:F:275:GLN:NE2	10:F:571:HOH:O	2.21	0.73
7:D:304:GOL:O1	10:D:544:HOH:O	2.08	0.71
1:G:104:HIS:NE2	4:G:307:SO4:O3	2.21	0.71
1:I:271:ASN:O	10:I:576:HOH:O	2.09	0.70
1:A:10:TYR:CE1	1:A:212:LYS:HE2	2.26	0.70
1:J:2:ILE:HB	1:L:275:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:ARG:HH12	3:E:305:EDO:H22	1.59	0.68
8:F:303:PEG:H41	10:F:458:HOH:O	1.93	0.67
7:G:302:GOL:H32	10:G:496:HOH:O	1.94	0.67
1:D:113[B]:ARG:NH2	10:D:527:HOH:O	2.28	0.67
1:G:283[A]:ARG:NH2	10:G:418:HOH:O	2.27	0.66
1:A:113[B]:ARG:NH2	10:A:563:HOH:O	2.28	0.66
1:G:283[B]:ARG:HH12	3:G:306:EDO:H22	1.60	0.66
7:J:303:GOL:O2	10:J:512:HOH:O	2.13	0.66
1:J:26:ARG:HH12	6:J:308:BCT:C	2.10	0.65
1:A:68:ASN:ND2	10:A:529:HOH:O	2.08	0.65
6:D:309:BCT:O2	10:D:537:HOH:O	2.14	0.65
1:L:280:LYS:NZ	10:L:574:HOH:O	2.02	0.64
1:E:78:GLY:H	3:E:305:EDO:H21	1.62	0.64
1:F:129:TYR:CE2	7:F:302:GOL:H12	2.32	0.64
1:I:1:MET:HE1	1:J:159[A]:VAL:HG13	1.79	0.63
1:G:233:LYS:HE3	10:I:523:HOH:O	2.00	0.61
1:A:219:ARG:O	1:A:223[B]:GLN:HG2	2.01	0.60
1:F:205:VAL:HG11	1:F:213[A]:GLU:HG3	1.84	0.58
1:I:219:ARG:O	1:I:223[B]:GLN:HG2	2.02	0.58
1:D:205:VAL:HG11	1:D:213:GLU:HG3	1.86	0.57
1:K:223:GLN:NE2	10:K:576:HOH:O	1.95	0.57
1:D:80:LYS:HA	7:D:302:GOL:H32	1.87	0.56
7:J:302:GOL:H32	10:J:508:HOH:O	2.06	0.56
1:G:205:VAL:HG11	1:G:213:GLU:HG3	1.88	0.54
1:I:80:LYS:HE3	7:I:302:GOL:H32	1.88	0.54
1:B:2:ILE:C	1:C:275:GLN:HE22	2.10	0.54
1:C:80:LYS:HA	7:C:302:GOL:O1	2.08	0.54
1:A:212:LYS:HE3	1:I:6:GLU:CD	2.28	0.54
1:L:282:LYS:NZ	10:L:575:HOH:O	2.32	0.53
1:I:1:MET:HE1	1:J:159[A]:VAL:CG1	2.38	0.53
1:H:128:GLY:HA2	3:H:306:EDO:H11	1.91	0.53
1:D:86:GLY:HA3	3:D:306:EDO:H21	1.90	0.53
1:E:16:HIS:NE2	1:E:31:THR:HG23	2.24	0.52
1:L:13:VAL:HG21	1:L:215:VAL:HG21	1.92	0.52
3:D:306:EDO:H22	10:D:523:HOH:O	2.10	0.52
1:F:219:ARG:O	1:F:223:GLN:HG2	2.09	0.51
1:J:219:ARG:O	1:J:223:GLN:HG2	2.11	0.51
1:C:110:ASP:OD1	1:C:113[A]:ARG:NH1	2.44	0.50
1:E:280:LYS:HE3	1:E:281:PHE:CZ	2.47	0.50
1:C:132:GLY:HA2	5:C:309:CL:CL	2.49	0.50
1:D:2:ILE:O	1:F:275:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ILE:N	10:D:525:HOH:O	2.45	0.49
1:G:219:ARG:O	1:G:223:GLN:HG2	2.11	0.49
1:D:26:ARG:NH2	10:D:505:HOH:O	2.38	0.49
1:K:132:GLY:HA2	5:K:305:CL:CL	2.49	0.49
7:B:302:GOL:O1	7:B:302:GOL:O3	2.29	0.49
1:H:13:VAL:HG21	1:H:215:VAL:HG21	1.94	0.49
1:H:256:LEU:HD23	1:H:259:MET:CE	2.43	0.49
1:A:10:TYR:CD1	1:A:212:LYS:HE2	2.48	0.49
1:A:26:ARG:NH2	10:A:533:HOH:O	2.31	0.49
1:C:104:HIS:NE2	4:C:308:SO4:O1	2.43	0.48
1:G:2:ILE:HG22	1:K:275:GLN:HE21	1.78	0.48
1:J:275:GLN:HE21	1:L:2:ILE:HG22	1.77	0.48
1:E:132:GLY:HA2	5:E:310:CL:CL	2.50	0.48
1:E:26:ARG:NH1	3:E:305:EDO:H22	2.26	0.48
1:I:26:ARG:HH12	6:I:310:BCT:C	2.26	0.48
9:C:310:BTB:H72	9:C:310:BTB:H61	1.50	0.48
1:E:78:GLY:N	3:E:305:EDO:H21	2.27	0.48
1:F:132:GLY:HA2	5:F:306:CL:CL	2.51	0.48
1:G:173:ARG:HH22	7:G:302:GOL:H2	1.78	0.48
1:A:132:GLY:HA2	5:A:304:CL:CL	2.50	0.47
1:A:89:LYS:HE2	2:A:301:1HA:N3	2.29	0.47
1:G:9:LEU:HB3	1:G:216:ARG:HG3	1.97	0.47
1:K:107:ASN:HB3	10:K:531:HOH:O	2.14	0.47
1:I:132:GLY:HA2	5:I:307:CL:CL	2.51	0.47
1:A:212:LYS:HE3	1:I:6:GLU:CG	2.44	0.47
1:L:132:GLY:HA2	5:L:308:CL:CL	2.51	0.46
1:G:132:GLY:HA2	5:G:308:CL:CL	2.52	0.46
1:C:21:GLY:HA3	3:C:307:EDO:H12	1.97	0.46
1:H:132:GLY:HA2	5:H:309:CL:CL	2.52	0.46
1:C:105:HIS:CE1	8:C:304:PEG:H31	2.50	0.46
1:E:219:ARG:O	1:E:223[B]:GLN:HG2	2.15	0.46
1:D:9:LEU:HB3	1:D:216:ARG:HG3	1.98	0.46
1:G:239:ASP:O	7:G:302:GOL:O2	2.34	0.45
1:E:26:ARG:HH12	3:E:305:EDO:C2	2.27	0.45
1:E:255:MET:HE3	7:E:303:GOL:H11	1.98	0.45
1:F:205:VAL:HG11	1:F:213[B]:GLU:HG2	1.99	0.45
1:H:224:ASN:OD1	1:K:158:LYS:HG2	2.16	0.45
1:L:104:HIS:NE2	4:L:306:SO4:O2	2.48	0.45
1:G:173:ARG:HH22	7:G:302:GOL:C2	2.29	0.45
1:I:109:LEU:O	1:I:113[B]:ARG:HG3	2.17	0.45
1:F:149:ASN:O	7:F:302:GOL:H32	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:TYR:HD1	1:I:4:PRO:HD2	1.82	0.45
1:B:157:PRO:HD2	1:B:187:CYS:SG	2.57	0.45
1:J:132:GLY:HA2	5:J:305:CL:CL	2.55	0.44
9:I:309:BTB:H82	9:I:309:BTB:H51	1.64	0.44
1:J:2:ILE:HB	1:L:275:GLN:HE21	1.80	0.44
1:E:205:VAL:HG11	1:E:213:GLU:HG3	1.99	0.44
1:G:5:ASP:OD2	1:G:7:ALA:HB3	2.17	0.44
1:A:283:ARG:NH2	10:A:449:HOH:O	2.51	0.44
1:H:247:GLN:HA	1:J:165:GLY:HA3	2.00	0.43
1:K:157:PRO:HD2	1:K:187:CYS:SG	2.58	0.43
1:L:58:GLN:HG3	10:L:504:HOH:O	2.17	0.43
1:B:132:GLY:HA2	5:B:307:CL:CL	2.56	0.43
1:D:133:GLY:HA3	3:D:306:EDO:H12	2.00	0.43
1:J:136:VAL:O	1:J:140:MET:HG2	2.19	0.43
1:C:9:LEU:HB3	1:C:216:ARG:HG3	2.00	0.43
1:D:2:ILE:HB	1:F:275:GLN:HE21	1.84	0.43
1:G:147:ALA:HB2	1:G:210:LEU:HD22	1.99	0.43
7:G:302:GOL:C3	10:G:497:HOH:O	2.62	0.43
1:H:158:LYS:HG2	1:L:224:ASN:OD1	2.19	0.43
1:C:4:PRO:HB2	1:C:9:LEU:HD11	2.00	0.43
1:H:110:ASP:OD1	1:H:113[A]:ARG:NH1	2.51	0.43
1:L:157:PRO:HD2	1:L:187:CYS:SG	2.58	0.42
1:K:219:ARG:O	1:K:223:GLN:HG2	2.19	0.42
1:H:104:HIS:NE2	4:H:307:SO4:O4	2.52	0.42
1:G:109:LEU:O	1:G:113[B]:ARG:HG3	2.20	0.42
1:K:54:LYS:HD2	8:K:303:PEG:H12	2.01	0.42
1:L:128:GLY:HA2	3:L:304:EDO:H12	2.01	0.42
1:L:5:ASP:OD1	1:L:6:GLU:N	2.53	0.42
1:G:159:VAL:CG1	1:J:1:MET:HE1	2.50	0.42
1:G:188:ARG:HH22	7:J:304:GOL:H31	1.85	0.42
1:K:212:LYS:HE3	10:K:577:HOH:O	2.20	0.42
1:F:54:LYS:HD2	8:F:303:PEG:H42	2.01	0.42
1:D:157:PRO:HD2	1:D:187:CYS:SG	2.60	0.41
1:F:155:THR:O	1:F:159[B]:VAL:HG23	2.20	0.41
1:L:13:VAL:CG2	1:L:215:VAL:HG11	2.50	0.41
1:L:282:LYS:NZ	10:L:491:HOH:O	2.12	0.41
1:A:157:PRO:HD2	1:A:187:CYS:SG	2.60	0.41
1:C:135:HIS:NE2	1:C:200:LEU:HD21	2.35	0.41
1:G:137:LEU:HD23	1:G:137:LEU:HA	1.92	0.41
1:I:9:LEU:HB3	1:I:216:ARG:HG3	2.01	0.41
1:J:275:GLN:HE22	1:L:2:ILE:C	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:280:LYS:HE3	1:J:281:PHE:CZ	2.56	0.41
1:H:256:LEU:HA	1:H:259:MET:CE	2.50	0.41
1:L:282:LYS:CE	10:L:491:HOH:O	2.67	0.41
1:B:9:LEU:HB3	1:B:216:ARG:HG3	2.02	0.41
1:F:157:PRO:HD2	1:F:187:CYS:SG	2.61	0.41
1:I:104:HIS:NE2	4:I:306:SO4:O2	2.50	0.41
1:J:87:ASP:OD1	1:J:89:LYS:HB3	2.22	0.41
1:J:157:PRO:HD2	1:J:187:CYS:SG	2.61	0.40
1:B:159[B]:VAL:HG13	1:F:1:MET:HE1	2.02	0.40
1:G:240:CYS:O	7:G:302:GOL:O3	2.40	0.40
1:D:283:ARG:NH1	10:D:425:HOH:O	2.55	0.40
1:F:136:VAL:O	1:F:140:MET:HG2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:567:HOH:O	10:C:619:HOH:O[4_555]	2.16	0.04
10:E:586:HOH:O	10:H:563:HOH:O[2_454]	2.16	0.04

## 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	285/285 (100%)	280 (98%)	5 (2%)	0	100	100
1	B	284/285 (100%)	278 (98%)	6 (2%)	0	100	100
1	C	281/285 (99%)	276 (98%)	5 (2%)	0	100	100
1	D	265/285 (93%)	261 (98%)	4 (2%)	0	100	100
1	E	285/285 (100%)	280 (98%)	5 (2%)	0	100	100
1	F	286/285 (100%)	281 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	286/285 (100%)	281 (98%)	5 (2%)	0	100	100
1	H	284/285 (100%)	279 (98%)	5 (2%)	0	100	100
1	I	285/285 (100%)	280 (98%)	5 (2%)	0	100	100
1	J	285/285 (100%)	279 (98%)	6 (2%)	0	100	100
1	K	284/285 (100%)	278 (98%)	6 (2%)	0	100	100
1	L	285/285 (100%)	278 (98%)	7 (2%)	0	100	100
All	All	3395/3420 (99%)	3331 (98%)	64 (2%)	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	230/229 (100%)	229 (100%)	1 (0%)	93	91
1	B	228/229 (100%)	227 (100%)	1 (0%)	93	91
1	C	227/229 (99%)	226 (100%)	1 (0%)	93	91
1	D	216/229 (94%)	215 (100%)	1 (0%)	91	88
1	E	231/229 (101%)	230 (100%)	1 (0%)	93	91
1	F	232/229 (101%)	231 (100%)	1 (0%)	93	91
1	G	230/229 (100%)	228 (99%)	2 (1%)	82	76
1	H	228/229 (100%)	226 (99%)	2 (1%)	82	76
1	I	231/229 (101%)	230 (100%)	1 (0%)	93	91
1	J	231/229 (101%)	230 (100%)	1 (0%)	93	91
1	K	230/229 (100%)	229 (100%)	1 (0%)	93	91
1	L	229/229 (100%)	228 (100%)	1 (0%)	93	91
All	All	2743/2748 (100%)	2729 (100%)	14 (0%)	91	88

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

Mol	Chain	Res	Type
1	A	138	HIS
1	B	138	HIS
1	C	138	HIS
1	D	138	HIS
1	E	138	HIS
1	F	138	HIS
1	G	5	ASP
1	G	138	HIS
1	H	138	HIS
1	H	275	GLN
1	I	138	HIS
1	J	138	HIS
1	K	138	HIS
1	L	138	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	275	GLN
1	F	275	GLN
1	J	275	GLN
1	K	275	GLN
1	L	275	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 19 are monoatomic - leaving 83 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	$\# Z  > 2$
2	1HA	A	301	-	58,65,65	2.01	18 (31%)	71,97,97	1.53	10 (14%)
3	EDO	A	302	-	3,3,3	0.44	0	2,2,2	0.44	0
4	SO4	A	303	-	4,4,4	0.13	0	6,6,6	0.12	0
6	BCT	A	307	-	0,3,3	0.00	-	0,3,3	0.00	-
2	1HA	B	301	-	58,65,65	2.03	17 (29%)	71,97,97	1.47	7 (9%)
7	GOL	B	302	-	5,5,5	0.34	0	5,5,5	0.18	0
8	PEG	B	303	-	6,6,6	0.62	0	5,5,5	1.41	0
3	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.38	0
4	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	B	306	-	4,4,4	0.14	0	6,6,6	0.04	0
2	1HA	C	301	-	58,65,65	1.97	17 (29%)	71,97,97	1.52	8 (11%)
7	GOL	C	302	-	5,5,5	0.33	0	5,5,5	1.14	1 (20%)
7	GOL	C	303	-	5,5,5	0.24	0	5,5,5	0.22	0
8	PEG	C	304	-	6,6,6	0.64	0	5,5,5	1.41	0
3	EDO	C	305	-	3,3,3	0.44	0	2,2,2	0.40	0
3	EDO	C	306	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	C	307	-	3,3,3	0.43	0	2,2,2	0.36	0
4	SO4	C	308	-	4,4,4	0.16	0	6,6,6	0.20	0
9	BTB	C	310	-	13,13,13	0.77	0	9,16,16	0.82	0
7	GOL	D	301	-	5,5,5	0.27	0	5,5,5	0.29	0
7	GOL	D	302	-	5,5,5	0.21	0	5,5,5	0.37	0
7	GOL	D	303	-	5,5,5	0.32	0	5,5,5	0.35	0
7	GOL	D	304	-	5,5,5	0.33	0	5,5,5	0.25	0
8	PEG	D	305	-	6,6,6	0.61	0	5,5,5	1.35	0
3	EDO	D	306	-	3,3,3	0.42	0	2,2,2	0.40	0
4	SO4	D	307	-	4,4,4	0.30	0	6,6,6	0.13	0
6	BCT	D	308	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	D	309	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BCT	D	310	-	0,3,3	0.00	-	0,3,3	0.00	-
2	1HA	E	301	-	58,65,65	2.05	17 (29%)	71,97,97	1.62	9 (12%)
7	GOL	E	302	-	5,5,5	0.23	0	5,5,5	0.32	0
7	GOL	E	303	-	5,5,5	0.31	0	5,5,5	0.34	0
8	PEG	E	304	-	6,6,6	0.61	0	5,5,5	1.44	0
3	EDO	E	305	-	3,3,3	0.45	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	E	306	-	3,3,3	0.40	0	2,2,2	0.42	0
3	EDO	E	307	-	3,3,3	0.45	0	2,2,2	0.38	0
4	SO4	E	308	-	4,4,4	0.10	0	6,6,6	0.13	0
4	SO4	E	309	-	4,4,4	0.12	0	6,6,6	0.15	0
2	1HA	F	301	-	58,65,65	1.99	17 (29%)	71,97,97	1.50	9 (12%)
7	GOL	F	302	-	5,5,5	0.26	0	5,5,5	0.85	0
8	PEG	F	303	-	6,6,6	0.63	0	5,5,5	1.43	0
8	PEG	F	304	-	6,6,6	0.63	0	5,5,5	1.35	0
4	SO4	F	305	-	4,4,4	0.13	0	6,6,6	0.06	0
9	BTB	F	308	-	13,13,13	0.82	0	9,16,16	0.40	0
6	BCT	F	309	-	0,3,3	0.00	-	0,3,3	0.00	-
2	1HA	G	301	-	58,65,65	2.02	18 (31%)	71,97,97	1.55	9 (12%)
7	GOL	G	302	-	5,5,5	0.38	0	5,5,5	0.25	0
7	GOL	G	303	-	5,5,5	0.28	0	5,5,5	0.36	0
3	EDO	G	304	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	G	305	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	G	306	-	3,3,3	0.46	0	2,2,2	0.39	0
4	SO4	G	307	-	4,4,4	0.17	0	6,6,6	0.12	0
2	1HA	H	301	-	58,65,65	2.02	16 (27%)	71,97,97	1.42	7 (9%)
7	GOL	H	302	-	5,5,5	0.32	0	5,5,5	0.37	0
7	GOL	H	303	-	5,5,5	0.25	0	5,5,5	0.32	0
8	PEG	H	304	-	6,6,6	0.62	0	5,5,5	1.44	0
3	EDO	H	305	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	H	306	-	3,3,3	0.43	0	2,2,2	0.41	0
4	SO4	H	307	-	4,4,4	0.10	0	6,6,6	0.14	0
4	SO4	H	308	-	4,4,4	0.15	0	6,6,6	0.09	0
2	1HA	I	301	-	58,65,65	2.00	15 (25%)	71,97,97	1.50	10 (14%)
7	GOL	I	302	-	5,5,5	0.31	0	5,5,5	0.36	0
7	GOL	I	303	-	5,5,5	0.30	0	5,5,5	0.31	0
8	PEG	I	304	-	6,6,6	0.63	0	5,5,5	1.43	0
3	EDO	I	305	-	3,3,3	0.46	0	2,2,2	0.37	0
4	SO4	I	306	-	4,4,4	0.12	0	6,6,6	0.14	0
9	BTB	I	309	-	13,13,13	0.79	0	9,16,16	0.65	0
6	BCT	I	310	-	0,3,3	0.00	-	0,3,3	0.00	-
2	1HA	J	301	-	58,65,65	2.05	18 (31%)	71,97,97	1.46	8 (11%)
7	GOL	J	302	-	5,5,5	0.31	0	5,5,5	0.40	0
7	GOL	J	303	-	5,5,5	0.31	0	5,5,5	0.53	0
7	GOL	J	304	-	5,5,5	0.24	0	5,5,5	0.32	0
6	BCT	J	308	-	0,3,3	0.00	-	0,3,3	0.00	-
2	1HA	K	301	-	58,65,65	2.08	19 (32%)	71,97,97	1.51	9 (12%)
7	GOL	K	302	-	5,5,5	0.34	0	5,5,5	0.17	0
8	PEG	K	303	-	6,6,6	0.60	0	5,5,5	1.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	1HA	L	301	-	58,65,65	2.00	16 (27%)	71,97,97	1.48	8 (11%)
7	GOL	L	302	-	5,5,5	0.31	0	5,5,5	0.31	0
8	PEG	L	303	-	6,6,6	0.61	0	5,5,5	1.43	0
3	EDO	L	304	-	3,3,3	0.41	0	2,2,2	0.46	0
3	EDO	L	305	-	3,3,3	0.52	0	2,2,2	0.44	0
4	SO4	L	306	-	4,4,4	0.12	0	6,6,6	0.22	0
3	EDO	L	307	-	3,3,3	0.46	0	2,2,2	0.38	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	1HA	A	301	-	-	0/51/71/71	0/5/5/5
3	EDO	A	302	-	-	0/1/1/1	0/0/0/0
4	SO4	A	303	-	-	0/0/0/0	0/0/0/0
6	BCT	A	307	-	-	0/0/0/0	0/0/0/0
2	1HA	B	301	-	-	0/51/71/71	0/5/5/5
7	GOL	B	302	-	-	0/4/4/4	0/0/0/0
8	PEG	B	303	-	-	0/4/4/4	0/0/0/0
3	EDO	B	304	-	-	0/1/1/1	0/0/0/0
4	SO4	B	305	-	-	0/0/0/0	0/0/0/0
4	SO4	B	306	-	-	0/0/0/0	0/0/0/0
2	1HA	C	301	-	-	0/51/71/71	0/5/5/5
7	GOL	C	302	-	-	0/4/4/4	0/0/0/0
7	GOL	C	303	-	-	0/4/4/4	0/0/0/0
8	PEG	C	304	-	-	0/4/4/4	0/0/0/0
3	EDO	C	305	-	-	0/1/1/1	0/0/0/0
3	EDO	C	306	-	-	0/1/1/1	0/0/0/0
3	EDO	C	307	-	-	0/1/1/1	0/0/0/0
4	SO4	C	308	-	-	0/0/0/0	0/0/0/0
9	BTB	C	310	-	-	0/21/21/21	0/0/0/0
7	GOL	D	301	-	-	0/4/4/4	0/0/0/0
7	GOL	D	302	-	-	0/4/4/4	0/0/0/0
7	GOL	D	303	-	-	0/4/4/4	0/0/0/0
7	GOL	D	304	-	-	0/4/4/4	0/0/0/0
8	PEG	D	305	-	-	0/4/4/4	0/0/0/0
3	EDO	D	306	-	-	0/1/1/1	0/0/0/0
4	SO4	D	307	-	-	0/0/0/0	0/0/0/0
6	BCT	D	308	-	-	0/0/0/0	0/0/0/0
6	BCT	D	309	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCT	D	310	-	-	0/0/0/0	0/0/0/0
2	1HA	E	301	-	-	0/51/71/71	0/5/5/5
7	GOL	E	302	-	-	0/4/4/4	0/0/0/0
7	GOL	E	303	-	-	0/4/4/4	0/0/0/0
8	PEG	E	304	-	-	0/4/4/4	0/0/0/0
3	EDO	E	305	-	-	0/1/1/1	0/0/0/0
3	EDO	E	306	-	-	0/1/1/1	0/0/0/0
3	EDO	E	307	-	-	0/1/1/1	0/0/0/0
4	SO4	E	308	-	-	0/0/0/0	0/0/0/0
4	SO4	E	309	-	-	0/0/0/0	0/0/0/0
2	1HA	F	301	-	-	0/51/71/71	0/5/5/5
7	GOL	F	302	-	-	0/4/4/4	0/0/0/0
8	PEG	F	303	-	-	0/4/4/4	0/0/0/0
8	PEG	F	304	-	-	0/4/4/4	0/0/0/0
4	SO4	F	305	-	-	0/0/0/0	0/0/0/0
9	BTB	F	308	-	-	0/21/21/21	0/0/0/0
6	BCT	F	309	-	-	0/0/0/0	0/0/0/0
2	1HA	G	301	-	-	0/51/71/71	0/5/5/5
7	GOL	G	302	-	-	0/4/4/4	0/0/0/0
7	GOL	G	303	-	-	0/4/4/4	0/0/0/0
3	EDO	G	304	-	-	0/1/1/1	0/0/0/0
3	EDO	G	305	-	-	0/1/1/1	0/0/0/0
3	EDO	G	306	-	-	0/1/1/1	0/0/0/0
4	SO4	G	307	-	-	0/0/0/0	0/0/0/0
2	1HA	H	301	-	-	0/51/71/71	0/5/5/5
7	GOL	H	302	-	-	0/4/4/4	0/0/0/0
7	GOL	H	303	-	-	0/4/4/4	0/0/0/0
8	PEG	H	304	-	-	0/4/4/4	0/0/0/0
3	EDO	H	305	-	-	0/1/1/1	0/0/0/0
3	EDO	H	306	-	-	0/1/1/1	0/0/0/0
4	SO4	H	307	-	-	0/0/0/0	0/0/0/0
4	SO4	H	308	-	-	0/0/0/0	0/0/0/0
2	1HA	I	301	-	-	0/51/71/71	0/5/5/5
7	GOL	I	302	-	-	0/4/4/4	0/0/0/0
7	GOL	I	303	-	-	0/4/4/4	0/0/0/0
8	PEG	I	304	-	-	0/4/4/4	0/0/0/0
3	EDO	I	305	-	-	0/1/1/1	0/0/0/0
4	SO4	I	306	-	-	0/0/0/0	0/0/0/0
9	BTB	I	309	-	-	0/21/21/21	0/0/0/0
6	BCT	I	310	-	-	0/0/0/0	0/0/0/0
2	1HA	J	301	-	-	0/51/71/71	0/5/5/5
7	GOL	J	302	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	J	303	-	-	0/4/4/4	0/0/0/0
7	GOL	J	304	-	-	0/4/4/4	0/0/0/0
6	BCT	J	308	-	-	0/0/0/0	0/0/0/0
2	1HA	K	301	-	-	0/51/71/71	0/5/5/5
7	GOL	K	302	-	-	0/4/4/4	0/0/0/0
8	PEG	K	303	-	-	0/4/4/4	0/0/0/0
2	1HA	L	301	-	-	0/51/71/71	0/5/5/5
7	GOL	L	302	-	-	0/4/4/4	0/0/0/0
8	PEG	L	303	-	-	0/4/4/4	0/0/0/0
3	EDO	L	304	-	-	0/1/1/1	0/0/0/0
3	EDO	L	305	-	-	0/1/1/1	0/0/0/0
4	SO4	L	306	-	-	0/0/0/0	0/0/0/0
3	EDO	L	307	-	-	0/1/1/1	0/0/0/0

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	1HA	C2'-C3'	-5.11	1.41	1.53
2	K	301	1HA	C2'-C3'	-5.03	1.41	1.53
2	B	301	1HA	O4'-C1'	-4.97	1.34	1.41
2	F	301	1HA	C2'-C3'	-4.95	1.42	1.53
2	K	301	1HA	O4'-C1'	-4.90	1.34	1.41
2	J	301	1HA	O4'-C1'	-4.88	1.34	1.41
2	L	301	1HA	C2'-C3'	-4.87	1.42	1.53
2	A	301	1HA	O4'-C1'	-4.86	1.34	1.41
2	L	301	1HA	O4'-C1'	-4.86	1.34	1.41
2	J	301	1HA	C2'-C3'	-4.81	1.42	1.53
2	G	301	1HA	C2'-C3'	-4.77	1.42	1.53
2	A	301	1HA	C2'-C3'	-4.76	1.42	1.53
2	B	301	1HA	C2'-C3'	-4.76	1.42	1.53
2	H	301	1HA	O4'-C1'	-4.73	1.34	1.41
2	I	301	1HA	C2'-C3'	-4.73	1.42	1.53
2	G	301	1HA	O4'-C1'	-4.67	1.34	1.41
2	H	301	1HA	C2'-C3'	-4.64	1.42	1.53
2	C	301	1HA	C2'-C3'	-4.62	1.42	1.53
2	I	301	1HA	O4'-C1'	-4.58	1.34	1.41
2	E	301	1HA	O4'-C1'	-4.45	1.35	1.41
2	C	301	1HA	O4'-C1'	-4.38	1.35	1.41
2	F	301	1HA	O4'-C1'	-4.34	1.35	1.41
2	C	301	1HA	PCG-OAN	-4.08	1.38	1.54
2	E	301	1HA	PCG-OAN	-4.07	1.38	1.54
2	G	301	1HA	PCG-OAN	-4.03	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	1HA	PCG-OAN	-4.01	1.38	1.54
2	L	301	1HA	PCG-OAN	-4.00	1.38	1.54
2	F	301	1HA	PCG-OAN	-3.99	1.38	1.54
2	K	301	1HA	PCG-OAN	-3.98	1.38	1.54
2	B	301	1HA	PCG-OAN	-3.94	1.38	1.54
2	A	301	1HA	PCG-OAN	-3.92	1.38	1.54
2	J	301	1HA	PCG-OAN	-3.91	1.38	1.54
2	I	301	1HA	PCG-OAN	-3.88	1.38	1.54
2	G	301	1HA	CBW-CBV	-3.53	1.36	1.43
2	J	301	1HA	CBW-CBV	-3.49	1.36	1.43
2	A	301	1HA	CBW-CBV	-3.49	1.36	1.43
2	E	301	1HA	CBW-CBV	-3.48	1.36	1.43
2	L	301	1HA	CBW-CBV	-3.44	1.36	1.43
2	K	301	1HA	CBW-CBV	-3.40	1.36	1.43
2	B	301	1HA	CBW-CBV	-3.35	1.36	1.43
2	I	301	1HA	CBW-CBV	-3.35	1.36	1.43
2	H	301	1HA	CBW-CBV	-3.31	1.36	1.43
2	F	301	1HA	CBW-CBV	-3.18	1.37	1.43
2	C	301	1HA	CBW-CBV	-3.17	1.37	1.43
2	H	301	1HA	PCI-OBK	-2.77	1.47	1.59
2	E	301	1HA	C4-N3	-2.77	1.31	1.35
2	B	301	1HA	CAZ-NBI	-2.72	1.39	1.46
2	J	301	1HA	PCI-OBK	-2.70	1.47	1.59
2	K	301	1HA	PCI-OBK	-2.63	1.48	1.59
2	C	301	1HA	PCI-OBK	-2.62	1.48	1.59
2	F	301	1HA	PCI-OBK	-2.62	1.48	1.59
2	G	301	1HA	C4-N3	-2.59	1.31	1.35
2	H	301	1HA	CAZ-NBI	-2.59	1.40	1.46
2	K	301	1HA	C4-N3	-2.53	1.31	1.35
2	A	301	1HA	PCI-OBK	-2.53	1.48	1.59
2	B	301	1HA	PCI-OBK	-2.53	1.48	1.59
2	L	301	1HA	PCI-OBK	-2.52	1.48	1.59
2	J	301	1HA	CAZ-NBI	-2.52	1.40	1.46
2	E	301	1HA	PCI-OBK	-2.51	1.48	1.59
2	F	301	1HA	C4-N3	-2.50	1.31	1.35
2	J	301	1HA	C4-N3	-2.47	1.31	1.35
2	F	301	1HA	CAZ-NBI	-2.47	1.40	1.46
2	I	301	1HA	PCI-OBK	-2.45	1.48	1.59
2	K	301	1HA	CAZ-NBI	-2.44	1.40	1.46
2	A	301	1HA	CAZ-NBI	-2.44	1.40	1.46
2	G	301	1HA	PCI-OBK	-2.43	1.48	1.59
2	A	301	1HA	C4-N3	-2.40	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	1HA	O2'-C2'	-2.39	1.37	1.43
2	L	301	1HA	PCI-OAI	-2.37	1.42	1.50
2	G	301	1HA	CAZ-NBI	-2.37	1.40	1.46
2	A	301	1HA	OAF-CBR	-2.36	1.16	1.21
2	I	301	1HA	C3'-C4'	-2.36	1.46	1.52
2	B	301	1HA	OAF-CBR	-2.35	1.17	1.21
2	H	301	1HA	PCI-OAI	-2.34	1.42	1.50
2	E	301	1HA	O2'-C2'	-2.33	1.37	1.43
2	F	301	1HA	C3'-C4'	-2.33	1.46	1.52
2	B	301	1HA	C3'-C4'	-2.33	1.46	1.52
2	B	301	1HA	PCI-OAI	-2.32	1.42	1.50
2	H	301	1HA	C3'-C4'	-2.31	1.46	1.52
2	K	301	1HA	PCI-OAI	-2.31	1.42	1.50
2	B	301	1HA	O2'-C2'	-2.31	1.37	1.43
2	G	301	1HA	C3'-C4'	-2.31	1.46	1.52
2	L	301	1HA	C4-N3	-2.30	1.32	1.35
2	A	301	1HA	C3'-C4'	-2.29	1.46	1.52
2	J	301	1HA	OAF-CBR	-2.27	1.17	1.21
2	E	301	1HA	PCI-OAI	-2.27	1.42	1.50
2	L	301	1HA	O2'-C2'	-2.27	1.37	1.43
2	J	301	1HA	PCI-OAI	-2.26	1.42	1.50
2	B	301	1HA	CAZ-CBB	-2.26	1.43	1.51
2	C	301	1HA	C4-N3	-2.26	1.32	1.35
2	L	301	1HA	CAZ-NBI	-2.25	1.41	1.46
2	B	301	1HA	C4-N3	-2.24	1.32	1.35
2	I	301	1HA	PCI-OAI	-2.24	1.42	1.50
2	K	301	1HA	O2'-C2'	-2.24	1.37	1.43
2	J	301	1HA	C3'-C4'	-2.24	1.46	1.52
2	I	301	1HA	C4-N3	-2.23	1.32	1.35
2	C	301	1HA	PCI-OAI	-2.23	1.42	1.50
2	A	301	1HA	PCI-OAI	-2.23	1.42	1.50
2	G	301	1HA	PCI-OAI	-2.23	1.42	1.50
2	F	301	1HA	PCI-OAI	-2.22	1.42	1.50
2	K	301	1HA	C3'-C4'	-2.22	1.46	1.52
2	C	301	1HA	CAZ-NBI	-2.21	1.41	1.46
2	H	301	1HA	O2'-C2'	-2.21	1.37	1.43
2	J	301	1HA	O2'-C2'	-2.21	1.37	1.43
2	C	301	1HA	O2'-C2'	-2.20	1.37	1.43
2	E	301	1HA	OAF-CBR	-2.20	1.17	1.21
2	G	301	1HA	O2'-C2'	-2.20	1.37	1.43
2	H	301	1HA	OAF-CBR	-2.20	1.17	1.21
2	F	301	1HA	CAZ-CBB	-2.20	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	1HA	C3'-C4'	-2.19	1.46	1.52
2	L	301	1HA	OAF-CBR	-2.19	1.17	1.21
2	K	301	1HA	CAZ-CBB	-2.19	1.44	1.51
2	E	301	1HA	CAZ-NBI	-2.18	1.41	1.46
2	A	301	1HA	O2'-C2'	-2.18	1.37	1.43
2	E	301	1HA	C3'-C4'	-2.15	1.46	1.52
2	I	301	1HA	CAZ-NBI	-2.15	1.41	1.46
2	L	301	1HA	CAZ-CBB	-2.15	1.44	1.51
2	I	301	1HA	CAZ-CBB	-2.13	1.44	1.51
2	K	301	1HA	PCH-OAH	-2.12	1.44	1.55
2	A	301	1HA	CAZ-CBB	-2.11	1.44	1.51
2	J	301	1HA	CAZ-CBB	-2.11	1.44	1.51
2	C	301	1HA	OAF-CBR	-2.10	1.17	1.21
2	H	301	1HA	PCH-OAH	-2.09	1.44	1.55
2	F	301	1HA	O2'-C2'	-2.09	1.38	1.43
2	E	301	1HA	CAZ-CBB	-2.09	1.44	1.51
2	G	301	1HA	CAZ-CBB	-2.08	1.44	1.51
2	A	301	1HA	C5-N7	-2.06	1.32	1.39
2	C	301	1HA	PCH-OAH	-2.06	1.44	1.55
2	C	301	1HA	C3'-C4'	-2.06	1.47	1.52
2	J	301	1HA	PCH-OAH	-2.06	1.44	1.55
2	E	301	1HA	C5-N7	-2.05	1.32	1.39
2	G	301	1HA	PCH-OAH	-2.05	1.44	1.55
2	G	301	1HA	C5-N7	-2.04	1.32	1.39
2	F	301	1HA	OAF-CBR	-2.04	1.17	1.21
2	H	301	1HA	CAZ-CBB	-2.04	1.44	1.51
2	K	301	1HA	C5-N7	-2.04	1.32	1.39
2	G	301	1HA	OAF-CBR	-2.02	1.17	1.21
2	F	301	1HA	PCH-OAH	-2.02	1.45	1.55
2	A	301	1HA	PCH-OAH	-2.02	1.45	1.55
2	K	301	1HA	OAF-CBR	-2.01	1.17	1.21
2	B	301	1HA	PCH-OAH	-2.00	1.45	1.55
2	J	301	1HA	OAK-CBZ	2.01	1.46	1.42
2	K	301	1HA	OAK-CBZ	2.06	1.46	1.42
2	C	301	1HA	OAK-CBZ	2.11	1.46	1.42
2	E	301	1HA	CAA-CCF	2.37	1.59	1.53
2	J	301	1HA	CAA-CCF	2.44	1.59	1.53
2	F	301	1HA	CAA-CCF	2.47	1.59	1.53
2	H	301	1HA	CAA-CCF	2.50	1.59	1.53
2	I	301	1HA	CAA-CCF	2.53	1.59	1.53
2	K	301	1HA	CAA-CCF	2.56	1.59	1.53
2	B	301	1HA	CAA-CCF	2.56	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	1HA	CAA-CCF	2.64	1.59	1.53
2	A	301	1HA	CAA-CCF	2.65	1.59	1.53
2	G	301	1HA	CAA-CCF	2.66	1.59	1.53
2	C	301	1HA	CAA-CCF	2.72	1.60	1.53
2	G	301	1HA	CBR-SBO	2.81	1.82	1.76
2	L	301	1HA	CBR-SBO	2.84	1.82	1.76
2	A	301	1HA	CBR-SBO	2.93	1.82	1.76
2	C	301	1HA	CBR-SBO	3.00	1.82	1.76
2	F	301	1HA	CBR-SBO	3.04	1.82	1.76
2	J	301	1HA	CBR-SBO	3.19	1.83	1.76
2	E	301	1HA	CBR-SBO	3.24	1.83	1.76
2	I	301	1HA	CBR-SBO	3.25	1.83	1.76
2	H	301	1HA	CBR-SBO	3.27	1.83	1.76
2	B	301	1HA	CBR-SBO	3.34	1.83	1.76
2	K	301	1HA	CBR-SBO	3.52	1.83	1.76
2	F	301	1HA	CBP-NBH	4.02	1.42	1.33
2	H	301	1HA	CBP-NBH	4.14	1.43	1.33
2	A	301	1HA	CBP-NBH	4.21	1.43	1.33
2	L	301	1HA	CBP-NBH	4.21	1.43	1.33
2	K	301	1HA	CBP-NBH	4.22	1.43	1.33
2	B	301	1HA	CBP-NBH	4.26	1.43	1.33
2	G	301	1HA	CBP-NBH	4.26	1.43	1.33
2	I	301	1HA	CBP-NBH	4.31	1.43	1.33
2	J	301	1HA	CBP-NBH	4.34	1.43	1.33
2	C	301	1HA	CBP-NBH	4.46	1.43	1.33
2	E	301	1HA	CBP-NBH	4.47	1.43	1.33
2	B	301	1HA	CBQ-NBI	5.33	1.44	1.33
2	C	301	1HA	CBQ-NBI	5.33	1.44	1.33
2	L	301	1HA	CBQ-NBI	5.34	1.44	1.33
2	A	301	1HA	CBQ-NBI	5.38	1.44	1.33
2	F	301	1HA	CBQ-NBI	5.40	1.44	1.33
2	G	301	1HA	CBQ-NBI	5.55	1.44	1.33
2	J	301	1HA	CBQ-NBI	5.66	1.45	1.33
2	H	301	1HA	CBQ-NBI	5.69	1.45	1.33
2	E	301	1HA	CBQ-NBI	5.73	1.45	1.33
2	I	301	1HA	CBQ-NBI	5.74	1.45	1.33
2	K	301	1HA	CBQ-NBI	5.80	1.45	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	1HA	N3-C2-N1	-6.94	122.81	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	1HA	N3-C2-N1	-6.90	122.85	128.86
2	L	301	1HA	N3-C2-N1	-6.80	122.94	128.86
2	I	301	1HA	N3-C2-N1	-6.74	122.99	128.86
2	J	301	1HA	N3-C2-N1	-6.66	123.05	128.86
2	K	301	1HA	N3-C2-N1	-6.63	123.09	128.86
2	C	301	1HA	N3-C2-N1	-6.60	123.11	128.86
2	H	301	1HA	N3-C2-N1	-6.57	123.14	128.86
2	F	301	1HA	N3-C2-N1	-6.19	123.47	128.86
2	B	301	1HA	N3-C2-N1	-6.16	123.50	128.86
2	G	301	1HA	N3-C2-N1	-5.79	123.82	128.86
2	E	301	1HA	C4-C5-N7	-4.80	104.77	109.41
2	A	301	1HA	C4-C5-N7	-4.72	104.85	109.41
2	G	301	1HA	C4-C5-N7	-4.69	104.88	109.41
2	J	301	1HA	C4-C5-N7	-4.57	104.99	109.41
2	F	301	1HA	C4-C5-N7	-4.38	105.18	109.41
2	L	301	1HA	C4-C5-N7	-4.32	105.23	109.41
2	K	301	1HA	C4-C5-N7	-4.26	105.29	109.41
2	B	301	1HA	C4-C5-N7	-4.07	105.48	109.41
2	H	301	1HA	C4-C5-N7	-3.99	105.56	109.41
2	C	301	1HA	C4-C5-N7	-3.96	105.59	109.41
2	I	301	1HA	C4-C5-N7	-3.87	105.67	109.41
2	L	301	1HA	OAF-CBR-SBO	-3.63	114.22	122.58
2	A	301	1HA	OAF-CBR-SBO	-3.45	114.64	122.58
2	I	301	1HA	OAF-CBR-SBO	-3.43	114.67	122.58
2	C	301	1HA	OAF-CBR-SBO	-3.30	114.97	122.58
2	G	301	1HA	OAF-CBR-SBO	-3.21	115.18	122.58
2	B	301	1HA	OAF-CBR-SBO	-3.02	115.61	122.58
2	E	301	1HA	OAF-CBR-SBO	-3.02	115.62	122.58
2	F	301	1HA	OAF-CBR-SBO	-2.75	116.24	122.58
2	J	301	1HA	OAF-CBR-SBO	-2.74	116.26	122.58
2	K	301	1HA	OAF-CBR-SBO	-2.61	116.57	122.58
2	H	301	1HA	OAF-CBR-SBO	-2.50	116.81	122.58
2	A	301	1HA	O3'-C3'-C4'	-2.31	101.35	110.04
2	F	301	1HA	O3'-C3'-C4'	-2.25	101.59	110.04
7	C	302	GOL	C3-C2-C1	-2.21	102.75	111.52
2	I	301	1HA	O3'-C3'-C4'	-2.13	102.05	110.04
2	G	301	1HA	O3'-C3'-C4'	-2.09	102.19	110.04
2	G	301	1HA	CAY-CBA-SBO	2.02	117.12	111.23
2	I	301	1HA	OBK-CBD-CCF	2.03	113.80	110.55
2	H	301	1HA	CBU-CBR-SBO	2.03	119.00	115.02
2	A	301	1HA	CBB-CAZ-NBI	2.05	116.10	111.87
2	K	301	1HA	CBB-CAZ-NBI	2.06	116.12	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301	1HA	CBB-CAZ-NBI	2.11	116.25	111.87
2	E	301	1HA	CAY-CBA-SBO	2.12	117.40	111.23
2	I	301	1HA	CBB-CAZ-NBI	2.12	116.27	111.87
2	B	301	1HA	CAY-CBA-SBO	2.19	117.60	111.23
2	A	301	1HA	CAY-CBA-SBO	2.20	117.62	111.23
2	K	301	1HA	CAY-CBA-SBO	2.20	117.62	111.23
2	J	301	1HA	O2'-C2'-C3'	2.20	117.45	111.18
2	F	301	1HA	OBK-CBD-CCF	2.20	114.09	110.55
2	C	301	1HA	CAY-CBA-SBO	2.23	117.72	111.23
2	L	301	1HA	CAY-CBA-SBO	2.28	117.87	111.23
2	H	301	1HA	CAB-CCF-CBD	2.29	111.74	108.37
2	A	301	1HA	OBK-CBD-CCF	2.31	114.26	110.55
2	L	301	1HA	CAB-CCF-CBD	2.32	111.78	108.37
2	K	301	1HA	OBK-CBD-CCF	2.34	114.31	110.55
2	I	301	1HA	CAY-CBA-SBO	2.36	118.08	111.23
2	H	301	1HA	CBB-CAZ-NBI	2.37	116.77	111.87
2	J	301	1HA	CAY-CBA-SBO	2.41	118.24	111.23
2	G	301	1HA	CBB-CAZ-NBI	2.44	116.91	111.87
2	L	301	1HA	CBB-CAZ-NBI	2.48	116.99	111.87
2	F	301	1HA	CBU-CBR-SBO	2.51	119.94	115.02
2	E	301	1HA	CBB-CAZ-NBI	2.54	117.13	111.87
2	C	301	1HA	CBB-CAZ-NBI	2.56	117.17	111.87
2	B	301	1HA	OBK-CBD-CCF	2.59	114.71	110.55
2	K	301	1HA	CAB-CCF-CBD	2.62	112.22	108.37
2	F	301	1HA	CBB-CAZ-NBI	2.65	117.36	111.87
2	A	301	1HA	CBU-CBR-SBO	2.68	120.27	115.02
2	L	301	1HA	CBA-SBO-CBR	2.69	102.98	99.68
2	E	301	1HA	CBU-CBR-SBO	2.70	120.33	115.02
2	E	301	1HA	OBK-CBD-CCF	2.71	114.90	110.55
2	J	301	1HA	CBU-CBR-SBO	2.83	120.58	115.02
2	G	301	1HA	OBK-CBD-CCF	2.92	115.24	110.55
2	I	301	1HA	CBU-CBR-SBO	2.94	120.79	115.02
2	B	301	1HA	CBU-CBR-SBO	2.96	120.83	115.02
2	I	301	1HA	CAB-CCF-CBD	2.99	112.76	108.37
2	K	301	1HA	CBU-CBR-SBO	3.01	120.92	115.02
2	L	301	1HA	CBU-CBR-SBO	3.02	120.95	115.02
2	C	301	1HA	CAB-CCF-CBD	3.04	112.83	108.37
2	A	301	1HA	CAB-CCF-CBD	3.11	112.93	108.37
2	C	301	1HA	CBU-CBR-SBO	3.18	121.27	115.02
2	J	301	1HA	CBA-SBO-CBR	3.22	103.64	99.68
2	F	301	1HA	CAB-CCF-CBD	3.28	113.18	108.37
2	G	301	1HA	CAB-CCF-CBD	3.42	113.39	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	1HA	CBA-SBO-CBR	3.45	103.92	99.68
2	A	301	1HA	CBA-SBO-CBR	3.48	103.96	99.68
2	H	301	1HA	CBA-SBO-CBR	3.63	104.14	99.68
2	B	301	1HA	CBA-SBO-CBR	3.75	104.29	99.68
2	F	301	1HA	CBA-SBO-CBR	3.77	104.31	99.68
2	E	301	1HA	CAB-CCF-CBD	3.85	114.02	108.37
2	C	301	1HA	CBA-SBO-CBR	3.86	104.42	99.68
2	K	301	1HA	CBA-SBO-CBR	4.19	104.82	99.68
2	G	301	1HA	CBA-SBO-CBR	4.82	105.60	99.68
2	E	301	1HA	CBA-SBO-CBR	5.00	105.82	99.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	1HA	2	0
7	B	302	GOL	1	0
7	C	302	GOL	1	0
8	C	304	PEG	1	0
3	C	307	EDO	1	0
4	C	308	SO4	1	0
9	C	310	BTB	1	0
7	D	302	GOL	1	0
7	D	304	GOL	1	0
8	D	305	PEG	1	0
3	D	306	EDO	3	0
6	D	309	BCT	1	0
7	E	303	GOL	1	0
3	E	305	EDO	5	0
7	F	302	GOL	2	0
8	F	303	PEG	2	0
7	G	302	GOL	6	0
3	G	306	EDO	1	0
4	G	307	SO4	1	0
3	H	306	EDO	1	0
4	H	307	SO4	1	0
7	I	302	GOL	1	0
4	I	306	SO4	1	0
9	I	309	BTB	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	310	BCT	1	0
7	J	302	GOL	1	0
7	J	303	GOL	1	0
7	J	304	GOL	1	0
6	J	308	BCT	1	0
8	K	303	PEG	1	0
3	L	304	EDO	1	0
4	L	306	SO4	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, 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	285/285 (100%)	-0.17	3 (1%) 80 80	14, 21, 39, 60	1 (0%)
1	B	284/285 (99%)	-0.11	7 (2%) 58 55	15, 25, 46, 67	0
1	C	282/285 (98%)	-0.39	7 (2%) 58 55	12, 16, 43, 75	0
1	D	268/285 (94%)	-0.12	10 (3%) 42 38	12, 24, 46, 81	1 (0%)
1	E	285/285 (100%)	-0.35	3 (1%) 80 80	12, 19, 37, 60	0
1	F	285/285 (100%)	-0.16	6 (2%) 64 62	12, 22, 46, 58	0
1	G	285/285 (100%)	-0.26	4 (1%) 75 75	14, 21, 41, 66	1 (0%)
1	H	284/285 (99%)	-0.04	9 (3%) 48 45	15, 25, 51, 65	0
1	I	285/285 (100%)	-0.16	10 (3%) 44 41	13, 21, 48, 67	0
1	J	285/285 (100%)	-0.02	13 (4%) 33 30	15, 26, 51, 69	1 (0%)
1	K	285/285 (100%)	-0.10	7 (2%) 58 55	15, 23, 47, 71	0
1	L	285/285 (100%)	-0.16	6 (2%) 64 62	14, 21, 43, 69	0
All	All	3398/3420 (99%)	-0.17	85 (2%) 58 55	12, 22, 47, 81	4 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	3	TYR	5.7
1	J	3	TYR	4.6
1	B	2	ILE	4.4
1	B	3	TYR	4.3
1	J	101	SER	4.3
1	D	20	GLU	4.1
1	D	280	LYS	4.1
1	F	3	TYR	3.9
1	G	100	ASP	3.7
1	E	3	TYR	3.7
1	K	100	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	2	ILE	3.6
1	J	2	ILE	3.6
1	B	4	PRO	3.6
1	J	4	PRO	3.5
1	H	2	ILE	3.5
1	C	275	GLN	3.5
1	B	16	HIS	3.4
1	J	14	GLU	3.4
1	L	3	TYR	3.3
1	F	14	GLU	3.2
1	H	3	TYR	3.2
1	C	4	PRO	3.2
1	I	16	HIS	3.2
1	H	4	PRO	3.2
1	D	89	LYS	3.2
1	J	1	MET	3.1
1	J	5	ASP	3.1
1	E	100	ASP	3.1
1	H	5	ASP	3.0
1	K	13	VAL	3.0
1	D	5	ASP	3.0
1	I	1	MET	2.9
1	L	100	ASP	2.9
1	I	2	ILE	2.8
1	J	89	LYS	2.8
1	I	282	LYS	2.8
1	K	14	GLU	2.8
1	L	20	GLU	2.8
1	K	12	PRO	2.7
1	D	15	TRP	2.7
1	L	16	HIS	2.7
1	D	14	GLU	2.7
1	J	16	HIS	2.7
1	J	100	ASP	2.7
1	D	2	ILE	2.6
1	D	4	PRO	2.6
1	H	100	ASP	2.6
1	F	113[A]	ARG	2.6
1	F	5	ASP	2.6
1	C	280	LYS	2.5
1	H	16	HIS	2.5
1	H	31	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	14	GLU	2.5
1	G	3	TYR	2.5
1	I	280	LYS	2.4
1	G	14	GLU	2.4
1	I	100	ASP	2.4
1	A	113[A]	ARG	2.4
1	H	280	LYS	2.3
1	A	12	PRO	2.3
1	C	282	LYS	2.3
1	K	3	TYR	2.3
1	J	113[A]	ARG	2.3
1	I	238	ALA	2.3
1	A	14	GLU	2.2
1	B	113[A]	ARG	2.2
1	K	240	CYS	2.2
1	C	281	PHE	2.2
1	F	275	GLN	2.2
1	D	16	HIS	2.1
1	C	283	ARG	2.1
1	B	5	ASP	2.1
1	E	14	GLU	2.1
1	D	113[A]	ARG	2.1
1	K	113[A]	ARG	2.1
1	J	7	ALA	2.1
1	L	19	SER	2.1
1	L	281	PHE	2.1
1	J	90	VAL	2.1
1	C	279	SER	2.1
1	H	14	GLU	2.0
1	G	101	SER	2.0
1	I	4	PRO	2.0
1	I	14	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CL	A	306	1/1	0.96	0.54	15.18	78,78,78,78	0
7	GOL	J	302	6/6	0.56	0.34	12.20	67,70,72,73	0
5	CL	J	307	1/1	0.84	0.45	10.53	75,75,75,75	0
3	EDO	C	306	4/4	0.78	0.18	10.11	46,47,50,55	0
7	GOL	H	303	6/6	0.92	0.15	10.07	28,31,38,39	0
7	GOL	C	303	6/6	0.93	0.13	7.81	20,31,37,42	0
7	GOL	C	302	6/6	0.92	0.17	7.69	14,26,39,40	0
7	GOL	G	302	6/6	0.88	0.31	6.82	51,54,58,61	0
4	SO4	D	307	5/5	0.96	0.14	6.72	12,38,44,48	0
9	BTB	F	308	14/14	0.69	0.26	6.44	36,59,64,67	0
6	BCT	D	308	4/4	0.77	0.21	6.40	50,58,59,60	0
9	BTB	I	309	14/14	0.66	0.30	6.12	41,57,66,68	0
7	GOL	F	302	6/6	0.79	0.24	6.06	30,45,46,50	0
8	PEG	C	304	7/7	0.82	0.17	4.81	39,41,46,47	0
4	SO4	E	309	5/5	0.84	0.25	4.74	86,88,89,90	0
4	SO4	H	308	5/5	0.89	0.27	4.62	96,97,98,99	0
9	BTB	C	310	14/14	0.81	0.20	4.06	33,40,55,57	0
7	GOL	H	302	6/6	0.89	0.23	4.04	42,47,48,48	0
3	EDO	C	305	4/4	0.80	0.15	4.04	56,56,61,69	0
7	GOL	G	303	6/6	0.92	0.14	3.92	23,31,33,34	0
6	BCT	F	309	4/4	0.65	0.24	3.91	61,61,61,62	0
7	GOL	J	303	6/6	0.83	0.22	3.89	35,38,46,49	0
3	EDO	D	306	4/4	0.88	0.16	3.82	42,46,54,60	0
7	GOL	J	304	6/6	0.89	0.15	3.68	22,35,36,41	0
8	PEG	E	304	7/7	0.91	0.12	3.59	41,44,48,51	0
3	EDO	H	305	4/4	0.86	0.17	3.57	41,51,55,60	0
7	GOL	D	302	6/6	0.82	0.20	3.43	35,46,50,52	0
3	EDO	H	306	4/4	0.90	0.16	2.94	28,31,31,37	0
7	GOL	B	302	6/6	0.89	0.16	2.91	28,37,42,42	0
7	GOL	D	301	6/6	0.94	0.10	2.80	24,31,32,32	0
7	GOL	E	303	6/6	0.68	0.25	2.66	33,37,40,47	0
3	EDO	B	304	4/4	0.71	0.20	2.60	66,66,67,75	0
7	GOL	L	302	6/6	0.94	0.16	2.54	31,32,33,34	0
3	EDO	G	306	4/4	0.84	0.14	2.44	55,56,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	PEG	K	303	7/7	0.86	0.19	2.24	49,51,59,65	0
7	GOL	I	303	6/6	0.92	0.16	2.24	25,32,42,48	0
8	PEG	H	304	7/7	0.85	0.15	2.13	53,56,61,64	0
7	GOL	I	302	6/6	0.87	0.17	2.05	39,42,46,46	0
3	EDO	E	306	4/4	0.92	0.14	1.42	29,31,35,36	0
4	SO4	C	308	5/5	0.95	0.14	1.31	37,46,49,50	0
4	SO4	B	306	5/5	0.93	0.20	1.28	72,80,80,83	0
7	GOL	E	302	6/6	0.95	0.08	1.16	21,28,31,34	0
8	PEG	I	304	7/7	0.93	0.12	1.11	36,39,46,48	0
3	EDO	L	304	4/4	0.88	0.12	1.02	25,28,33,37	0
8	PEG	F	303	7/7	0.93	0.10	0.91	38,42,45,46	0
2	1HA	G	301	61/61	0.94	0.14	0.79	19,30,42,51	0
8	PEG	D	305	7/7	0.84	0.18	0.73	51,54,57,57	0
8	PEG	F	304	7/7	0.90	0.13	0.73	44,48,55,64	0
7	GOL	K	302	6/6	0.92	0.13	0.71	38,45,46,50	0
2	1HA	H	301	61/61	0.95	0.10	0.59	19,27,34,44	0
2	1HA	J	301	61/61	0.92	0.15	0.50	25,37,44,58	0
3	EDO	G	305	4/4	0.76	0.18	0.47	47,47,52,56	0
2	1HA	B	301	61/61	0.94	0.12	0.41	18,30,39,45	0
8	PEG	L	303	7/7	0.81	0.14	0.37	51,53,56,61	0
2	1HA	K	301	61/61	0.94	0.11	0.33	25,35,50,58	0
2	1HA	I	301	61/61	0.95	0.10	0.32	17,24,33,43	0
2	1HA	F	301	61/61	0.95	0.10	0.29	17,25,37,45	0
3	EDO	A	302	4/4	0.90	0.10	0.09	43,47,48,50	0
2	1HA	A	301	61/61	0.95	0.10	0.05	17,25,36,45	0
2	1HA	E	301	61/61	0.95	0.10	0.04	17,28,36,53	0
5	CL	E	310	1/1	0.99	0.07	0.00	22,22,22,22	0
2	1HA	C	301	61/61	0.98	0.07	-0.29	11,18,24,36	0
5	CL	J	305	1/1	0.98	0.08	-0.48	26,26,26,26	0
2	1HA	L	301	61/61	0.97	0.08	-0.51	16,23,27,38	0
4	SO4	G	307	5/5	0.96	0.14	-0.51	52,53,58,58	0
8	PEG	B	303	7/7	0.93	0.09	-0.53	44,46,48,50	0
5	CL	K	305	1/1	0.98	0.07	-0.78	27,27,27,27	0
5	CL	B	307	1/1	0.99	0.07	-0.93	22,22,22,22	0
5	CL	C	309	1/1	0.99	0.07	-1.15	17,17,17,17	0
5	CL	I	307	1/1	0.98	0.05	-1.45	19,19,19,19	0
5	CL	H	309	1/1	0.98	0.05	-1.71	21,21,21,21	0
5	CL	G	308	1/1	0.99	0.05	-1.87	22,22,22,22	0
5	CL	L	308	1/1	0.99	0.05	-1.97	19,19,19,19	0
5	CL	A	304	1/1	1.00	0.04	-2.00	21,21,21,21	0
5	CL	F	306	1/1	0.98	0.05	-3.52	20,20,20,20	0
7	GOL	D	304	6/6	0.89	0.18	-	44,48,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	E	307	4/4	0.89	0.12	-	60,61,63,66	0
4	SO4	E	308	5/5	0.97	0.12	-	46,48,58,66	0
3	EDO	G	304	4/4	0.83	0.17	-	46,48,48,52	0
3	EDO	C	307	4/4	0.89	0.12	-	44,47,51,52	0
5	CL	I	308	1/1	0.91	0.11	-	66,66,66,66	0
5	CL	J	306	1/1	0.95	0.14	-	51,51,51,51	0
6	BCT	D	310	4/4	0.91	0.08	-	46,48,50,53	0
3	EDO	L	307	4/4	0.77	0.29	-	43,51,57,61	0
5	CL	K	304	1/1	0.96	0.12	-	56,56,56,56	0
7	GOL	D	303	6/6	0.61	0.25	-	67,69,69,70	0
6	BCT	A	307	4/4	0.88	0.10	-	61,64,64,66	0
3	EDO	E	305	4/4	0.83	0.11	-	48,50,51,53	0
4	SO4	B	305	5/5	0.98	0.13	-	53,53,55,55	0
4	SO4	H	307	5/5	0.95	0.12	-	45,48,54,62	0
5	CL	A	305	1/1	0.69	0.11	-	84,84,84,84	0
6	BCT	J	308	4/4	0.88	0.13	-	50,53,53,54	0
4	SO4	I	306	5/5	0.94	0.17	-	58,66,67,71	0
4	SO4	F	305	5/5	0.98	0.09	-	41,42,52,54	0
5	CL	F	307	1/1	0.86	0.12	-	65,65,65,65	0
6	BCT	D	309	4/4	0.74	0.22	-	58,60,62,66	0
6	BCT	I	310	4/4	0.88	0.10	-	55,60,60,61	0
3	EDO	L	305	4/4	0.93	0.14	-	20,31,32,35	0
4	SO4	A	303	5/5	0.97	0.14	-	54,55,63,64	0
4	SO4	L	306	5/5	0.98	0.11	-	42,43,53,54	0
3	EDO	I	305	4/4	0.74	0.15	-	52,55,58,58	0
5	CL	L	309	1/1	0.82	0.12	-	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.