



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 10:47 AM EDT

PDB ID : 3E8M  
Title : Structure-function Analysis of 2-Keto-3-deoxy-D-glycero-D-galacto-nononate-9-phosphate (KDN) Phosphatase Defines a New Clad Within the Type C0 HAD Subfamily  
Authors : Lu, Z.; Wang, L.; Dunaway-Mariano, D.; Allen, K.N.  
Deposited on : 2008-08-20  
Resolution : 1.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

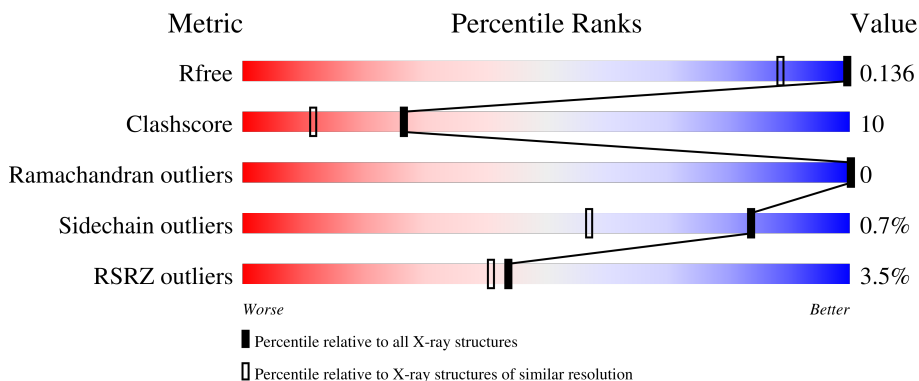
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	164	 3% 90% 10%
1	B	164	 3% 92% 7%
1	C	164	 4% 88% 11%
1	D	164	 4% 87% 12%

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
5	PEG	A	171	-	-	X	-
6	PG4	A	172	-	-	X	-
7	EDO	B	169	-	-	X	-
7	EDO	B	171	-	-	-	X
7	EDO	C	169	-	-	X	-
7	EDO	D	171	-	-	X	-
7	EDO	D	172	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12179 atoms, of which 5401 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 Acylneuraminate cytidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	164	2716	902	1312	235	264	3	0	25	0
1	B	164	2695	884	1312	236	260	3	0	21	0
1	C	164	2688	884	1312	230	259	3	0	19	0
1	D	164	2712	896	1312	235	266	3	0	23	0

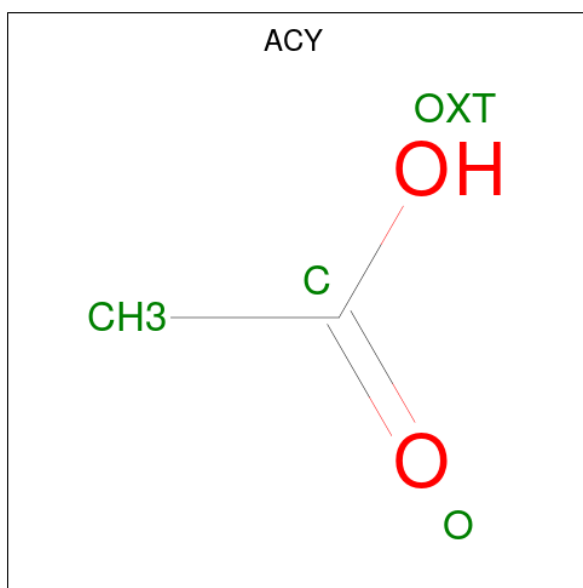
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



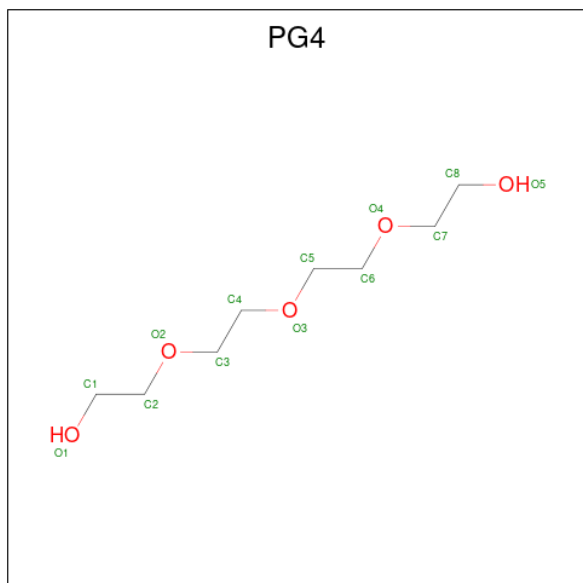
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	7	2	3	2	0	0
4	A	1	7	2	3	2	0	0
4	B	1	7	2	3	2	0	0
4	C	1	7	2	3	2	0	0
4	D	1	7	2	3	2	0	0
4	D	1	7	2	3	2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



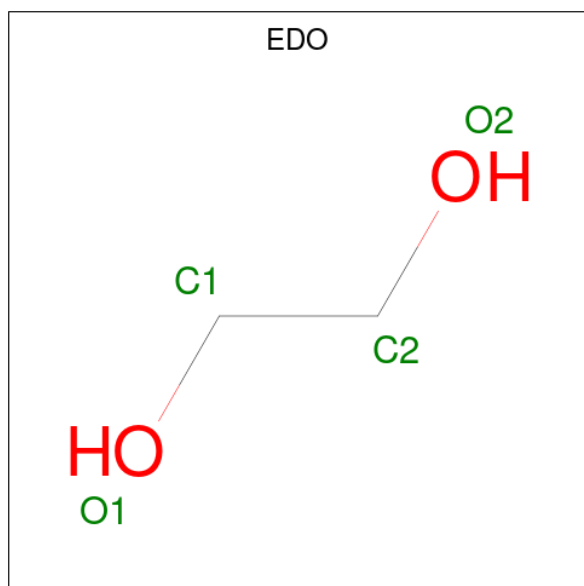
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	17	4	10	3	0	0
5	A	1	17	4	10	3	0	0
5	B	1	17	4	10	3	0	0
5	C	1	17	4	10	3	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



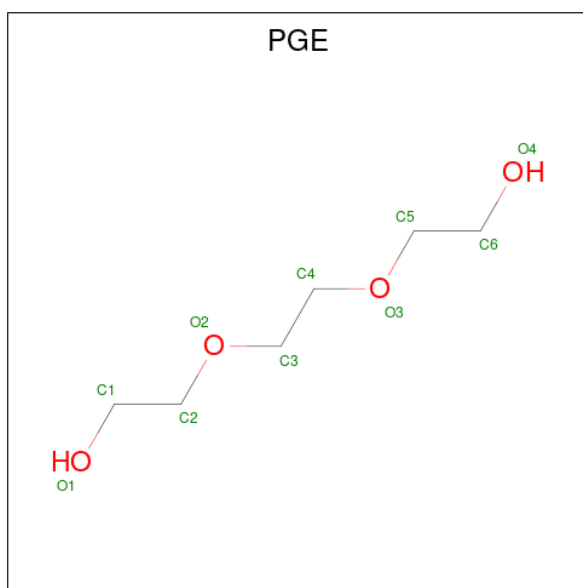
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	30	8	17	5	0	0

- Molecule 7 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
			Total	C	H	O		
7	A	1	10	2	6	2	0	0
7	A	1	10	2	6	2	0	0
7	A	1	10	2	6	2	0	0
7	B	1	10	2	6	2	0	0
7	B	1	10	2	6	2	0	0
7	B	1	10	2	6	2	0	0
7	C	1	9	2	5	2	0	0
7	C	1	9	2	5	2	0	0
7	D	1	10	2	6	2	0	0
7	D	1	10	2	6	2	0	0
7	D	1	10	2	6	2	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	D	1	24	6	14	4	0	0

- Molecule 9 is water.

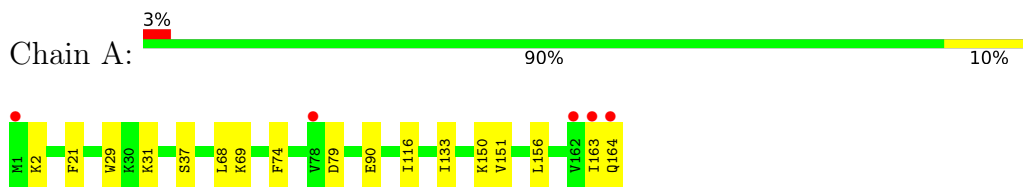
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	283	283	283	0	0
9	B	272	272	272	0	0
9	C	277	277	277	0	0
9	D	255	255	255	0	0



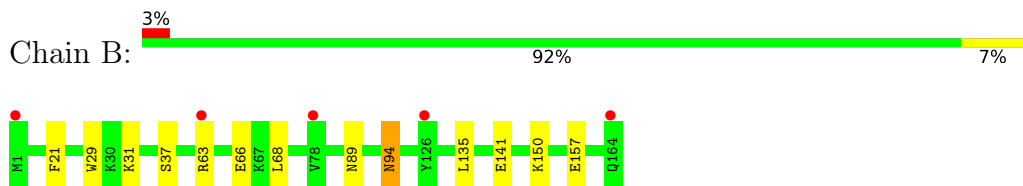
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

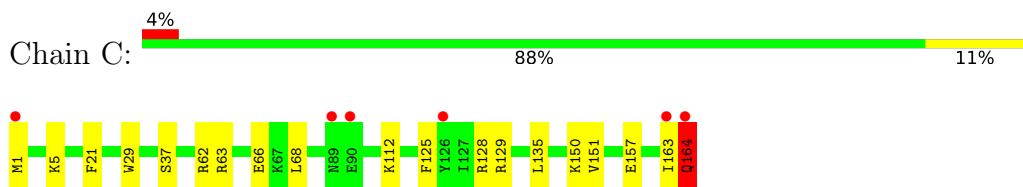
- Molecule 1: Acylneuraminate cytidyltransferase



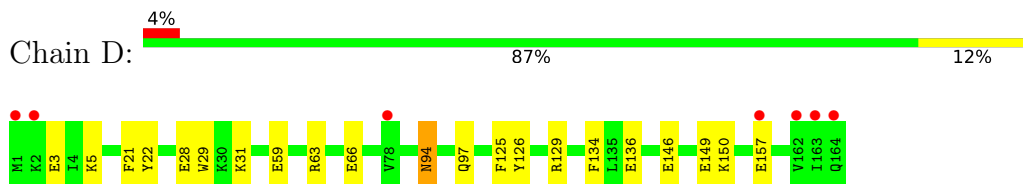
- Molecule 1: Acylneuraminate cytidyltransferase



- Molecule 1: Acylneuraminate cytidyltransferase



- Molecule 1: Acylneuraminate cytidyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.24Å 107.48Å 75.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.78 – 1.10 28.78 – 1.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (28.78-1.10) 97.2 (28.78-1.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.10Å)	Xtrriage
Refinement program	PHENIX, REFMAC	Depositor
R, $R_{free}$	0.127 , 0.141 0.122 , 0.136	Depositor DCC
$R_{free}$ test set	12970 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.9	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	12179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, MG, EDO, PGE, CL, ACY, 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	0.54	0/1426	0.68	1/1917 (0.1%)
1	B	0.55	1/1405 (0.1%)	0.67	0/1890
1	C	0.52	0/1399	0.81	2/1884 (0.1%)
1	D	0.53	0/1423	0.68	1/1913 (0.1%)
All	All	0.53	1/5653 (0.0%)	0.71	4/7604 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	GLU	CD-OE1	5.42	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	GLN	CA-C-O	-17.52	83.31	120.10
1	C	129[A]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	79	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	22	TYR	CB-CG-CD1	5.12	124.07	121.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1404	1312	1349	27	1
1	B	1383	1312	1320	14	0
1	C	1376	1312	1307	36	0
1	D	1400	1312	1297	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	6	6	0	0
4	B	4	3	3	0	0
4	C	4	3	3	0	0
4	D	8	6	6	0	0
5	A	14	20	20	5	0
5	B	7	10	10	0	0
5	C	7	10	10	1	0
6	A	13	17	17	8	0
7	A	12	18	18	6	0
7	B	12	18	18	6	0
7	C	8	10	12	6	0
7	D	12	18	16	10	0
8	D	10	14	14	4	0
9	A	283	0	0	14	0
9	B	272	0	0	10	0
9	C	277	0	0	8	1
9	D	255	0	0	13	0
All	All	6778	5401	5426	117	1

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 10.

All (117) 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:C:66[B]:GLU:HG2	9:C:415:HOH:O	1.38	1.20
1:A:163[B]:ILE:HD11	9:A:303:HOH:O	1.69	0.92
1:D:150:LYS:HG3	7:D:171:EDO:O2	1.70	0.89
1:C:5:LYS:HB3	7:C:169:EDO:H12	1.59	0.85
1:D:134:PHE:CE2	1:D:136[A]:GLU:HG2	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66[A]:GLU:HG3	9:C:257:HOH:O	1.79	0.81
1:A:74:PHE:CE2	5:A:171:PEG:H11	2.17	0.79
1:C:163:ILE:O	1:C:164:GLN:HB3	1.83	0.77
1:C:62:ARG:HD3	7:C:170:EDO:H22	1.65	0.77
1:A:163[A]:ILE:HD11	7:A:174:EDO:O2	1.85	0.76
1:D:126[B]:TYR:CD2	9:D:405:HOH:O	2.38	0.76
7:C:169:EDO:H21	9:C:337:HOH:O	1.91	0.69
1:D:126[B]:TYR:CE2	9:D:405:HOH:O	2.46	0.68
1:B:63[B]:ARG:NH2	9:B:290:HOH:O	2.26	0.67
1:C:157:GLU:HG3	9:C:419:HOH:O	1.94	0.67
6:A:172:PG4:H81	9:D:283:HOH:O	1.96	0.65
1:C:62:ARG:NH2	1:C:66[A]:GLU:OE1	2.30	0.65
1:A:163[B]:ILE:CD1	9:A:303:HOH:O	2.34	0.64
1:D:5[B]:LYS:HE2	9:D:396:HOH:O	1.96	0.64
1:A:163[B]:ILE:C	1:A:163[B]:ILE:HD12	2.19	0.63
9:B:321:HOH:O	1:D:59[B]:GLU:HG3	2.00	0.62
1:B:66:GLU:O	7:B:170:EDO:H12	2.01	0.60
1:B:63[A]:ARG:HD2	9:B:418:HOH:O	2.01	0.59
5:C:168:PEG:H32	9:C:406:HOH:O	2.03	0.57
1:C:62:ARG:HD3	7:C:170:EDO:C2	2.33	0.57
1:C:5:LYS:CB	7:C:169:EDO:H12	2.34	0.57
1:D:149:GLU:HB2	7:D:171:EDO:H22	1.88	0.56
1:C:1:MET:HG2	1:C:151[A]:VAL:O	2.06	0.55
1:A:163[A]:ILE:HD12	1:C:112:LYS:HZ1	1.72	0.55
1:A:2[B]:LYS:HG3	9:A:271:HOH:O	2.06	0.55
1:C:125[B]:PHE:HD1	1:C:128[B]:ARG:HH21	1.55	0.54
1:C:37[B]:SER:OG	1:C:68[B]:LEU:CD2	2.56	0.54
1:D:63:ARG:NH1	9:D:452:HOH:O	2.41	0.54
7:B:169:EDO:H12	9:B:185:HOH:O	2.07	0.54
1:D:5[A]:LYS:HE3	9:D:462:HOH:O	2.08	0.53
1:D:149:GLU:HB2	7:D:171:EDO:C2	2.39	0.53
5:A:171:PEG:H12	9:A:443:HOH:O	2.09	0.53
7:A:173:EDO:H22	9:A:267:HOH:O	2.08	0.52
1:C:29:TRP:NE1	1:D:29:TRP:CH2	2.76	0.52
1:D:94:ASN:ND2	9:D:350:HOH:O	2.43	0.52
1:C:125[B]:PHE:HD1	1:C:128[B]:ARG:NH2	2.06	0.51
6:A:172:PG4:H12	9:A:184:HOH:O	2.10	0.51
1:A:163[A]:ILE:HD12	1:C:112:LYS:HE2	1.92	0.51
1:A:21:PHE:HB2	1:A:29:TRP:HB2	1.93	0.51
1:D:94:ASN:ND2	1:D:97[A]:GLN:HG3	2.27	0.50
1:B:89[B]:ASN:OD1	9:B:281:HOH:O	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HZ2	6:A:172:PG4:C2	2.25	0.49
1:B:21:PHE:HB2	1:B:29:TRP:HB2	1.93	0.49
5:A:170:PEG:H32	9:A:355:HOH:O	2.11	0.49
1:C:21:PHE:HB2	1:C:29:TRP:HB2	1.93	0.49
1:D:21:PHE:HB2	1:D:29:TRP:HB2	1.92	0.49
1:B:66:GLU:O	7:B:170:EDO:C1	2.61	0.49
1:D:3:GLU:OE1	1:D:97[B]:GLN:CG	2.60	0.49
1:D:146:GLU:HA	7:D:171:EDO:H22	1.94	0.49
7:B:169:EDO:H11	9:B:210:HOH:O	2.11	0.49
1:B:135:LEU:HG	9:B:372:HOH:O	2.11	0.49
1:D:146:GLU:HG3	7:D:171:EDO:H11	1.94	0.48
6:A:172:PG4:H11	9:A:242:HOH:O	2.14	0.48
1:C:37[B]:SER:OG	1:C:68[B]:LEU:HD21	2.13	0.48
1:C:163:ILE:O	1:C:164:GLN:CB	2.57	0.48
1:D:3:GLU:OE1	1:D:97[B]:GLN:HG2	2.13	0.48
1:A:163[A]:ILE:HD12	1:C:112:LYS:CE	2.44	0.47
1:D:66[A]:GLU:HG3	9:D:511:HOH:O	2.15	0.47
7:D:172:EDO:C2	9:D:327:HOH:O	2.63	0.47
1:A:74:PHE:CZ	5:A:171:PEG:H11	2.49	0.47
1:A:163[A]:ILE:HD12	1:C:112:LYS:NZ	2.30	0.47
6:A:172:PG4:C8	9:D:283:HOH:O	2.57	0.47
1:A:150:LYS:HG3	9:A:235:HOH:O	2.15	0.46
1:B:150:LYS:HG3	9:B:346:HOH:O	2.14	0.46
1:D:28:GLU:OE1	8:D:169:PGE:H5	2.14	0.46
1:C:150:LYS:HG3	9:C:212:HOH:O	2.15	0.46
1:A:29:TRP:NE1	1:C:29:TRP:CH2	2.81	0.45
7:D:172:EDO:H22	9:D:324:HOH:O	2.15	0.45
1:A:163[A]:ILE:CD1	1:C:112:LYS:HZ1	2.29	0.45
1:A:133:ILE:HB	7:A:175:EDO:H11	1.99	0.45
7:D:171:EDO:O1	7:D:172:EDO:H12	2.16	0.45
1:B:29:TRP:CH2	1:D:29:TRP:NE1	2.82	0.44
6:A:172:PG4:H82	9:D:335:HOH:O	2.17	0.44
1:C:37[B]:SER:OG	1:C:68[B]:LEU:HD22	2.17	0.44
9:B:403:HOH:O	1:D:157:GLU:HG3	2.17	0.44
7:A:174:EDO:H22	9:A:244:HOH:O	2.17	0.44
1:B:37[B]:SER:OG	1:B:68[B]:LEU:HD21	2.17	0.44
1:A:116:ILE:HG21	1:A:151[B]:VAL:HG12	1.99	0.43
1:C:5:LYS:O	7:C:169:EDO:H12	2.18	0.43
1:B:94:ASN:C	1:B:94:ASN:HD22	2.22	0.43
7:D:171:EDO:O1	7:D:172:EDO:H21	2.19	0.43
1:A:69[B]:LYS:HD3	9:A:356:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163[A]:ILE:CD1	1:C:112:LYS:HE2	2.48	0.42
7:B:169:EDO:C1	9:B:185:HOH:O	2.67	0.42
1:D:125:PHE:O	1:D:129[B]:ARG:HG3	2.19	0.41
6:A:172:PG4:O4	1:D:31:LYS:NZ	2.46	0.41
1:A:150:LYS:HD3	7:A:175:EDO:H12	2.03	0.41
7:A:174:EDO:H11	9:A:303:HOH:O	2.20	0.41
1:C:63:ARG:HD3	8:D:169:PGE:H1	2.01	0.41
1:A:37[B]:SER:OG	1:A:68[B]:LEU:CD2	2.69	0.41
1:A:90[B]:GLU:OE1	5:A:171:PEG:H31	2.21	0.41
1:B:37[B]:SER:OG	1:B:68[B]:LEU:CD2	2.68	0.41
1:A:163[B]:ILE:CD1	1:A:163[B]:ILE:C	2.86	0.41
1:B:31:LYS:NZ	7:B:169:EDO:O2	2.47	0.41
1:C:135:LEU:HG	9:C:320:HOH:O	2.20	0.41
1:C:164:GLN:HE21	1:C:164:GLN:C	2.25	0.41
1:A:29:TRP:CH2	1:B:29:TRP:NE1	2.84	0.40
6:A:172:PG4:C7	1:D:31:LYS:HZ3	2.33	0.40
7:D:171:EDO:H11	9:D:372:HOH:O	2.21	0.40

All (1) 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)
1:A:164[A]:GLN:OE1	9:C:415:HOH:O[4_454]	2.18	0.02

## 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	176/164 (107%)	170 (97%)	6 (3%)	0	100	100
1	B	173/164 (106%)	169 (98%)	4 (2%)	0	100	100
1	C	172/164 (105%)	167 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	174/164 (106%)	169 (97%)	5 (3%)	0	100	100
All	All	695/656 (106%)	675 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/136 (110%)	150 (100%)	0	100	100
1	B	147/136 (108%)	145 (99%)	2 (1%)	67	30
1	C	146/136 (107%)	145 (99%)	1 (1%)	84	57
1	D	148/136 (109%)	147 (99%)	1 (1%)	84	57
All	All	591/544 (109%)	587 (99%)	4 (1%)	84	57

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	ASN
1	B	157	GLU
1	C	164	GLN
1	D	94	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	ASN
1	C	164	GLN
1	D	45	ASN
1	D	94	ASN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 9 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACY	C	167	-	3,3,3	1.14	0	3,3,3	0.76	0
4	ACY	D	168	-	3,3,3	1.32	0	3,3,3	0.84	0
7	EDO	A	175	-	3,3,3	0.58	0	2,2,2	0.47	0
7	EDO	D	171	-	3,3,3	1.14	0	2,2,2	1.45	1 (50%)
7	EDO	A	173	-	3,3,3	0.64	0	2,2,2	0.36	0
5	PEG	A	170	-	6,6,6	0.49	0	5,5,5	0.63	0
7	EDO	B	171	-	3,3,3	0.55	0	2,2,2	0.16	0
4	ACY	D	167	-	3,3,3	1.02	0	3,3,3	0.69	0
7	EDO	B	169	-	3,3,3	0.53	0	2,2,2	0.78	0
4	ACY	A	168	-	3,3,3	1.04	0	3,3,3	0.75	0
7	EDO	D	172	-	3,3,3	0.68	0	2,2,2	1.03	0
7	EDO	B	170	-	3,3,3	0.57	0	2,2,2	0.51	0
8	PGE	D	169	-	9,9,9	0.89	0	8,8,8	1.21	1 (12%)
6	PG4	A	172	-	12,12,12	1.42	1 (8%)	11,11,11	1.07	1 (9%)
5	PEG	C	168	-	6,6,6	0.50	0	5,5,5	0.60	0
5	PEG	B	168	-	6,6,6	0.52	0	5,5,5	0.44	0
4	ACY	A	169	-	3,3,3	1.53	1 (33%)	3,3,3	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	A	171	-	6,6,6	0.52	0	5,5,5	0.75	0
7	EDO	C	169	-	3,3,3	0.67	0	2,2,2	0.47	0
4	ACY	B	167	-	3,3,3	1.12	0	3,3,3	0.62	0
7	EDO	A	174	-	3,3,3	0.61	0	2,2,2	0.48	0
7	EDO	D	170	-	3,3,3	0.62	0	2,2,2	0.39	0
7	EDO	C	170	-	3,3,3	0.72	0	2,2,2	0.96	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	172	-	-	1/1/1/1	-
7	EDO	B	170	-	-	1/1/1/1	-
7	EDO	C	170	-	-	1/1/1/1	-
7	EDO	B	171	-	-	1/1/1/1	-
8	PGE	D	169	-	-	2/7/7/7	-
7	EDO	D	171	-	-	0/1/1/1	-
6	PG4	A	172	-	-	5/10/10/10	-
5	PEG	A	171	-	-	2/4/4/4	-
7	EDO	A	173	-	-	1/1/1/1	-
5	PEG	C	168	-	-	2/4/4/4	-
5	PEG	B	168	-	-	0/4/4/4	-
7	EDO	B	169	-	-	1/1/1/1	-
7	EDO	C	169	-	-	0/1/1/1	-
5	PEG	A	170	-	-	2/4/4/4	-
7	EDO	A	174	-	-	1/1/1/1	-
7	EDO	D	170	-	-	1/1/1/1	-
7	EDO	A	175	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	172	PG4	O1-C1	-4.53	1.18	1.42
4	A	169	ACY	OXT-C	-2.23	1.20	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	172	PG4	O4-C7-C8	2.42	120.72	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	169	PGE	O1-C1-C2	2.17	124.39	111.81
7	D	171	EDO	O1-C1-C2	-2.00	97.49	111.91

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	172	PG4	O1-C1-C2-O2
6	A	172	PG4	O4-C7-C8-O5
6	A	172	PG4	O3-C5-C6-O4
5	A	171	PEG	O1-C1-C2-O2
7	A	173	EDO	O1-C1-C2-O2
7	B	169	EDO	O1-C1-C2-O2
7	B	171	EDO	O1-C1-C2-O2
7	D	172	EDO	O1-C1-C2-O2
7	A	174	EDO	O1-C1-C2-O2
7	B	170	EDO	O1-C1-C2-O2
5	C	168	PEG	C1-C2-O2-C3
8	D	169	PGE	O2-C3-C4-O3
5	A	170	PEG	C1-C2-O2-C3
8	D	169	PGE	C6-C5-O3-C4
7	D	170	EDO	O1-C1-C2-O2
5	A	170	PEG	O2-C3-C4-O4
7	C	170	EDO	O1-C1-C2-O2
6	A	172	PG4	C5-C6-O4-C7
5	A	171	PEG	C1-C2-O2-C3
6	A	172	PG4	O2-C3-C4-O3
5	C	168	PEG	O2-C3-C4-O4

There are no ring outliers.

14 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	175	EDO	2	0
7	D	171	EDO	8	0
7	A	173	EDO	1	0
5	A	170	PEG	1	0
7	B	169	EDO	4	0
7	D	172	EDO	4	0
7	B	170	EDO	2	0
8	D	169	PGE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	172	PG4	8	0
5	C	168	PEG	1	0
5	A	171	PEG	4	0
7	C	169	EDO	4	0
7	A	174	EDO	3	0
7	C	170	EDO	2	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	164/164 (100%)	0.04	5 (3%) 50 47	9, 11, 19, 32	0
1	B	164/164 (100%)	0.22	5 (3%) 50 47	9, 12, 24, 47	0
1	C	164/164 (100%)	0.17	6 (3%) 41 38	9, 13, 27, 74	0
1	D	164/164 (100%)	0.13	7 (4%) 35 32	9, 13, 28, 68	0
All	All	656/656 (100%)	0.14	23 (3%) 44 41	9, 13, 25, 74	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	GLN	8.7
1	D	1	MET	7.4
1	A	163[A]	ILE	5.8
1	B	1	MET	5.3
1	A	1	MET	5.2
1	C	1	MET	4.8
1	B	78	VAL	4.7
1	A	164[A]	GLN	4.7
1	B	164	GLN	4.0
1	D	163	ILE	3.6
1	B	126	TYR	3.3
1	C	126[A]	TYR	3.2
1	D	164	GLN	3.1
1	D	162	VAL	2.9
1	A	162	VAL	2.6
1	D	2	LYS	2.5
1	C	89	ASN	2.5
1	C	163	ILE	2.4
1	A	78	VAL	2.3
1	D	78	VAL	2.2
1	D	157	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	63[A]	ARG	2.1
1	C	90	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	PEG	A	171	7/7	0.66	0.29	29,35,47,49	0
7	EDO	D	170	4/4	0.69	0.33	22,27,29,30	0
8	PGE	D	169	10/10	0.70	0.31	16,23,25,27	0
7	EDO	A	174	4/4	0.71	0.33	27,33,34,35	0
5	PEG	C	168	7/7	0.73	0.16	32,39,48,49	0
5	PEG	A	170	7/7	0.73	0.25	28,34,44,46	0
4	ACY	A	169	4/4	0.74	0.34	22,24,27,27	0
7	EDO	B	171	4/4	0.79	0.46	22,27,29,30	0
7	EDO	C	170	4/4	0.81	0.52	21,25,28,28	0
7	EDO	B	169	4/4	0.82	0.23	21,26,27,30	0
4	ACY	D	168	4/4	0.83	0.28	18,19,22,22	0
6	PG4	A	172	13/13	0.85	0.41	18,24,29,30	0
5	PEG	B	168	7/7	0.89	0.21	27,33,43,44	0
7	EDO	A	175	4/4	0.89	0.45	22,26,27,29	0
7	EDO	D	171	4/4	0.89	0.31	22,26,27,27	0
7	EDO	D	172	4/4	0.89	0.44	21,25,27,28	0
7	EDO	C	169	4/4	0.89	0.36	21,24,26,26	0
7	EDO	B	170	4/4	0.91	0.40	23,28,29,30	0
7	EDO	A	173	4/4	0.92	0.31	18,22,24,25	0
4	ACY	B	167	4/4	0.98	0.07	10,11,16,16	0
4	ACY	A	168	4/4	0.99	0.06	10,12,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACY	C	167	4/4	0.99	0.07	11,12,16,16	0
4	ACY	D	167	4/4	0.99	0.06	11,12,16,16	0
3	CL	A	167	1/1	1.00	0.04	12,12,12,12	0
3	CL	B	166	1/1	1.00	0.04	12,12,12,12	0
3	CL	C	166	1/1	1.00	0.04	13,13,13,13	0
3	CL	D	166	1/1	1.00	0.04	12,12,12,12	0
2	MG	A	165	1/1	1.00	0.06	9,9,9,9	0
2	MG	B	165	1/1	1.00	0.08	10,10,10,10	0
2	MG	C	165	1/1	1.00	0.07	10,10,10,10	0
2	MG	D	165	1/1	1.00	0.05	10,10,10,10	0
3	CL	A	166	1/1	1.00	0.04	11,11,11,11	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.