



wwPDB X-ray Structure Validation Summary Report i

Mar 10, 2024 – 07:34 AM EDT

PDB ID : 4KTR
Title : Crystal structure of 2-O-alpha-glucosylglycerol phosphorylase in complex with isofagomine and glycerol
Authors : Touhara, K.K.; Nihira, T.; Kitaoka, M.; Nakai, H.; Fushinobu, S.
Deposited on : 2013-05-21
Resolution : 2.30 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

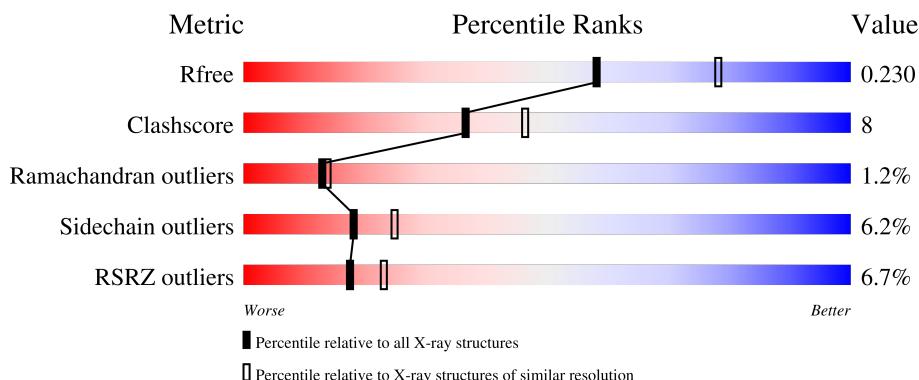
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



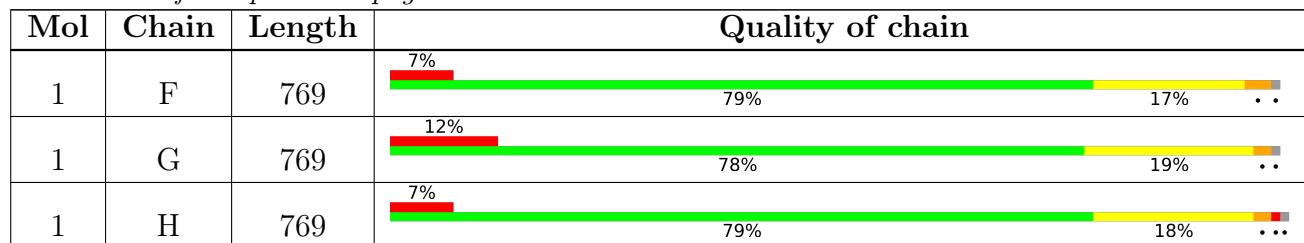
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



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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
4	GOL	B	804	-	X	X	-
4	GOL	D	809	-	-	X	-
4	GOL	H	807	-	-	X	-
6	PGE	A	812	-	-	X	-

2 Entry composition [\(i\)](#)

There are 12 unique types of molecules in this entry. The entry contains 51264 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 Glycoside hydrolase family 65 central catalytic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total 6093	C 3850	N 1036	O 1185	S 22	0	0	0
1	B	761	Total 6085	C 3844	N 1035	O 1184	S 22	0	0	0
1	C	761	Total 6085	C 3844	N 1035	O 1184	S 22	0	0	0
1	D	761	Total 6085	C 3844	N 1035	O 1184	S 22	0	0	0
1	E	761	Total 6085	C 3844	N 1035	O 1184	S 22	0	0	0
1	F	761	Total 6085	C 3844	N 1035	O 1184	S 22	0	0	0
1	G	762	Total 6093	C 3850	N 1036	O 1185	S 22	0	0	0
1	H	761	Total 6085	C 3844	N 1035	O 1184	S 22	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	GLU	engineered mutation	UNP D6XZ22
A	762	LEU	-	expression tag	UNP D6XZ22
A	763	GLU	-	expression tag	UNP D6XZ22
A	764	HIS	-	expression tag	UNP D6XZ22
A	765	HIS	-	expression tag	UNP D6XZ22
A	766	HIS	-	expression tag	UNP D6XZ22
A	767	HIS	-	expression tag	UNP D6XZ22
A	768	HIS	-	expression tag	UNP D6XZ22
A	769	HIS	-	expression tag	UNP D6XZ22
B	475	GLN	GLU	engineered mutation	UNP D6XZ22
B	762	LEU	-	expression tag	UNP D6XZ22
B	763	GLU	-	expression tag	UNP D6XZ22
B	764	HIS	-	expression tag	UNP D6XZ22

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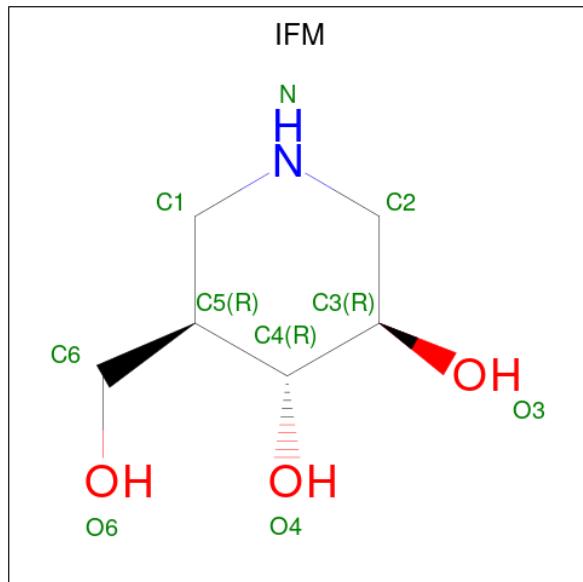
Chain	Residue	Modelled	Actual	Comment	Reference
B	765	HIS	-	expression tag	UNP D6XZ22
B	766	HIS	-	expression tag	UNP D6XZ22
B	767	HIS	-	expression tag	UNP D6XZ22
B	768	HIS	-	expression tag	UNP D6XZ22
B	769	HIS	-	expression tag	UNP D6XZ22
C	475	GLN	GLU	engineered mutation	UNP D6XZ22
C	762	LEU	-	expression tag	UNP D6XZ22
C	763	GLU	-	expression tag	UNP D6XZ22
C	764	HIS	-	expression tag	UNP D6XZ22
C	765	HIS	-	expression tag	UNP D6XZ22
C	766	HIS	-	expression tag	UNP D6XZ22
C	767	HIS	-	expression tag	UNP D6XZ22
C	768	HIS	-	expression tag	UNP D6XZ22
C	769	HIS	-	expression tag	UNP D6XZ22
D	475	GLN	GLU	engineered mutation	UNP D6XZ22
D	762	LEU	-	expression tag	UNP D6XZ22
D	763	GLU	-	expression tag	UNP D6XZ22
D	764	HIS	-	expression tag	UNP D6XZ22
D	765	HIS	-	expression tag	UNP D6XZ22
D	766	HIS	-	expression tag	UNP D6XZ22
D	767	HIS	-	expression tag	UNP D6XZ22
D	768	HIS	-	expression tag	UNP D6XZ22
D	769	HIS	-	expression tag	UNP D6XZ22
E	475	GLN	GLU	engineered mutation	UNP D6XZ22
E	762	LEU	-	expression tag	UNP D6XZ22
E	763	GLU	-	expression tag	UNP D6XZ22
E	764	HIS	-	expression tag	UNP D6XZ22
E	765	HIS	-	expression tag	UNP D6XZ22
E	766	HIS	-	expression tag	UNP D6XZ22
E	767	HIS	-	expression tag	UNP D6XZ22
E	768	HIS	-	expression tag	UNP D6XZ22
E	769	HIS	-	expression tag	UNP D6XZ22
F	475	GLN	GLU	engineered mutation	UNP D6XZ22
F	762	LEU	-	expression tag	UNP D6XZ22
F	763	GLU	-	expression tag	UNP D6XZ22
F	764	HIS	-	expression tag	UNP D6XZ22
F	765	HIS	-	expression tag	UNP D6XZ22
F	766	HIS	-	expression tag	UNP D6XZ22
F	767	HIS	-	expression tag	UNP D6XZ22
F	768	HIS	-	expression tag	UNP D6XZ22
F	769	HIS	-	expression tag	UNP D6XZ22
G	475	GLN	GLU	engineered mutation	UNP D6XZ22

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Chain	Residue	Modelled	Actual	Comment	Reference
G	762	LEU	-	expression tag	UNP D6XZ22
G	763	GLU	-	expression tag	UNP D6XZ22
G	764	HIS	-	expression tag	UNP D6XZ22
G	765	HIS	-	expression tag	UNP D6XZ22
G	766	HIS	-	expression tag	UNP D6XZ22
G	767	HIS	-	expression tag	UNP D6XZ22
G	768	HIS	-	expression tag	UNP D6XZ22
G	769	HIS	-	expression tag	UNP D6XZ22
H	475	GLN	GLU	engineered mutation	UNP D6XZ22
H	762	LEU	-	expression tag	UNP D6XZ22
H	763	GLU	-	expression tag	UNP D6XZ22
H	764	HIS	-	expression tag	UNP D6XZ22
H	765	HIS	-	expression tag	UNP D6XZ22
H	766	HIS	-	expression tag	UNP D6XZ22
H	767	HIS	-	expression tag	UNP D6XZ22
H	768	HIS	-	expression tag	UNP D6XZ22
H	769	HIS	-	expression tag	UNP D6XZ22

- Molecule 2 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: C₆H₁₃NO₃).



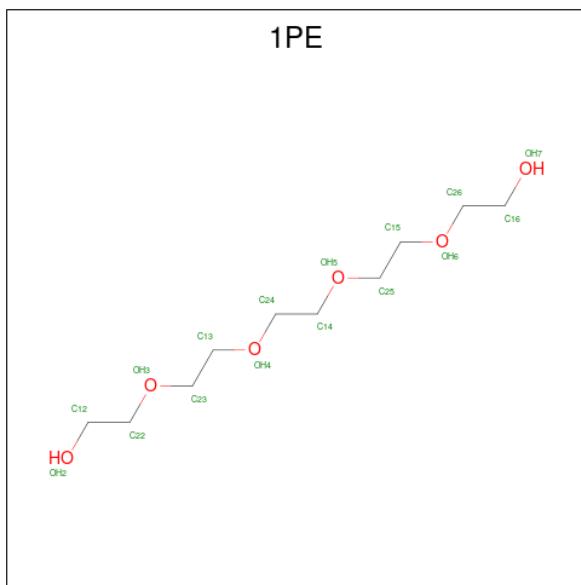
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	D	1	Total	C	N	O	0	0
			10	6	1	3		

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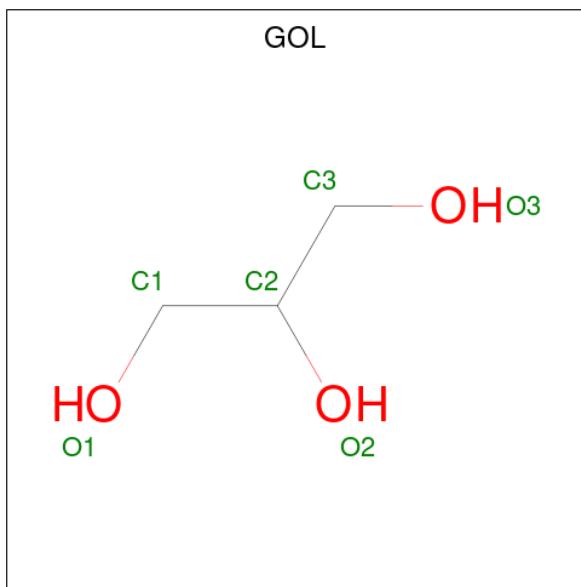
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C N O 10 6 1 3	0	0
2	F	1	Total C N O 10 6 1 3	0	0
2	G	1	Total C N O 10 6 1 3	0	0
2	H	1	Total C N O 10 6 1 3	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	C	1	Total C O 16 10 6	0	0
3	E	1	Total C O 16 10 6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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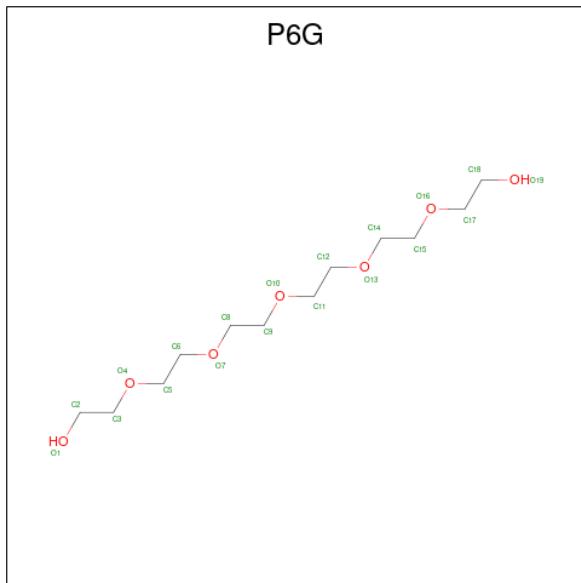
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0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

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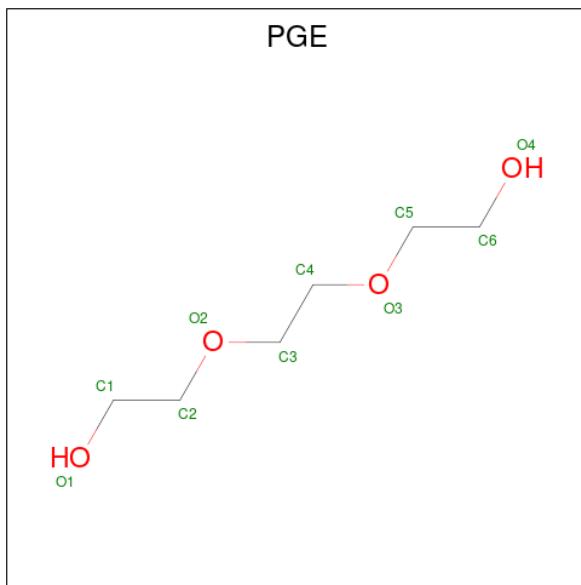
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).

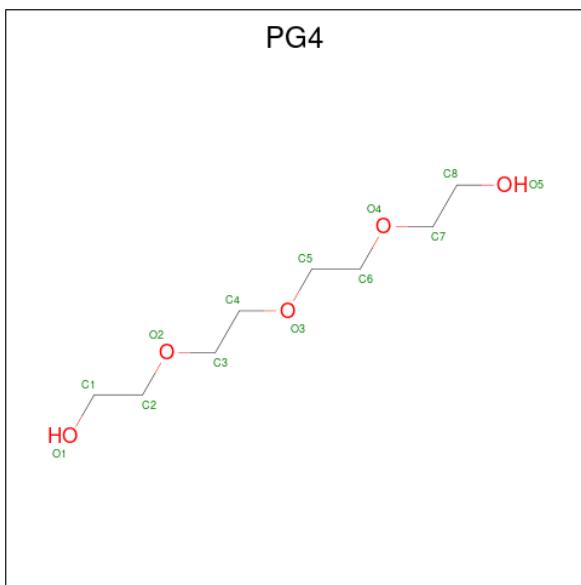


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0
6	F	1	Total C O 10 6 4	0	0
6	G	1	Total C O 10 6 4	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

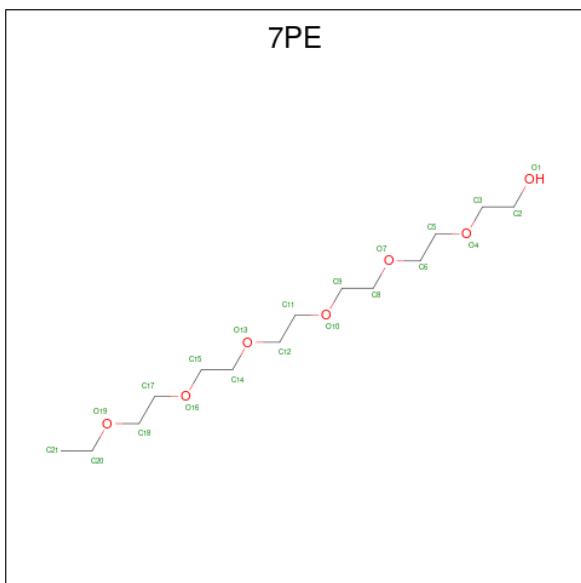
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	D	2	Total Ca 2 2	0	0
7	E	1	Total Ca 1 1	0	0
7	G	1	Total Ca 1 1	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



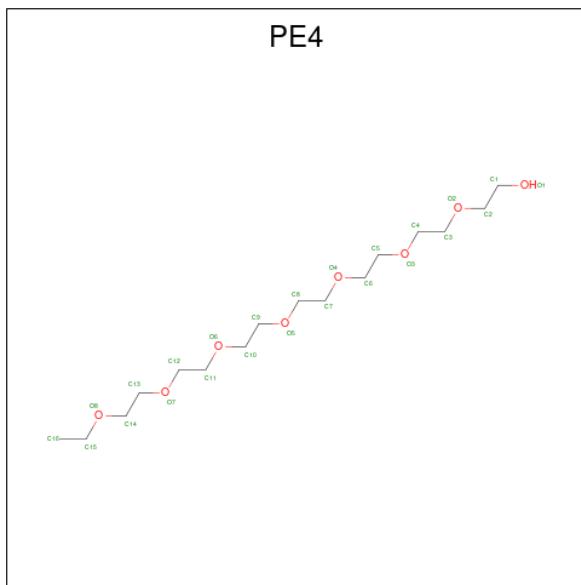
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 13 8 5	0	0
8	D	1	Total C O 13 8 5	0	0
8	F	1	Total C O 13 8 5	0	0
8	H	1	Total C O 13 8 5	0	0

- Molecule 9 is 2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (three-letter code: 7PE) (formula: C₁₄H₃₀O₇).



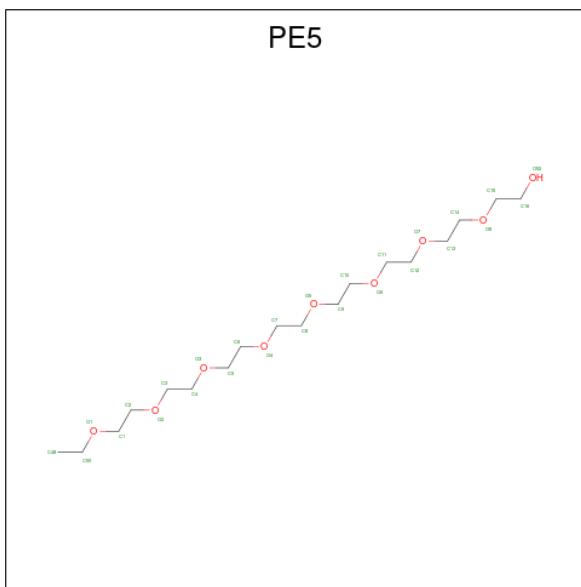
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 21 14 7	0	0
9	D	1	Total C O 21 14 7	0	0

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 24 16 8	0	0

- Molecule 11 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C₁₈H₃₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	H	1	27	18	9	0	0

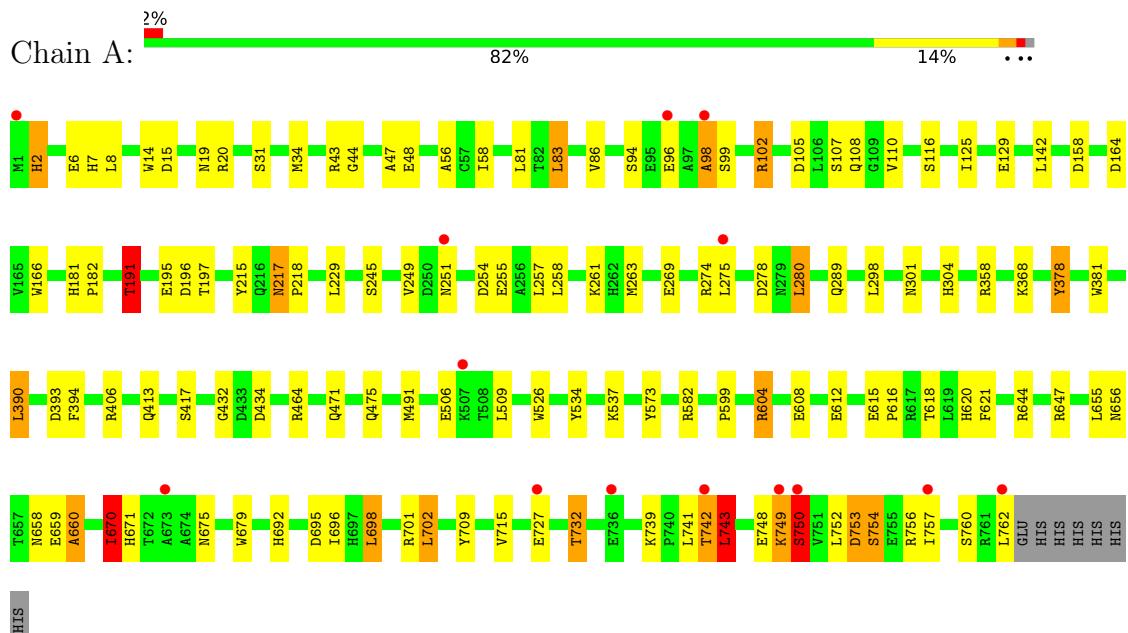
- Molecule 12 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
12	A	182	182	182		0	0
12	B	303	303	303		0	0
12	C	286	286	286		0	0
12	D	348	348	348		0	0
12	E	185	185	185		0	0
12	F	247	247	247		0	0
12	G	197	197	197		0	0
12	H	218	218	218		0	0

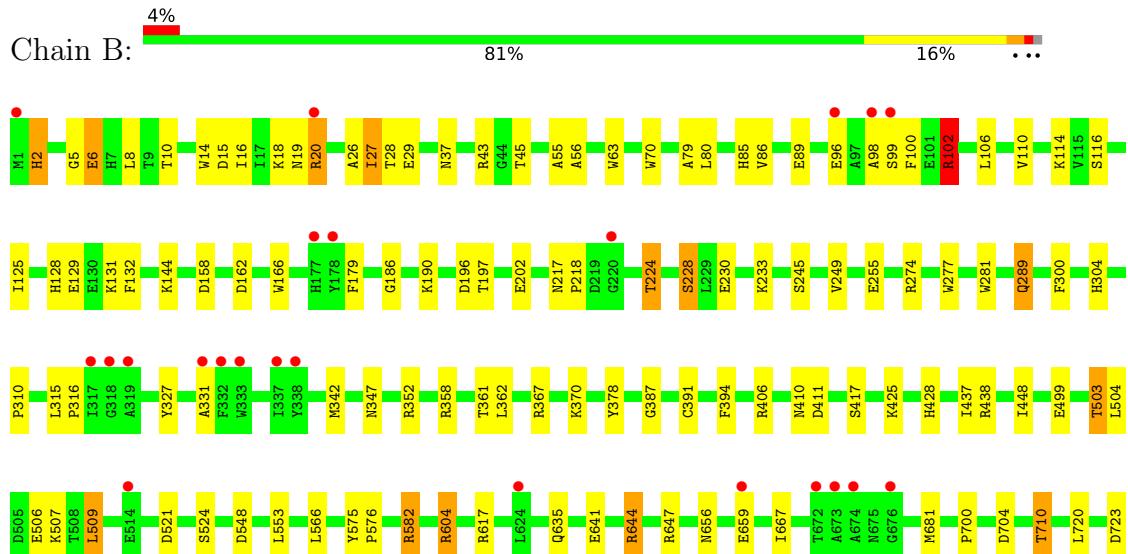
3 Residue-property plots

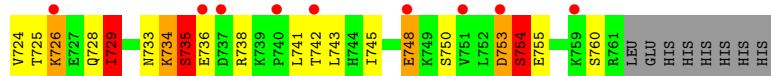
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycoside hydrolase family 65 central catalytic

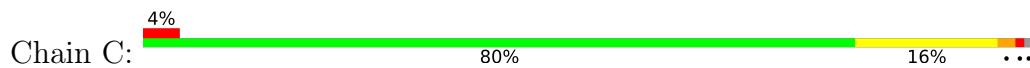


- Molecule 1: Glycoside hydrolase family 65 central catalytic

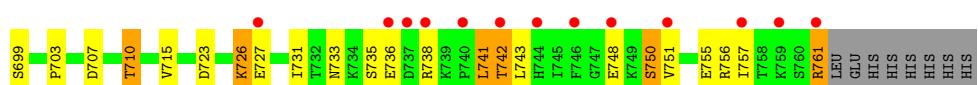




- Molecule 1: Glycoside hydrolase family 65 central catalytic

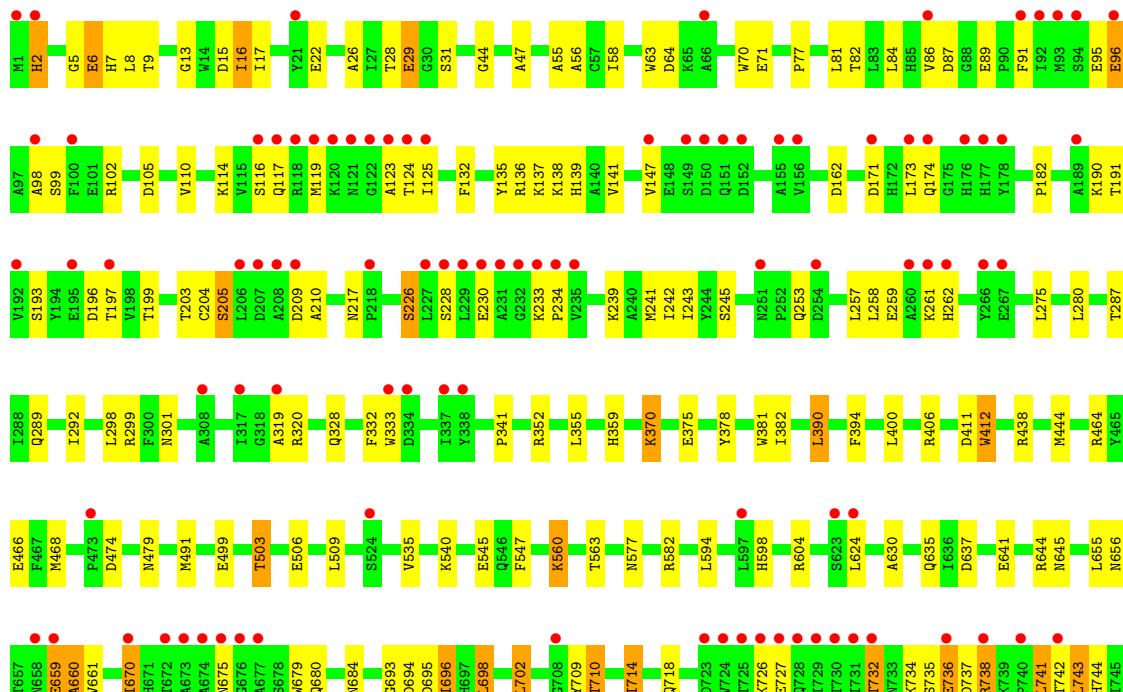


- Molecule 1: Glycoside hydrolase family 65 central catalytic

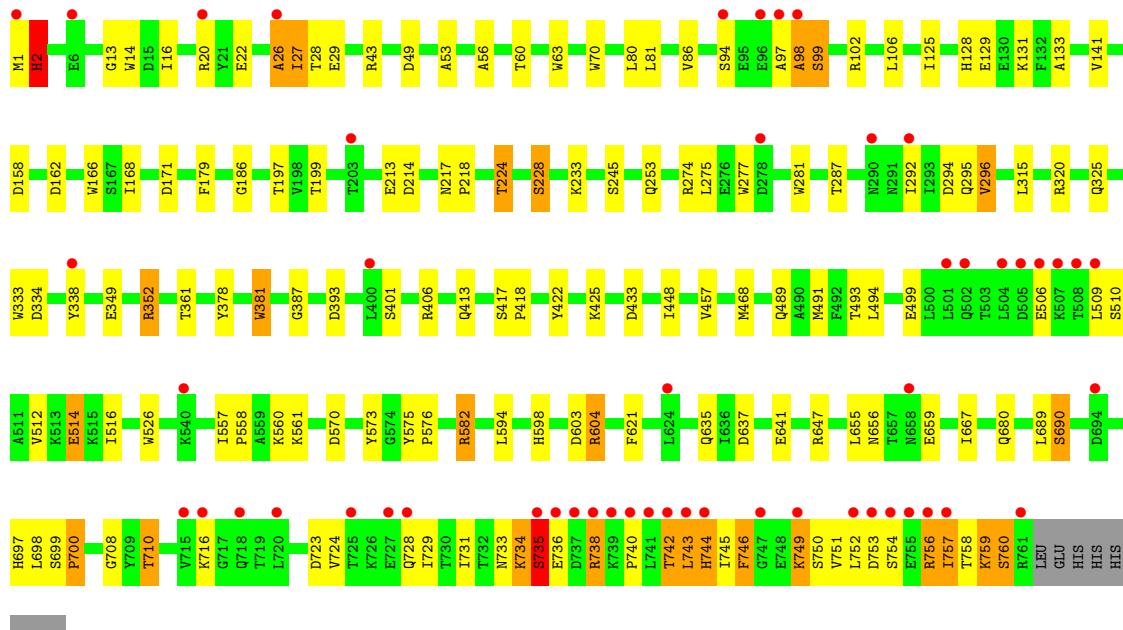
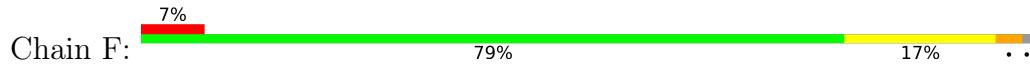


- Molecule 1: Glycoside hydrolase family 65 central catalytic

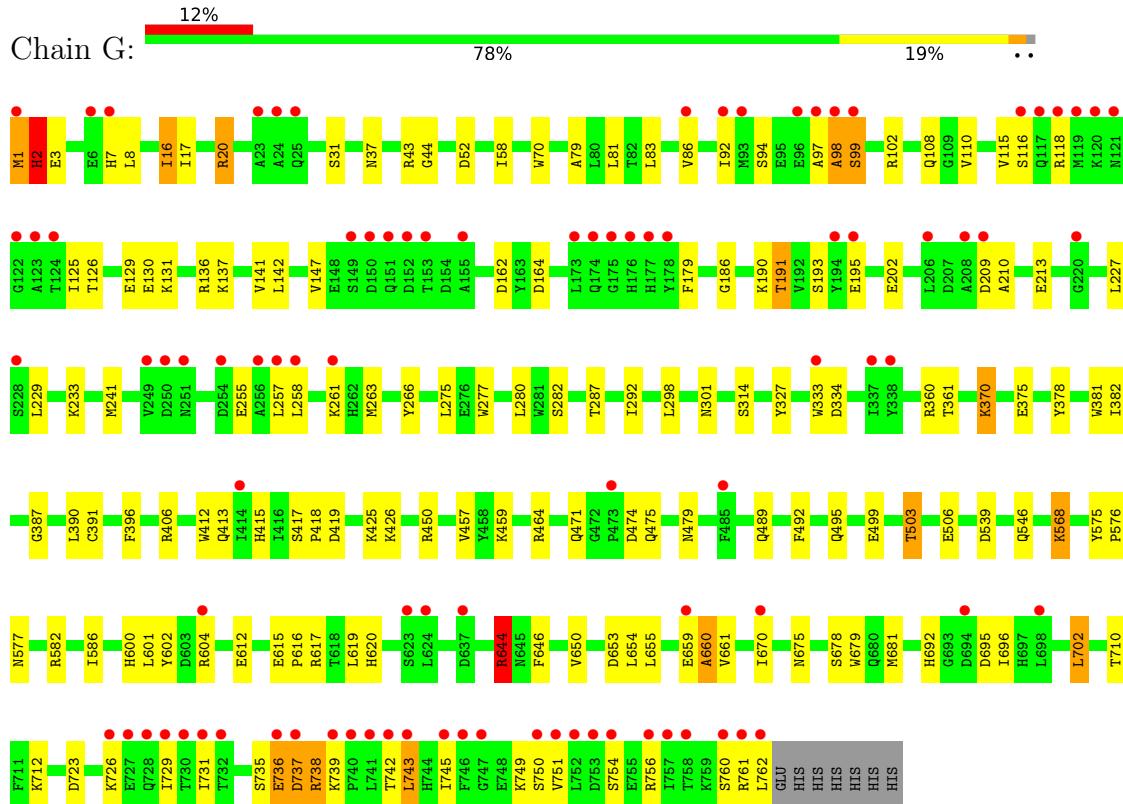




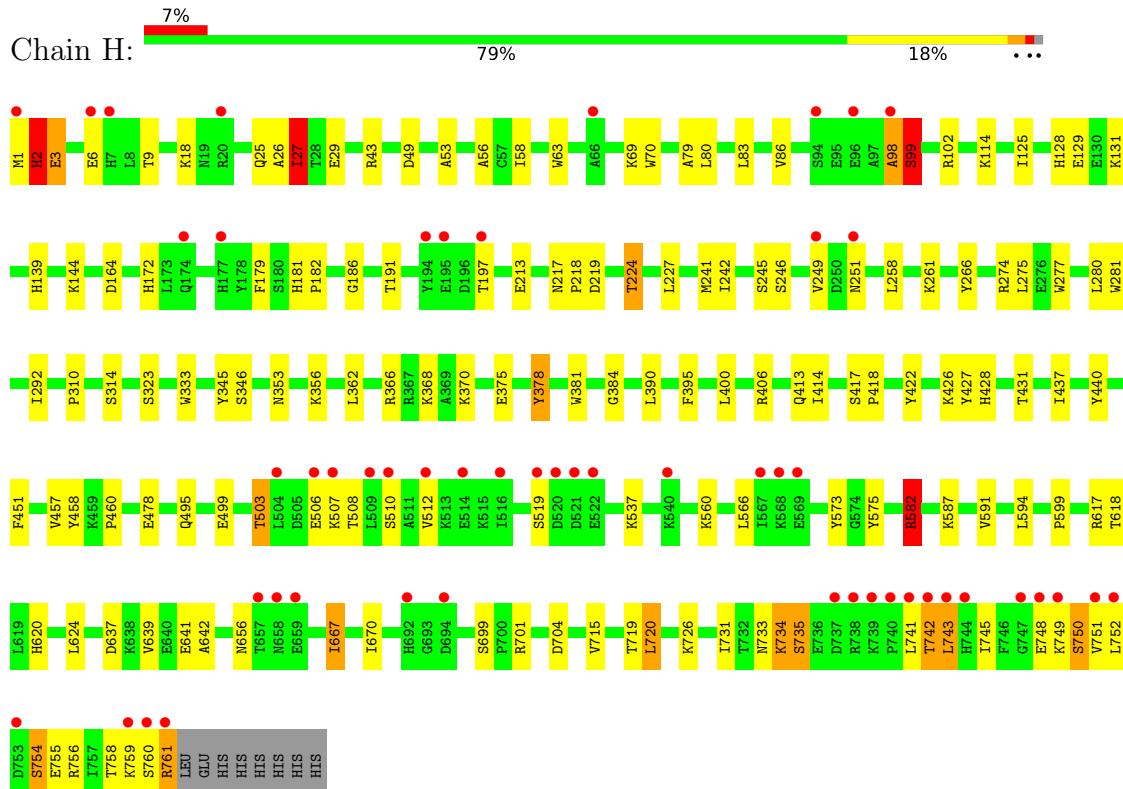
- Molecule 1: Glycoside hydrolase family 65 central catalytic



- Molecule 1: Glycoside hydrolase family 65 central catalytic



- Molecule 1: Glycoside hydrolase family 65 central catalytic



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.00Å 263.21Å 138.79Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	48.99 – 2.30 48.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.99-2.30) 99.8 (48.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ ¹	2.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R , R_{free}	0.167 , 0.228 0.168 , 0.230	Depositor DCC
R_{free} test set	16702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.6	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51264	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGE, PE5, GOL, IFM, CA, P6G, 7PE, PG4, 1PE, PE4

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	0.99	6/6236 (0.1%)	0.98	14/8456 (0.2%)
1	B	0.97	8/6228 (0.1%)	0.99	26/8445 (0.3%)
1	C	0.99	3/6228 (0.0%)	0.99	20/8445 (0.2%)
1	D	1.01	5/6228 (0.1%)	1.00	21/8445 (0.2%)
1	E	0.85	6/6228 (0.1%)	0.90	15/8445 (0.2%)
1	F	0.87	9/6228 (0.1%)	0.91	4/8445 (0.0%)
1	G	0.83	4/6236 (0.1%)	0.88	8/8456 (0.1%)
1	H	0.84	3/6228 (0.0%)	0.87	4/8445 (0.0%)
All	All	0.92	44/49840 (0.1%)	0.94	112/67582 (0.2%)

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	2
1	C	0	2
1	F	0	1
1	G	0	1
All	All	0	6

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	TRP	CD2-CE2	7.43	1.50	1.41
1	B	754	SER	CB-OG	6.83	1.51	1.42
1	E	70	TRP	CD2-CE2	6.81	1.49	1.41
1	F	333	TRP	CD2-CE2	6.40	1.49	1.41
1	F	63	TRP	CD2-CE2	6.39	1.49	1.41

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ARG	NE-CZ-NH2	12.77	126.69	120.30
1	D	102	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	A	670	ILE	CG1-CB-CG2	-11.80	85.43	111.40
1	E	438	ARG	NE-CZ-NH1	-9.91	115.35	120.30
1	B	644	ARG	NE-CZ-NH1	9.13	124.86	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	HIS	Peptide
1	A	748	GLU	Peptide
1	C	1	MET	Peptide
1	C	694	ASP	Peptide
1	F	26	ALA	Peptide

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	6093	0	5855	81	0
1	B	6085	0	5844	94	0
1	C	6085	0	5844	88	0
1	D	6085	0	5844	76	0
1	E	6085	0	5844	108	0
1	F	6085	0	5844	113	0
1	G	6093	0	5855	96	0
1	H	6085	0	5844	104	0
2	A	10	0	13	4	0
2	D	10	0	12	3	0
2	E	10	0	13	0	0
2	F	10	0	13	2	0
2	G	10	0	13	3	0
2	H	10	0	13	1	0
3	A	16	0	22	0	0
3	C	16	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	16	0	22	2	0
4	A	48	0	64	12	0
4	B	36	0	47	9	0
4	C	36	0	48	2	0
4	D	54	0	72	14	0
4	E	24	0	32	1	0
4	F	18	0	24	2	0
4	G	18	0	24	4	0
4	H	30	0	40	10	0
5	A	19	0	26	3	0
5	E	19	0	26	5	0
6	A	10	0	14	7	0
6	C	10	0	14	0	0
6	F	10	0	14	2	0
6	G	10	0	14	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	B	13	0	18	1	0
8	D	13	0	18	1	0
8	F	13	0	18	0	0
8	H	13	0	18	1	0
9	B	21	0	30	5	0
9	D	21	0	30	3	0
10	C	24	0	34	6	0
11	H	27	0	38	12	0
12	A	182	0	0	8	0
12	B	303	0	0	8	0
12	C	286	0	0	10	0
12	D	348	0	0	11	0
12	E	185	0	0	8	0
12	F	247	0	0	13	0
12	G	197	0	0	3	0
12	H	218	0	0	7	0
All	All	51264	0	47580	765	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 8.

The worst 5 of 765 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)
2:D:801:IFM:H2C2	12:D:1243:HOH:O	1.38	1.23
2:A:801:IFM:H2C2	12:A:917:HOH:O	1.35	1.21
1:B:352:ARG:HD3	12:B:1019:HOH:O	1.45	1.17
1:A:278:ASP:HB3	12:A:1031:HOH:O	1.45	1.14
1:F:756:ARG:HH11	1:F:756:ARG:HG3	1.09	1.12

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	760/769 (99%)	721 (95%)	29 (4%)	10 (1%)	12 12
1	B	759/769 (99%)	720 (95%)	33 (4%)	6 (1%)	19 23
1	C	759/769 (99%)	728 (96%)	25 (3%)	6 (1%)	19 23
1	D	759/769 (99%)	723 (95%)	34 (4%)	2 (0%)	41 50
1	E	759/769 (99%)	696 (92%)	48 (6%)	15 (2%)	7 6
1	F	759/769 (99%)	701 (92%)	44 (6%)	14 (2%)	8 7
1	G	760/769 (99%)	718 (94%)	31 (4%)	11 (1%)	11 11
1	H	759/769 (99%)	715 (94%)	35 (5%)	9 (1%)	13 14
All	All	6074/6152 (99%)	5722 (94%)	279 (5%)	73 (1%)	13 14

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	THR
1	A	750	SER
1	A	754	SER
1	B	6	GLU
1	B	27	ILE

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	651/658 (99%)	616 (95%)	35 (5%)	22 30
1	B	650/658 (99%)	615 (95%)	35 (5%)	22 30
1	C	650/658 (99%)	609 (94%)	41 (6%)	18 24
1	D	650/658 (99%)	615 (95%)	35 (5%)	22 30
1	E	650/658 (99%)	598 (92%)	52 (8%)	12 15
1	F	650/658 (99%)	609 (94%)	41 (6%)	18 24
1	G	651/658 (99%)	600 (92%)	51 (8%)	12 16
1	H	650/658 (99%)	616 (95%)	34 (5%)	23 32
All	All	5202/5264 (99%)	4878 (94%)	324 (6%)	18 25

5 of 324 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	736	GLU
1	G	750	SER
1	F	759	LYS
1	G	275	LEU
1	H	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	7	HIS
1	G	475	GLN
1	H	680	GLN
1	H	7	HIS
1	C	429	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 74 ligands modelled in this entry, 7 are monoatomic - leaving 67 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GOL	E	804	-	5,5,5	0.21	0	5,5,5	0.67	0
4	GOL	A	811	-	5,5,5	0.45	0	5,5,5	1.21	0
4	GOL	C	809	-	5,5,5	0.60	0	5,5,5	2.29	1 (20%)
10	PE4	C	805	-	23,23,23	0.91	0	22,22,22	1.33	2 (9%)
2	IFM	E	801	-	9,10,10	1.51	2 (22%)	9,13,13	3.09	4 (44%)
4	GOL	B	807	-	5,5,5	0.59	0	5,5,5	0.89	0
8	PG4	F	803	-	12,12,12	0.54	0	11,11,11	0.48	0
4	GOL	F	805	-	5,5,5	0.65	0	5,5,5	0.66	0
4	GOL	D	807	-	5,5,5	0.32	0	5,5,5	0.53	0
4	GOL	H	806	-	5,5,5	0.49	0	5,5,5	1.03	0
9	7PE	B	802	-	20,20,20	0.61	0	19,19,19	0.99	1 (5%)
4	GOL	G	804	-	5,5,5	0.33	0	5,5,5	0.55	0
4	GOL	A	807	-	5,5,5	0.57	0	5,5,5	1.10	0
4	GOL	A	804	-	5,5,5	0.80	0	5,5,5	2.09	2 (40%)
2	IFM	H	801	-	9,10,10	1.27	2 (22%)	9,13,13	3.81	4 (44%)
4	GOL	H	805	-	5,5,5	0.43	0	5,5,5	1.00	1 (20%)
4	GOL	G	802	-	5,5,5	0.19	0	5,5,5	0.78	0
5	P6G	E	803	-	18,18,18	0.66	0	17,17,17	0.79	0
4	GOL	B	808	-	5,5,5	0.55	0	5,5,5	1.91	1 (20%)
4	GOL	D	811	-	5,5,5	0.35	0	5,5,5	0.29	0
8	PG4	B	801	-	12,12,12	0.57	0	11,11,11	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	H	804	-	5,5,5	0.36	0	5,5,5	0.61	0
4	GOL	H	802	-	5,5,5	0.31	0	5,5,5	0.53	0
4	GOL	B	803	-	5,5,5	0.55	0	5,5,5	1.70	2 (40%)
4	GOL	D	804	-	5,5,5	0.35	0	5,5,5	0.45	0
4	GOL	D	809	-	5,5,5	0.37	0	5,5,5	1.35	1 (20%)
4	GOL	D	806	-	5,5,5	0.75	0	5,5,5	1.08	0
4	GOL	H	807	-	5,5,5	0.44	0	5,5,5	0.64	0
9	7PE	D	808	-	20,20,20	0.73	0	19,19,19	1.43	3 (15%)
4	GOL	C	808	-	5,5,5	0.48	0	5,5,5	0.66	0
4	GOL	G	803	-	5,5,5	0.20	0	5,5,5	0.77	0
4	GOL	E	805	-	5,5,5	0.42	0	5,5,5	0.21	0
2	IFM	D	801	-	9,10,10	2.40	5 (55%)	9,13,13	3.56	6 (66%)
4	GOL	C	806	-	5,5,5	0.64	0	5,5,5	0.75	0
6	PGE	F	806	-	9,9,9	0.50	0	8,8,8	0.48	0
3	1PE	A	802	-	15,15,15	0.72	0	14,14,14	0.71	0
4	GOL	B	804	-	5,5,5	0.72	0	5,5,5	1.56	2 (40%)
5	P6G	A	806	-	18,18,18	0.59	0	17,17,17	0.83	0
4	GOL	E	806	-	5,5,5	0.51	0	5,5,5	0.78	0
4	GOL	E	807	-	5,5,5	0.22	0	5,5,5	0.93	0
4	GOL	D	802	-	5,5,5	0.49	0	5,5,5	0.76	0
3	1PE	C	801	-	15,15,15	0.65	0	14,14,14	0.96	0
8	PG4	H	803	-	12,12,12	0.68	0	11,11,11	0.48	0
4	GOL	A	810	-	5,5,5	0.56	0	5,5,5	0.85	0
6	PGE	A	812	-	9,9,9	0.56	0	8,8,8	0.45	0
8	PG4	D	803	-	12,12,12	0.60	0	11,11,11	0.62	0
4	GOL	D	812	-	5,5,5	1.29	0	5,5,5	1.95	2 (40%)
11	PE5	H	808	-	26,26,26	0.77	0	25,25,25	0.90	0
4	GOL	C	802	-	5,5,5	0.52	0	5,5,5	0.36	0
4	GOL	C	803	-	5,5,5	0.22	0	5,5,5	1.24	1 (20%)
4	GOL	A	803	-	5,5,5	0.58	0	5,5,5	1.10	0
4	GOL	B	806	-	5,5,5	0.31	0	5,5,5	0.54	0
2	IFM	G	801	-	9,10,10	1.22	1 (11%)	9,13,13	3.17	5 (55%)
4	GOL	F	804	-	5,5,5	0.55	0	5,5,5	0.52	0
4	GOL	F	802	-	5,5,5	0.26	0	5,5,5	0.80	0
2	IFM	A	801	-	9,10,10	1.75	3 (33%)	9,13,13	3.85	3 (33%)
2	IFM	F	801	-	9,10,10	1.36	2 (22%)	9,13,13	3.26	3 (33%)
4	GOL	A	809	-	5,5,5	0.53	0	5,5,5	0.45	0
6	PGE	C	807	-	9,9,9	0.45	0	8,8,8	0.85	0
4	GOL	D	810	-	5,5,5	0.38	0	5,5,5	1.77	1 (20%)
4	GOL	D	805	-	5,5,5	0.08	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	805	-	5,5,5	0.26	0	5,5,5	0.67	0
4	GOL	A	808	-	5,5,5	0.44	0	5,5,5	0.72	0
6	PGE	G	805	-	9,9,9	0.71	0	8,8,8	0.60	0
3	1PE	E	802	-	15,15,15	0.70	0	14,14,14	0.40	0
4	GOL	C	804	-	5,5,5	0.42	0	5,5,5	1.25	1 (20%)
4	GOL	B	805	-	5,5,5	0.53	0	5,5,5	0.88	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
4	GOL	E	804	-	-	2/4/4/4	-
4	GOL	A	811	-	-	4/4/4/4	-
4	GOL	C	809	-	-	2/4/4/4	-
10	PE4	C	805	-	-	8/21/21/21	-
2	IFM	E	801	-	-	0/2/16/16	0/1/1/1
4	GOL	B	807	-	-	0/4/4/4	-
8	PG4	F	803	-	-	8/10/10/10	-
4	GOL	F	805	-	-	2/4/4/4	-
4	GOL	D	807	-	-	2/4/4/4	-
4	GOL	H	806	-	-	0/4/4/4	-
9	7PE	B	802	-	-	8/18/18/18	-
4	GOL	G	804	-	-	0/4/4/4	-
4	GOL	A	807	-	-	4/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-
2	IFM	H	801	-	-	0/2/16/16	1/1/1/1
4	GOL	H	805	-	-	2/4/4/4	-
4	GOL	G	802	-	-	2/4/4/4	-
5	P6G	E	803	-	-	10/16/16/16	-
4	GOL	B	808	-	-	3/4/4/4	-
4	GOL	D	811	-	-	4/4/4/4	-
8	PG4	B	801	-	-	3/10/10/10	-
4	GOL	H	804	-	-	4/4/4/4	-
4	GOL	H	802	-	-	0/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	D	804	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	809	-	-	3/4/4/4	-
4	GOL	D	806	-	-	3/4/4/4	-
4	GOL	H	807	-	-	4/4/4/4	-
9	7PE	D	808	-	-	4/18/18/18	-
4	GOL	C	808	-	-	0/4/4/4	-
4	GOL	G	803	-	-	3/4/4/4	-
4	GOL	E	805	-	-	2/4/4/4	-
2	IFM	D	801	-	-	0/2/16/16	0/1/1/1
4	GOL	C	806	-	-	0/4/4/4	-
6	PGE	F	806	-	-	4/7/7/7	-
3	1PE	A	802	-	-	9/13/13/13	-
4	GOL	B	804	-	-	4/4/4/4	-
5	P6G	A	806	-	-	11/16/16/16	-
4	GOL	E	806	-	-	1/4/4/4	-
4	GOL	E	807	-	-	2/4/4/4	-
4	GOL	D	802	-	-	2/4/4/4	-
3	1PE	C	801	-	-	5/13/13/13	-
8	PG4	H	803	-	-	6/10/10/10	-
4	GOL	A	810	-	-	1/4/4/4	-
6	PGE	A	812	-	-	4/7/7/7	-
8	PG4	D	803	-	-	4/10/10/10	-
4	GOL	D	812	-	-	0/4/4/4	-
11	PE5	H	808	-	-	21/24/24/24	-
4	GOL	C	802	-	-	0/4/4/4	-
4	GOL	C	803	-	-	0/4/4/4	-
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-
2	IFM	G	801	-	-	0/2/16/16	0/1/1/1
4	GOL	F	804	-	-	2/4/4/4	-
4	GOL	F	802	-	-	2/4/4/4	-
2	IFM	A	801	-	-	1/2/16/16	0/1/1/1
2	IFM	F	801	-	-	0/2/16/16	1/1/1/1
4	GOL	A	809	-	-	2/4/4/4	-
6	PGE	C	807	-	-	3/7/7/7	-
4	GOL	D	810	-	-	4/4/4/4	-
4	GOL	D	805	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	805	-	-	4/4/4/4	-
4	GOL	A	808	-	-	4/4/4/4	-
6	PGE	G	805	-	-	4/7/7/7	-
3	1PE	E	802	-	-	9/13/13/13	-
4	GOL	C	804	-	-	2/4/4/4	-
4	GOL	B	805	-	-	3/4/4/4	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	IFM	C2-N	-3.71	1.41	1.46
2	A	801	IFM	C5-C4	-3.20	1.49	1.53
2	D	801	IFM	C5-C4	-3.10	1.49	1.53
2	D	801	IFM	O4-C4	-3.04	1.35	1.43
2	E	801	IFM	C3-C4	2.80	1.56	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	IFM	C1-N-C2	9.07	121.66	111.70
2	F	801	IFM	C1-N-C2	8.43	120.96	111.70
2	A	801	IFM	C1-N-C2	8.10	120.59	111.70
2	D	801	IFM	O4-C4-C5	-7.59	97.27	110.08
2	G	801	IFM	C1-N-C2	7.34	119.75	111.70

There are no chirality outliers.

5 of 217 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	808	GOL	O1-C1-C2-C3
4	A	808	GOL	C1-C2-C3-O3
4	A	809	GOL	O1-C1-C2-O2
4	A	809	GOL	O1-C1-C2-C3
4	A	811	GOL	C1-C2-C3-O3

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	801	IFM	C1-C2-C3-C4-C5-N
2	H	801	IFM	C1-C2-C3-C4-C5-N

46 monomers are involved in 114 short contacts:

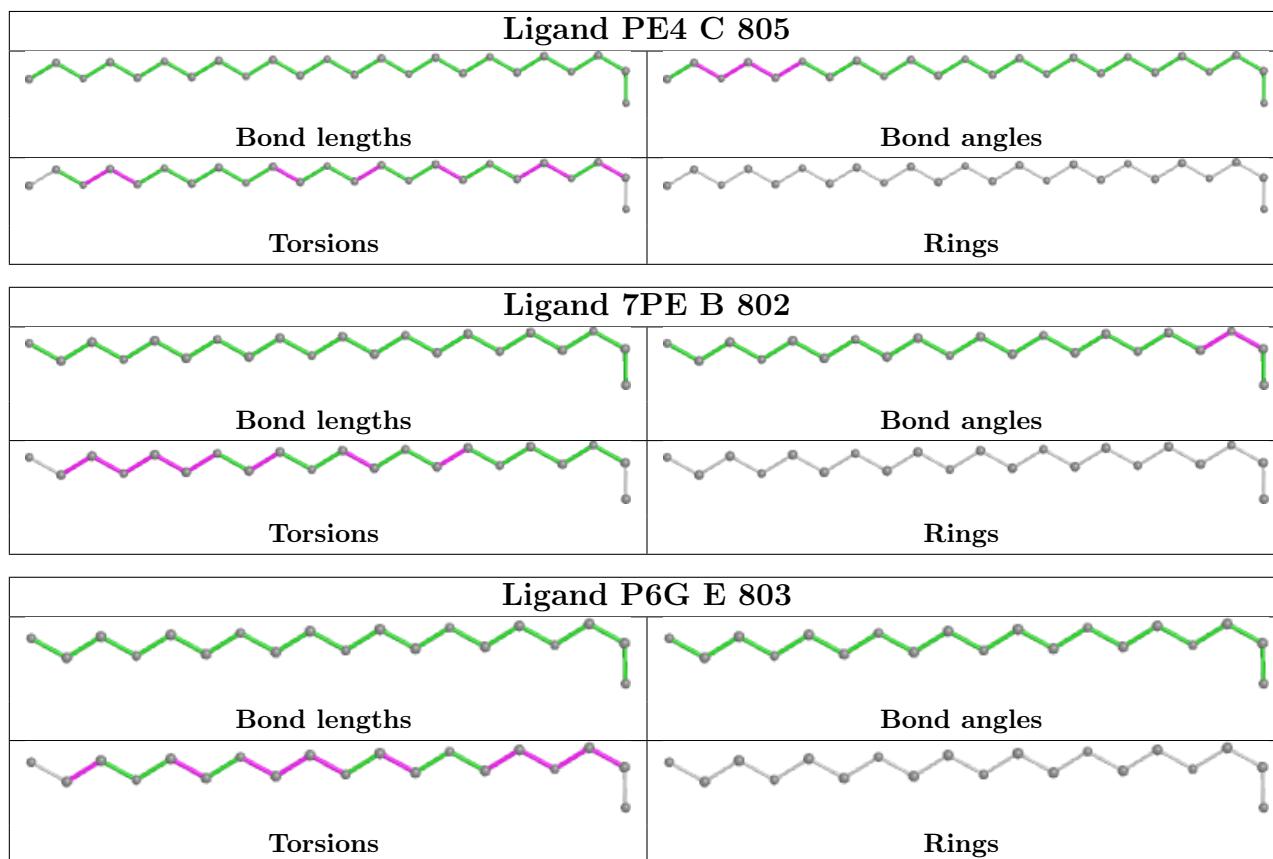
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	811	GOL	2	0
4	C	809	GOL	1	0
10	C	805	PE4	6	0
4	B	807	GOL	1	0
4	F	805	GOL	1	0
4	D	807	GOL	1	0
9	B	802	7PE	5	0
2	H	801	IFM	1	0
4	H	805	GOL	2	0
4	G	802	GOL	2	0
5	E	803	P6G	5	0
4	B	808	GOL	1	0
8	B	801	PG4	1	0
4	H	804	GOL	2	0
4	H	802	GOL	2	0
4	B	803	GOL	2	0
4	D	804	GOL	2	0
4	D	809	GOL	4	0
4	D	806	GOL	2	0
4	H	807	GOL	4	0
9	D	808	7PE	3	0
4	G	803	GOL	2	0
4	E	805	GOL	1	0
2	D	801	IFM	3	0
4	C	806	GOL	1	0
6	F	806	PGE	2	0
4	B	804	GOL	4	0
5	A	806	P6G	3	0
4	D	802	GOL	1	0
3	C	801	1PE	1	0
8	H	803	PG4	1	0
6	A	812	PGE	7	0
8	D	803	PG4	1	0
4	D	812	GOL	2	0
11	H	808	PE5	12	0
4	A	803	GOL	3	0
2	G	801	IFM	3	0
4	F	802	GOL	1	0
2	A	801	IFM	4	0
2	F	801	IFM	2	0
4	A	809	GOL	1	0
4	D	805	GOL	2	0

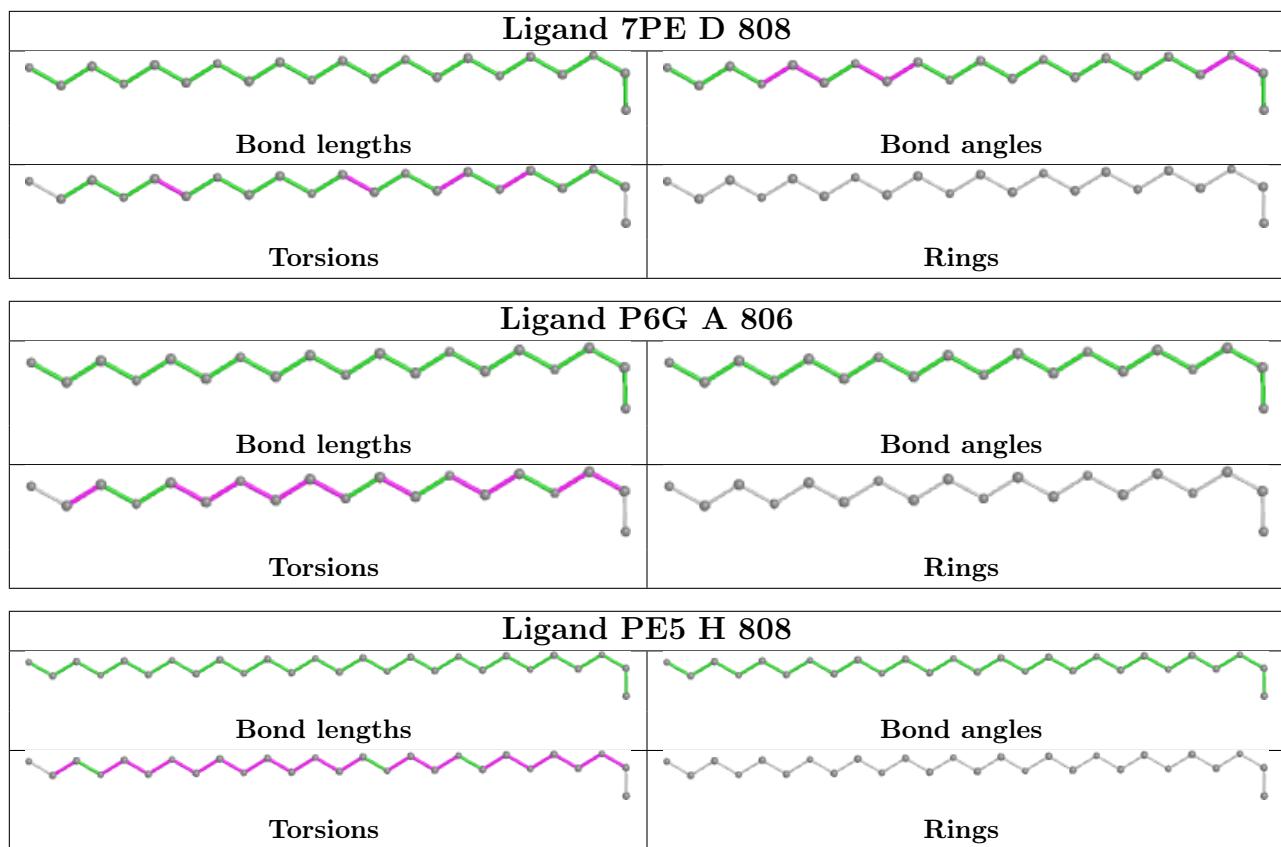
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	GOL	3	0
4	A	808	GOL	3	0
3	E	802	1PE	2	0
4	B	805	GOL	1	0

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 than 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.





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	762/769 (99%)	0.04	14 (1%) 68 74	30, 40, 65, 98	0
1	B	761/769 (98%)	0.22	32 (4%) 36 43	28, 40, 64, 97	0
1	C	761/769 (98%)	0.18	28 (3%) 41 48	28, 40, 64, 99	0
1	D	761/769 (98%)	0.13	29 (3%) 40 47	28, 39, 68, 97	0
1	E	761/769 (98%)	0.68	108 (14%) 2 3	35, 53, 101, 142	0
1	F	761/769 (98%)	0.33	52 (6%) 17 22	32, 49, 86, 131	0
1	G	762/769 (99%)	0.56	91 (11%) 4 6	38, 52, 83, 110	0
1	H	761/769 (98%)	0.32	53 (6%) 16 21	37, 50, 85, 115	0
All	All	6090/6152 (98%)	0.31	407 (6%) 17 23	28, 46, 80, 142	0

The worst 5 of 407 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ALA	12.3
1	G	98	ALA	9.7
1	H	751	VAL	8.4
1	E	753	ASP	7.9
1	F	754	SER	7.4

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.

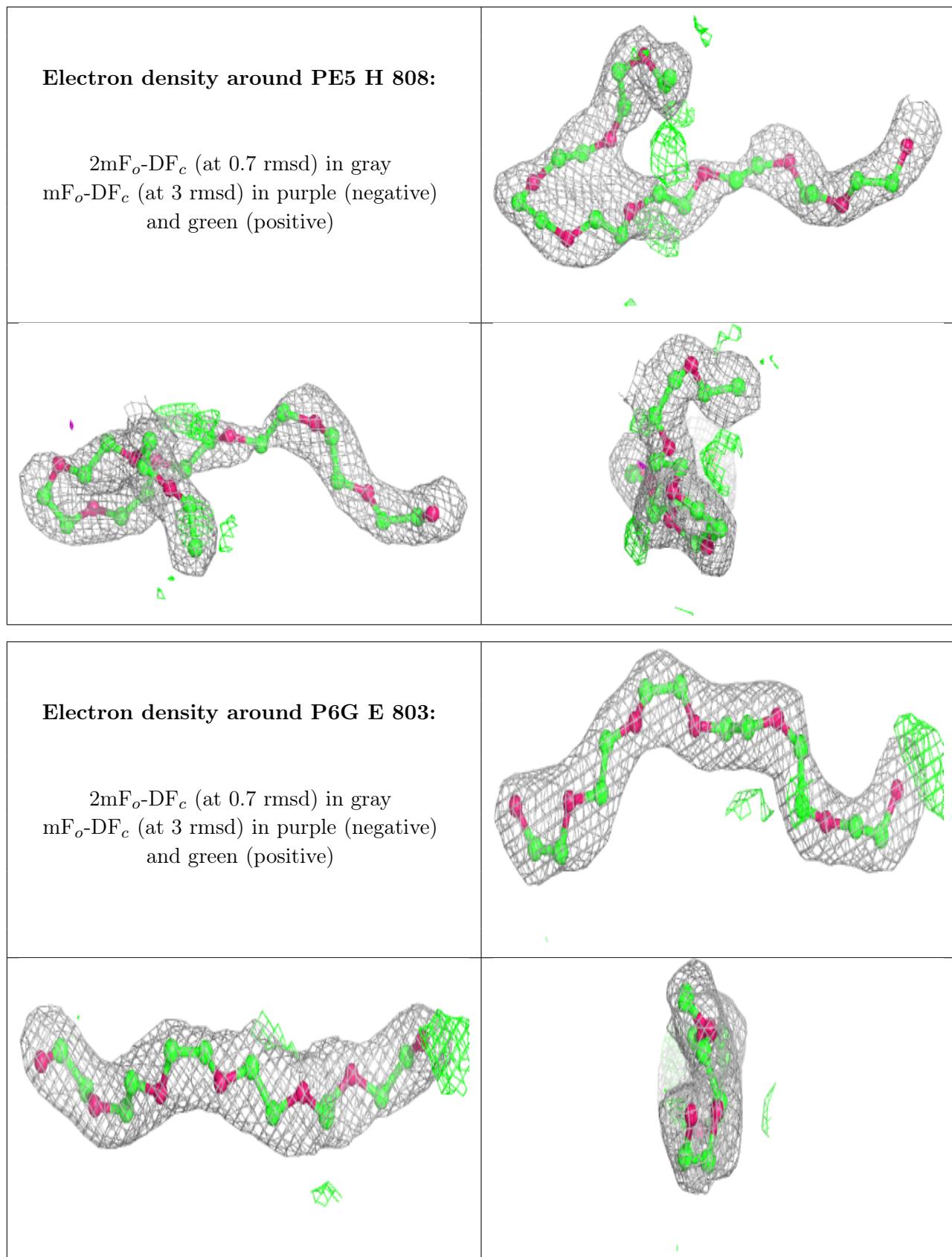
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	806	6/6	0.66	0.24	64,77,87,89	0
4	GOL	H	807	6/6	0.70	0.17	70,70,73,76	0
4	GOL	B	805	6/6	0.74	0.24	59,73,75,75	0
4	GOL	A	807	6/6	0.80	0.19	57,59,72,79	0
4	GOL	D	806	6/6	0.82	0.12	56,64,67,71	0
4	GOL	G	803	6/6	0.82	0.10	65,76,86,86	0
4	GOL	H	806	6/6	0.82	0.15	48,62,65,73	0
4	GOL	A	809	6/6	0.82	0.14	58,66,67,73	0
4	GOL	F	805	6/6	0.83	0.15	39,62,67,70	0
2	IFM	G	801	10/10	0.83	0.38	55,79,87,98	0
6	PGE	G	805	10/10	0.83	0.23	54,66,73,78	0
3	1PE	E	802	16/16	0.84	0.23	62,75,101,104	0
11	PE5	H	808	27/27	0.85	0.22	53,72,84,96	0
2	IFM	E	801	10/10	0.86	0.35	44,59,71,73	0
8	PG4	H	803	13/13	0.86	0.18	57,68,83,88	0
4	GOL	B	807	6/6	0.86	0.22	59,65,74,82	0
4	GOL	A	808	6/6	0.87	0.19	59,61,66,85	0
8	PG4	D	803	13/13	0.87	0.17	48,65,75,77	0
5	P6G	E	803	19/19	0.88	0.30	52,67,71,73	0
3	1PE	A	802	16/16	0.88	0.23	50,62,83,101	0
4	GOL	D	805	6/6	0.88	0.14	63,64,69,70	0
3	1PE	C	801	16/16	0.88	0.16	44,61,79,82	0
4	GOL	E	805	6/6	0.88	0.18	63,77,85,87	0
4	GOL	D	811	6/6	0.89	0.13	49,56,61,71	0
6	PGE	A	812	10/10	0.89	0.22	40,51,58,60	0
2	IFM	H	801	10/10	0.89	0.25	56,70,75,82	0
2	IFM	F	801	10/10	0.90	0.28	49,56,65,72	0
4	GOL	D	807	6/6	0.90	0.19	55,64,71,72	0
4	GOL	G	804	6/6	0.91	0.21	68,68,70,72	0
4	GOL	B	806	6/6	0.91	0.23	57,64,70,77	0
4	GOL	A	803	6/6	0.91	0.28	46,60,72,75	0
6	PGE	F	806	10/10	0.92	0.24	62,65,71,74	0
6	PGE	C	807	10/10	0.93	0.15	42,51,57,59	0
2	IFM	A	801	10/10	0.93	0.22	38,51,60,62	0
4	GOL	G	802	6/6	0.93	0.38	52,64,71,76	0
8	PG4	B	801	13/13	0.93	0.18	46,57,87,88	0
5	P6G	A	806	19/19	0.93	0.21	41,49,64,70	0

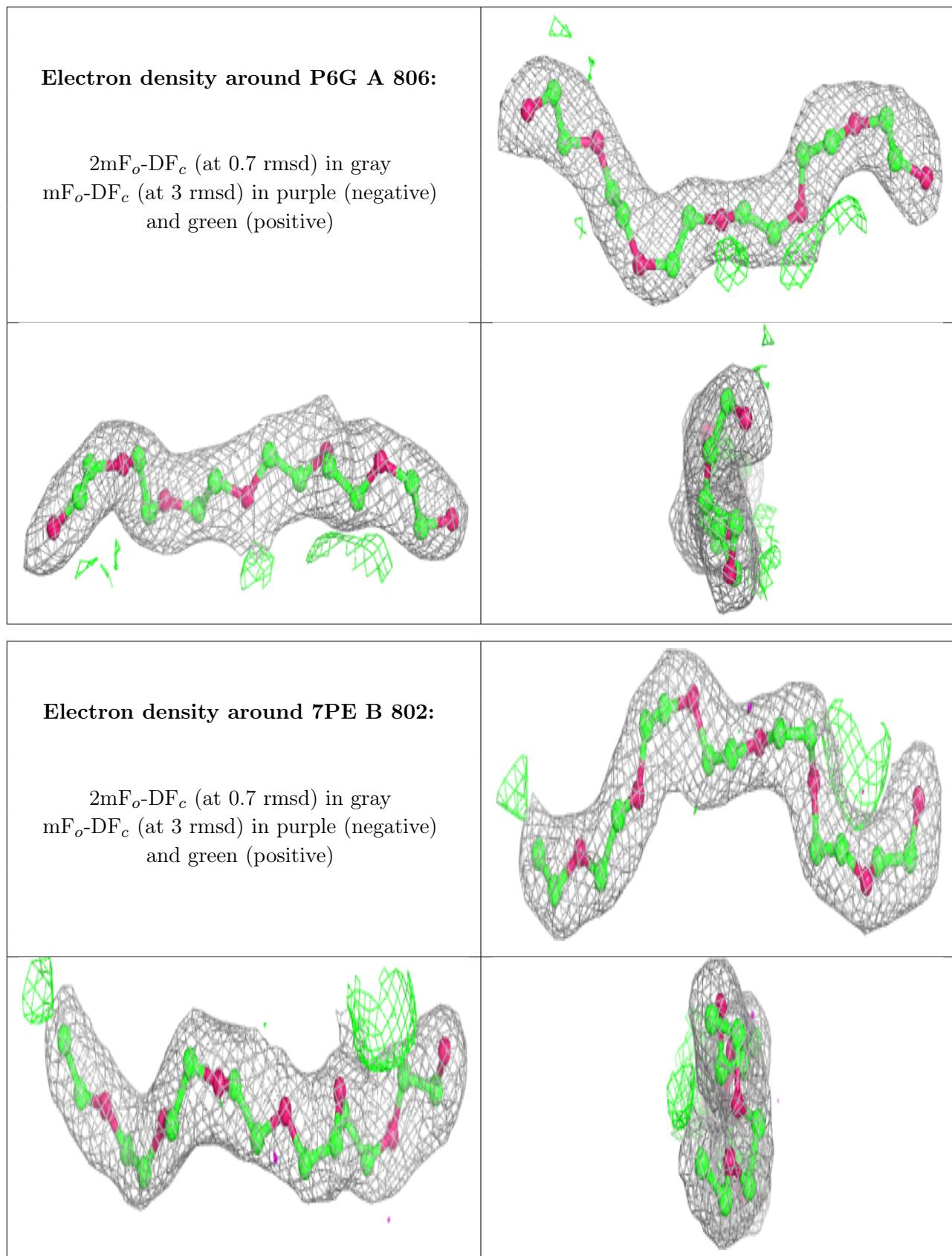
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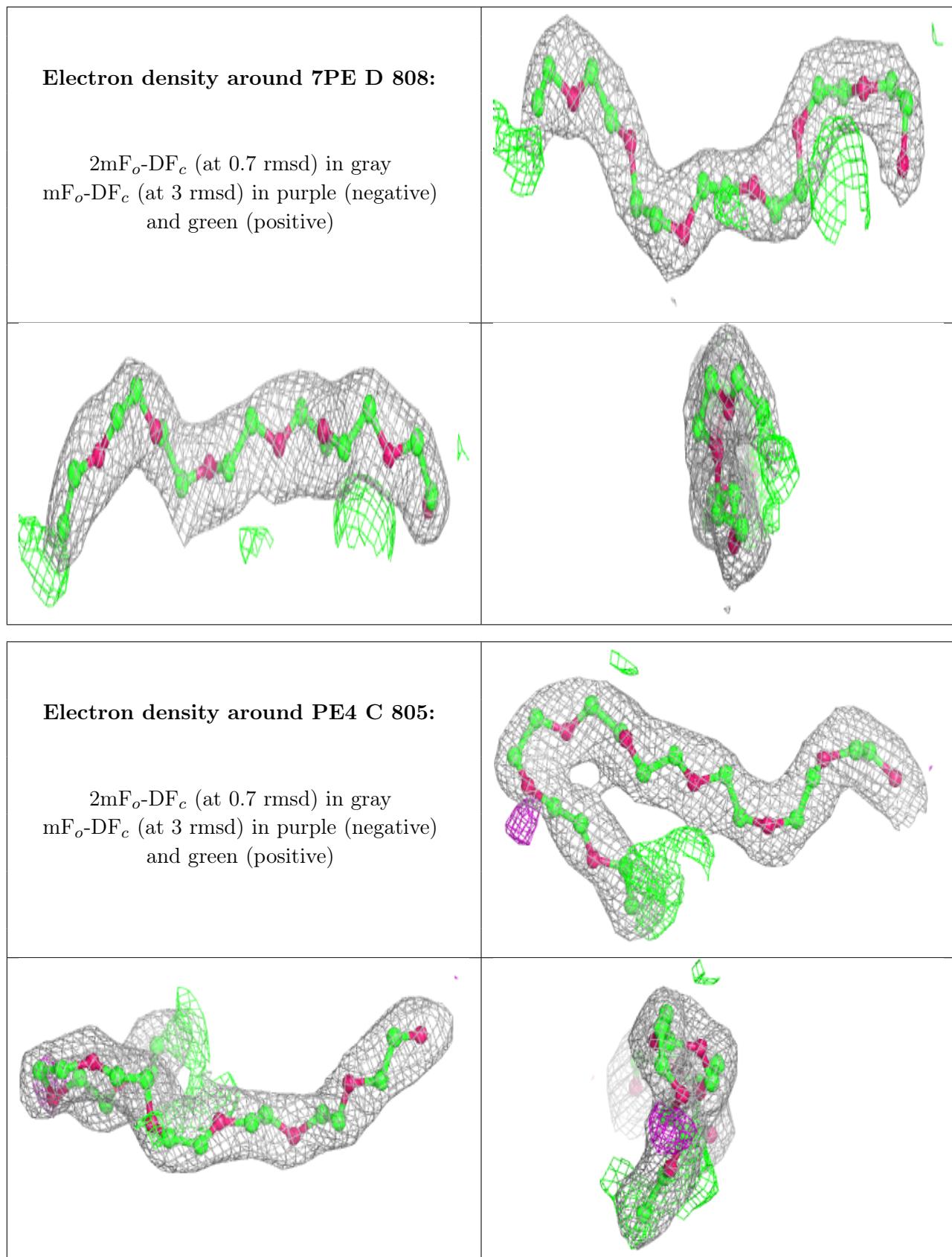
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PG4	F	803	13/13	0.93	0.16	56,62,75,77	0
4	GOL	E	804	6/6	0.93	0.19	54,59,62,63	0
4	GOL	A	805	6/6	0.93	0.09	57,64,74,75	0
4	GOL	D	812	6/6	0.94	0.23	32,38,40,45	0
4	GOL	F	802	6/6	0.94	0.25	52,58,61,65	0
7	CA	G	806	1/1	0.94	0.11	55,55,55,55	0
9	7PE	B	802	21/21	0.94	0.22	36,45,52,55	0
9	7PE	D	808	21/21	0.94	0.17	41,48,54,59	0
10	PE4	C	805	24/24	0.94	0.27	39,48,59,68	0
4	GOL	H	802	6/6	0.94	0.24	58,73,84,85	0
4	GOL	B	804	6/6	0.95	0.20	33,35,40,47	0
4	GOL	H	804	6/6	0.95	0.17	46,52,57,61	0
4	GOL	H	805	6/6	0.95	0.20	51,52,59,60	0
4	GOL	E	806	6/6	0.95	0.17	46,47,50,54	0
2	IFM	D	801	10/10	0.95	0.21	35,44,50,63	0
4	GOL	F	804	6/6	0.95	0.20	47,48,50,53	0
4	GOL	D	809	6/6	0.95	0.16	45,54,57,60	0
4	GOL	C	809	6/6	0.95	0.21	37,42,49,52	0
4	GOL	D	804	6/6	0.95	0.18	47,54,57,62	0
4	GOL	A	804	6/6	0.95	0.18	42,43,46,52	0
4	GOL	C	802	6/6	0.96	0.16	43,57,62,73	0
4	GOL	D	802	6/6	0.96	0.33	50,58,60,62	0
7	CA	D	813	1/1	0.96	0.04	54,54,54,54	0
4	GOL	C	804	6/6	0.96	0.24	43,46,53,57	0
4	GOL	B	808	6/6	0.96	0.28	36,43,46,48	0
4	GOL	E	807	6/6	0.96	0.20	43,53,60,60	0
4	GOL	B	803	6/6	0.97	0.16	35,41,44,46	0
4	GOL	A	811	6/6	0.97	0.14	45,50,51,51	0
7	CA	D	814	1/1	0.97	0.16	45,45,45,45	0
4	GOL	C	803	6/6	0.98	0.13	45,48,52,59	0
4	GOL	C	808	6/6	0.98	0.14	35,38,39,42	0
4	GOL	A	810	6/6	0.98	0.14	37,37,39,40	0
7	CA	A	813	1/1	0.98	0.10	44,44,44,44	0
4	GOL	D	810	6/6	0.98	0.21	33,37,40,41	0
7	CA	E	808	1/1	0.99	0.11	54,54,54,54	0
7	CA	C	810	1/1	0.99	0.13	36,36,36,36	0
7	CA	B	809	1/1	1.00	0.12	43,43,43,43	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.







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

There are no such residues in this entry.