Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2022 – 10:24 pm GMT

|		
PDB ID	:	7QI3
Title	:	Structure of Fusarium verticillioides NAT1 (FDB2) N-malonyltransferase
Authors	:	Lowe, E.D.; Kotomina, E.; Karagianni, E.; Boukouvala, S.
Deposited on	:	2021-12-14
Resolution	:	1.80 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
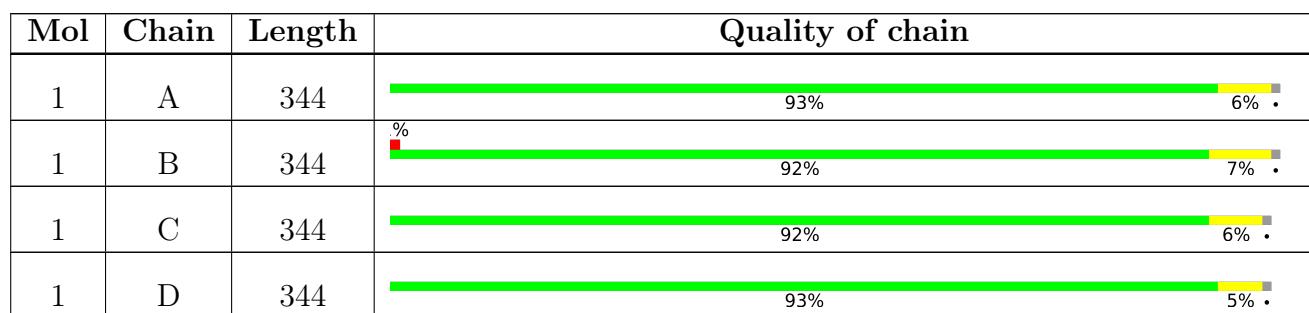
The reported resolution of this entry is 1.80 Å.

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	Percentile Ranks	Value
Rfree		0.222
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		1.4%
RSRZ outliers		0.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	344	93% 6% ·
1	B	344	% 92% 7% ·
1	C	344	92% 6% ·
1	D	344	93% 5% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	B	405	-	-	X	-
3	EDO	A	402	-	-	-	X
3	EDO	B	406	-	-	-	X

2 Entry composition ⓘ
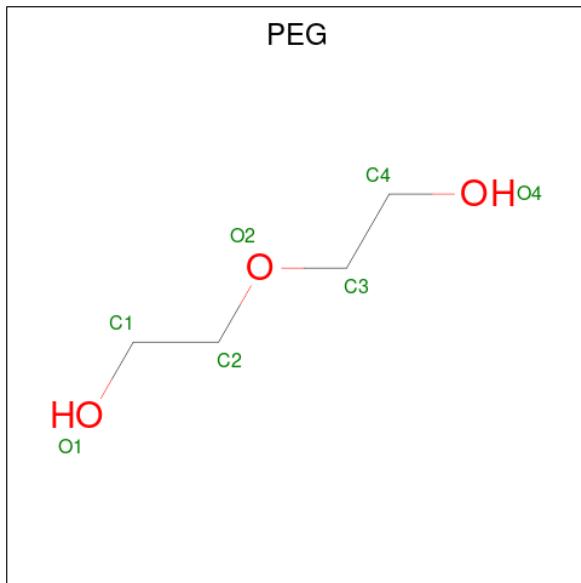
There are 6 unique types of molecules in this entry. The entry contains 12925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Arylamine N-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	15	0
			2867	1810	492	548	17			
1	B	340	Total	C	N	O	S	0	13	0
			2847	1804	485	541	17			
1	C	340	Total	C	N	O	S	0	15	0
			2867	1816	488	546	17			
1	D	340	Total	C	N	O	S	0	13	0
			2847	1798	486	546	17			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
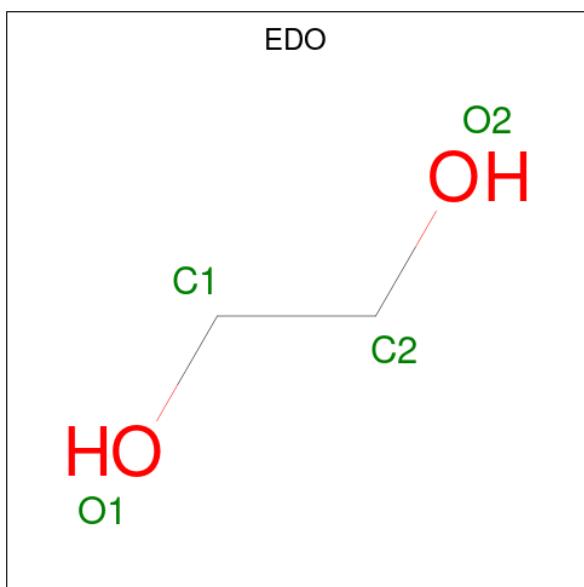
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
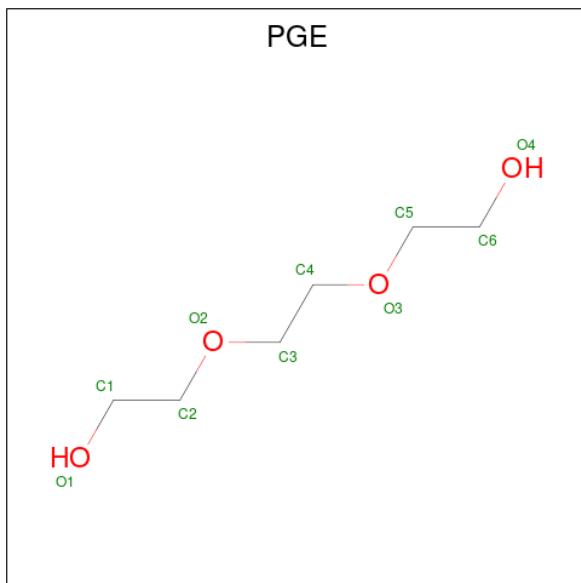
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0

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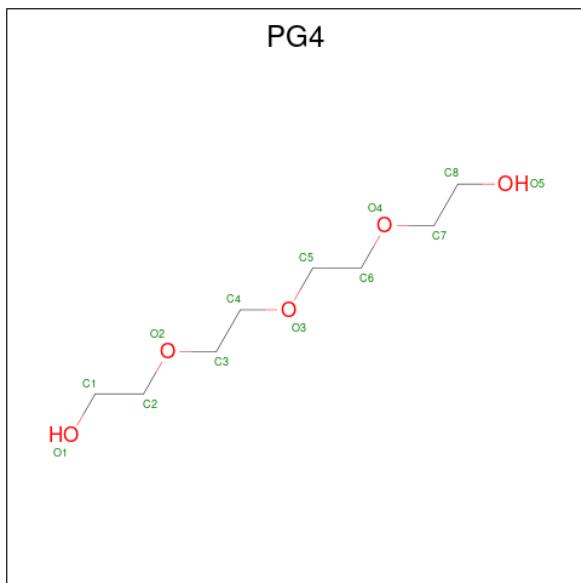
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 4	C 2	O 2	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 13	C 8	O 5	0	0
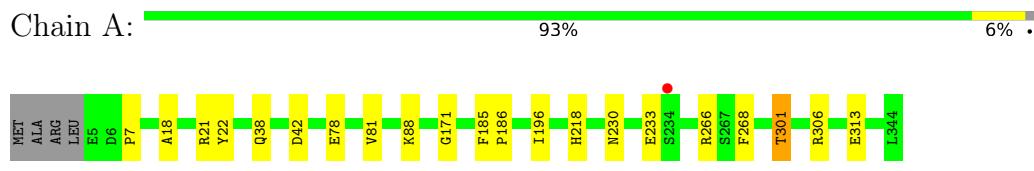
- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	357	Total 359	O 359	0	2
6	B	341	Total 344	O 344	0	3
6	C	350	Total 351	O 351	0	1
6	D	342	Total 343	O 343	0	1
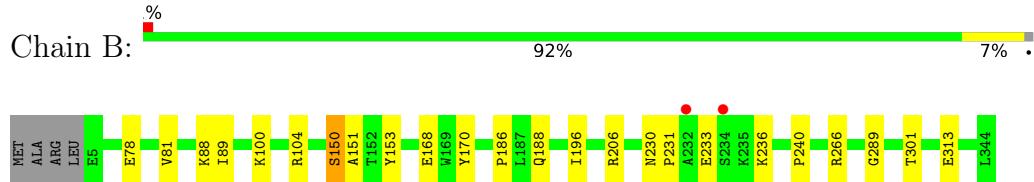
3 Residue-property plots ⓘ

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.
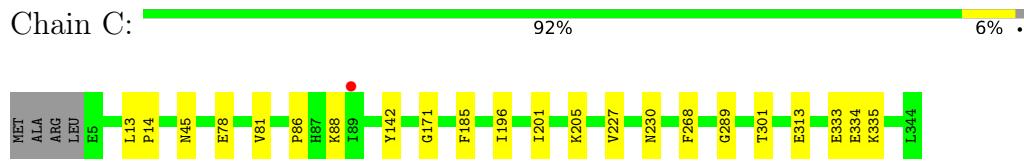
- Molecule 1: Arylamine N-acetyltransferase
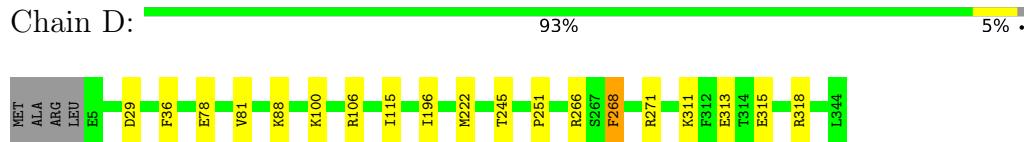
Chain A:

- Molecule 1: Arylamine N-acetyltransferase

Chain B:

- Molecule 1: Arylamine N-acetyltransferase

Chain C:

- Molecule 1: Arylamine N-acetyltransferase

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.58Å 76.88Å 92.54Å 76.22° 73.06° 72.49°	Depositor
Resolution (Å)	87.32 – 1.80 87.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (87.32-1.80) 95.1 (87.32-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.20rc4_4425	Depositor
R, R_{free}	0.178 , 0.222 0.179 , 0.222	Depositor DCC
R_{free} test set	7764 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12925	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0/2932	0.59	0/3971
1	B	0.36	0/2914	0.59	0/3949
1	C	0.38	0/2932	0.59	0/3971
1	D	0.36	0/2912	0.59	0/3944
All	All	0.36	0/11690	0.59	0/15835

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	2867	0	2800	11	0
1	B	2847	0	2773	17	0
1	C	2867	0	2823	11	0
1	D	2847	0	2761	14	0
2	A	14	0	20	0	0
2	B	28	0	40	10	0
2	C	7	0	10	0	0
3	A	8	0	12	1	0
3	B	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	12	0	0
3	D	4	0	6	1	0
4	D	10	0	14	4	0
5	D	13	0	18	2	0
6	A	359	0	0	3	1
6	B	344	0	0	5	0
6	C	351	0	0	2	0
6	D	343	0	0	3	1
All	All	12925	0	11301	55	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 2.

All (55) 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:B:240:PRO:HG3	2:B:405:PEG:H22	1.73	0.71
2:B:405:PEG:O2	6:B:501:HOH:O	2.09	0.71
1:D:222[B]:MET:HG2	1:D:245:THR:HG22	1.73	0.71
1:D:251:PRO:HG3	4:D:401:PGE:H4	1.78	0.66
1:B:151:ALA:HA	2:B:405:PEG:H21	1.79	0.63
1:B:100[A]:LYS:NZ	6:B:503:HOH:O	2.28	0.61
1:B:153:TYR:CZ	2:B:405:PEG:H11	2.36	0.61
1:D:115:ILE:HG23	4:D:401:PGE:H6	1.85	0.58
1:C:333[B]:GLU:HG2	1:C:334:GLU:N	2.21	0.56
1:D:29:ASP:OD1	6:D:502:HOH:O	2.18	0.56
1:A:186:PRO:HD3	3:A:402:EDO:H22	1.87	0.55
1:A:301:THR:HG22	1:A:306:ARG:HG3	1.89	0.53
1:B:104:ARG:HA	3:B:403:EDO:H11	1.91	0.53
1:B:266:ARG:NH1	6:B:508:HOH:O	2.36	0.51
1:B:206:ARG:HH21	2:B:405:PEG:C3	2.25	0.50
1:B:230[A]:ASN:ND2	1:B:233:GLU:HG3	2.27	0.50
1:A:38[B]:GLN:NE2	1:A:42:ASP:OD1	2.45	0.49
1:D:115:ILE:HG23	4:D:401:PGE:C6	2.43	0.48
1:C:335:LYS:NZ	6:C:516:HOH:O	2.45	0.48
1:A:218:HIS:ND1	6:A:505:HOH:O	2.35	0.48
1:C:13[B]:LEU:HD12	1:C:14:PRO:HD2	1.95	0.48
1:B:168:GLU:HG3	1:B:170:TYR:CE1	2.50	0.47
1:A:18:ALA:O	6:A:501:HOH:O	2.20	0.47
1:B:150:SER:HB3	2:B:404:PEG:H32	1.96	0.47
1:A:81:VAL:O	1:A:88:LYS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:PHE:CE2	5:D:403:PG4:H61	2.50	0.46
1:D:81:VAL:O	1:D:88:LYS:HA	2.17	0.45
1:D:311:LYS:NZ	6:D:512:HOH:O	2.39	0.45
1:D:251:PRO:HB3	4:D:401:PGE:O2	2.16	0.45
1:D:100[A]:LYS:HG3	1:D:106:ARG:HB2	1.98	0.45
1:D:266[A]:ARG:NH1	6:D:523:HOH:O	2.48	0.45
1:D:315:GLU:OE2	1:D:318:ARG:NH2	2.49	0.44
1:C:201:ILE:HG22	1:C:227:VAL:HG12	1.98	0.44
1:B:240:PRO:CG	2:B:405:PEG:H22	2.43	0.44
1:A:266:ARG:NH1	6:A:522:HOH:O	2.50	0.44
2:B:402:PEG:H22	2:B:402:PEG:H41	1.75	0.43
1:A:171:GLY:HA3	1:A:185:PHE:CZ	2.54	0.43
1:C:45:ASN:OD1	6:C:501:HOH:O	2.21	0.43
1:A:7:PRO:HD2	1:C:142:TYR:CZ	2.54	0.43
1:C:81:VAL:O	1:C:88[B]:LYS:HA	2.20	0.42
1:B:240:PRO:HG3	2:B:405:PEG:C2	2.47	0.42
1:B:206:ARG:HH21	2:B:405:PEG:C4	2.32	0.42
6:B:505:HOH:O	1:D:271:ARG:NH1	2.49	0.42
1:B:81:VAL:O	1:B:88:LYS:HA	2.20	0.42
1:C:171:GLY:HA3	1:C:185:PHE:CZ	2.55	0.42
1:C:86:PRO:HG3	1:C:333[B]:GLU:HG3	2.01	0.41
1:A:230[A]:ASN:ND2	1:A:233:GLU:HG3	2.36	0.41
1:B:231:PRO:HB3	1:B:236:LYS:HE2	2.02	0.41
1:B:186:PRO:HB2	1:B:188[B]:GLN:CG	2.51	0.41
1:C:81:VAL:O	1:C:88[A]:LYS:HA	2.20	0.41
1:C:289:GLY:HA3	1:C:301:THR:O	2.20	0.41
1:D:268:PHE:HE2	5:D:403:PG4:H71	1.86	0.41
6:B:724:HOH:O	3:D:402:EDO:H21	2.20	0.41
1:A:21:ARG:NH1	1:A:22:TYR:O	2.55	0.40
1:B:289:GLY:HA3	1:B:301:THR: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)
6:A:710:HOH:O	6:D:759:HOH:O[1_564]	2.14	0.06

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	353/344 (103%)	346 (98%)	6 (2%)	1 (0%)	41	27
1	B	351/344 (102%)	342 (97%)	8 (2%)	1 (0%)	41	27
1	C	353/344 (103%)	344 (98%)	8 (2%)	1 (0%)	41	27
1	D	351/344 (102%)	343 (98%)	7 (2%)	1 (0%)	41	27
All	All	1408/1376 (102%)	1375 (98%)	29 (2%)	4 (0%)	41	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ILE
1	B	196	ILE
1	C	196	ILE
1	D	196	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/312 (103%)	317 (99%)	4 (1%)	71	65
1	B	317/312 (102%)	313 (99%)	4 (1%)	69	62
1	C	323/312 (104%)	317 (98%)	6 (2%)	57	46
1	D	316/312 (101%)	312 (99%)	4 (1%)	69	62
All	All	1277/1248 (102%)	1259 (99%)	18 (1%)	67	59

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	268	PHE
1	A	301	THR
1	A	313	GLU
1	B	78	GLU
1	B	89	ILE
1	B	150	SER
1	B	313	GLU
1	C	78	GLU
1	C	205	LYS
1	C	230[A]	ASN
1	C	230[B]	ASN
1	C	268	PHE
1	C	313	GLU
1	D	36	PHE
1	D	78	GLU
1	D	268	PHE
1	D	313	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	#$|Z| > 2$
3	EDO	B	406	-	3,3,3	0.52	0	2,2,2	0.30	0
3	EDO	B	403	-	3,3,3	0.51	0	2,2,2	0.21	0
2	PEG	B	405	-	6,6,6	0.22	0	5,5,5	0.35	0
3	EDO	C	402	-	3,3,3	0.49	0	2,2,2	0.39	0
2	PEG	B	404	-	6,6,6	0.20	0	5,5,5	0.05	0
3	EDO	A	404	-	3,3,3	0.51	0	2,2,2	0.28	0
2	PEG	B	401	-	6,6,6	0.17	0	5,5,5	0.14	0
5	PG4	D	403	-	12,12,12	0.17	0	11,11,11	0.64	0
2	PEG	C	401	-	6,6,6	0.21	0	5,5,5	0.12	0
2	PEG	B	402	-	6,6,6	0.12	0	5,5,5	0.12	0
3	EDO	C	403	-	3,3,3	0.48	0	2,2,2	0.27	0
4	PGE	D	401	-	9,9,9	0.35	0	8,8,8	0.55	0
2	PEG	A	401	-	6,6,6	0.13	0	5,5,5	0.08	0
2	PEG	A	403	-	6,6,6	0.20	0	5,5,5	0.15	0
3	EDO	A	402	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	D	402	-	3,3,3	0.47	0	2,2,2	0.19	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
3	EDO	B	406	-	-	0/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
2	PEG	B	405	-	-	2/4/4/4	-
3	EDO	C	402	-	-	1/1/1/1	-
2	PEG	B	404	-	-	4/4/4/4	-
3	EDO	A	404	-	-	1/1/1/1	-
2	PEG	B	401	-	-	2/4/4/4	-
5	PG4	D	403	-	-	6/10/10/10	-
2	PEG	C	401	-	-	2/4/4/4	-
2	PEG	B	402	-	-	3/4/4/4	-
3	EDO	C	403	-	-	0/1/1/1	-
4	PGE	D	401	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	401	-	-	4/4/4/4	-
2	PEG	A	403	-	-	1/4/4/4	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	D	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	PEG	C1-C2-O2-C3
2	B	404	PEG	O2-C3-C4-O4
5	D	403	PG4	O2-C3-C4-O3
2	A	401	PEG	O1-C1-C2-O2
2	B	402	PEG	O1-C1-C2-O2
2	C	401	PEG	O1-C1-C2-O2
2	A	401	PEG	O2-C3-C4-O4
2	B	401	PEG	O1-C1-C2-O2
2	B	402	PEG	O2-C3-C4-O4
2	B	405	PEG	O2-C3-C4-O4
5	D	403	PG4	O4-C7-C8-O5
2	B	402	PEG	C4-C3-O2-C2
3	B	403	EDO	O1-C1-C2-O2
4	D	401	PGE	O2-C3-C4-O3
2	A	401	PEG	C1-C2-O2-C3
2	B	404	PEG	C1-C2-O2-C3
2	B	405	PEG	C1-C2-O2-C3
5	D	403	PG4	C4-C3-O2-C2
4	D	401	PGE	C1-C2-O2-C3
2	B	404	PEG	O1-C1-C2-O2
2	B	401	PEG	C1-C2-O2-C3
2	C	401	PEG	C1-C2-O2-C3
4	D	401	PGE	O3-C5-C6-O4
5	D	403	PG4	C8-C7-O4-C6
3	A	404	EDO	O1-C1-C2-O2
5	D	403	PG4	C3-C4-O3-C5
3	C	402	EDO	O1-C1-C2-O2
5	D	403	PG4	O3-C5-C6-O4
2	A	401	PEG	C4-C3-O2-C2
2	B	404	PEG	C4-C3-O2-C2

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	EDO	1	0
2	B	405	PEG	8	0
2	B	404	PEG	1	0
5	D	403	PG4	2	0
2	B	402	PEG	1	0
4	D	401	PGE	4	0
3	A	402	EDO	1	0
3	D	402	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	340/344 (98%)	-0.51	1 (0%)	94	92	16, 28, 47, 65	0
1	B	340/344 (98%)	-0.46	2 (0%)	89	87	17, 30, 51, 82	0
1	C	340/344 (98%)	-0.49	1 (0%)	94	92	17, 27, 48, 65	0
1	D	340/344 (98%)	-0.53	0	100	100	17, 29, 51, 65	0
All	All	1360/1376 (98%)	-0.50	4 (0%)	94	92	16, 29, 49, 82	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	ALA	2.3
1	B	234	SER	2.3
1	A	234	SER	2.2
1	C	89[A]	ILE	2.1

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	EDO	B	406	4/4	0.66	0.47	56,57,66,69	0
3	EDO	B	403	4/4	0.71	0.18	39,41,47,50	4
3	EDO	C	403	4/4	0.71	0.15	61,62,63,63	0
3	EDO	A	402	4/4	0.74	0.42	47,48,55,57	0
3	EDO	C	402	4/4	0.80	0.16	52,55,56,62	0
2	PEG	B	404	7/7	0.80	0.31	45,47,57,61	0
5	PG4	D	403	13/13	0.82	0.18	37,45,51,57	13
2	PEG	C	401	7/7	0.83	0.14	41,46,52,52	0
4	PGE	D	401	10/10	0.84	0.21	18,24,28,30	10
2	PEG	B	405	7/7	0.84	0.25	19,29,38,39	7
3	EDO	A	404	4/4	0.86	0.13	54,59,60,64	0
3	EDO	D	402	4/4	0.86	0.14	21,34,43,48	0
2	PEG	B	401	7/7	0.87	0.14	34,40,42,49	7
2	PEG	B	402	7/7	0.88	0.14	32,36,44,44	7
2	PEG	A	401	7/7	0.89	0.15	38,48,56,58	0
2	PEG	A	403	7/7	0.89	0.15	44,48,57,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.