Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 09:45 PM JST

PDB ID	:	7BUG
Title	:	Reduced oxygenase of carbazole 1,9a-dioxygenase
Authors	:	Matsuzawa, J.; Wang, Y.X.; Suzuki-Minakuchi, C.; Nojiri, H.
Deposited on	:	2020-04-06
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

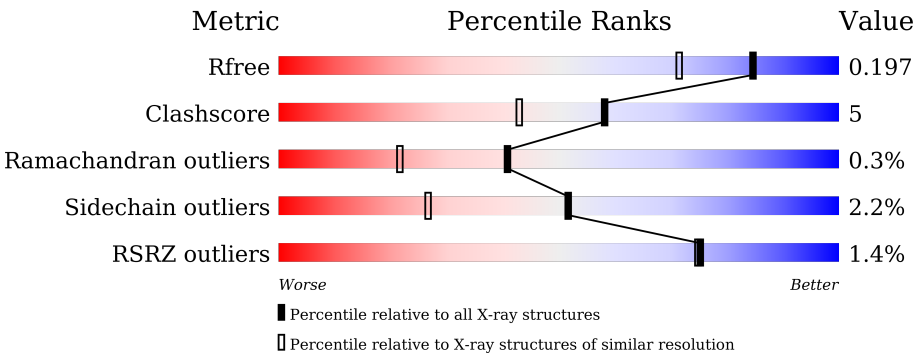
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	.% 85% 12% •
1	B	392	2% 88% 10% •
1	C	392	2% 88% 9% • •

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
11	MXE	A	411	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10529 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
			Total	C	N	O	S			
1	A	383	3125	2000	528	584	13	0	7	0
1	B	383	3164	2028	534	588	14	0	13	0
1	C	383	3134	2005	532	584	13	0	8	0

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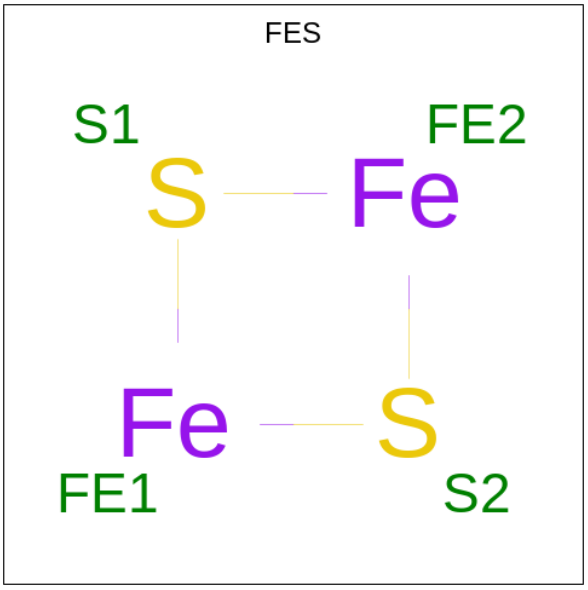
Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP Q84II6

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



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

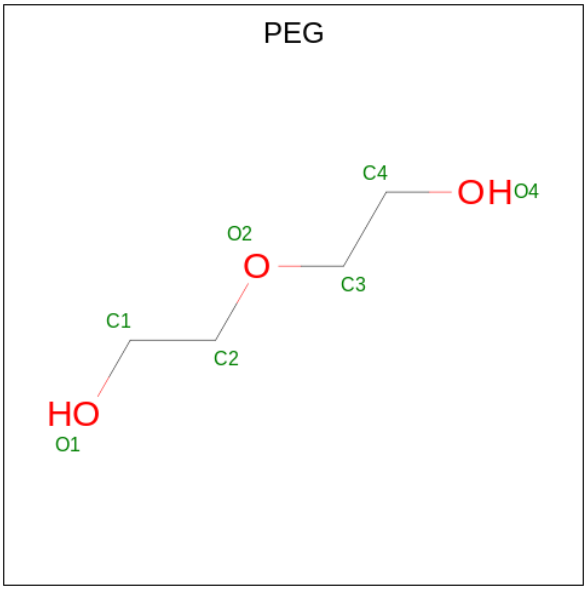
- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

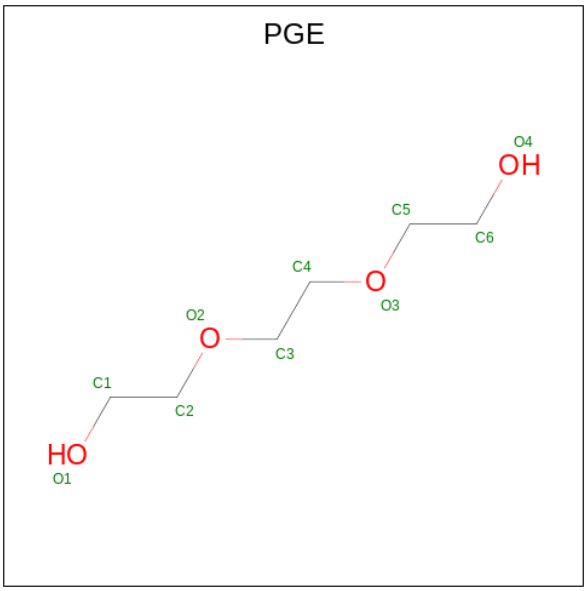
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	3	3	3	0	0
4	C	1	1	1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



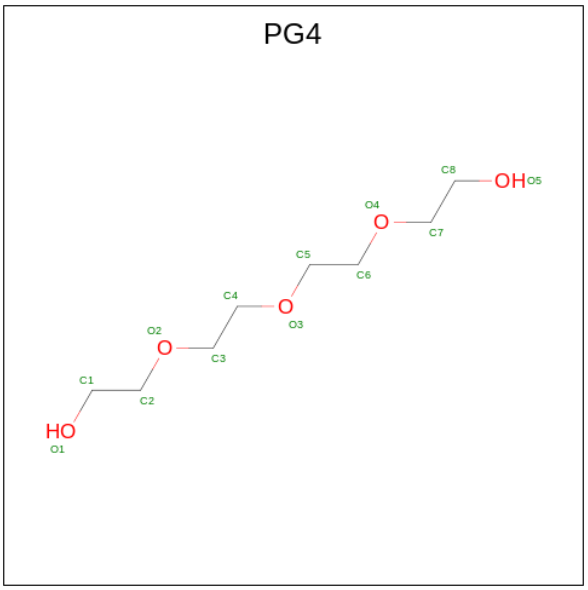
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	4	3	0	0
5	B	1	7	4	3	0	0
5	B	1	7	4	3	0	0
5	B	1	7	4	3	0	0
5	C	1	7	4	3	0	0
5	C	1	7	4	3	0	0
5	C	1	7	4	3	0	0
5	C	1	7	4	3	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



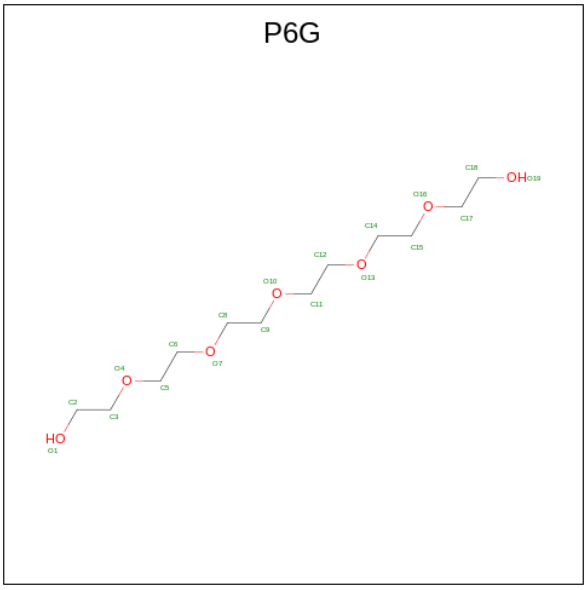
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			10	6	4			
6	A	1	Total	C	O		0	0
			10	6	4			
6	B	1	Total	C	O		0	0
			10	6	4			
6	C	1	Total	C	O		0	0
			10	6	4			

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



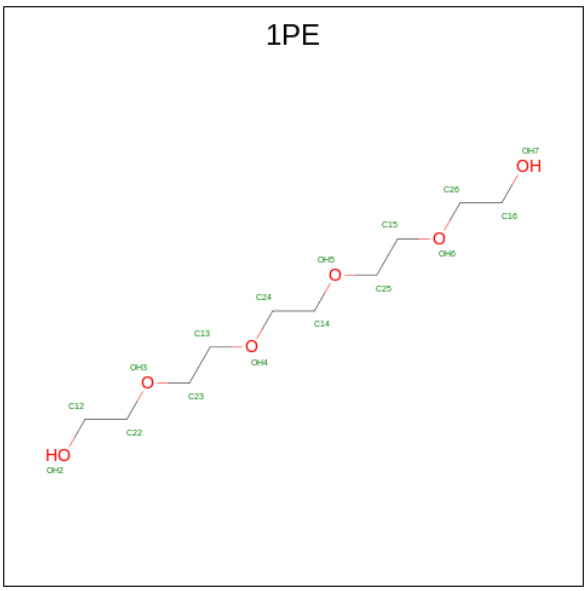
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	13	8	5	0	0

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



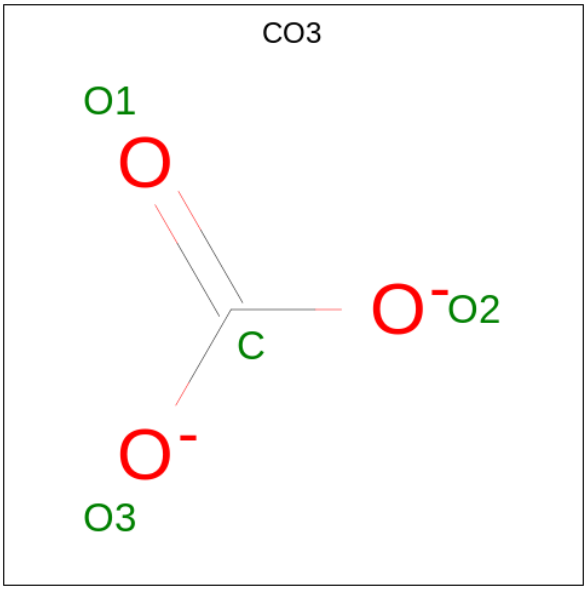
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	19	12	7	0	0

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



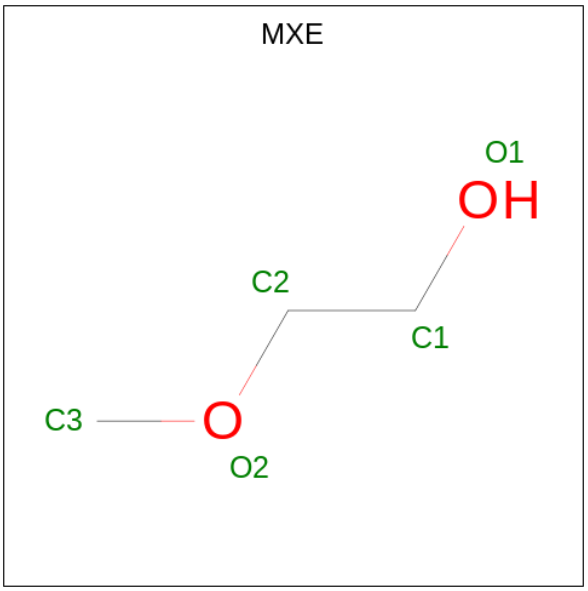
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	16	10	6	0	0
			Total	C	O		
9	B	1	16	10	6	0	0
			Total	C	O		
9	C	1	16	10	6	0	0

- Molecule 10 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



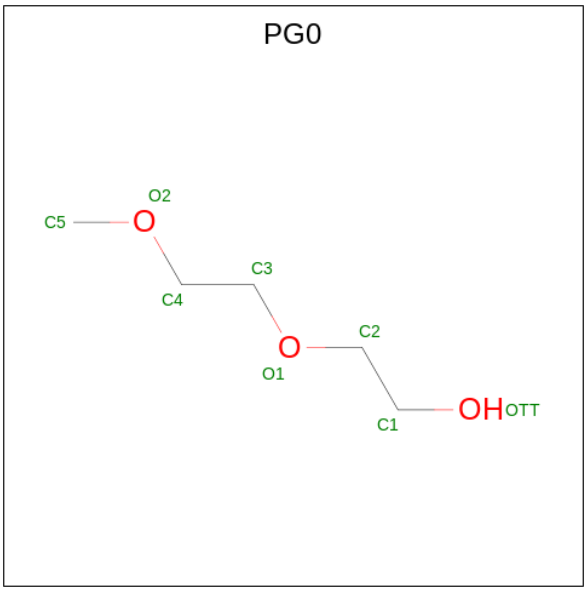
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	4	1	3	0	0
			Total	C	O		
10	B	1	4	1	3	0	0

- Molecule 11 is 2-METHOXYETHANOL (three-letter code: MXE) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	5	3	2	0	0
			Total	C	O		
11	C	1	5	3	2	0	0

- Molecule 12 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	A	1	8	5	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	B	1	8	5	3	0	0
			Total	C	O		
12	B	1	8	5	3	0	0
			Total	C	O		
12	C	1	8	5	3	0	0

- Molecule 13 is water.

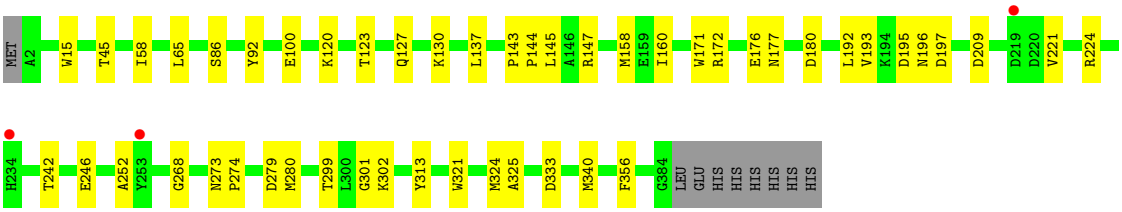
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	302	302	302	0	0
			Total	O		
13	B	299	299	299	0	0
			Total	O		
13	C	259	259	259	0	0

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.

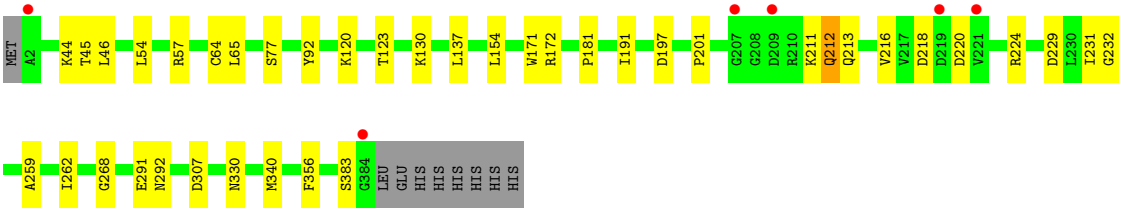
• Molecule 1: Terminal oxygenase component of carbazole

Chain A:



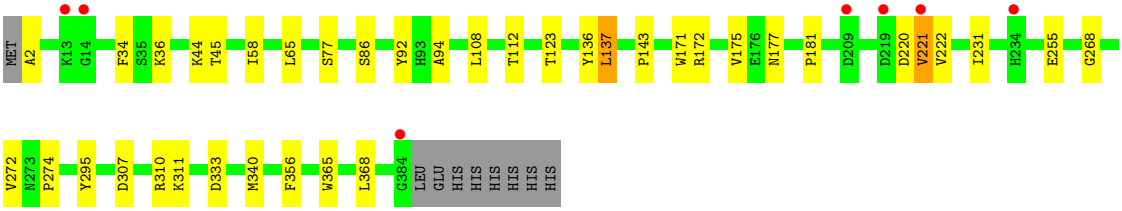
• Molecule 1: Terminal oxygenase component of carbazole

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	91.94Å 91.94Å 243.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.01 – 1.60 45.97 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.01-1.60) 100.0 (45.97-1.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.154 , 0.188 0.165 , 0.197	Depositor DCC
R_{free} test set	7679 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10529	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FES, PG0, P6G, PGE, MXE, CO3, FE2, 1PE, PG4, 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	0.76	0/3219	0.90	2/4368 (0.0%)
1	B	0.76	1/3264 (0.0%)	0.93	2/4425 (0.0%)
1	C	0.73	0/3231	0.90	2/4382 (0.0%)
All	All	0.75	1/9714 (0.0%)	0.91	6/13175 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	GLU	CD-OE2	6.40	1.32	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	340	MET	CG-SD-CE	-6.20	90.28	100.20
1	A	340	MET	CG-SD-CE	-6.12	90.41	100.20
1	B	57	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	224	ARG	CG-CD-NE	-5.38	100.49	111.80
1	C	295	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	C	340	MET	CG-SD-CE	-5.25	91.81	100.20

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	3125	0	3045	36	0
1	B	3164	0	3102	23	0
1	C	3134	0	3061	28	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	1	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
5	A	7	0	10	0	0
5	B	21	0	30	2	0
5	C	28	0	40	5	0
6	A	20	0	28	1	0
6	B	10	0	14	0	0
6	C	10	0	14	3	0
7	A	13	0	18	0	0
8	A	19	0	26	5	0
9	A	16	0	22	0	0
9	B	16	0	22	0	0
9	C	16	0	22	3	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
11	A	5	0	8	4	0
11	C	5	0	8	0	0
12	A	8	0	12	1	0
12	B	16	0	24	4	0
12	C	8	0	12	1	0
13	A	302	0	0	5	0
13	B	299	0	0	9	0
13	C	259	0	0	5	0
All	All	10529	0	9518	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (93) 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:330:ASN:HD21	12:B:412:PG0:H12	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:H	11:A:411:MXE:H33	1.25	0.97
1:A:279:ASP:OD2	1:A:302:LYS:HE2	1.84	0.77
1:A:145:LEU:N	11:A:411:MXE:H33	2.01	0.76
1:A:192:LEU:HA	1:A:324:MET:CE	2.16	0.75
1:B:229:ASP:OD1	13:B:501:HOH:O	2.09	0.70
1:A:192:LEU:HA	1:A:324:MET:HE2	1.74	0.68
1:C:177:ASN:ND2	13:C:501:HOH:O	1.97	0.68
12:B:412:PG0:H11	13:B:717:HOH:O	1.95	0.67
1:A:192:LEU:HD12	1:A:324:MET:HE2	1.76	0.66
1:A:127:GLN:OE1	11:A:411:MXE:H31	1.95	0.65
1:B:213:GLN:HG3	13:B:757:HOH:O	1.96	0.65
12:A:412:PG0:H51	13:A:749:HOH:O	1.97	0.65
1:B:330:ASN:ND2	12:B:412:PG0:H12	2.06	0.64
1:C:45:THR:H	6:C:405:PGE:H5	1.63	0.64
1:B:292:ASN:OD1	13:B:502:HOH:O	2.15	0.64
1:B:201:PRO:HD3	5:B:407:PEG:H31	1.81	0.62
1:C:44:LYS:HD2	6:C:405:PGE:H32	1.83	0.61
1:A:280:MET:CE	1:A:313:TYR:HE1	2.13	0.60
1:A:45:THR:HB	13:A:512:HOH:O	2.01	0.60
1:B:197:ASP:OD1	13:B:503:HOH:O	2.16	0.59
1:A:177:ASN:HD21	1:A:333:ASP:HB3	1.67	0.59
1:A:242:THR:HA	1:A:246[A]:GLU:O	2.02	0.58
1:A:100:GLU:HB2	8:A:408:P6G:H31	1.86	0.58
1:A:177:ASN:ND2	13:A:501:HOH:O	2.07	0.58
1:A:192:LEU:HA	1:A:324:MET:HE3	1.86	0.57
1:B:212:GLN:O	1:B:212:GLN:HG3	2.04	0.57
1:C:45:THR:HB	13:C:538:HOH:O	2.03	0.57
1:C:177:ASN:HD21	1:C:333:ASP:HB3	1.69	0.57
1:A:195:ASP:HB2	1:A:324:MET:HE3	1.87	0.57
1:C:255:GLU:OE1	13:C:502:HOH:O	2.17	0.57
1:A:195:ASP:HB2	1:A:324:MET:CE	2.35	0.56
1:C:36:LYS:HE2	5:C:406:PEG:O2	2.05	0.56
1:B:231:ILE:HG23	1:B:232:GLY:N	2.22	0.55
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.88	0.54
1:C:86:SER:CB	9:C:407:1PE:H231	2.38	0.54
1:B:44:LYS:HE3	13:B:523:HOH:O	2.08	0.53
1:B:231:ILE:CG2	1:B:232:GLY:N	2.72	0.53
1:C:34:PHE:CG	5:C:406:PEG:H21	2.45	0.52
1:C:44:LYS:HD2	6:C:405:PGE:C3	2.39	0.52
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.93	0.51
1:A:86:SER:CB	8:A:408:P6G:H51	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.46	0.51
8:A:408:P6G:H21	13:A:664:HOH:O	2.12	0.49
1:B:181:PRO:HB3	1:B:231:ILE:HG21	1.94	0.49
1:C:58:ILE:HG21	9:C:407:1PE:H232	1.93	0.49
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.95	0.48
1:B:220:ASP:CG	1:B:224:ARG:HG2	2.35	0.47
1:B:130[B]:LYS:HE3	1:B:154:LEU:HA	1.96	0.47
1:B:45:THR:CG2	1:B:77:SER:CB	2.93	0.47
1:A:280:MET:HE1	1:A:313:TYR:HE1	1.80	0.46
1:A:280:MET:HE3	1:A:313:TYR:CE1	2.52	0.45
1:C:307:ASP:OD1	1:C:310[B]:ARG:NH1	2.49	0.45
1:A:144:PRO:HB3	11:A:411:MXE:H22	1.99	0.44
1:C:112:THR:O	5:C:408:PEG:H41	2.18	0.44
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.53	0.44
1:C:45:THR:CG2	1:C:77:SER:CB	2.95	0.44
1:C:310[A]:ARG:HH12	1:C:311:LYS:HE2	1.82	0.44
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.48	0.44
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.53	0.44
1:A:176:GLU:O	1:A:180:ASP:HB2	2.18	0.44
5:C:409:PEG:H21	13:C:638:HOH:O	2.17	0.43
1:A:280:MET:HE3	1:A:313:TYR:HE1	1.82	0.43
1:B:191[B]:ILE:HG22	13:B:510:HOH:O	2.18	0.43
1:A:130[B]:LYS:NZ	1:A:158:MET:HB3	2.34	0.43
1:C:272:VAL:HG21	12:C:411:PG0:H31	2.01	0.43
1:B:45:THR:CG2	1:B:77:SER:HB2	2.49	0.43
1:A:321:TRP:O	1:A:325:ALA:HB3	2.19	0.43
1:B:216:VAL:HG21	5:B:410:PEG:H41	2.00	0.43
1:A:196:ASN:N	1:A:324:MET:HE1	2.34	0.43
1:C:181:PRO:HB3	1:C:231:ILE:HG21	2.01	0.42
1:A:58:ILE:HG21	8:A:408:P6G:H52	2.02	0.42
1:A:86:SER:HB3	8:A:408:P6G:H51	2.00	0.42
1:C:86:SER:HB3	9:C:407:1PE:H231	2.00	0.42
1:C:136:TYR:CE1	1:C:143:PRO:HD2	2.54	0.42
1:A:120[B]:LYS:NZ	13:A:503:HOH:O	2.25	0.42
1:C:45:THR:HG21	1:C:77:SER:CB	2.50	0.42
1:C:221:VAL:HG22	1:C:222:VAL:HG13	2.02	0.42
1:A:160:ILE:HG23	1:A:299:THR:HB	2.01	0.42
1:B:120[A]:LYS:HD3	13:B:615:HOH:O	2.19	0.42
1:B:54:LEU:O	1:B:64:CYS:HA	2.21	0.41
1:C:36:LYS:CE	5:C:406:PEG:O2	2.68	0.41
1:A:193:VAL:CG1	1:A:252:ALA:CB	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ALA:HB1	1:C:108:LEU:HB2	2.03	0.41
1:C:175:VAL:HG11	1:C:365:TRP:CE2	2.56	0.41
1:A:273:ASN:HA	1:A:274:PRO:HA	1.92	0.41
1:C:2:ALA:N	13:C:520:HOH:O	2.53	0.41
1:A:280:MET:CE	1:A:313:TYR:CE1	3.00	0.40
1:C:137:LEU:HD22	1:C:137:LEU:HA	1.98	0.40
6:A:407:PGE:H52	6:A:407:PGE:H3	1.76	0.40
12:B:412:PG0:H31	13:B:717:HOH:O	2.21	0.40
1:B:259:ALA:HB1	1:B:262:ILE:HD11	2.03	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	388/392 (99%)	371 (96%)	15 (4%)	2 (0%)	29	11
1	B	394/392 (100%)	377 (96%)	16 (4%)	1 (0%)	41	21
1	C	389/392 (99%)	373 (96%)	15 (4%)	1 (0%)	41	21
All	All	1171/1176 (100%)	1121 (96%)	46 (4%)	4 (0%)	41	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLY
1	B	268	GLY
1	C	268	GLY
1	A	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	336/339 (99%)	330 (98%)	6 (2%)	59	36
1	B	342/339 (101%)	333 (97%)	9 (3%)	46	21
1	C	337/339 (99%)	330 (98%)	7 (2%)	53	29
All	All	1015/1017 (100%)	993 (98%)	22 (2%)	52	27

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	TYR
1	A	137	LEU
1	A	197	ASP
1	A	209	ASP
1	A	221	VAL
1	A	356	PHE
1	B	46	LEU
1	B	92	TYR
1	B	137	LEU
1	B	211	LYS
1	B	212	GLN
1	B	218	ASP
1	B	307	ASP
1	B	356	PHE
1	B	383	SER
1	C	92	TYR
1	C	137	LEU
1	C	220	ASP
1	C	221	VAL
1	C	274	PRO
1	C	356	PHE
1	C	368	LEU

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

Mol	Chain	Res	Type
1	A	177	ASN
1	A	352	ASN
1	B	292	ASN
1	B	352	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 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
9	1PE	A	409	-	15,15,15	0.74	0	14,14,14	0.75	0
9	1PE	B	408	-	15,15,15	0.59	0	14,14,14	0.84	0
5	PEG	B	409	-	6,6,6	0.24	0	5,5,5	0.11	0
5	PEG	A	404	-	6,6,6	0.44	0	5,5,5	0.36	0
12	PG0	A	412	-	7,7,7	0.25	0	6,6,6	0.53	0
11	MXE	C	410	-	4,4,4	0.34	0	3,3,3	0.27	0
6	PGE	C	405	-	9,9,9	0.22	0	8,8,8	0.14	0
2	FES	A	401	1	0,4,4	-	-	-		
6	PGE	B	406	-	9,9,9	0.20	0	8,8,8	0.17	0
12	PG0	C	411	-	7,7,7	0.26	0	6,6,6	0.18	0
2	FES	C	401	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	1PE	C	407	-	15,15,15	0.76	0	14,14,14	1.03	2 (14%)
10	CO3	B	411	-	2,3,3	0.56	0	2,3,3	0.18	0
7	PG4	A	406	-	12,12,12	0.24	0	11,11,11	0.22	0
5	PEG	C	409	-	6,6,6	0.13	0	5,5,5	0.31	0
2	FES	B	401	1	0,4,4	-	-	-		
12	PG0	B	412	-	7,7,7	0.37	0	6,6,6	0.30	0
12	PG0	B	413	-	7,7,7	0.35	0	6,6,6	0.43	0
6	PGE	A	405	-	9,9,9	0.35	0	8,8,8	0.22	0
5	PEG	B	407	-	6,6,6	0.23	0	5,5,5	0.23	0
8	P6G	A	408	-	18,18,18	0.75	0	17,17,17	0.86	0
5	PEG	C	406	-	6,6,6	0.15	0	5,5,5	0.27	0
10	CO3	A	410	-	2,3,3	0.12	0	2,3,3	0.42	0
11	MXE	A	411	-	4,4,4	0.47	0	3,3,3	1.12	0
5	PEG	C	408	-	6,6,6	0.17	0	5,5,5	0.23	0
6	PGE	A	407	-	9,9,9	0.30	0	8,8,8	0.29	0
5	PEG	B	410	-	6,6,6	0.27	0	5,5,5	0.25	0
5	PEG	C	404	-	6,6,6	0.36	0	5,5,5	0.37	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
9	1PE	A	409	-	-	6/13/13/13	-
9	1PE	B	408	-	-	5/13/13/13	-
5	PEG	B	409	-	-	2/4/4/4	-
5	PEG	A	404	-	-	1/4/4/4	-
12	PG0	A	412	-	-	2/5/5/5	-
11	MXE	C	410	-	-	1/2/2/2	-
6	PGE	C	405	-	-	4/7/7/7	-
2	FES	A	401	1	-	-	0/1/1/1
6	PGE	B	406	-	-	1/7/7/7	-
12	PG0	C	411	-	-	1/5/5/5	-
2	FES	C	401	1	-	-	0/1/1/1
9	1PE	C	407	-	-	8/13/13/13	-
7	PG4	A	406	-	-	3/10/10/10	-
5	PEG	C	409	-	-	1/4/4/4	-
12	PG0	B	412	-	-	2/5/5/5	-
2	FES	B	401	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PG0	B	413	-	-	3/5/5/5	-
6	PGE	A	405	-	-	2/7/7/7	-
5	PEG	B	407	-	-	3/4/4/4	-
8	P6G	A	408	-	-	11/16/16/16	-
5	PEG	C	406	-	-	2/4/4/4	-
11	MXE	A	411	-	-	2/2/2/2	-
5	PEG	C	408	-	-	3/4/4/4	-
6	PGE	A	407	-	-	4/7/7/7	-
5	PEG	B	410	-	-	3/4/4/4	-
5	PEG	C	404	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	407	1PE	OH3-C23-C13	2.49	121.62	110.39
9	C	407	1PE	OH3-C22-C12	2.09	119.26	110.07

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	407	PGE	C3-C4-O3-C5
9	C	407	1PE	OH7-C16-C26-OH6
5	B	410	PEG	C1-C2-O2-C3
8	A	408	P6G	O7-C8-C9-O10
8	A	408	P6G	O13-C14-C15-O16
12	B	413	PG0	O1-C3-C4-O2
6	A	407	PGE	C1-C2-O2-C3
9	B	408	1PE	OH5-C14-C24-OH4
9	C	407	1PE	OH4-C13-C23-OH3
6	A	405	PGE	O2-C3-C4-O3
5	C	409	PEG	O1-C1-C2-O2
6	A	405	PGE	O3-C5-C6-O4
6	C	405	PGE	O1-C1-C2-O2
11	C	410	MXE	O1-C1-C2-O2
12	C	411	PG0	OTT-C1-C2-O1
6	C	405	PGE	O2-C3-C4-O3
5	B	410	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	410	PEG	O2-C3-C4-O4
5	A	404	PEG	O2-C3-C4-O4
8	A	408	P6G	O1-C2-C3-O4
9	C	407	1PE	OH2-C12-C22-OH3
11	A	411	MXE	O1-C1-C2-O2
8	A	408	P6G	O4-C5-C6-O7
9	A	409	1PE	OH4-C13-C23-OH3
12	A	412	PG0	OTT-C1-C2-O1
9	B	408	1PE	OH6-C15-C25-OH5
9	C	407	1PE	OH6-C15-C25-OH5
5	B	409	PEG	O2-C3-C4-O4
5	C	406	PEG	O1-C1-C2-O2
5	C	408	PEG	O2-C3-C4-O4
6	A	407	PGE	O1-C1-C2-O2
8	A	408	P6G	C2-C3-O4-C5
8	A	408	P6G	C6-C5-O4-C3
6	A	407	PGE	O2-C3-C4-O3
9	A	409	1PE	OH6-C15-C25-OH5
9	C	407	1PE	C12-C22-OH3-C23
12	A	412	PG0	C3-C4-O2-C5
9	C	407	1PE	C13-C23-OH3-C22
5	B	407	PEG	C1-C2-O2-C3
5	B	407	PEG	C4-C3-O2-C2
8	A	408	P6G	O16-C17-C18-O19
8	A	408	P6G	C14-C15-O16-C17
9	C	407	1PE	C23-C13-OH4-C24
5	C	408	PEG	C4-C3-O2-C2
7	A	406	PG4	C1-C2-O2-C3
7	A	406	PG4	C8-C7-O4-C6
7	A	406	PG4	O4-C7-C8-O5
8	A	408	P6G	C12-C11-O10-C9
5	C	406	PEG	C1-C2-O2-C3
11	A	411	MXE	C1-C2-O2-C3
9	A	409	1PE	OH5-C14-C24-OH4
5	B	407	PEG	O2-C3-C4-O4
9	B	408	1PE	OH7-C16-C26-OH6
12	B	413	PG0	OTT-C1-C2-O1
9	A	409	1PE	C13-C23-OH3-C22
9	B	408	1PE	C23-C13-OH4-C24
6	B	406	PGE	C1-C2-O2-C3
9	A	409	1PE	OH7-C16-C26-OH6
9	A	409	1PE	C16-C26-OH6-C15

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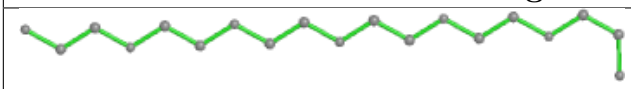
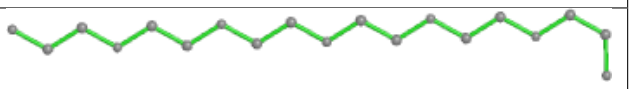
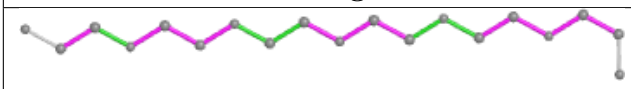
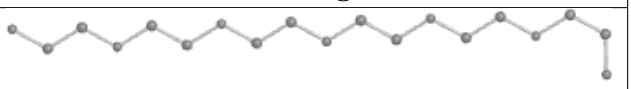
Mol	Chain	Res	Type	Atoms
5	C	408	PEG	C1-C2-O2-C3
9	C	407	1PE	OH5-C14-C24-OH4
6	C	405	PGE	O3-C5-C6-O4
5	B	409	PEG	C4-C3-O2-C2
8	A	408	P6G	C15-C14-O13-C12
12	B	412	PG0	C1-C2-O1-C3
9	B	408	1PE	C25-C15-OH6-C26
12	B	413	PG0	C3-C4-O2-C5
12	B	412	PG0	O1-C3-C4-O2
8	A	408	P6G	C8-C9-O10-C11
6	C	405	PGE	C1-C2-O2-C3

There are no ring outliers.

13 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	412	PG0	1	0
6	C	405	PGE	3	0
12	C	411	PG0	1	0
9	C	407	1PE	3	0
5	C	409	PEG	1	0
12	B	412	PG0	4	0
5	B	407	PEG	1	0
8	A	408	P6G	5	0
5	C	406	PEG	3	0
11	A	411	MXE	4	0
5	C	408	PEG	1	0
6	A	407	PGE	1	0
5	B	410	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand P6G A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 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	383/392 (97%)	-0.35	3 (0%)	86	86	9, 19, 43, 58	0
1	B	383/392 (97%)	-0.35	6 (1%)	72	71	10, 18, 38, 67	0
1	C	383/392 (97%)	-0.37	7 (1%)	68	67	13, 21, 40, 61	0
All	All	1149/1176 (97%)	-0.36	16 (1%)	75	75	9, 19, 42, 67	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	VAL	4.6
1	B	384	GLY	4.2
1	C	234	HIS	3.2
1	A	253	TYR	3.0
1	C	221	VAL	2.9
1	C	13[A]	LYS	2.7
1	A	219	ASP	2.7
1	B	207	GLY	2.6
1	C	384	GLY	2.5
1	B	219	ASP	2.4
1	A	234	HIS	2.4
1	C	14[A]	GLY	2.4
1	B	2	ALA	2.2
1	B	209	ASP	2.1
1	C	219	ASP	2.1
1	C	209	ASP	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, 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(Å^2)	Q<0.9
6	PGE	A	405	10/10	0.71	0.21	41,45,47,53	0
5	PEG	C	406	7/7	0.72	0.13	49,51,54,57	0
5	PEG	A	404	7/7	0.72	0.18	33,39,43,45	0
9	1PE	A	409	16/16	0.72	0.13	41,47,53,53	0
5	PEG	B	410	7/7	0.74	0.14	46,47,49,49	0
12	PG0	B	413	8/8	0.77	0.12	44,46,48,50	0
5	PEG	B	407	7/7	0.78	0.13	44,52,54,55	0
5	PEG	B	409	7/7	0.79	0.13	41,49,51,56	0
6	PGE	A	407	10/10	0.79	0.22	45,49,53,56	0
5	PEG	C	409	7/7	0.80	0.11	46,47,48,53	0
6	PGE	C	405	10/10	0.80	0.14	43,48,54,56	0
12	PG0	A	412	8/8	0.81	0.13	36,40,43,50	0
8	P6G	A	408	19/19	0.82	0.22	44,47,61,62	0
9	1PE	C	407	16/16	0.83	0.18	37,41,48,49	0
5	PEG	C	408	7/7	0.83	0.23	49,52,54,59	0
9	1PE	B	408	16/16	0.83	0.13	43,50,60,60	0
11	MXE	C	410	5/5	0.87	0.09	43,45,49,55	0
7	PG4	A	406	13/13	0.88	0.18	25,36,50,54	0
12	PG0	B	412	8/8	0.89	0.10	19,26,35,40	0
11	MXE	A	411	5/5	0.89	0.14	25,26,36,37	0
10	CO3	B	411	4/4	0.90	0.17	34,36,38,39	0
4	MG	B	403	1/1	0.90	0.21	39,39,39,39	0
10	CO3	A	410	4/4	0.90	0.10	21,25,29,36	0
6	PGE	B	406	10/10	0.91	0.13	35,40,48,48	0
5	PEG	C	404	7/7	0.91	0.11	25,26,39,50	0
12	PG0	C	411	8/8	0.92	0.10	25,27,42,45	0
4	MG	B	405	1/1	0.95	0.15	29,29,29,29	0
4	MG	A	403	1/1	0.99	0.10	18,18,18,18	0
2	FES	B	401	4/4	0.99	0.07	13,13,13,14	0
4	MG	B	404	1/1	0.99	0.14	20,20,20,20	0
2	FES	C	401	4/4	0.99	0.06	13,15,15,15	0
4	MG	C	403	1/1	0.99	0.08	21,21,21,21	0

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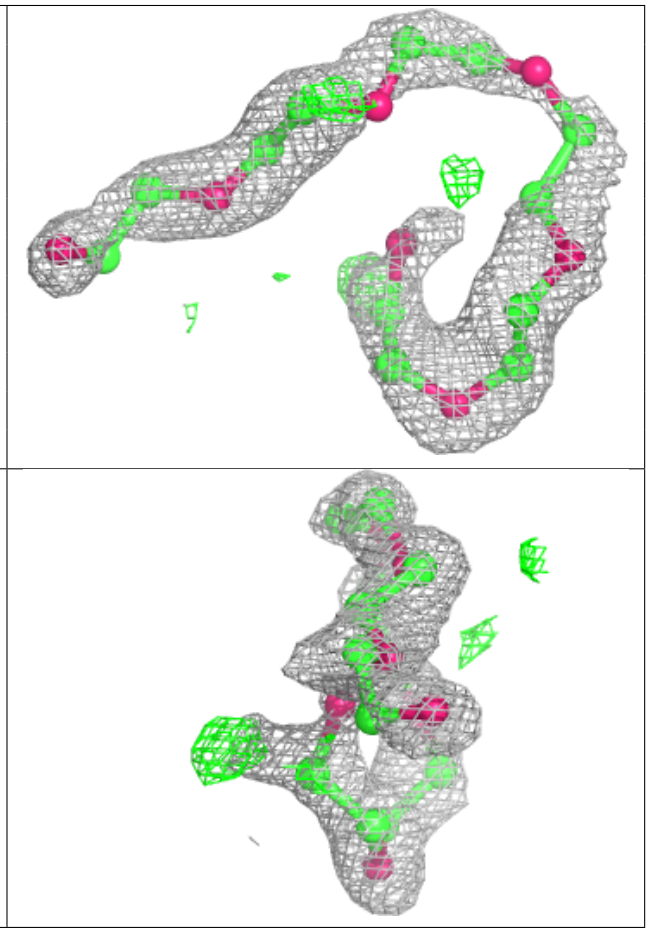
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE2	A	402	1/1	0.99	0.05	19,19,19,19	0
2	FES	A	401	4/4	1.00	0.07	9,9,9,9	0
3	FE2	B	402	1/1	1.00	0.04	13,13,13,13	0
3	FE2	C	402	1/1	1.00	0.04	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

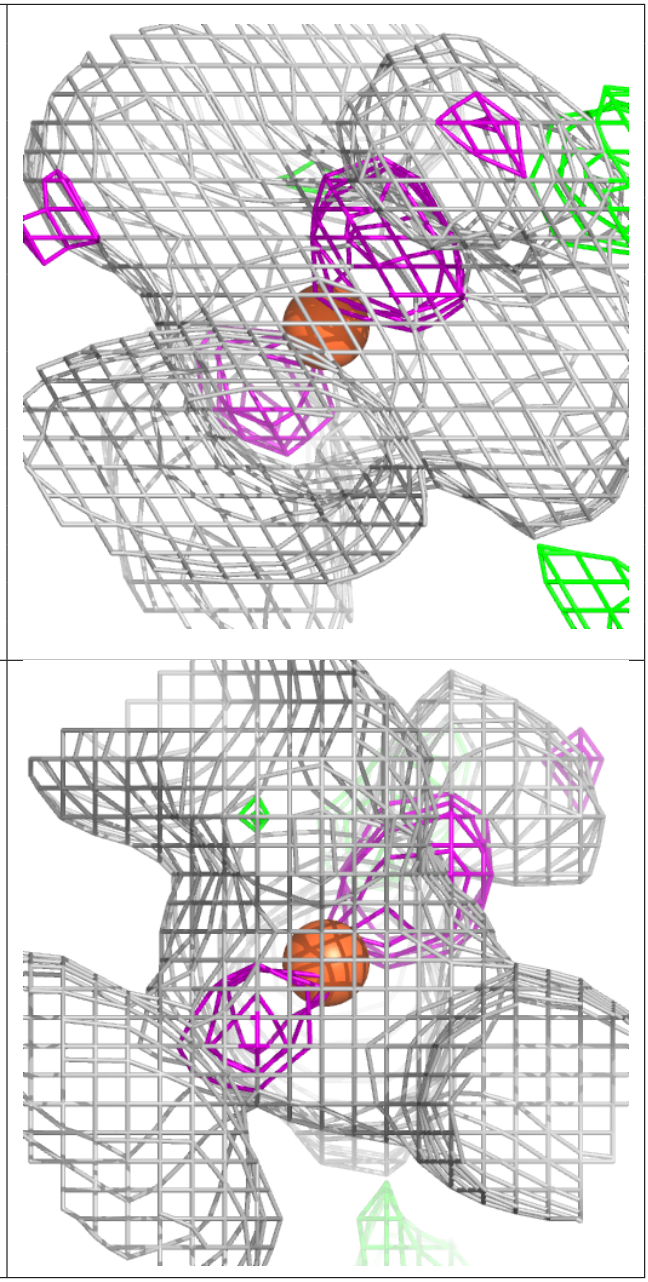
Electron density around P6G A 408:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



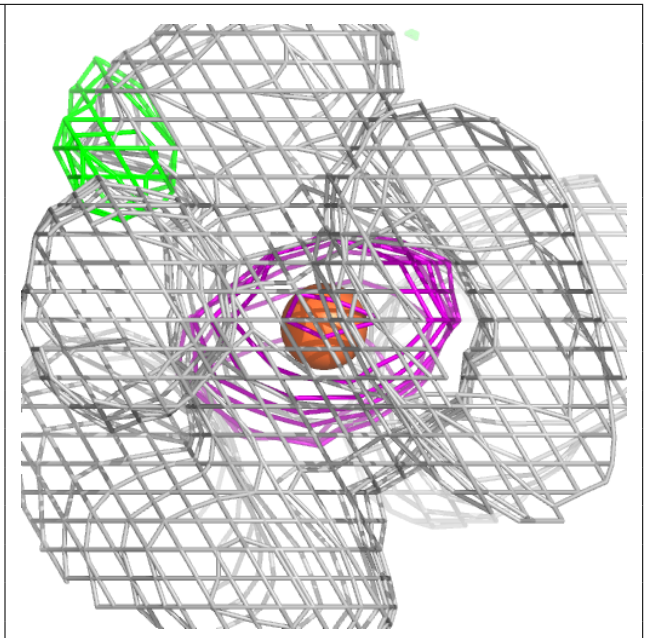
Electron density around FE2 A 402:

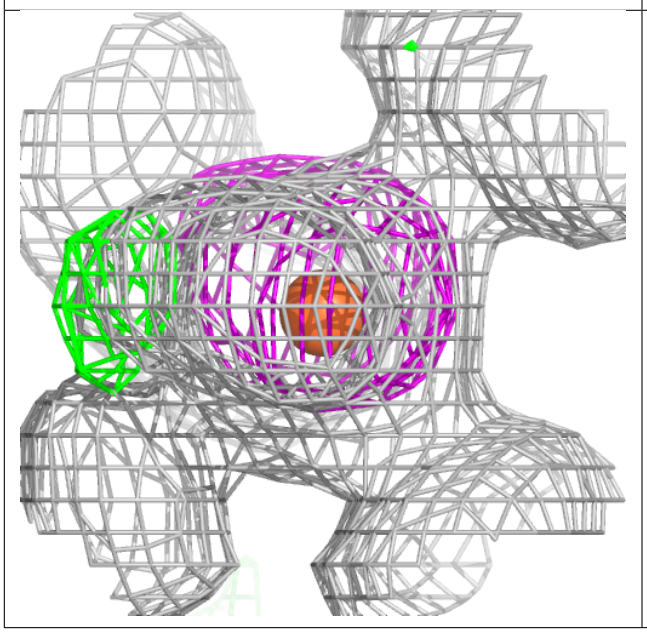
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

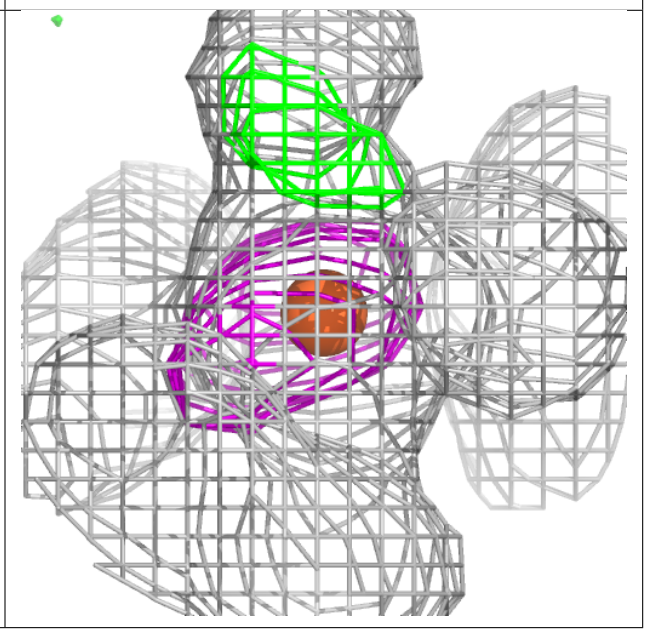


Electron density around FE2 B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

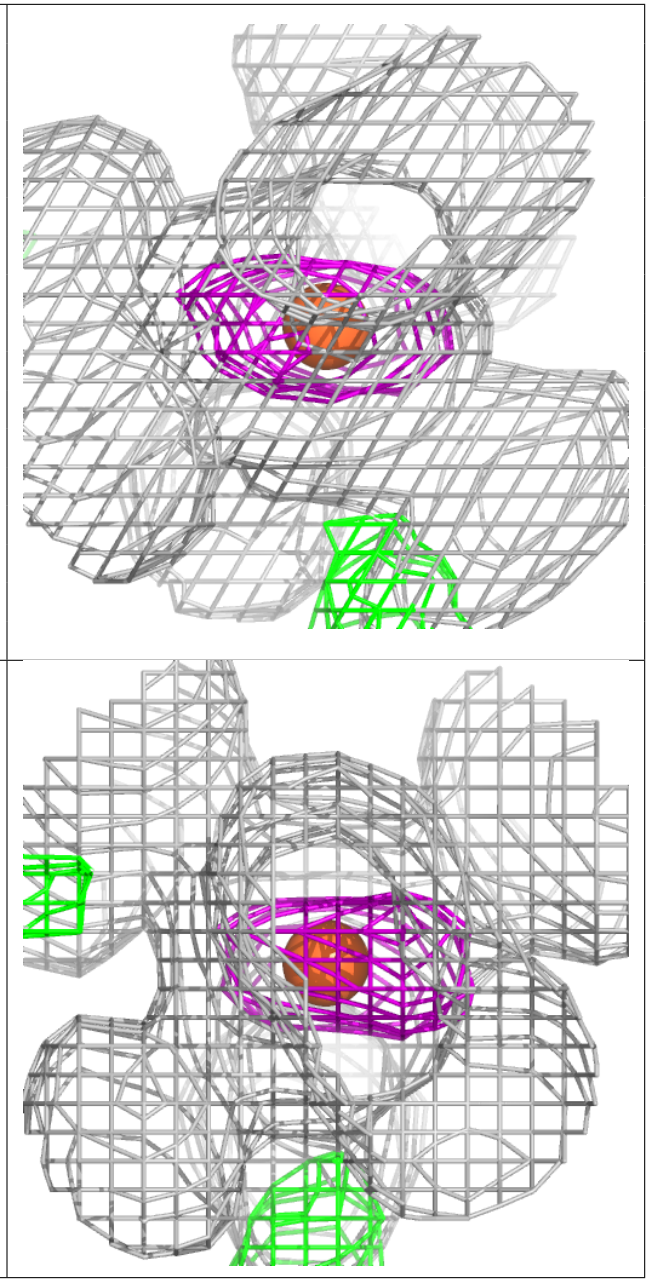






Electron density around FE2 C 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.