



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:16 am BST

PDB ID : 6OQA  
Title : Crystal structure of CEP250 bound to FKBP12 in the presence of FK506-like novel natural product  
Authors : Lee, S.-J.; Shigdel, U.K.; Townson, S.A.; Verdine, G.L.  
Deposited on : 2019-04-26  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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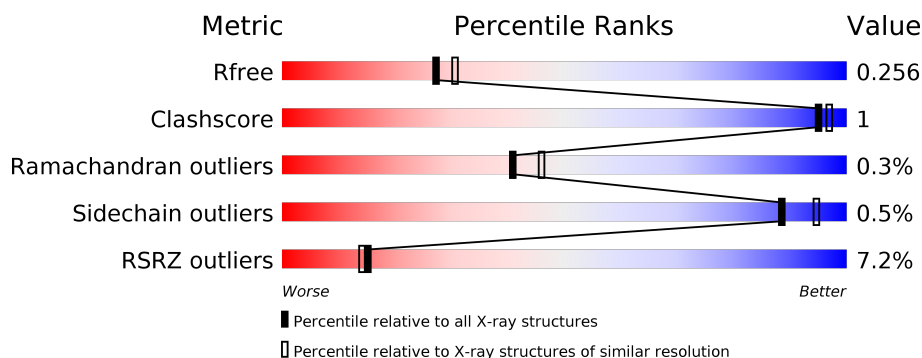
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

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## X-RAY DIFFRACTION

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
R <sub>free</sub>	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	<div> <div></div> <div>99%</div> <div>.</div> </div>
1	B	108	<div> <div></div> <div>96%</div> <div>..</div> </div>
1	E	108	<div> <div>5%</div> <div>97%</div> <div>..</div> </div>
1	F	108	<div> <div>16%</div> <div>94%</div> <div>5% ..</div> </div>
2	C	98	<div> <div>6%</div> <div>81%</div> <div>. 15%</div> </div>
2	D	98	<div> <div>9%</div> <div>82%</div> <div>. 15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	98	<div><div></div><div>7%</div><div>86%</div><div>11%</div></div>
2	H	98	<div><div></div><div>9%</div><div>83%</div><div>13%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6829 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.

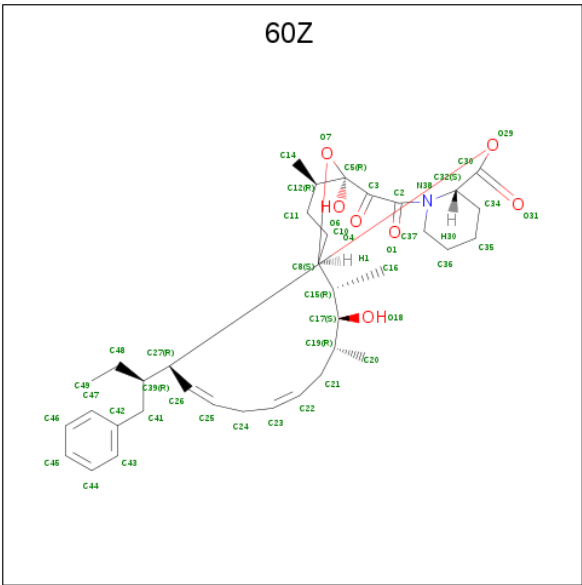
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	1	0
			851	538	151	157	5			
1	B	107	Total	C	N	O	S	7	0	0
			832	527	146	155	4			
1	E	107	Total	C	N	O	S	8	1	0
			843	533	150	156	4			
1	F	107	Total	C	N	O	S	22	0	0
			832	527	146	155	4			

- Molecule 2 is a protein called Centrosome-associated protein CEP250.

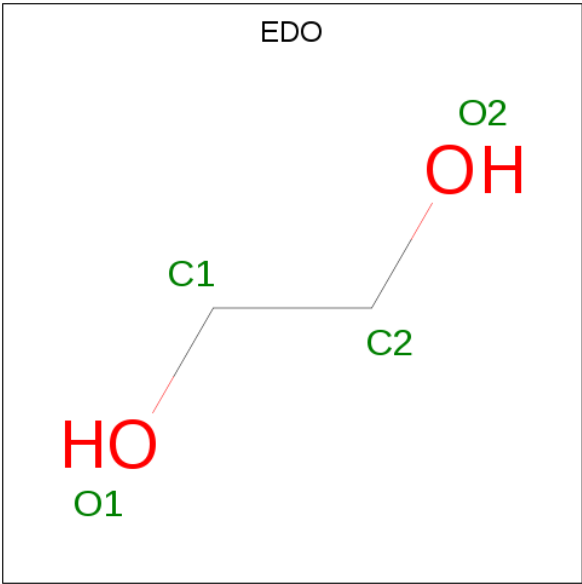
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	83	Total	C	N	O	S	7	0	0
			685	418	132	134	1			
2	D	83	Total	C	N	O	S	29	0	0
			685	418	132	134	1			
2	G	87	Total	C	N	O	S	43	0	0
			716	436	136	143	1			
2	H	85	Total	C	N	O	S	9	0	0
			702	429	134	138	1			

- Molecule 3 is (3R,4E,7E,10R,11S,12R,13S,16R,17R,24aS)-11,17-dihydroxy-10,12,16-trimethyl-3-[(2R)-1-phenylbutan-2-yl]-6,9,10,11,12,13,14,15,16,17,22,23,24,24a-tetradecahydro-3H-13,17-epoxypyrido[2,1-c][1,4]oxazacyclohenicosine-1,18,19(21H)-trione (three-letter code: 60Z) (formula: C<sub>36</sub>H<sub>51</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			44	36	1	7		
3	B	1	Total	C	N	O	0	0
			44	36	1	7		
3	E	1	Total	C	N	O	0	0
			44	36	1	7		
3	F	1	Total	C	N	O	0	0
			44	36	1	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



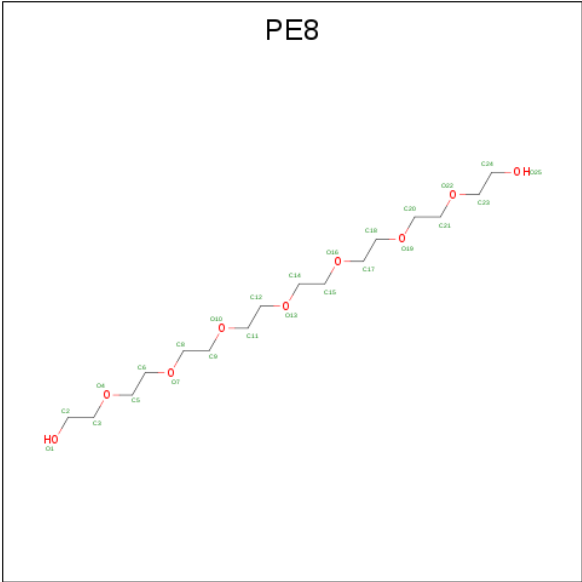
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

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



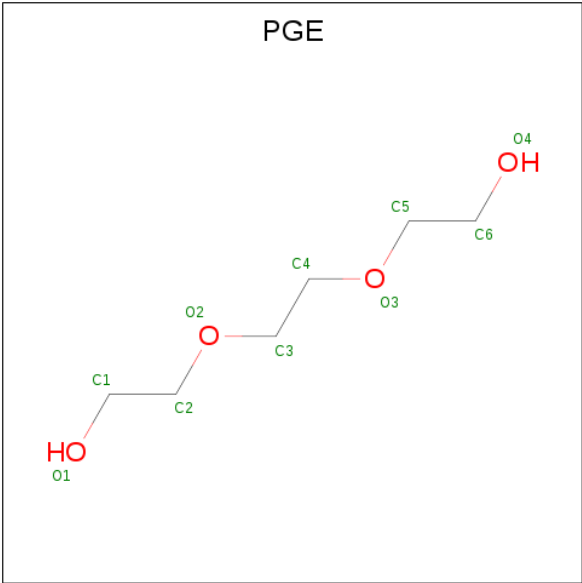
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total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

- Molecule 6 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula:  $C_{16}H_{34}O_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			25	16	9		
6	B	1	Total	C	O	0	0
			22	14	8		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

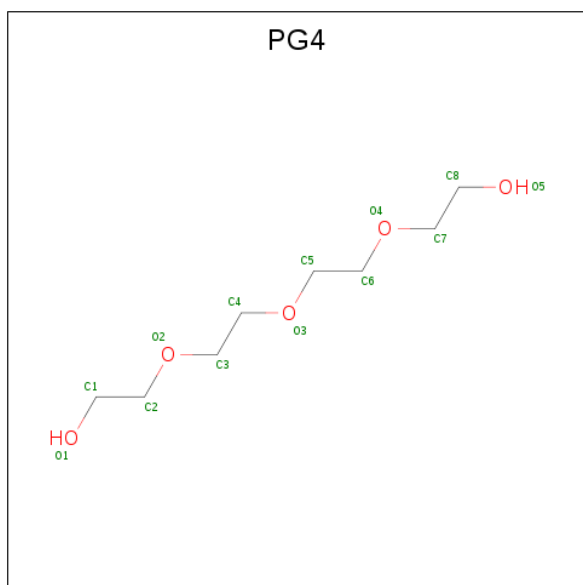
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).

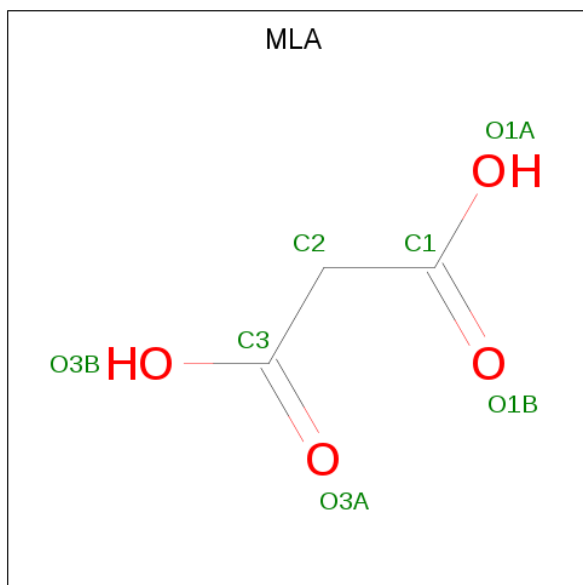


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	8	5		
8	C	1	Total	C	O	0	0
			13	8	5		
8	C	1	Total	C	O	0	0
			13	8	5		
8	G	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is MALONIC ACID (three-letter code: MLA) (formula:  $C_3H_4O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			7	3	4		

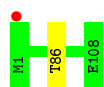
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	70	Total	O	0	0
			70	70		
11	B	64	Total	O	0	0
			64	64		
11	C	27	Total	O	0	0
			27	27		
11	D	26	Total	O	0	0
			26	26		
11	E	4	Total	O	0	0
			4	4		
11	F	5	Total	O	0	0
			5	5		
11	G	16	Total	O	0	0
			16	16		
11	H	14	Total	O	0	0
			14	14		

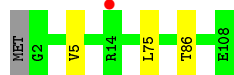
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Peptidyl-prolyl cis-trans isomerase FKBP1A



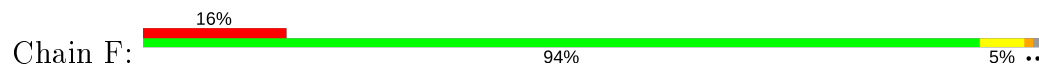
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



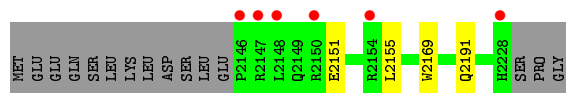
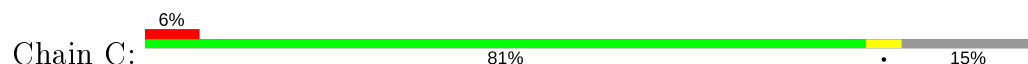
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



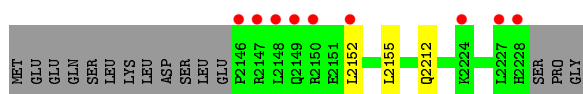
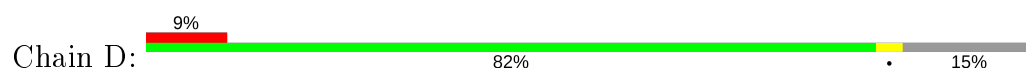
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



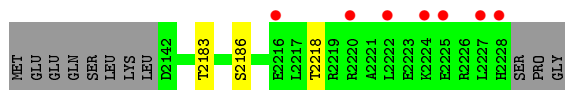
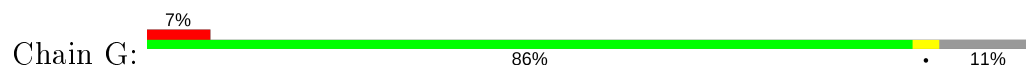
- Molecule 2: Centrosome-associated protein CEP250



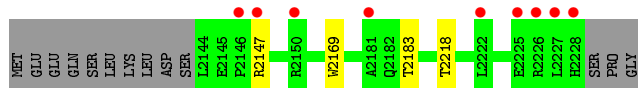
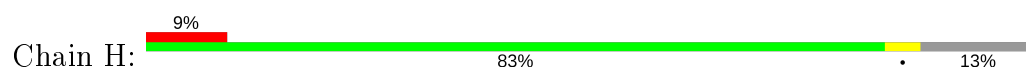
- Molecule 2: Centrosome-associated protein CEP250



- Molecule 2: Centrosome-associated protein CEP250



- Molecule 2: Centrosome-associated protein CEP250



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.83Å 64.95Å 136.06Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	136.05 – 2.20 30.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (136.05-2.20) 98.6 (30.42-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.256 0.211 , 0.256	Depositor DCC
$R_{free}$ test set	2726 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PGE, PE8, EDO, 60Z, PG4, MLA, 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	0.49	0/870	0.61	0/1170
1	B	0.50	0/851	0.63	0/1146
1	E	0.46	0/862	0.55	0/1160
1	F	0.48	0/851	0.59	0/1146
2	C	0.51	1/689 (0.1%)	0.62	0/922
2	D	0.49	0/689	0.60	0/922
2	G	0.46	0/720	0.59	0/965
2	H	0.48	1/706 (0.1%)	0.61	0/946
All	All	0.48	2/6238 (0.0%)	0.60	0/8377

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2169	TRP	CD2-CE2	5.41	1.47	1.41
2	C	2169	TRP	CD2-CE2	5.35	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	851	0	852	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	832	0	828	4	0
1	E	843	0	840	1	0
1	F	832	0	828	3	0
2	C	685	0	698	3	0
2	D	685	0	698	5	0
2	G	716	0	723	2	0
2	H	702	0	714	2	0
3	A	44	0	0	0	0
3	B	44	0	0	0	0
3	E	44	0	0	0	0
3	F	44	0	0	1	0
4	A	12	0	18	0	0
4	B	28	0	42	0	0
4	C	4	0	6	0	0
4	D	8	0	12	0	0
4	E	8	0	12	0	0
4	G	4	0	6	0	0
5	A	7	0	10	0	0
5	B	21	0	30	1	0
5	C	7	0	10	0	0
5	D	14	0	20	0	0
5	F	7	0	10	0	0
5	G	7	0	10	0	0
5	H	7	0	10	0	0
6	A	25	0	34	0	0
6	B	22	0	29	1	0
7	B	10	0	14	0	0
7	C	10	0	14	0	0
7	D	10	0	14	2	0
7	G	10	0	14	0	0
8	C	39	0	54	0	0
8	G	13	0	18	0	0
9	D	1	0	0	0	0
10	H	7	0	2	0	0
11	A	70	0	0	1	0
11	B	64	0	0	0	0
11	C	27	0	0	0	0
11	D	26	0	0	0	0
11	E	4	0	0	0	0
11	F	5	0	0	0	0
11	G	16	0	0	0	0
11	H	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6829	0	6570	16	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 1.

All (16) 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:G:2218:THR:HG22	2:H:2218:THR:HG22	1.82	0.61
1:B:5:VAL:HG22	1:B:75:LEU:CD2	2.37	0.55
2:G:2183:THR:HG22	2:H:2183:THR:HG22	1.90	0.53
2:D:2212:GLN:HE22	7:D:2306:PGE:C2	2.22	0.53
2:D:2212:GLN:HE22	7:D:2306:PGE:H22	1.75	0.51
1:B:86:THR:HG21	6:B:212:PE8:H211	1.93	0.51
2:C:2151:GLU:HG2	2:D:2152:LEU:HD11	1.94	0.49
1:B:5:VAL:HG22	1:B:75:LEU:HD22	1.95	0.48
1:A:86:THR:HG22	11:A:354:HOH:O	2.14	0.46
2:C:2151:GLU:CG	2:D:2152:LEU:HD11	2.48	0.44
1:F:17:PRO:HB2	1:F:51:LEU:HD12	2.00	0.43
1:F:77:ILE:HG22	1:F:82:ALA:HB2	2.01	0.42
2:C:2155:LEU:HB3	2:D:2155:LEU:HD23	2.00	0.42
1:E:25:VAL:HG12	1:E:104:LEU:HA	2.01	0.42
1:F:57:ILE:HG23	3:F:201:60Z:O31	2.20	0.41
1:B:86:THR:HG23	5:B:210:PEG:H11	2.02	0.41

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	107/108 (99%)	104 (97%)	3 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	E	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
1	F	105/108 (97%)	98 (93%)	5 (5%)	2 (2%)	8	5
2	C	81/98 (83%)	80 (99%)	1 (1%)	0	100	100
2	D	81/98 (83%)	81 (100%)	0	0	100	100
2	G	85/98 (87%)	85 (100%)	0	0	100	100
2	H	83/98 (85%)	83 (100%)	0	0	100	100
All	All	753/824 (91%)	735 (98%)	16 (2%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	14	ARG
1	F	82	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/90 (101%)	91 (100%)	0	100	100
1	B	89/90 (99%)	89 (100%)	0	100	100
1	E	90/90 (100%)	90 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
2	C	73/87 (84%)	72 (99%)	1 (1%)	67	80
2	D	73/87 (84%)	73 (100%)	0	100	100
2	G	77/87 (88%)	76 (99%)	1 (1%)	69	81
2	H	75/87 (86%)	74 (99%)	1 (1%)	69	81
All	All	657/708 (93%)	654 (100%)	3 (0%)	88	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	2191	GLN
2	G	2186	SER
2	H	2147	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	2191	GLN
2	H	2191	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 1 is monoatomic - leaving 41 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	$\# Z  > 2$
7	PGE	D	2306	9	9,9,9	0.44	0	8,8,8	0.48	0
8	PG4	C	2305	-	12,12,12	0.45	0	11,11,11	0.24	0
3	60Z	A	201	-	43,47,47	1.05	3 (6%)	48,66,66	1.93	10 (20%)
4	EDO	B	206	-	3,3,3	0.50	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	B	210	-	6,6,6	0.47	0	5,5,5	0.22	0
5	PEG	B	211	-	6,6,6	0.46	0	5,5,5	0.20	0
4	EDO	B	202	-	3,3,3	0.46	0	2,2,2	0.15	0
8	PG4	C	2304	-	12,12,12	0.50	0	11,11,11	0.16	0
10	MLA	H	2301	-	0,6,6	0.00	-	0,7,7	0.00	-
4	EDO	D	2303	-	3,3,3	0.52	0	2,2,2	0.20	0
3	60Z	E	201	-	43,47,47	0.98	3 (6%)	48,66,66	1.55	8 (16%)
6	PE8	B	212	-	21,21,24	0.46	0	20,20,23	0.30	0
5	PEG	C	2302	-	6,6,6	0.50	0	5,5,5	0.23	0
8	PG4	C	2303	-	12,12,12	0.41	0	11,11,11	0.45	0
5	PEG	H	2302	-	6,6,6	0.45	0	5,5,5	0.22	0
5	PEG	D	2305	-	6,6,6	0.48	0	5,5,5	0.15	0
5	PEG	A	205	-	6,6,6	0.51	0	5,5,5	0.18	0
3	60Z	B	201	-	43,47,47	0.99	3 (6%)	48,66,66	1.35	6 (12%)
7	PGE	B	213	-	9,9,9	0.48	0	8,8,8	0.23	0
4	EDO	A	202	-	3,3,3	0.54	0	2,2,2	0.25	0
4	EDO	A	203	-	3,3,3	0.51	0	2,2,2	0.24	0
5	PEG	B	209	-	6,6,6	0.54	0	5,5,5	0.32	0
4	EDO	B	205	-	3,3,3	0.50	0	2,2,2	0.28	0
8	PG4	G	2303	-	12,12,12	0.49	0	11,11,11	0.31	0
4	EDO	D	2302	-	3,3,3	0.54	0	2,2,2	0.22	0
4	EDO	B	203	-	3,3,3	0.48	0	2,2,2	0.28	0
4	EDO	A	204	-	3,3,3	0.49	0	2,2,2	0.16	0
6	PE8	A	206	-	24,24,24	0.48	0	23,23,23	0.52	0
5	PEG	G	2302	-	6,6,6	0.45	0	5,5,5	0.13	0
5	PEG	F	202	-	6,6,6	0.50	0	5,5,5	0.14	0
5	PEG	D	2304	-	6,6,6	0.47	0	5,5,5	0.25	0
4	EDO	E	203	-	3,3,3	0.48	0	2,2,2	0.21	0
7	PGE	C	2306	-	9,9,9	0.50	0	8,8,8	0.24	0
4	EDO	B	208	-	3,3,3	0.49	0	2,2,2	0.20	0
4	EDO	G	2301	-	3,3,3	0.47	0	2,2,2	0.24	0
7	PGE	G	2304	-	9,9,9	0.49	0	8,8,8	0.14	0
4	EDO	E	202	-	3,3,3	0.51	0	2,2,2	0.21	0
4	EDO	C	2301	-	3,3,3	0.52	0	2,2,2	0.13	0
4	EDO	B	207	-	3,3,3	0.50	0	2,2,2	0.21	0
3	60Z	F	201	-	43,47,47	0.90	3 (6%)	48,66,66	1.56	8 (16%)
4	EDO	B	204	-	3,3,3	0.50	0	2,2,2	0.25	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
7	PGE	D	2306	9	-	4/7/7/7	-
8	PG4	C	2305	-	-	1/10/10/10	-
3	60Z	A	201	-	-	3/50/80/80	0/3/4/4
4	EDO	B	206	-	-	1/1/1/1	-
5	PEG	B	210	-	-	1/4/4/4	-
5	PEG	B	211	-	-	1/4/4/4	-
4	EDO	B	202	-	-	0/1/1/1	-
8	PG4	C	2304	-	-	4/10/10/10	-
10	MLA	H	2301	-	-	0/0/4/4	-
4	EDO	D	2303	-	-	1/1/1/1	-
3	60Z	E	201	-	-	4/50/80/80	0/3/4/4
6	PE8	B	212	-	-	4/19/19/22	-
5	PEG	C	2302	-	-	1/4/4/4	-
8	PG4	C	2303	-	-	2/10/10/10	-
5	PEG	H	2302	-	-	0/4/4/4	-
5	PEG	D	2305	-	-	2/4/4/4	-
5	PEG	A	205	-	-	3/4/4/4	-
3	60Z	B	201	-	-	6/50/80/80	0/3/4/4
7	PGE	B	213	-	-	4/7/7/7	-
4	EDO	A	202	-	-	1/1/1/1	-
4	EDO	A	203	-	-	1/1/1/1	-
5	PEG	B	209	-	-	3/4/4/4	-
4	EDO	B	205	-	-	1/1/1/1	-
8	PG4	G	2303	-	-	3/10/10/10	-
4	EDO	D	2302	-	-	0/1/1/1	-
4	EDO	B	203	-	-	1/1/1/1	-
4	EDO	A	204	-	-	0/1/1/1	-
6	PE8	A	206	-	-	7/22/22/22	-
5	PEG	G	2302	-	-	0/4/4/4	-
5	PEG	F	202	-	-	1/4/4/4	-
5	PEG	D	2304	-	-	1/4/4/4	-
4	EDO	E	203	-	-	1/1/1/1	-
7	PGE	C	2306	-	-	4/7/7/7	-
4	EDO	B	208	-	-	0/1/1/1	-
4	EDO	G	2301	-	-	0/1/1/1	-
7	PGE	G	2304	-	-	0/7/7/7	-
4	EDO	E	202	-	-	0/1/1/1	-
4	EDO	C	2301	-	-	0/1/1/1	-
4	EDO	B	207	-	-	0/1/1/1	-
3	60Z	F	201	-	-	6/50/80/80	0/3/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	204	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	60Z	C2-C3	-4.33	1.48	1.53
3	A	201	60Z	C2-C3	-3.79	1.48	1.53
3	E	201	60Z	C2-C3	-3.26	1.49	1.53
3	E	201	60Z	C32-N38	3.25	1.51	1.47
3	F	201	60Z	C2-C3	-3.06	1.49	1.53
3	F	201	60Z	O6-C5	2.93	1.44	1.39
3	A	201	60Z	O6-C5	2.90	1.44	1.39
3	B	201	60Z	O6-C5	2.83	1.44	1.39
3	E	201	60Z	O6-C5	2.83	1.44	1.39
3	A	201	60Z	C32-N38	2.82	1.50	1.47
3	F	201	60Z	C32-N38	2.66	1.50	1.47
3	B	201	60Z	C32-N38	2.21	1.49	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	60Z	C34-C32-N38	-5.32	103.14	110.53
3	A	201	60Z	C3-C2-N38	5.02	124.99	119.25
3	A	201	60Z	C34-C32-C30	4.99	124.22	110.53
3	F	201	60Z	C34-C32-C30	4.77	123.62	110.53
3	E	201	60Z	C34-C32-C30	4.71	123.46	110.53
3	F	201	60Z	O29-C30-C32	4.39	120.45	110.78
3	A	201	60Z	O29-C30-C32	4.34	120.35	110.78
3	B	201	60Z	C27-O29-C30	4.21	122.54	117.34
3	E	201	60Z	O29-C30-C32	4.12	119.86	110.78
3	F	201	60Z	C3-C2-N38	3.95	123.76	119.25
3	A	201	60Z	O31-C30-C32	-3.87	115.77	124.49
3	E	201	60Z	C3-C2-N38	3.86	123.67	119.25
3	A	201	60Z	C27-O29-C30	3.71	121.92	117.34
3	F	201	60Z	O31-C30-C32	-3.70	116.17	124.49
3	E	201	60Z	C27-O29-C30	3.47	121.62	117.34
3	E	201	60Z	O31-C30-C32	-3.29	117.08	124.49
3	B	201	60Z	C3-C2-N38	3.12	122.82	119.25
3	B	201	60Z	C16-C15-C8	-3.01	107.03	111.43
3	A	201	60Z	C16-C15-C8	-2.83	107.29	111.43
3	B	201	60Z	O29-C30-C32	2.80	116.95	110.78
3	F	201	60Z	C27-O29-C30	2.77	120.75	117.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	60Z	C16-C15-C8	-2.64	107.57	111.43
3	E	201	60Z	C16-C15-C8	-2.42	107.89	111.43
3	E	201	60Z	C35-C34-C32	-2.40	106.75	111.23
3	E	201	60Z	C27-C26-C25	-2.30	117.94	124.60
3	B	201	60Z	C27-C26-C25	-2.26	118.06	124.60
3	A	201	60Z	C27-C26-C25	-2.19	118.27	124.60
3	A	201	60Z	C21-C19-C17	2.18	114.64	110.39
3	F	201	60Z	C35-C34-C32	-2.16	107.19	111.23
3	A	201	60Z	O4-C3-C2	-2.09	116.73	119.08
3	F	201	60Z	C27-C26-C25	-2.07	118.60	124.60
3	B	201	60Z	O31-C30-C32	-2.06	119.84	124.49

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	60Z	C23-C24-C25-C26
3	A	201	60Z	C25-C26-C27-O29
3	A	201	60Z	C25-C26-C27-C39
3	E	201	60Z	C25-C26-C27-O29
3	E	201	60Z	C25-C26-C27-C39
3	B	201	60Z	C23-C24-C25-C26
3	B	201	60Z	C25-C26-C27-O29
3	F	201	60Z	C25-C26-C27-O29
3	F	201	60Z	C25-C26-C27-C39
6	A	206	PE8	O19-C20-C21-O22
6	A	206	PE8	O4-C5-C6-O7
8	C	2304	PG4	O2-C3-C4-O3
5	F	202	PEG	O1-C1-C2-O2
5	B	210	PEG	O2-C3-C4-O4
6	B	212	PE8	O1-C2-C3-O4
7	B	213	PGE	O3-C5-C6-O4
6	A	206	PE8	O1-C2-C3-O4
7	C	2306	PGE	O3-C5-C6-O4
5	D	2304	PEG	O2-C3-C4-O4
7	B	213	PGE	O2-C3-C4-O3
5	C	2302	PEG	O2-C3-C4-O4
5	D	2305	PEG	O1-C1-C2-O2
5	B	209	PEG	O1-C1-C2-O2
8	G	2303	PG4	O1-C1-C2-O2
7	C	2306	PGE	O2-C3-C4-O3
4	D	2303	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	202	EDO	O1-C1-C2-O2
4	A	203	EDO	O1-C1-C2-O2
3	B	201	60Z	C25-C26-C27-C39
6	B	212	PE8	O16-C17-C18-O19
8	C	2303	PG4	O3-C5-C6-O4
5	B	211	PEG	O1-C1-C2-O2
7	C	2306	PGE	O1-C1-C2-O2
4	B	206	EDO	O1-C1-C2-O2
3	F	201	60Z	C17-C15-C8-O7
7	D	2306	PGE	O2-C3-C4-O3
3	E	201	60Z	C23-C24-C25-C26
3	F	201	60Z	C23-C24-C25-C26
4	B	203	EDO	O1-C1-C2-O2
6	B	212	PE8	O19-C20-C21-O22
5	A	205	PEG	O1-C1-C2-O2
6	A	206	PE8	C6-C5-O4-C3
6	A	206	PE8	C5-C6-O7-C8
6	B	212	PE8	C2-C3-O4-C5
7	C	2306	PGE	C3-C4-O3-C5
8	G	2303	PG4	O2-C3-C4-O3
7	B	213	PGE	C4-C3-O2-C2
6	A	206	PE8	C12-C11-O10-C9
7	B	213	PGE	C6-C5-O3-C4
8	C	2304	PG4	C8-C7-O4-C6
8	C	2305	PG4	O1-C1-C2-O2
4	B	205	EDO	O1-C1-C2-O2
6	A	206	PE8	C8-C9-O10-C11
8	C	2304	PG4	C6-C5-O3-C4
5	B	209	PEG	C1-C2-O2-C3
5	B	209	PEG	O2-C3-C4-O4
8	C	2304	PG4	C1-C2-O2-C3
5	A	205	PEG	C4-C3-O2-C2
8	G	2303	PG4	C3-C4-O3-C5
3	F	201	60Z	C16-C15-C8-O7
7	D	2306	PGE	O3-C5-C6-O4
8	C	2303	PG4	C1-C2-O2-C3
7	D	2306	PGE	C6-C5-O3-C4
7	D	2306	PGE	C1-C2-O2-C3
3	E	201	60Z	C17-C15-C8-O7
4	E	203	EDO	O1-C1-C2-O2
5	D	2305	PEG	C4-C3-O2-C2
3	B	201	60Z	O29-C30-C32-C34

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Mol	Chain	Res	Type	Atoms
3	B	201	60Z	C39-C27-O29-C30
3	F	201	60Z	C39-C27-O29-C30
3	B	201	60Z	O31-C30-C32-C34
5	A	205	PEG	O2-C3-C4-O4

There are no ring outliers.

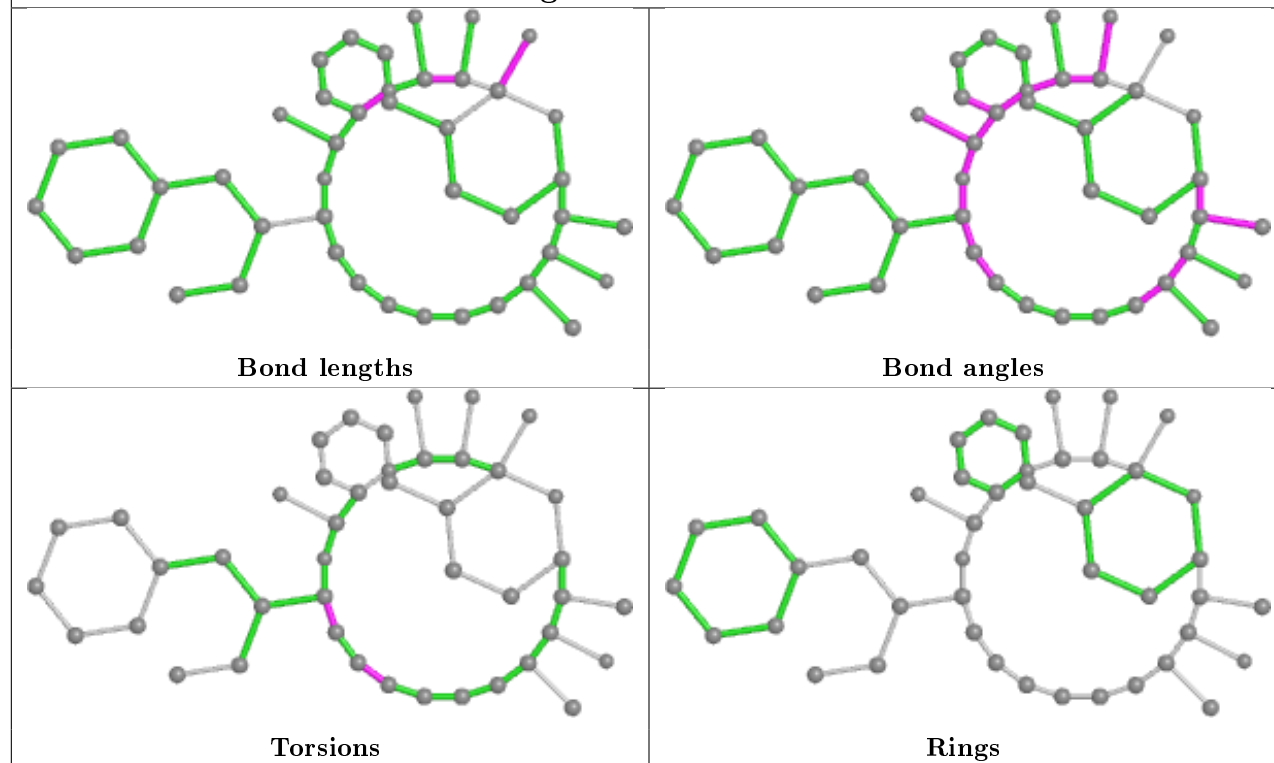
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	2306	PGE	2	0
5	B	210	PEG	1	0
6	B	212	PE8	1	0
3	F	201	60Z	1	0

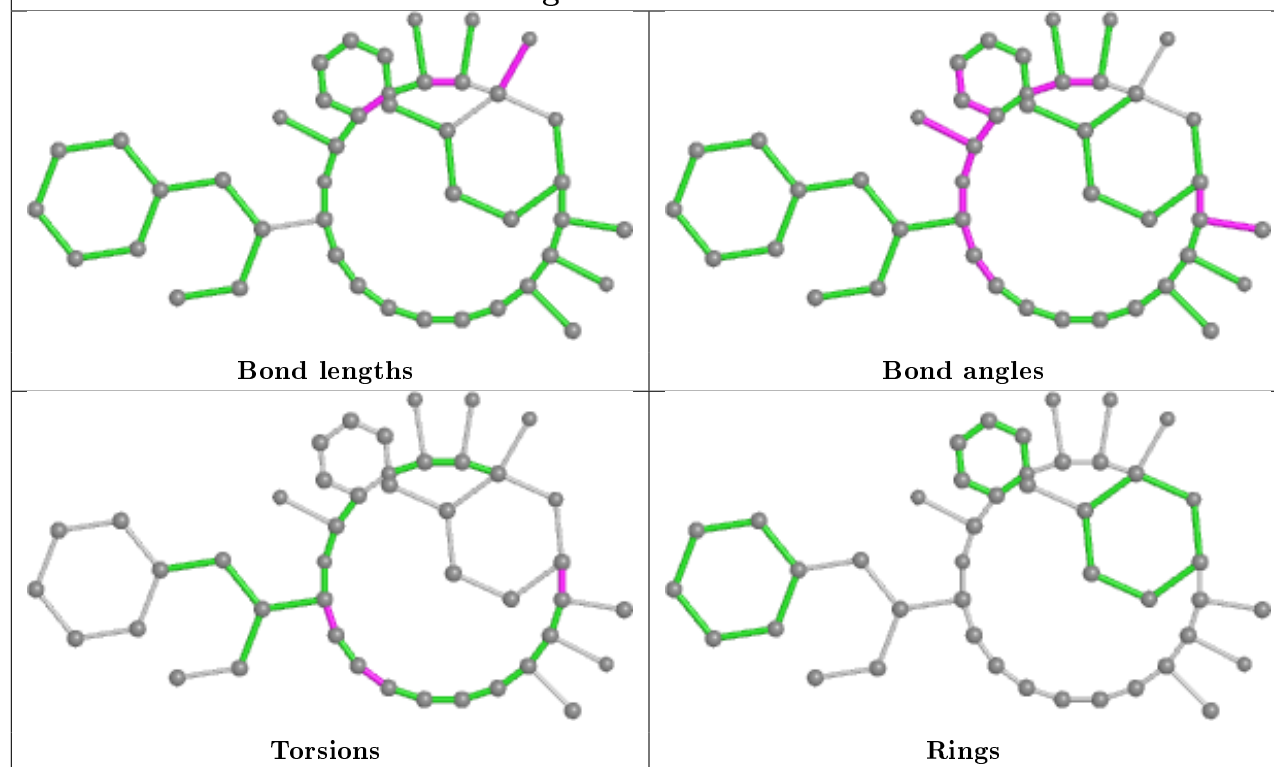
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

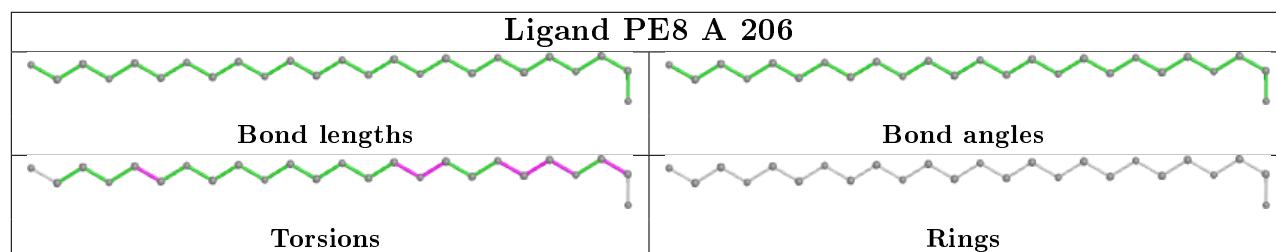
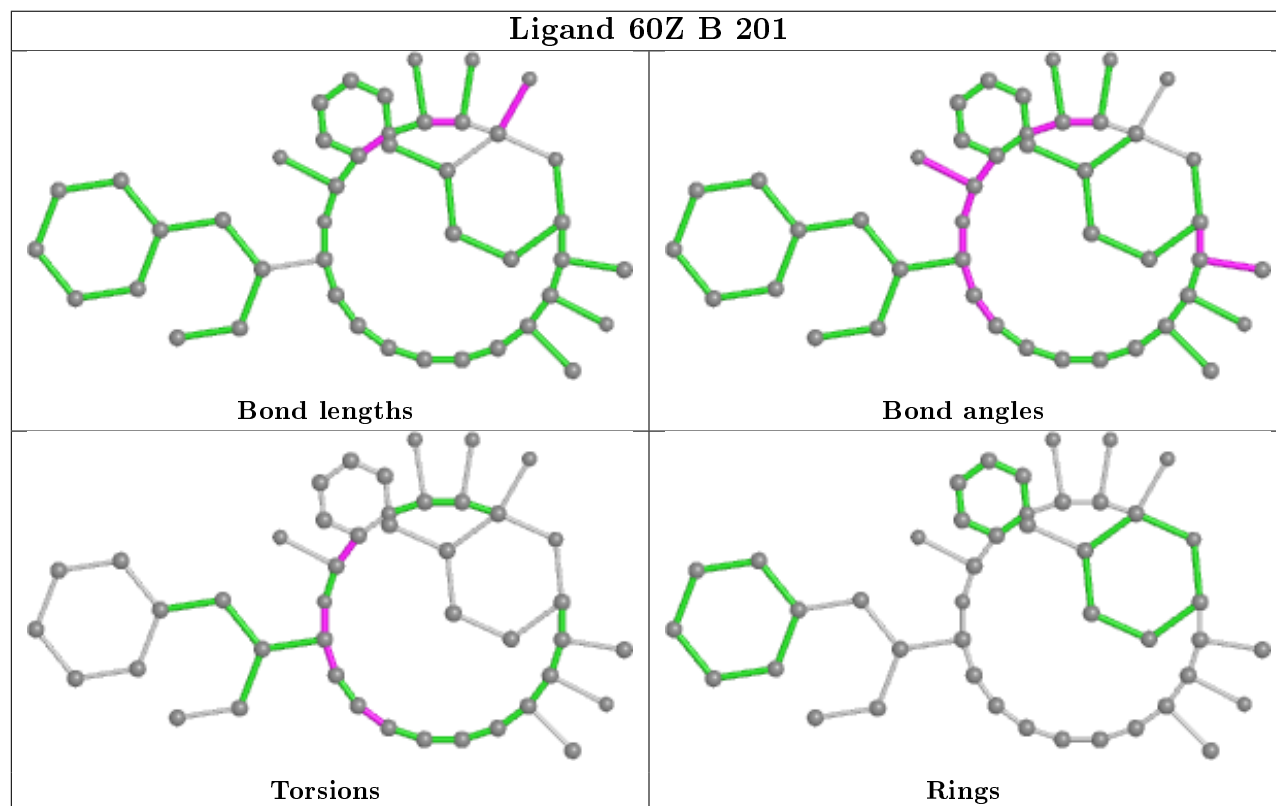
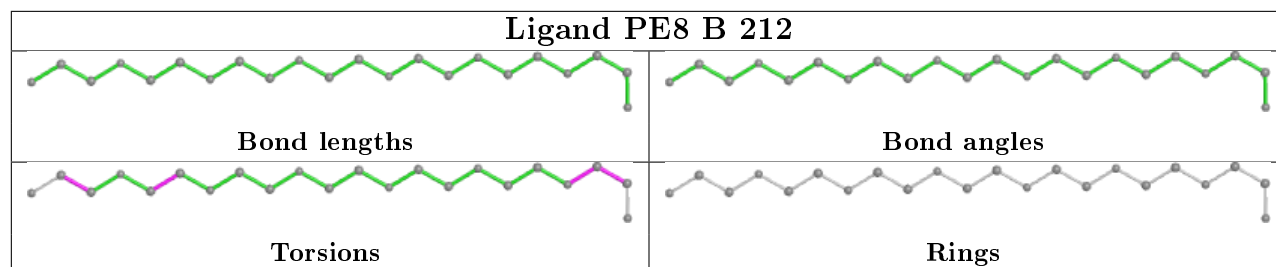


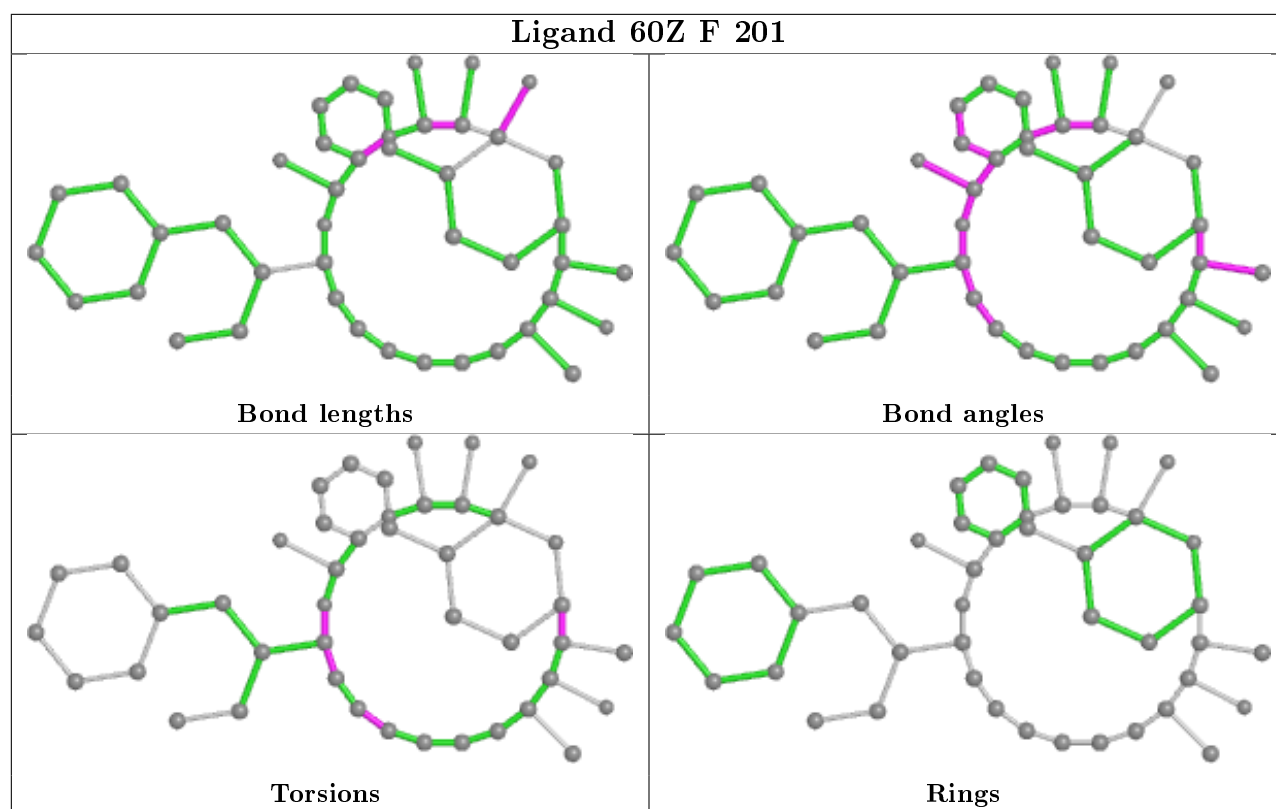
## Ligand 60Z A 201



## Ligand 60Z E 201







## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	108/108 (100%)	-0.11	1 (0%) 84 83	28, 38, 54, 74	0
1	B	107/108 (99%)	-0.16	1 (0%) 84 83	27, 37, 51, 75	3 (2%)
1	E	107/108 (99%)	0.18	5 (4%) 31 30	50, 64, 82, 97	3 (2%)
1	F	107/108 (99%)	0.64	17 (15%) 1 1	52, 77, 98, 116	6 (5%)
2	C	83/98 (84%)	-0.08	6 (7%) 15 14	26, 40, 92, 126	3 (3%)
2	D	83/98 (84%)	0.40	9 (10%) 5 5	26, 47, 104, 145	8 (9%)
2	G	87/98 (88%)	0.49	7 (8%) 12 11	31, 59, 98, 127	11 (12%)
2	H	85/98 (86%)	0.33	9 (10%) 6 5	35, 60, 85, 109	3 (3%)
All	All	767/824 (93%)	0.20	55 (7%) 15 14	26, 54, 93, 145	37 (4%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	2227	LEU	8.3
1	F	14	ARG	5.4
1	F	16	PHE	5.3
2	D	2146	PRO	5.3
1	F	8	ILE	5.0
2	H	2227	LEU	4.7
2	D	2227	LEU	4.4
2	D	2228	HIS	4.4
2	D	2148	LEU	4.0
2	G	2222	LEU	3.9
1	F	81	TYR	3.7
1	E	44	ASN	3.6
1	F	19	ARG	3.6
1	E	15	THR	3.5
2	D	2147	ARG	3.3
2	C	2148	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	2222	LEU	3.2
2	H	2146	PRO	3.1
2	H	2228	HIS	3.1
1	F	10	PRO	3.1
2	D	2150	ARG	3.1
2	G	2228	HIS	3.0
2	D	2149	GLN	2.8
2	C	2146	PRO	2.8
2	C	2147	ARG	2.8
2	D	2152	LEU	2.7
1	F	18	LYS	2.7
1	F	7	THR	2.6
2	D	2224	LYS	2.6
1	E	14	ARG	2.5
1	B	14	ARG	2.5
2	H	2181	ALA	2.4
1	F	13	GLY	2.4
1	A	1	MET	2.4
2	C	2154	ARG	2.4
1	F	85	ALA	2.3
1	F	11	GLY	2.3
1	F	33	ASP	2.3
1	F	2	GLY	2.3
2	G	2216	GLU	2.3
1	E	69	VAL	2.3
1	F	66	GLN	2.3
1	F	71	GLN	2.2
1	F	9	SER	2.2
2	H	2147	ARG	2.2
2	G	2224	LYS	2.2
2	C	2228	HIS	2.1
2	G	2220	ARG	2.1
2	H	2150	ARG	2.1
2	G	2225	GLU	2.1
1	E	12	ASP	2.1
2	H	2225	GLU	2.1
1	F	73	ALA	2.0
2	H	2226	ARG	2.0
2	C	2150	ARG	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PGE	C	2306	10/10	0.68	0.23	55,68,73,74	0
5	PEG	A	205	7/7	0.69	0.23	56,68,72,83	0
4	EDO	B	204	4/4	0.72	0.17	70,70,72,75	0
5	PEG	C	2302	7/7	0.75	0.17	74,75,78,81	0
5	PEG	H	2302	7/7	0.76	0.18	82,85,97,102	0
5	PEG	F	202	7/7	0.76	0.26	75,79,86,87	0
4	EDO	B	207	4/4	0.78	0.25	70,70,74,76	0
4	EDO	E	202	4/4	0.78	0.15	84,85,85,86	0
8	PG4	G	2303	13/13	0.79	0.22	72,79,86,87	0
4	EDO	D	2302	4/4	0.80	0.21	64,65,65,65	0
4	EDO	B	203	4/4	0.80	0.25	59,65,67,74	0
4	EDO	A	203	4/4	0.81	0.27	86,88,89,95	0
8	PG4	C	2304	13/13	0.81	0.17	66,71,77,78	0
4	EDO	C	2301	4/4	0.83	0.27	51,52,58,58	0
4	EDO	B	205	4/4	0.84	0.14	64,65,73,74	0
5	PEG	B	210	7/7	0.85	0.20	62,79,88,90	0
4	EDO	E	203	4/4	0.85	0.17	71,72,73,78	0
5	PEG	D	2305	7/7	0.85	0.18	74,78,83,83	0
7	PGE	G	2304	10/10	0.85	0.17	63,70,77,79	0
7	PGE	D	2306	10/10	0.86	0.18	33,42,51,53	0
5	PEG	B	209	7/7	0.86	0.16	49,55,60,62	0
4	EDO	D	2303	4/4	0.86	0.13	63,66,71,80	0
5	PEG	B	211	7/7	0.86	0.24	72,80,90,91	0
4	EDO	B	208	4/4	0.86	0.18	76,79,82,86	0
5	PEG	D	2304	7/7	0.87	0.18	64,68,75,76	0
8	PG4	C	2305	13/13	0.87	0.14	50,59,71,72	0
6	PE8	B	212	22/25	0.87	0.17	42,52,64,67	0

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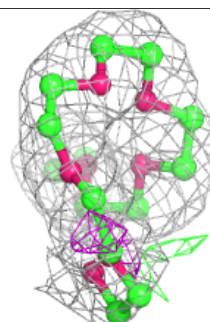
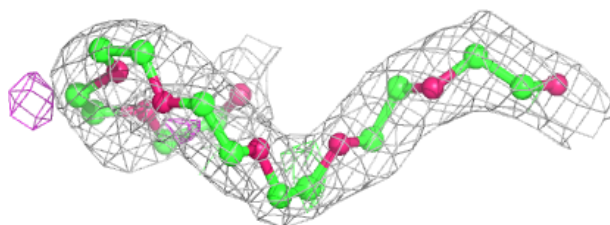
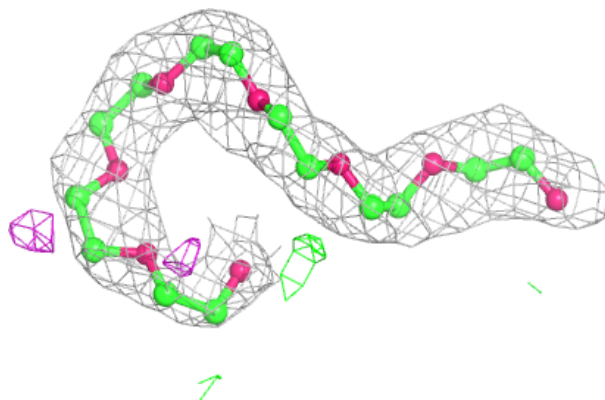
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	206	4/4	0.88	0.19	67,75,80,84	0
6	PE8	A	206	25/25	0.89	0.15	46,62,71,74	0
5	PEG	G	2302	7/7	0.89	0.17	54,58,62,63	0
3	60Z	F	201	44/44	0.90	0.20	56,68,80,87	0
4	EDO	B	202	4/4	0.90	0.41	61,62,64,70	0
8	PG4	C	2303	13/13	0.91	0.15	39,52,65,69	0
4	EDO	A	202	4/4	0.91	0.13	74,75,78,81	0
7	PGE	B	213	10/10	0.92	0.22	65,73,79,82	0
3	60Z	E	201	44/44	0.92	0.16	50,58,73,78	0
4	EDO	G	2301	4/4	0.92	0.16	68,70,76,77	0
4	EDO	A	204	4/4	0.94	0.10	61,63,65,78	0
3	60Z	A	201	44/44	0.95	0.19	30,35,46,64	0
3	60Z	B	201	44/44	0.96	0.18	28,34,48,68	0
9	MG	D	2301	1/1	0.97	0.07	34,34,34,34	0
10	MLA	H	2301	7/7	0.98	0.08	37,39,46,49	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.

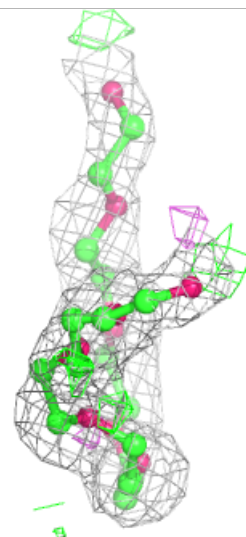
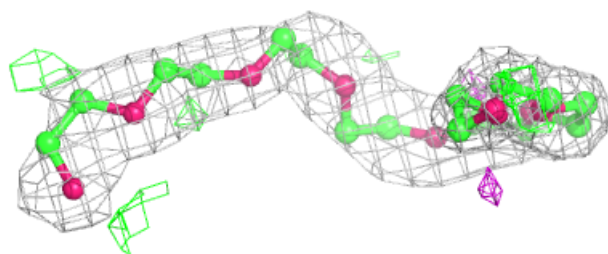
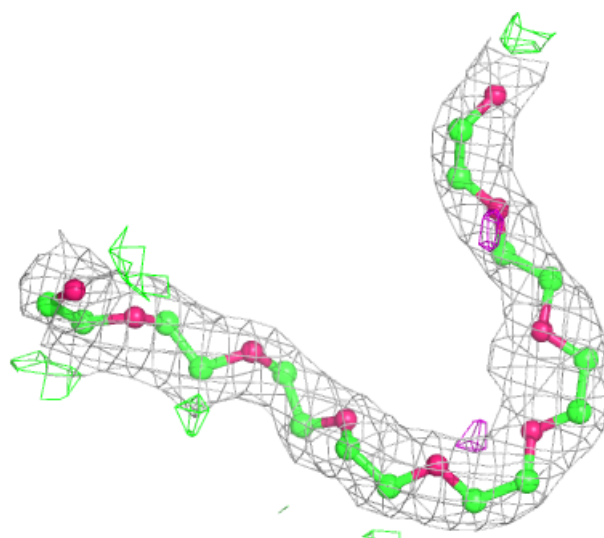
#### Electron density around PE8 B 212:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PE8 A 206:**

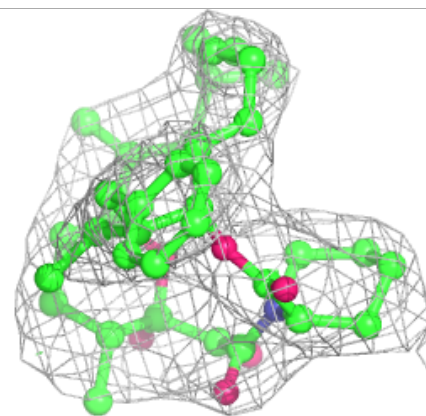
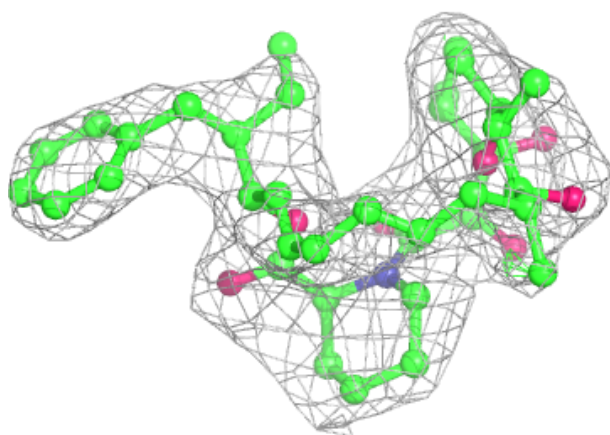
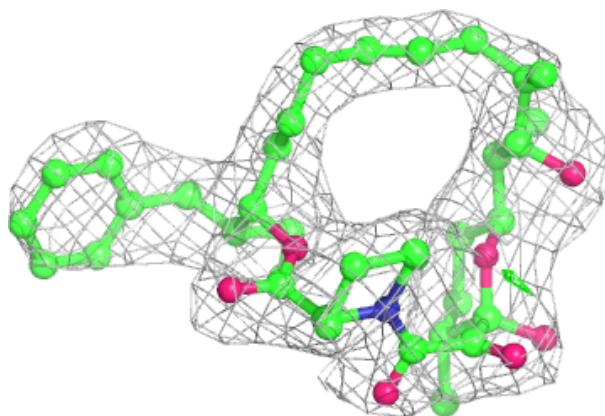
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





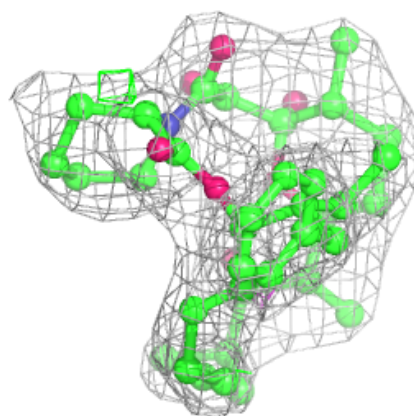
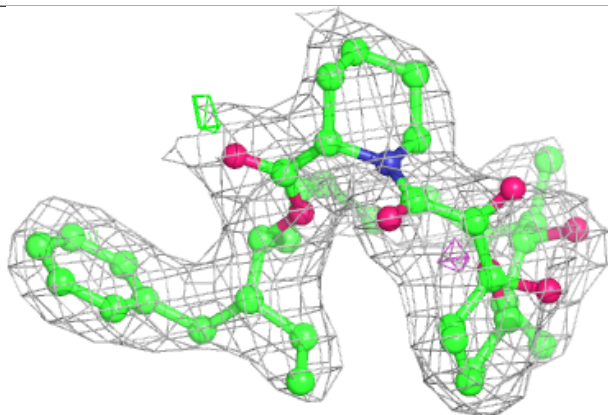
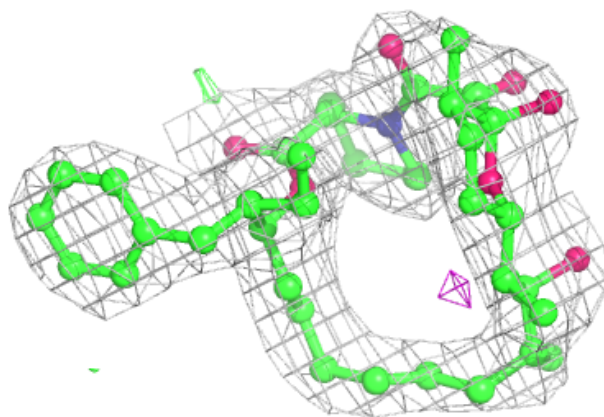
**Electron density around 60Z F 201:**

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



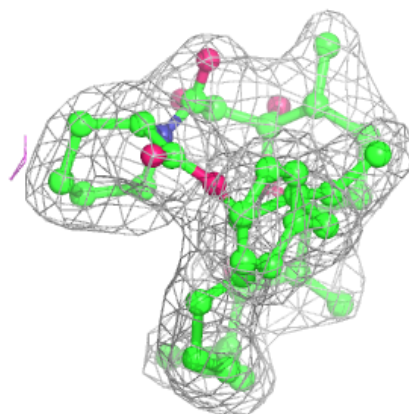
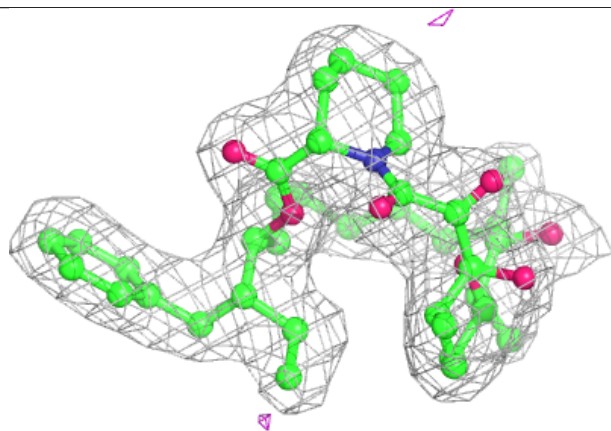
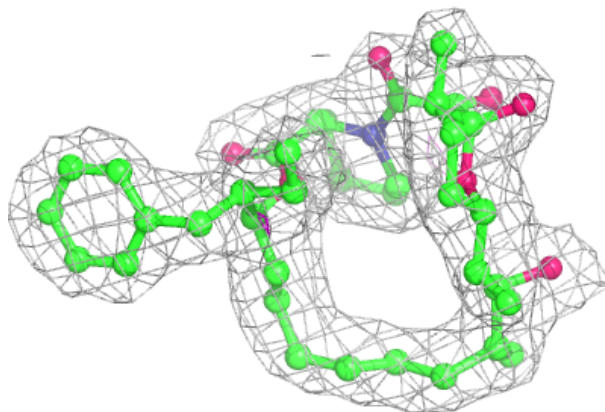
**Electron density around 6OZ E 201:**

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



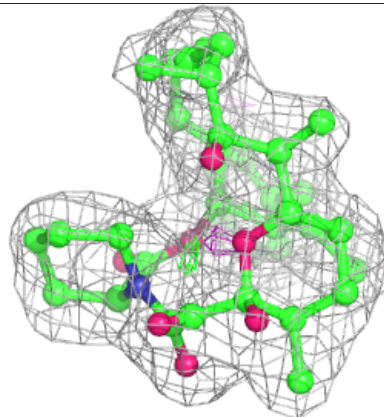
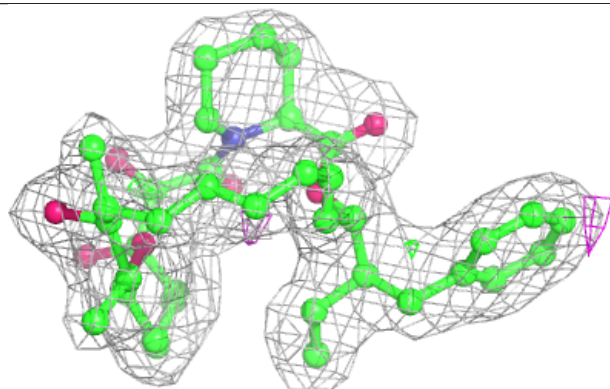
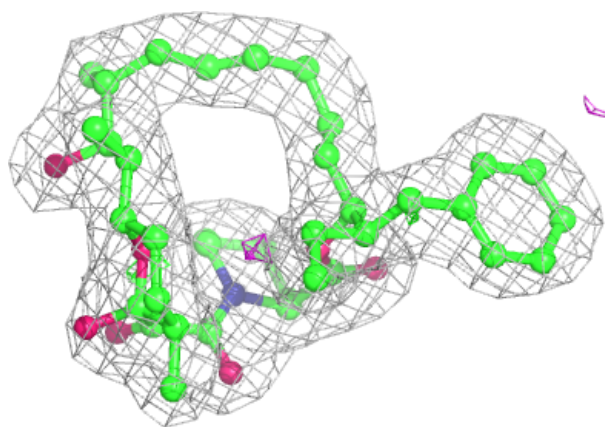
**Electron density around 6OZ A 201:**

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



**Electron density around 60Z B 201:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.