Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 10:29 AM JST

PDB ID	:	6LL4
Title	:	Oxygen-exposed carbazole-soaked reduced terminal oxygenase of carbazole 1,9a-dioxygenase
Authors	:	Wang, Y.X.; Suzuki-Minakuchi, C.; Nojiri, H.
Deposited on	:	2019-12-21
Resolution	:	2.20 Å(reported)

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

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

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

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

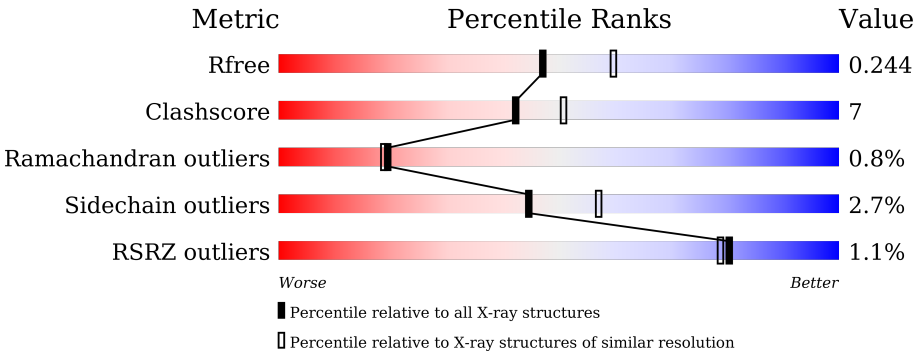
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	392	2% 79% 17%
1	B	392	3% 84% 13%
1	C	392	3% 84% 13%

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	EDO	B	410	-	-	X	-
5	EDO	B	414	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 10038 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 Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	18	0
			3207	2049	545	600	13			
1	B	383	Total	C	N	O	S	0	0	0
			3081	1970	523	575	13			
1	C	383	Total	C	N	O	S	0	2	0
			3092	1978	524	577	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP Q84II6
A	386	GLU	-	expression tag	UNP Q84II6
A	387	HIS	-	expression tag	UNP Q84II6
A	388	HIS	-	expression tag	UNP Q84II6
A	389	HIS	-	expression tag	UNP Q84II6
A	390	HIS	-	expression tag	UNP Q84II6
A	391	HIS	-	expression tag	UNP Q84II6
A	392	HIS	-	expression tag	UNP Q84II6
B	385	LEU	-	expression tag	UNP Q84II6
B	386	GLU	-	expression tag	UNP Q84II6
B	387	HIS	-	expression tag	UNP Q84II6
B	388	HIS	-	expression tag	UNP Q84II6
B	389	HIS	-	expression tag	UNP Q84II6
B	390	HIS	-	expression tag	UNP Q84II6
B	391	HIS	-	expression tag	UNP Q84II6
B	392	HIS	-	expression tag	UNP Q84II6
C	385	LEU	-	expression tag	UNP Q84II6
C	386	GLU	-	expression tag	UNP Q84II6
C	387	HIS	-	expression tag	UNP Q84II6
C	388	HIS	-	expression tag	UNP Q84II6
C	389	HIS	-	expression tag	UNP Q84II6
C	390	HIS	-	expression tag	UNP Q84II6
C	391	HIS	-	expression tag	UNP Q84II6

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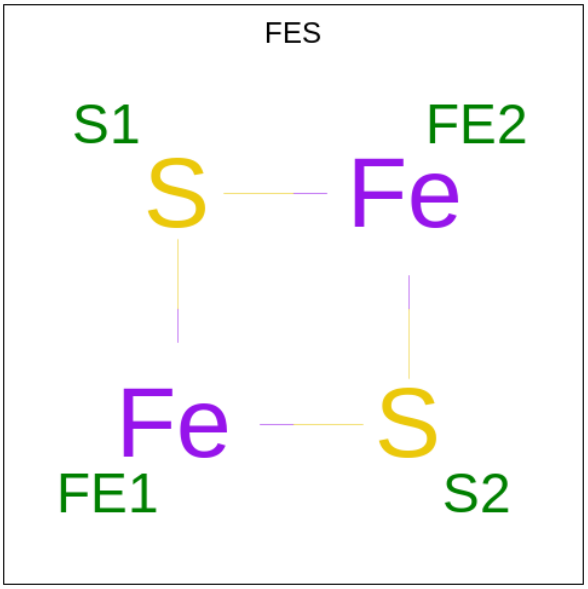
Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP Q84II6

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

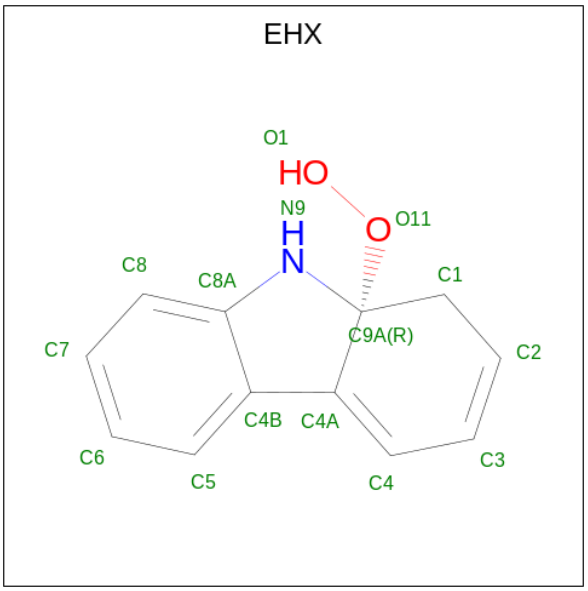


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

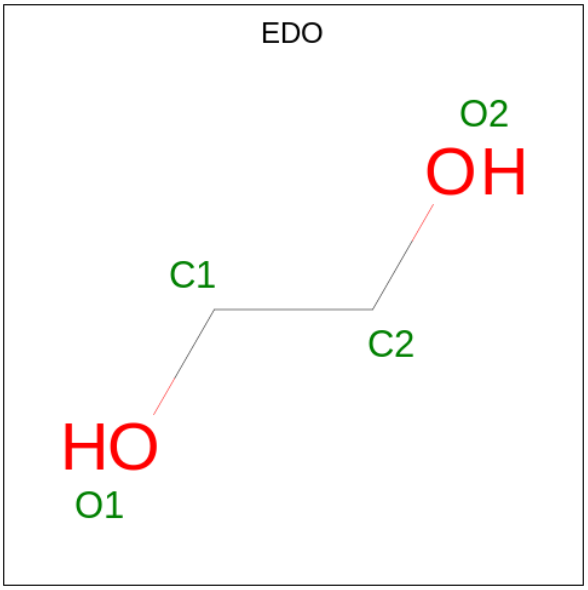
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

- Molecule 4 is (9aR)-9a-(dioxidanyl)-1,9-dihydrocarbazole (three-letter code: EHX) (formula: $C_{12}H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 12 1 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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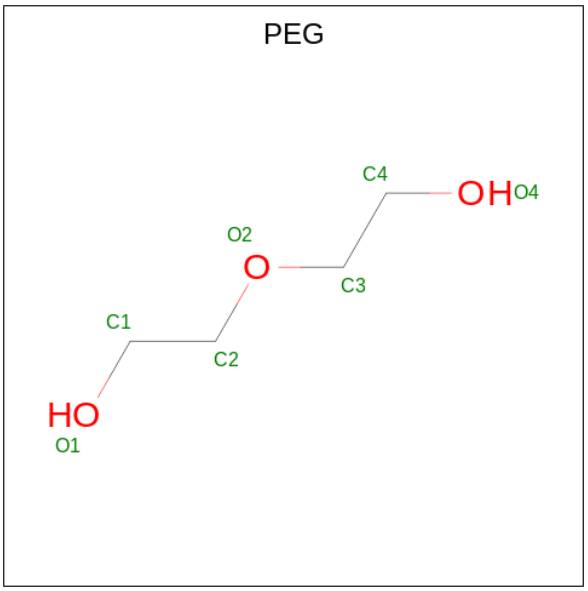
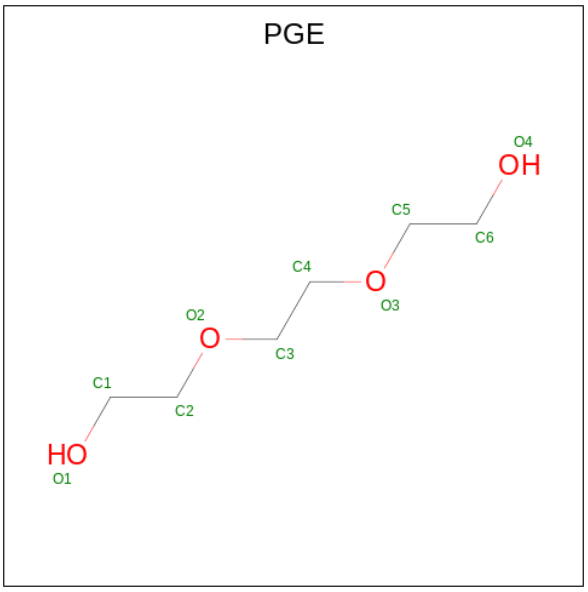
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



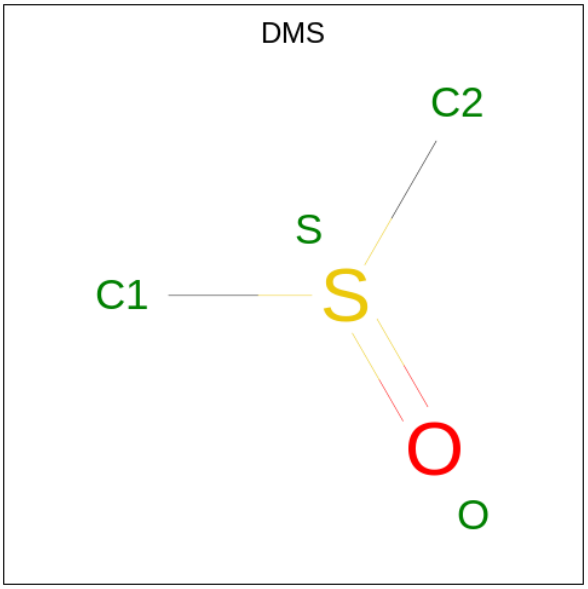
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0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

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



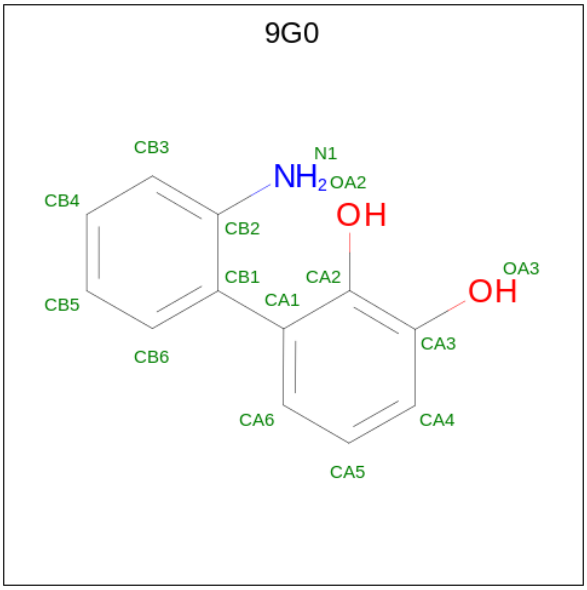
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0
7	A	1	Total C O 10 6 4	0	0
7	A	1	Total C O 10 6 4	0	0
7	B	1	Total C O 10 6 4	0	0
7	C	1	Total C O 10 6 4	0	0

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 9 is 2'-amino[1,1'-biphenyl]-2,3-diol (three-letter code: 9G0) (formula: $C_{12}H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O 15 12 1 2	0	0
9	C	1	Total C N O 15 12 1 2	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Mg 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	126	Total O 126 126	0	0

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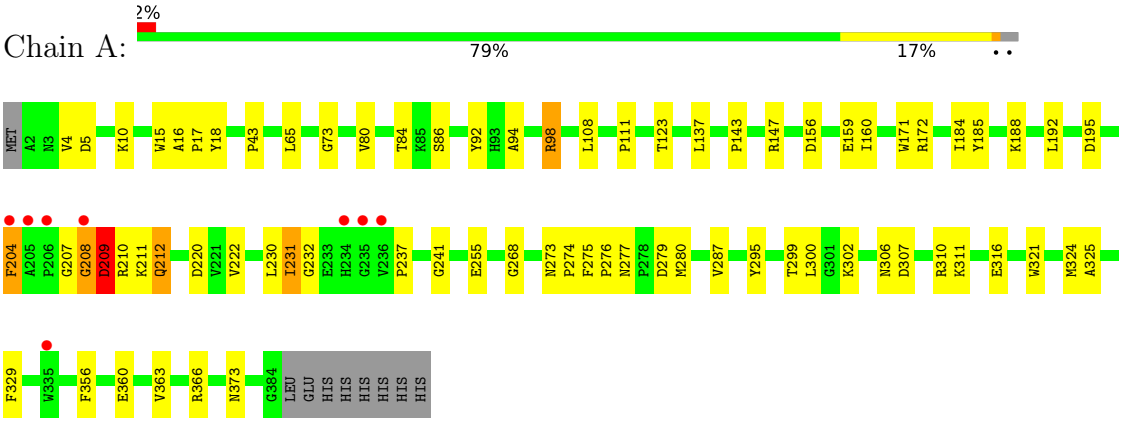
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	140	Total O 140 140	0	0
11	C	112	Total O 112 112	0	0

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.

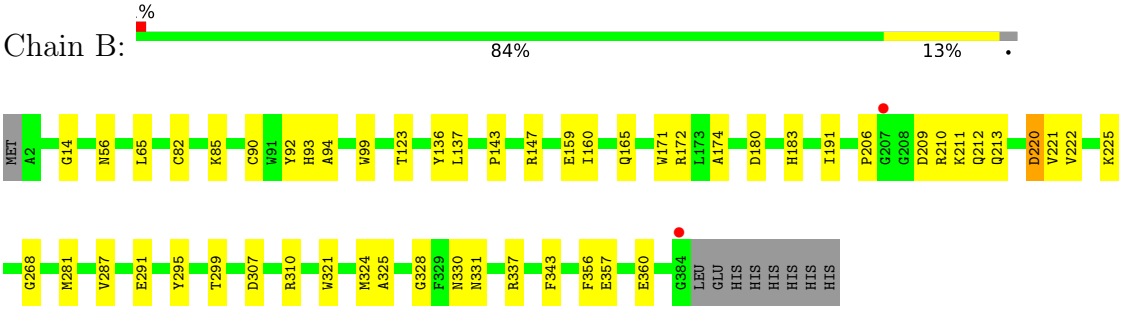
• Molecule 1: Terminal oxygenase component of carbazole

Chain A:



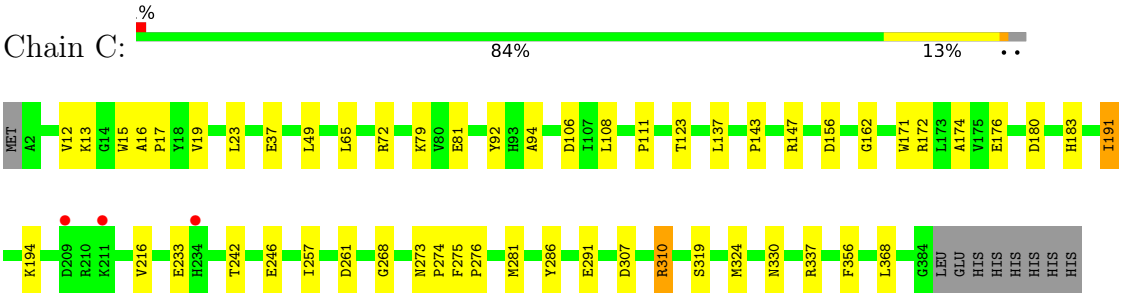
• Molecule 1: Terminal oxygenase component of carbazole

Chain B:



• Molecule 1: Terminal oxygenase component of carbazole

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	91.89Å 91.89Å 242.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.23 – 2.20 48.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.23-2.20) 97.9 (48.18-2.20)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.169 , 0.240 0.177 , 0.244	Depositor DCC
R_{free} test set	2969 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10038	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EHX, 9G0, MG, EDO, FE, PGE, DMS, PEG, FES

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	0.49	0/3297	0.66	0/4473
1	B	0.51	0/3163	0.68	0/4294
1	C	0.48	0/3180	0.66	0/4317
All	All	0.49	0/9640	0.67	0/13084

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	ARG	Sidechain
1	C	310	ARG	Sidechain
1	C	337	ARG	Sidechain
1	C	72	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3207	0	3114	70	0
1	B	3081	0	2992	35	0
1	C	3092	0	3009	29	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	0	0	0
5	A	20	0	30	2	0
5	B	40	0	60	8	0
5	C	20	0	30	4	0
6	A	28	0	40	2	0
6	B	42	0	60	4	0
6	C	7	0	10	0	0
7	A	30	0	42	2	0
7	B	10	0	14	0	0
7	C	10	0	14	1	0
8	A	4	0	6	0	0
8	B	8	0	12	0	0
9	B	15	0	0	1	0
9	C	15	0	0	2	0
10	B	1	0	0	0	0
11	A	126	0	0	1	0
11	B	140	0	0	2	0
11	C	112	0	0	1	0
All	All	10038	0	9433	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204[B]:PHE:CD2	1:A:231[B]:ILE:HD12	1.42	1.53
1:A:204[B]:PHE:CE2	1:A:231[B]:ILE:HD12	1.62	1.33
1:A:204[B]:PHE:CD2	1:A:231[B]:ILE:CD1	2.24	1.20
1:A:204[B]:PHE:CE2	1:A:231[B]:ILE:CD1	2.28	1.15
1:A:204[B]:PHE:CG	1:A:231[B]:ILE:HD12	1.99	0.96
1:A:210[B]:ARG:HD3	1:A:210[B]:ARG:H	1.38	0.87
1:A:207[B]:GLY:O	1:A:208[B]:GLY:O	1.94	0.84
1:A:204[B]:PHE:CB	1:A:231[B]:ILE:HB	2.18	0.73
1:A:204[B]:PHE:CZ	1:A:231[B]:ILE:HD12	2.23	0.71
1:C:330:ASN:HD21	9:C:403:9G0:CA4	2.05	0.70
1:A:210[B]:ARG:H	1:A:210[B]:ARG:CD	2.01	0.69
1:A:204[B]:PHE:HB3	1:A:231[B]:ILE:HB	1.75	0.68
1:B:331:ASN:OD1	5:B:414:EDO:C1	2.42	0.68
1:A:210[A]:ARG:C	1:A:212[A]:GLN:H	1.99	0.64
1:A:209[A]:ASP:OD2	1:A:211[A]:LYS:HE3	1.97	0.63
1:B:191:ILE:HB	6:B:419:PEG:H42	1.81	0.63
1:A:279:ASP:OD2	1:A:302:LYS:NZ	2.31	0.62
1:A:212[B]:GLN:HG2	1:A:212[B]:GLN:O	2.00	0.61
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.83	0.60
1:B:82:CYS:HB3	5:B:410:EDO:H11	1.83	0.59
1:A:204[B]:PHE:CG	1:A:231[B]:ILE:HB	2.37	0.59
1:A:210[B]:ARG:HD3	1:A:210[B]:ARG:N	2.15	0.59
1:A:84:THR:HG21	5:A:408:EDO:H11	1.84	0.58
1:B:331:ASN:OD1	5:B:414:EDO:H11	2.04	0.57
1:A:204[B]:PHE:CE2	1:A:231[B]:ILE:HD11	2.36	0.56
1:B:221:VAL:HG13	1:B:222:VAL:HG13	1.87	0.56
1:A:192:LEU:HA	1:A:324:MET:CE	2.36	0.56
1:A:86:SER:HG	5:A:408:EDO:HO1	1.54	0.56
1:A:207[B]:GLY:O	1:A:208[B]:GLY:C	2.42	0.56
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.89	0.55
1:A:210[A]:ARG:O	1:A:212[A]:GLN:N	2.40	0.54
1:A:230[B]:LEU:O	1:A:231[B]:ILE:C	2.45	0.54
1:A:195:ASP:HB2	1:A:324:MET:HE3	1.89	0.54
1:B:331:ASN:OD1	5:B:414:EDO:H12	2.07	0.54
1:A:204[B]:PHE:CD2	1:A:231[B]:ILE:HD13	2.35	0.54
1:A:210[A]:ARG:C	1:A:212[A]:GLN:N	2.62	0.53
1:B:93:HIS:NE2	1:C:180:ASP:OD2	2.33	0.53
1:B:206:PRO:HB3	1:B:213:GLN:OE1	2.08	0.52
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.91	0.52
1:C:194:LYS:N	1:C:194:LYS:HD3	2.25	0.52
1:A:185:TYR:CZ	1:A:188:LYS:HE3	2.46	0.52
1:A:212[B]:GLN:O	1:A:212[B]:GLN:CG	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LYS:HA	5:B:410:EDO:H22	1.92	0.51
1:A:18:TYR:CE2	1:A:366:ARG:HG2	2.46	0.51
1:B:174:ALA:HA	1:B:337:ARG:HG2	1.93	0.50
1:A:195:ASP:HB2	1:A:324:MET:CE	2.42	0.50
1:A:15:TRP:CZ3	1:A:363:VAL:HG13	2.46	0.50
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.47	0.49
1:B:210:ARG:HH12	1:B:357:GLU:HA	1.77	0.49
1:C:275:PHE:CG	1:C:276:PRO:HA	2.47	0.49
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.94	0.49
1:A:210[A]:ARG:HD3	1:A:360:GLU:OE1	2.12	0.49
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.47	0.48
1:A:192:LEU:HA	1:A:324:MET:HE2	1.94	0.48
1:C:108:LEU:HA	5:C:404:EDO:O2	2.14	0.48
1:B:136:TYR:CE1	1:B:143:PRO:HD2	2.49	0.47
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.49	0.47
1:C:16:ALA:N	1:C:17:PRO:CD	2.77	0.47
1:B:165:GLN:OE1	5:B:414:EDO:H21	2.14	0.47
1:A:241:GLY:HA2	11:C:516:HOH:O	2.15	0.47
1:B:82:CYS:SG	5:B:410:EDO:H12	2.55	0.47
1:A:230[B]:LEU:O	1:A:232[B]:GLY:N	2.47	0.47
1:A:306:ASN:O	1:A:310:ARG:HG3	2.14	0.47
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.97	0.47
1:B:82:CYS:HB3	5:B:410:EDO:C1	2.44	0.46
1:A:98:ARG:HH12	7:A:415:PGE:H6	1.81	0.46
1:B:14:GLY:C	6:B:417:PEG:H12	2.35	0.46
1:C:216:VAL:HG13	1:C:368:LEU:HD23	1.97	0.46
1:C:307:ASP:HA	1:C:310:ARG:HH11	1.80	0.46
1:A:204[B]:PHE:CD1	1:A:231[B]:ILE:HD12	2.49	0.46
1:A:280:MET:CE	1:A:300:LEU:HD13	2.46	0.46
1:B:328:GLY:HA3	6:B:419:PEG:H41	1.98	0.46
1:B:330:ASN:HD21	9:B:403:9G0:CA4	2.28	0.46
1:C:176:GLU:O	1:C:180:ASP:HB2	2.16	0.46
1:A:43:PRO:HG2	1:A:80:VAL:HG11	1.98	0.46
1:C:106:ASP:HB3	5:C:404:EDO:H12	1.98	0.46
1:A:321:TRP:O	1:A:325:ALA:HB3	2.17	0.45
1:A:192:LEU:HD23	1:A:329:PHE:CD1	2.52	0.45
1:A:207[B]:GLY:C	1:A:208[B]:GLY:O	2.55	0.45
1:A:277:ASN:HD21	6:A:410:PEG:H21	1.82	0.45
1:A:307:ASP:HA	1:A:310:ARG:HB2	1.99	0.45
1:C:23:LEU:O	1:C:49:LEU:HG	2.17	0.44
1:C:174:ALA:HB1	1:C:286:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:HG21	1:C:19:VAL:HG21	1.99	0.44
1:C:183:HIS:CE1	9:C:403:9G0:OA2	2.71	0.44
1:A:204[B]:PHE:CZ	1:A:231[B]:ILE:CD1	2.91	0.44
1:A:373:ASN:HD21	6:A:412:PEG:H22	1.82	0.44
1:A:209[A]:ASP:HB2	1:A:212[A]:GLN:HB2	2.00	0.44
1:B:291:GLU:HG3	11:B:580:HOH:O	2.17	0.44
1:C:291:GLU:H	1:C:291:GLU:CD	2.22	0.43
1:B:159:GLU:HG3	1:B:310:ARG:HG2	2.00	0.43
1:A:16:ALA:N	1:A:17:PRO:CD	2.82	0.43
1:C:79:LYS:NZ	1:C:81:GLU:OE2	2.52	0.43
1:C:191:ILE:HG23	1:C:324:MET:HG3	2.01	0.43
1:C:273:ASN:HA	1:C:274:PRO:HA	1.77	0.43
1:B:209:ASP:OD2	1:B:212:GLN:OE1	2.35	0.43
1:A:98:ARG:HH12	7:A:415:PGE:C6	2.31	0.43
1:A:273:ASN:HA	1:A:274:PRO:HA	1.86	0.43
1:C:368:LEU:C	1:C:368:LEU:HD13	2.38	0.43
1:A:316:GLU:HG2	1:A:321:TRP:NE1	2.34	0.43
1:A:325:ALA:O	1:A:329:PHE:HB3	2.19	0.43
1:C:111:PRO:HA	5:C:404:EDO:H11	2.01	0.43
1:C:143:PRO:HG3	1:C:147:ARG:NH1	2.34	0.43
1:A:111:PRO:O	11:A:502:HOH:O	2.21	0.42
1:B:210:ARG:HB3	1:B:360:GLU:OE1	2.19	0.42
1:A:4:VAL:O	1:A:5:ASP:C	2.58	0.42
1:A:287:VAL:HB	1:A:295:TYR:HB2	2.01	0.42
1:B:180:ASP:HB3	1:B:183:HIS:HB3	2.00	0.42
1:A:192:LEU:HD12	1:A:324:MET:HE2	2.02	0.42
1:B:90:CYS:O	1:B:94:ALA:HA	2.20	0.42
1:C:242:THR:HA	1:C:246:GLU:O	2.20	0.42
1:A:160:ILE:HG23	1:A:299:THR:HB	2.01	0.41
1:B:143:PRO:HG3	1:B:147:ARG:CZ	2.49	0.41
1:B:160:ILE:HG23	1:B:299:THR:HB	2.01	0.41
1:C:37:GLU:OE2	5:C:407:EDO:H22	2.20	0.41
1:C:162:GLY:H	7:C:410:PGE:C3	2.32	0.41
1:A:73:GLY:HA3	1:B:343:PHE:CG	2.54	0.41
1:B:225:LYS:HE2	11:B:634:HOH:O	2.21	0.41
1:C:257:ILE:N	1:C:257:ILE:HD12	2.34	0.41
1:A:209[A]:ASP:OD2	1:A:211[A]:LYS:CE	2.66	0.41
1:C:171:TRP:O	1:C:174:ALA:HB3	2.20	0.41
1:A:275:PHE:CG	1:A:276:PRO:HA	2.55	0.41
1:B:220:ASP:OD1	1:B:221:VAL:N	2.53	0.41
1:A:307:ASP:O	1:A:311:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:VAL:HB	1:B:295:TYR:HB2	2.01	0.41
1:B:56:ASN:HB2	1:B:99:TRP:CH2	2.56	0.41
1:B:324:MET:O	6:B:419:PEG:H41	2.20	0.40
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.51	0.40
1:A:280:MET:HE2	1:A:300:LEU:HD13	2.04	0.40
1:A:159:GLU:OE1	1:A:310:ARG:HD3	2.21	0.40
1:B:321:TRP:O	1:B:325:ALA:HB3	2.21	0.40
1:A:204[A]:PHE:CE2	1:A:237:PRO:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	399/392 (102%)	360 (90%)	29 (7%)	10 (2%)	5 3
1	B	381/392 (97%)	363 (95%)	17 (4%)	1 (0%)	41 46
1	C	383/392 (98%)	364 (95%)	17 (4%)	2 (0%)	29 31
All	All	1163/1176 (99%)	1087 (94%)	63 (5%)	13 (1%)	19 12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208[A]	GLY
1	A	208[B]	GLY
1	A	209[A]	ASP
1	A	209[B]	ASP
1	A	231[A]	ILE
1	A	231[B]	ILE
1	A	268	GLY
1	C	268	GLY
1	A	184	ILE

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Mol	Chain	Res	Type
1	B	268	GLY
1	A	204[A]	PHE
1	A	204[B]	PHE
1	C	15	TRP

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	342/339 (101%)	330 (96%)	12 (4%)	36	46
1	B	330/339 (97%)	323 (98%)	7 (2%)	53	67
1	C	332/339 (98%)	322 (97%)	10 (3%)	41	53
All	All	1004/1017 (99%)	975 (97%)	29 (3%)	44	54

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	92	TYR
1	A	137	LEU
1	A	156	ASP
1	A	209[A]	ASP
1	A	209[B]	ASP
1	A	212[A]	GLN
1	A	212[B]	GLN
1	A	220	ASP
1	A	222	VAL
1	A	255	GLU
1	A	356	PHE
1	B	92	TYR
1	B	137	LEU
1	B	211	LYS
1	B	220	ASP
1	B	281	MET
1	B	307	ASP

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Mol	Chain	Res	Type
1	B	356	PHE
1	C	13	LYS
1	C	92	TYR
1	C	137	LEU
1	C	156	ASP
1	C	191	ILE
1	C	233	GLU
1	C	261	ASP
1	C	281	MET
1	C	319	SER
1	C	356	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	315	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 4 are monoatomic - leaving 45 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	$\#\|Z\|>2$
6	PEG	B	418	-	6,6,6	0.37	0	5,5,5	0.79	0
7	PGE	A	413	-	9,9,9	0.47	0	8,8,8	0.37	0
5	EDO	C	408	-	3,3,3	0.74	0	2,2,2	0.43	0
5	EDO	B	410	-	3,3,3	0.20	0	2,2,2	0.48	0
5	EDO	A	408	-	3,3,3	0.46	0	2,2,2	0.14	0
5	EDO	B	411	-	3,3,3	0.53	0	2,2,2	0.36	0
6	PEG	B	419	-	6,6,6	0.54	0	5,5,5	0.76	0
5	EDO	B	413	-	3,3,3	0.44	0	2,2,2	0.21	0
5	EDO	B	407	-	3,3,3	0.47	0	2,2,2	0.43	0
2	FES	B	401	1	0,4,4	-	-	-		
5	EDO	A	406	-	3,3,3	0.32	0	2,2,2	0.58	0
8	DMS	A	416	-	3,3,3	0.40	0	3,3,3	0.87	0
8	DMS	B	422	-	3,3,3	0.63	0	3,3,3	0.82	0
5	EDO	B	406	-	3,3,3	0.36	0	2,2,2	0.26	0
5	EDO	A	405	-	3,3,3	0.53	0	2,2,2	0.27	0
2	FES	C	401	1	0,4,4	-	-	-		
6	PEG	B	416	-	6,6,6	0.42	0	5,5,5	0.28	0
5	EDO	B	409	-	3,3,3	0.54	0	2,2,2	0.30	0
5	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.59	0
4	EHX	A	403	3	13,17,17	3.98	5 (38%)	14,25,25	2.76	5 (35%)
6	PEG	B	415	-	6,6,6	0.53	0	5,5,5	0.98	0
6	PEG	A	411	-	6,6,6	0.50	0	5,5,5	0.23	0
6	PEG	B	417	-	6,6,6	0.64	0	5,5,5	0.90	0
7	PGE	A	415	-	9,9,9	0.58	0	8,8,8	0.36	0
9	9G0	C	403	3	16,16,16	2.30	4 (25%)	22,22,22	1.28	3 (13%)
5	EDO	B	414	-	3,3,3	0.62	0	2,2,2	0.17	0
5	EDO	C	406	-	3,3,3	0.48	0	2,2,2	0.50	0
6	PEG	B	420	-	6,6,6	0.54	0	5,5,5	0.51	0
5	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.46	0
5	EDO	C	407	-	3,3,3	0.39	0	2,2,2	0.32	0
6	PEG	A	409	-	6,6,6	0.60	0	5,5,5	0.58	0
8	DMS	B	423	-	3,3,3	0.51	0	3,3,3	0.79	0
6	PEG	A	410	-	6,6,6	0.48	0	5,5,5	0.38	0
7	PGE	B	421	-	9,9,9	0.51	0	8,8,8	0.56	0
5	EDO	C	405	-	3,3,3	0.35	0	2,2,2	0.46	0
7	PGE	C	410	-	9,9,9	0.46	0	8,8,8	0.48	0
2	FES	A	401	1	0,4,4	-	-	-		
5	EDO	B	405	-	3,3,3	0.55	0	2,2,2	0.39	0
5	EDO	B	412	-	3,3,3	0.68	0	2,2,2	0.30	0
6	PEG	A	412	-	6,6,6	0.61	0	5,5,5	0.36	0
5	EDO	C	404	-	3,3,3	0.30	0	2,2,2	0.52	0
5	EDO	B	408	-	3,3,3	0.43	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PGE	A	414	-	9,9,9	0.79	0	8,8,8	0.75	0
9	9G0	B	403	3	16,16,16	2.18	4 (25%)	22,22,22	1.73	5 (22%)
6	PEG	C	409	-	6,6,6	0.39	0	5,5,5	0.61	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
6	PEG	B	418	-	-	2/4/4/4	-
7	PGE	A	413	-	-	5/7/7/7	-
5	EDO	C	408	-	-	1/1/1/1	-
5	EDO	B	410	-	-	1/1/1/1	-
5	EDO	A	408	-	-	1/1/1/1	-
5	EDO	B	411	-	-	0/1/1/1	-
6	PEG	B	419	-	-	2/4/4/4	-
5	EDO	B	413	-	-	1/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
5	EDO	A	406	-	-	1/1/1/1	-
2	FES	B	401	1	-	-	0/1/1/1
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	A	405	-	-	0/1/1/1	-
2	FES	C	401	1	-	-	0/1/1/1
6	PEG	B	416	-	-	2/4/4/4	-
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	A	407	-	-	1/1/1/1	-
4	EHX	A	403	3	-	0/0/26/26	0/3/3/3
6	PEG	B	415	-	-	4/4/4/4	-
6	PEG	A	411	-	-	1/4/4/4	-
6	PEG	B	417	-	-	1/4/4/4	-
7	PGE	A	415	-	-	4/7/7/7	-
9	9G0	C	403	3	-	0/4/4/4	0/2/2/2
5	EDO	B	414	-	-	1/1/1/1	-
5	EDO	C	406	-	-	0/1/1/1	-
6	PEG	B	420	-	-	1/4/4/4	-
5	EDO	A	404	-	-	0/1/1/1	-
5	EDO	C	407	-	-	1/1/1/1	-
6	PEG	A	409	-	-	4/4/4/4	-
6	PEG	A	410	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	B	421	-	-	3/7/7/7	-
5	EDO	C	405	-	-	1/1/1/1	-
7	PGE	C	410	-	-	4/7/7/7	-
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	B	412	-	-	1/1/1/1	-
6	PEG	A	412	-	-	3/4/4/4	-
2	FES	A	401	1	-	-	0/1/1/1
5	EDO	C	404	-	-	0/1/1/1	-
5	EDO	B	408	-	-	1/1/1/1	-
7	PGE	A	414	-	-	5/7/7/7	-
9	9G0	B	403	3	-	0/4/4/4	0/2/2/2
6	PEG	C	409	-	-	1/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	EHX	C4-C4A	11.42	1.47	1.35
4	A	403	EHX	C4B-C8A	7.29	1.50	1.41
9	C	403	9G0	CA1-CA2	5.93	1.50	1.40
9	B	403	9G0	CA1-CA2	5.29	1.49	1.40
9	C	403	9G0	CA3-CA2	4.87	1.45	1.40
9	B	403	9G0	CA3-CA2	4.42	1.45	1.40
9	B	403	9G0	CB1-CB2	3.52	1.49	1.40
9	B	403	9G0	CB2-N1	3.46	1.49	1.37
9	C	403	9G0	CB1-CB2	3.37	1.48	1.40
9	C	403	9G0	CB2-N1	3.14	1.48	1.37
4	A	403	EHX	O1-O11	-2.55	1.36	1.45
4	A	403	EHX	C3-C4	2.38	1.47	1.40
4	A	403	EHX	C4B-C4A	2.01	1.48	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	EHX	C4B-C8A-N9	-6.51	108.45	111.74
4	A	403	EHX	C8-C8A-C4B	-4.62	117.55	122.19
4	A	403	EHX	C8A-C4B-C4A	-3.98	104.23	106.56
9	B	403	9G0	CA6-CA1-CB1	3.98	126.94	118.74
9	B	403	9G0	CB1-CA1-CA2	-3.87	115.25	121.85
4	A	403	EHX	C8-C8A-N9	3.64	133.97	128.20
9	B	403	9G0	OA3-CA3-CA4	3.63	129.20	119.33
9	C	403	9G0	OA3-CA3-CA4	2.86	127.12	119.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	EHX	C5-C4B-C8A	2.80	121.84	118.83
9	B	403	9G0	OA3-CA3-CA2	-2.49	111.47	117.90
9	C	403	9G0	CA6-CA1-CB1	2.42	123.73	118.74
9	B	403	9G0	OA2-CA2-CA1	2.39	125.22	119.37
9	C	403	9G0	OA2-CA2-CA1	2.25	124.87	119.37

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	415	PEG	C4-C3-O2-C2
7	A	415	PGE	O2-C3-C4-O3
7	B	421	PGE	O2-C3-C4-O3
7	A	414	PGE	O2-C3-C4-O3
6	A	410	PEG	O2-C3-C4-O4
6	A	411	PEG	O2-C3-C4-O4
7	C	410	PGE	O3-C5-C6-O4
7	A	413	PGE	O2-C3-C4-O3
6	A	409	PEG	O1-C1-C2-O2
6	A	409	PEG	O2-C3-C4-O4
6	A	412	PEG	O2-C3-C4-O4
6	B	415	PEG	O2-C3-C4-O4
6	B	420	PEG	O1-C1-C2-O2
7	A	415	PGE	O1-C1-C2-O2
7	C	410	PGE	O2-C3-C4-O3
6	B	418	PEG	O2-C3-C4-O4
7	A	413	PGE	O3-C5-C6-O4
5	B	406	EDO	O1-C1-C2-O2
5	B	408	EDO	O1-C1-C2-O2
5	B	410	EDO	O1-C1-C2-O2
5	B	412	EDO	O1-C1-C2-O2
5	B	413	EDO	O1-C1-C2-O2
5	C	407	EDO	O1-C1-C2-O2
6	B	417	PEG	O1-C1-C2-O2
7	A	414	PGE	O1-C1-C2-O2
6	C	409	PEG	O2-C3-C4-O4
5	B	409	EDO	O1-C1-C2-O2
6	A	409	PEG	C1-C2-O2-C3
6	B	419	PEG	O2-C3-C4-O4
6	B	416	PEG	O1-C1-C2-O2
7	A	413	PGE	O1-C1-C2-O2
6	B	415	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
7	B	421	PGE	C1-C2-O2-C3
7	C	410	PGE	C3-C4-O3-C5
7	A	415	PGE	C4-C3-O2-C2
7	B	421	PGE	C4-C3-O2-C2
6	A	409	PEG	C4-C3-O2-C2
6	A	412	PEG	O1-C1-C2-O2
6	A	410	PEG	O1-C1-C2-O2
5	A	406	EDO	O1-C1-C2-O2
5	A	407	EDO	O1-C1-C2-O2
5	C	408	EDO	O1-C1-C2-O2
7	A	415	PGE	C3-C4-O3-C5
7	A	414	PGE	C1-C2-O2-C3
6	B	416	PEG	O2-C3-C4-O4
6	B	418	PEG	C4-C3-O2-C2
7	A	414	PGE	O3-C5-C6-O4
6	A	412	PEG	C4-C3-O2-C2
7	C	410	PGE	C4-C3-O2-C2
7	A	413	PGE	C1-C2-O2-C3
7	A	413	PGE	C3-C4-O3-C5
5	C	405	EDO	O1-C1-C2-O2
7	A	414	PGE	C3-C4-O3-C5
5	A	408	EDO	O1-C1-C2-O2
6	B	415	PEG	O1-C1-C2-O2
5	B	414	EDO	O1-C1-C2-O2
6	B	419	PEG	C1-C2-O2-C3

There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	410	EDO	4	0
5	A	408	EDO	2	0
6	B	419	PEG	3	0
6	B	417	PEG	1	0
7	A	415	PGE	2	0
9	C	403	9G0	2	0
5	B	414	EDO	4	0
5	C	407	EDO	1	0
6	A	410	PEG	1	0
7	C	410	PGE	1	0
6	A	412	PEG	1	0
5	C	404	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	403	9G0	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^{th} 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	383/392 (97%)	-0.45	8 (2%)	63	61	20, 33, 61, 97	0
1	B	383/392 (97%)	-0.59	2 (0%)	91	90	20, 29, 53, 83	0
1	C	383/392 (97%)	-0.49	3 (0%)	86	85	22, 35, 59, 79	0
All	All	1149/1176 (97%)	-0.51	13 (1%)	80	79	20, 33, 59, 97	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	3.7
1	A	206[A]	PRO	3.2
1	C	234	HIS	3.1
1	C	209	ASP	3.0
1	A	208[A]	GLY	3.0
1	B	384	GLY	2.8
1	A	205[A]	ALA	2.5
1	A	204[A]	PHE	2.3
1	A	236	VAL	2.3
1	A	235	GLY	2.3
1	A	335	TRP	2.2
1	C	211	LYS	2.1
1	A	234	HIS	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 (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PGE	A	415	10/10	0.68	0.26	55,68,71,72	0
5	EDO	C	408	4/4	0.69	0.18	48,51,51,52	0
6	PEG	A	410	7/7	0.70	0.20	57,58,66,66	0
5	EDO	B	411	4/4	0.75	0.14	53,53,53,56	0
6	PEG	C	409	7/7	0.76	0.17	48,51,56,56	0
5	EDO	B	412	4/4	0.77	0.22	40,47,48,53	0
5	EDO	B	409	4/4	0.78	0.24	60,61,62,64	0
9	9G0	C	403	15/15	0.78	0.28	48,54,62,65	0
6	PEG	A	411	7/7	0.79	0.20	59,63,66,66	0
9	9G0	B	403	15/15	0.79	0.28	42,56,61,63	0
5	EDO	B	405	4/4	0.79	0.17	57,60,62,63	0
6	PEG	B	415	7/7	0.80	0.20	34,42,50,53	0
7	PGE	A	414	10/10	0.81	0.21	50,59,63,65	0
6	PEG	A	412	7/7	0.81	0.21	54,59,61,62	0
7	PGE	A	413	10/10	0.84	0.17	62,65,68,69	0
6	PEG	A	409	7/7	0.85	0.14	43,47,54,55	0
6	PEG	B	420	7/7	0.86	0.17	46,55,61,63	0
5	EDO	A	408	4/4	0.87	0.20	54,55,55,57	0
7	PGE	B	421	10/10	0.87	0.15	40,52,59,60	0
6	PEG	B	416	7/7	0.87	0.17	45,46,49,53	0
5	EDO	B	406	4/4	0.87	0.17	43,43,43,44	0
6	PEG	B	418	7/7	0.88	0.21	37,42,45,47	0
7	PGE	C	410	10/10	0.88	0.16	44,54,62,66	0
5	EDO	C	406	4/4	0.88	0.13	50,53,57,60	0
5	EDO	A	404	4/4	0.88	0.13	40,40,40,40	0
6	PEG	B	419	7/7	0.89	0.20	39,44,50,55	0
5	EDO	B	413	4/4	0.89	0.26	38,46,48,53	0
5	EDO	B	414	4/4	0.90	0.21	46,49,49,50	0
5	EDO	B	410	4/4	0.91	0.33	38,42,42,52	0
5	EDO	C	405	4/4	0.91	0.16	55,57,57,60	0
5	EDO	B	407	4/4	0.91	0.13	39,49,51,54	0
8	DMS	A	416	4/4	0.91	0.17	65,66,68,70	0
6	PEG	B	417	7/7	0.91	0.17	25,36,43,46	0
5	EDO	C	407	4/4	0.91	0.23	41,45,47,53	0
5	EDO	C	404	4/4	0.92	0.40	39,41,41,42	0
5	EDO	A	406	4/4	0.93	0.15	46,50,53,59	0
5	EDO	A	407	4/4	0.93	0.18	54,57,58,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EHX	A	403	15/15	0.93	0.23	43,51,63,64	0
5	EDO	A	405	4/4	0.93	0.26	34,40,41,42	0
8	DMS	B	423	4/4	0.95	0.12	76,76,79,80	0
5	EDO	B	408	4/4	0.96	0.14	43,44,46,48	0
10	MG	B	404	1/1	0.97	0.08	28,28,28,28	0
8	DMS	B	422	4/4	0.98	0.14	37,37,37,39	0
3	FE	A	402	1/1	0.99	0.06	46,46,46,46	0
3	FE	C	402	1/1	0.99	0.08	32,32,32,32	0
2	FES	C	401	4/4	0.99	0.05	32,33,34,34	0
3	FE	B	402	1/1	1.00	0.12	23,23,23,23	0
2	FES	A	401	4/4	1.00	0.09	20,20,21,21	0
2	FES	B	401	4/4	1.00	0.07	25,26,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.