



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:26 am BST

PDB ID : 6I5G
Title : X-ray structure of human soluble Epoxide Hydrolase C-terminal Domain (hsEH CTD)in complex with 15d-PGJ2
Authors : Abis, G.; Kopec, J.; Yue, W.W.; Conte, M.R.
Deposited on : 2018-11-13
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

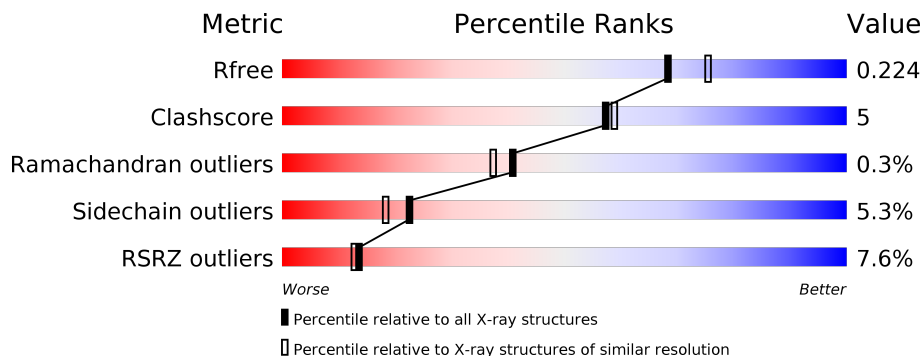
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 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	344	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">8% 79% 11% • 8%</p>
1	B	344	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">6% 81% 9% • 8%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	601	-	-	X	-
2	EDO	A	603	-	-	X	-
2	EDO	B	604	-	-	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5421 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 Bifunctional epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2547	1639	426	459	23	0	1	0
1	B	316	2554	1645	426	460	23	0	3	0

There are 36 discrepancies between the modelled and reference sequences:

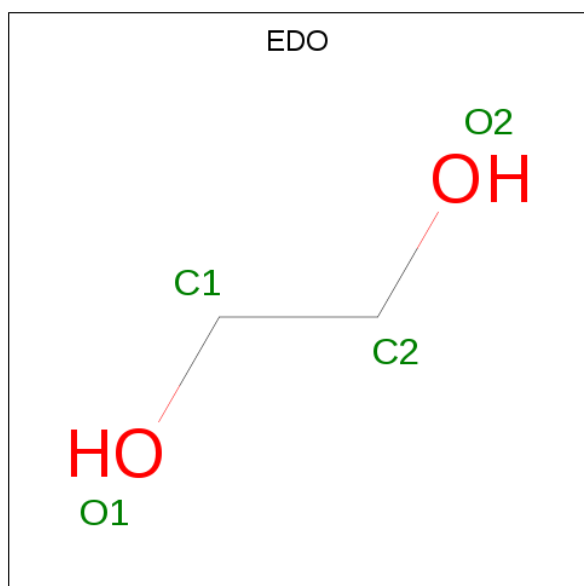
Chain	Residue	Modelled	Actual	Comment	Reference
A	212	MET	-	initiating methionine	UNP P34913
A	213	HIS	-	expression tag	UNP P34913
A	214	HIS	-	expression tag	UNP P34913
A	215	HIS	-	expression tag	UNP P34913
A	216	HIS	-	expression tag	UNP P34913
A	217	HIS	-	expression tag	UNP P34913
A	218	HIS	-	expression tag	UNP P34913
A	219	SER	-	expression tag	UNP P34913
A	220	THR	-	expression tag	UNP P34913
A	221	GLU	-	expression tag	UNP P34913
A	222	ASN	-	expression tag	UNP P34913
A	223	LEU	-	expression tag	UNP P34913
A	224	TYR	-	expression tag	UNP P34913
A	225	PHE	-	expression tag	UNP P34913
A	226	GLN	-	expression tag	UNP P34913
A	227	GLY	-	expression tag	UNP P34913
A	228	SER	-	expression tag	UNP P34913
A	229	SER	-	expression tag	UNP P34913
B	212	MET	-	initiating methionine	UNP P34913
B	213	HIS	-	expression tag	UNP P34913
B	214	HIS	-	expression tag	UNP P34913
B	215	HIS	-	expression tag	UNP P34913
B	216	HIS	-	expression tag	UNP P34913
B	217	HIS	-	expression tag	UNP P34913
B	218	HIS	-	expression tag	UNP P34913

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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	SER	-	expression tag	UNP P34913
B	220	THR	-	expression tag	UNP P34913
B	221	GLU	-	expression tag	UNP P34913
B	222	ASN	-	expression tag	UNP P34913
B	223	LEU	-	expression tag	UNP P34913
B	224	TYR	-	expression tag	UNP P34913
B	225	PHE	-	expression tag	UNP P34913
B	226	GLN	-	expression tag	UNP P34913
B	227	GLY	-	expression tag	UNP P34913
B	228	SER	-	expression tag	UNP P34913
B	229	SER	-	expression tag	UNP P34913

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



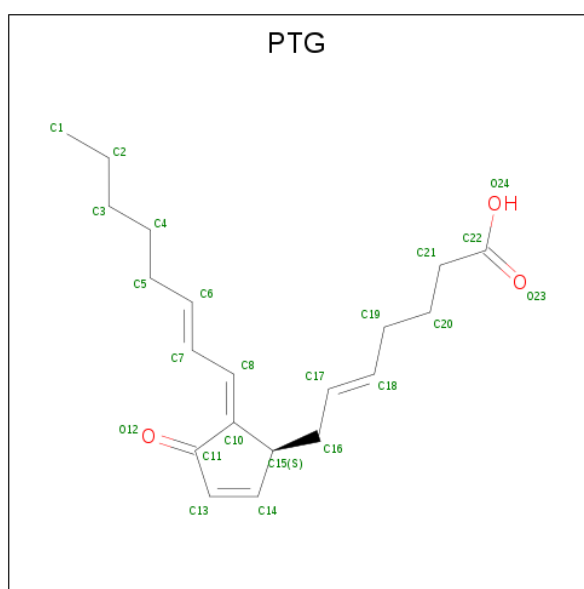
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			4	2 2		
2	A	1	Total	C O	0	0
			4	2 2		
2	A	1	Total	C O	0	0
			4	2 2		
2	A	1	Total	C O	0	0
			4	2 2		

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

- Molecule 3 is (5E,14E)-11-oxoprostano-5,9,12,14-tetraen-1-oic acid (three-letter code: PTG) (formula: C₂₀H₂₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	20	3		
3	B	1	Total	C	O	0	0
			23	20	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		

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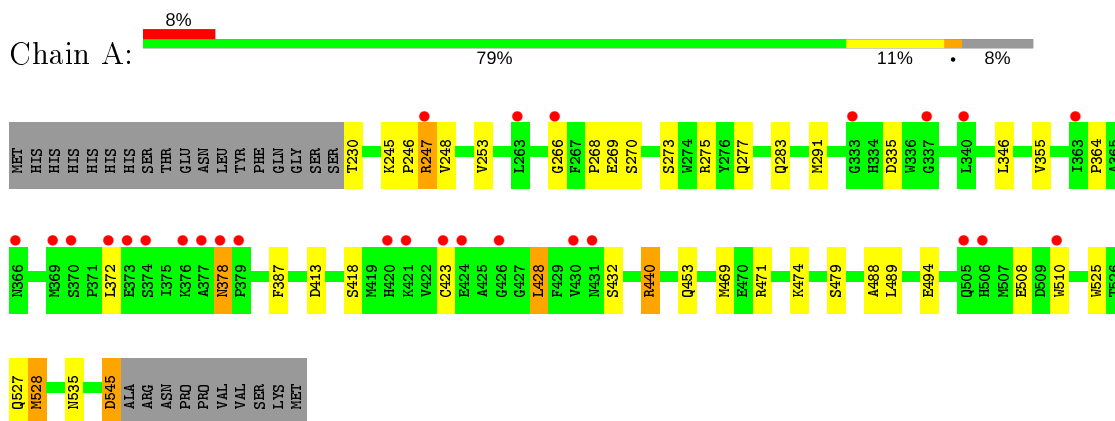
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	118	Total 118	O 118	0	0

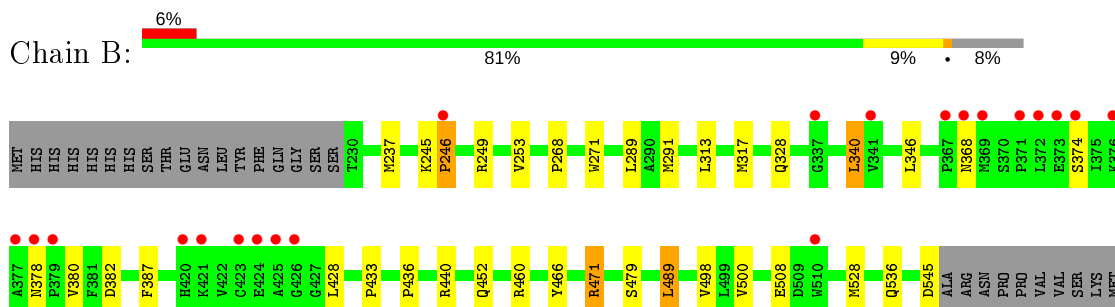
3 Residue-property plots [i](#)

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: Bifunctional epoxide hydrolase 2



- Molecule 1: Bifunctional epoxide hydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.49Å 79.99Å 104.54Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	71.83 – 2.00 29.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (71.83-2.00) 99.2 (29.73-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.172 , 0.217 0.181 , 0.224	Depositor DCC
R_{free} test set	2403 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtrriage
Anisotropy	0.477	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5421	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PTG, EDO

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	0.86	1/2626 (0.0%)	0.98	6/3563 (0.2%)
1	B	0.85	0/2639	0.99	9/3582 (0.3%)
All	All	0.86	1/5265 (0.0%)	0.98	15/7145 (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	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	GLU	CG-CD	5.87	1.60	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	B	440	ARG	NE-CZ-NH1	14.40	127.50	120.30
1	A	440	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	A	440	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	428	LEU	CB-CG-CD1	8.11	124.78	111.00
1	A	275	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	528	MET	CG-SD-CE	6.89	111.23	100.20
1	B	440	ARG	CD-NE-CZ	6.16	132.23	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	LEU	CA-CB-CG	6.03	129.17	115.30
1	B	471	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	528	MET	CG-SD-CE	5.85	109.56	100.20
1	B	460	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	489	LEU	CB-CG-CD2	5.65	120.60	111.00
1	A	469	MET	CG-SD-CE	5.59	109.14	100.20
1	B	440	ARG	CG-CD-NE	-5.41	100.44	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	ARG	Peptide
1	A	291	MET	Peptide
1	B	291	MET	Peptide

5.2 Too-close contacts

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	2547	0	2474	31	0
1	B	2554	0	2488	17	0
2	A	24	0	36	14	0
2	B	24	0	36	9	0
3	A	23	0	27	1	0
3	B	23	0	27	1	0
4	A	108	0	0	5	0
4	B	118	0	0	8	0
All	All	5421	0	5088	50	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 (50) 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:466:TYR:OH	4:B:701:HOH:O	1.92	0.86
1:A:270:SER:CB	2:A:603:EDO:H21	2.06	0.85
1:A:432:SER:CB	4:A:701:HOH:O	2.33	0.77
2:B:603:EDO:H11	4:B:737:HOH:O	1.93	0.69
1:A:283:GLN:HG2	4:A:807:HOH:O	1.95	0.67
1:A:270:SER:CB	2:A:603:EDO:C2	2.75	0.64
1:A:527:GLN:HB2	2:A:601:EDO:H22	1.80	0.61
1:A:270:SER:OG	2:A:603:EDO:C2	2.50	0.59
1:A:270:SER:HB2	2:A:603:EDO:H21	1.81	0.59
1:A:510:TRP:O	4:A:702:HOH:O	2.17	0.59
1:A:432:SER:HB2	4:A:701:HOH:O	2.00	0.59
1:A:453:GLN:HB3	2:A:603:EDO:C1	2.33	0.59
1:A:527:GLN:HB2	2:A:601:EDO:C2	2.34	0.58
1:A:270:SER:HB2	2:A:603:EDO:C2	2.34	0.57
1:A:247:ARG:HB2	1:A:248:VAL:HG23	1.87	0.57
1:A:270:SER:CA	2:A:603:EDO:H21	2.34	0.57
1:B:368:ASN:ND2	4:B:704:HOH:O	2.39	0.56
1:B:271:TRP:HE1	2:B:604:EDO:C1	2.19	0.55
2:B:603:EDO:C1	4:B:737:HOH:O	2.54	0.55
1:B:271:TRP:HE1	2:B:604:EDO:H22	1.72	0.54
1:A:270:SER:HA	2:A:603:EDO:H21	1.88	0.54
1:B:536:GLN:HG3	4:B:750:HOH:O	2.08	0.53
1:A:528:MET:HG3	2:A:601:EDO:O2	2.09	0.53
1:B:237:MET:HB3	1:B:253:VAL:HG13	1.92	0.52
1:A:413:ASP:OD2	1:A:440:ARG:NH2	2.43	0.52
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.91	0.51
1:A:545:ASP:N	1:A:545:ASP:OD1	2.45	0.49
1:A:230:THR:O	4:A:703:HOH:O	2.20	0.48
1:A:525:TRP:HB3	2:A:601:EDO:H11	1.95	0.47
1:A:387:PHE:HZ	3:A:607:PTG:C1	2.26	0.47
1:B:271:TRP:HE1	2:B:604:EDO:C2	2.28	0.47
1:A:277:GLN:HG3	1:A:535:ASN:ND2	2.30	0.47
1:A:270:SER:OG	2:A:603:EDO:H21	2.13	0.46
1:B:317:MET:HG2	2:B:601:EDO:H22	1.97	0.46
1:B:387:PHE:HZ	3:B:607:PTG:H1	1.82	0.45
1:A:355:VAL:O	1:A:488:ALA:HA	2.17	0.44
1:A:364:PRO:HG2	1:A:510:TRP:CE2	2.53	0.44
1:A:378:ASN:C	1:A:378:ASN:HD22	2.22	0.44
1:A:453:GLN:HB3	2:A:603:EDO:H12	2.00	0.44
1:B:433:PRO:O	1:B:436:PRO:HD3	2.19	0.42
1:A:245:LYS:HB2	1:A:246:PRO:HD2	2.02	0.42
1:B:328:GLN:NE2	4:B:702:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:HD22	2:B:601:EDO:H11	2.02	0.41
1:B:382:ASP:HB2	4:B:792:HOH:O	2.20	0.41
1:A:245:LYS:HB2	1:A:246:PRO:CD	2.51	0.41
1:A:269:GLU:HB3	1:A:273:SER:OG	2.20	0.41
1:B:271:TRP:NE1	2:B:604:EDO:H22	2.34	0.41
1:B:452:GLN:NE2	4:B:703:HOH:O	2.52	0.41
1:B:271:TRP:HE1	2:B:604:EDO:H11	1.85	0.41
1:B:245:LYS:HB2	1:B:246:PRO:CD	2.51	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	315/344 (92%)	302 (96%)	12 (4%)	1 (0%)	41	37
1	B	317/344 (92%)	309 (98%)	7 (2%)	1 (0%)	41	37
All	All	632/688 (92%)	611 (97%)	19 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	PRO
1	B	268	PRO

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	277/304 (91%)	264 (95%)	13 (5%)	26	22
1	B	279/304 (92%)	261 (94%)	18 (6%)	17	12
All	All	556/608 (91%)	525 (94%)	31 (6%)	22	17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	VAL
1	A	346	LEU
1	A	372	LEU
1	A	378	ASN
1	A	418	SER
1	A	423	CYS
1	A	428	LEU
1	A	471	ARG
1	A	474	LYS
1	A	479	SER
1	A	489	LEU
1	A	508	GLU
1	A	545	ASP
1	B	246	PRO
1	B	249	ARG
1	B	289	LEU
1	B	340	LEU
1	B	346	LEU
1	B	374	SER
1	B	378	ASN
1	B	380	VAL
1	B	428	LEU
1	B	471	ARG
1	B	479	SER
1	B	489	LEU
1	B	498[A]	VAL
1	B	498[B]	VAL
1	B	500[A]	VAL
1	B	500[B]	VAL
1	B	508	GLU
1	B	545	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	378	ASN
1	A	384	GLN
1	A	535	ASN
1	B	328	GLN
1	B	378	ASN
1	B	452	GLN
1	B	505	GLN
1	B	535	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	B	601	-	3,3,3	0.79	0	2,2,2	0.64	0
2	EDO	B	605	-	3,3,3	0.55	0	2,2,2	0.38	0
3	PTG	A	607	-	16,23,23	1.89	3 (18%)	15,27,27	3.05	7 (46%)
2	EDO	B	602	-	3,3,3	0.50	0	2,2,2	0.40	0
2	EDO	A	602	-	3,3,3	0.50	0	2,2,2	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PTG	B	607	-	16,23,23	1.76	3 (18%)	15,27,27	2.76	7 (46%)
2	EDO	B	603	-	3,3,3	0.88	0	2,2,2	1.11	0
2	EDO	B	606	-	3,3,3	0.41	0	2,2,2	0.79	0
2	EDO	A	606	-	3,3,3	0.50	0	2,2,2	0.76	0
2	EDO	A	601	-	3,3,3	0.35	0	2,2,2	0.59	0
2	EDO	A	605	-	3,3,3	0.74	0	2,2,2	0.12	0
2	EDO	A	604	-	3,3,3	0.66	0	2,2,2	0.02	0
2	EDO	B	604	-	3,3,3	0.71	0	2,2,2	1.02	0
2	EDO	A	603	-	3,3,3	0.43	0	2,2,2	1.33	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
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	B	605	-	-	1/1/1/1	-
3	PTG	A	607	-	-	6/15/30/30	0/1/1/1
2	EDO	B	602	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
3	PTG	B	607	-	-	7/15/30/30	0/1/1/1
2	EDO	B	603	-	-	1/1/1/1	-
2	EDO	B	606	-	-	0/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	A	605	-	-	1/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	B	604	-	-	1/1/1/1	-
2	EDO	A	603	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	PTG	C15-C10	-4.70	1.45	1.54
3	B	607	PTG	C15-C10	-4.64	1.45	1.54
3	B	607	PTG	C7-C8	-4.14	1.30	1.43
3	A	607	PTG	C13-C14	4.02	1.41	1.33
3	A	607	PTG	C7-C8	-3.91	1.31	1.43
3	B	607	PTG	C13-C14	2.58	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	607	PTG	C14-C13-C11	-5.77	104.50	109.84
3	A	607	PTG	C14-C13-C11	-5.75	104.51	109.84
3	A	607	PTG	C8-C7-C6	5.58	136.71	123.63
3	A	607	PTG	O12-C11-C10	-4.96	120.61	126.95
3	A	607	PTG	C15-C10-C11	4.73	113.89	107.05
3	B	607	PTG	C15-C10-C11	4.08	112.95	107.05
3	B	607	PTG	C8-C7-C6	4.00	133.01	123.63
3	B	607	PTG	O12-C11-C10	-3.84	122.04	126.95
3	B	607	PTG	C5-C6-C7	-3.28	109.91	125.90
3	A	607	PTG	C5-C6-C7	-3.17	110.43	125.90
3	B	607	PTG	C16-C17-C18	-2.64	116.59	126.40
3	A	607	PTG	C16-C17-C18	-2.60	116.75	126.40
3	B	607	PTG	C14-C15-C10	-2.38	97.21	100.82
3	A	607	PTG	C14-C15-C10	-2.36	97.24	100.82

There are no chirality outliers.

All (23) torsion outliers are listed below:

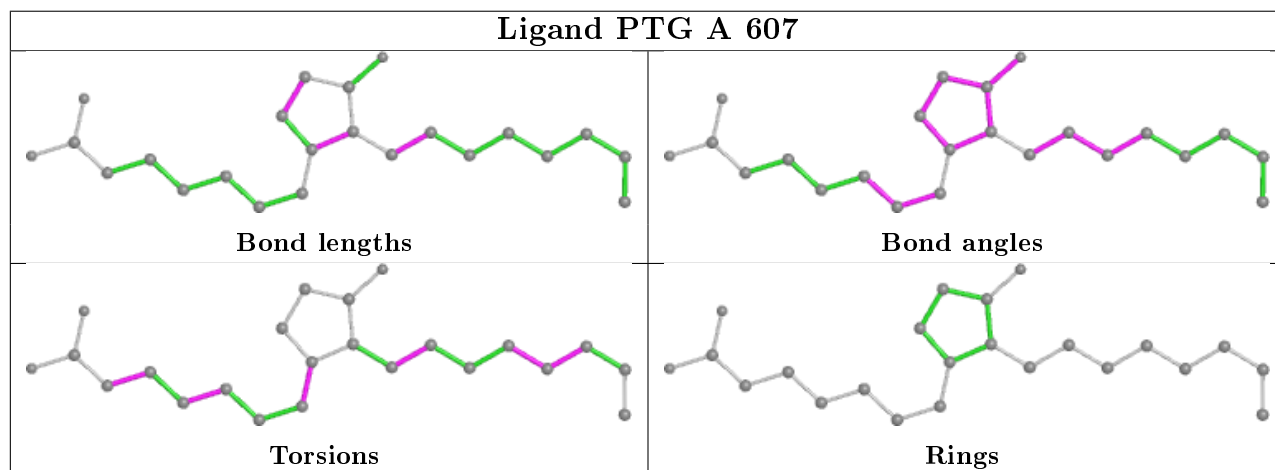
Mol	Chain	Res	Type	Atoms
3	A	607	PTG	C19-C20-C21-C22
3	B	607	PTG	C19-C20-C21-C22
3	A	607	PTG	C6-C7-C8-C10
3	B	607	PTG	C6-C7-C8-C10
3	A	607	PTG	C2-C3-C4-C5
2	A	606	EDO	O1-C1-C2-O2
2	A	605	EDO	O1-C1-C2-O2
2	B	604	EDO	O1-C1-C2-O2
2	A	603	EDO	O1-C1-C2-O2
3	A	607	PTG	C3-C4-C5-C6
2	A	602	EDO	O1-C1-C2-O2
2	B	602	EDO	O1-C1-C2-O2
3	B	607	PTG	C14-C15-C16-C17
3	B	607	PTG	C1-C2-C3-C4
2	B	603	EDO	O1-C1-C2-O2
3	B	607	PTG	C2-C3-C4-C5
3	B	607	PTG	C17-C18-C19-C20
2	B	601	EDO	O1-C1-C2-O2
2	B	605	EDO	O1-C1-C2-O2
3	B	607	PTG	C4-C5-C6-C7
2	A	601	EDO	O1-C1-C2-O2
3	A	607	PTG	C17-C18-C19-C20
3	A	607	PTG	C14-C15-C16-C17

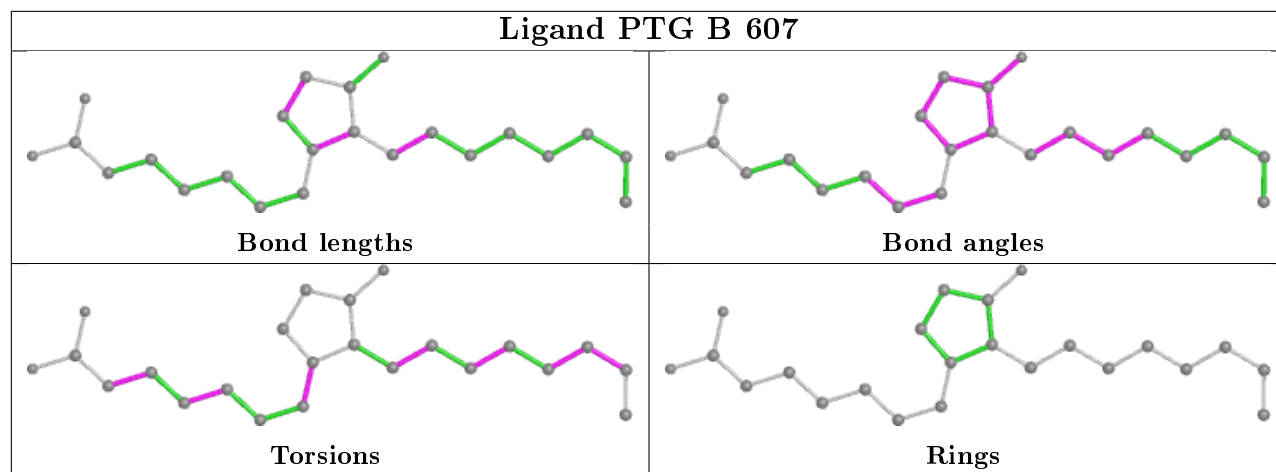
There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	EDO	2	0
3	A	607	PTG	1	0
3	B	607	PTG	1	0
2	B	603	EDO	2	0
2	A	601	EDO	4	0
2	B	604	EDO	5	0
2	A	603	EDO	10	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	316/344 (91%)	0.06	27 (8%) 10 10	18, 29, 71, 94	0
1	B	316/344 (91%)	-0.02	21 (6%) 18 17	18, 27, 70, 94	0
All	All	632/688 (91%)	0.02	48 (7%) 13 13	18, 28, 71, 94	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	GLY	7.8
1	A	369	MET	5.3
1	A	372	LEU	5.1
1	B	423	CYS	4.7
1	A	423	CYS	4.5
1	B	377	ALA	4.4
1	B	421	LYS	4.4
1	B	426	GLY	4.3
1	B	424	GLU	4.3
1	B	369	MET	4.0
1	B	425	ALA	3.8
1	B	368	ASN	3.8
1	A	424	GLU	3.7
1	A	420	HIS	3.6
1	A	370	SER	3.5
1	B	372	LEU	3.4
1	A	431	ASN	3.1
1	B	373	GLU	3.0
1	A	421	LYS	2.9
1	A	505	GLN	2.9
1	A	376	LYS	2.8
1	B	374	SER	2.8
1	A	266	GLY	2.8
1	A	374	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	247	ARG	2.7
1	B	337	GLY	2.7
1	A	373	GLU	2.7
1	A	340	LEU	2.6
1	A	337	GLY	2.6
1	B	341	VAL	2.6
1	B	367	PRO	2.6
1	A	378	ASN	2.5
1	B	420	HIS	2.5
1	A	377	ALA	2.5
1	B	510	TRP	2.4
1	A	510	TRP	2.3
1	B	371	PRO	2.3
1	A	263	LEU	2.3
1	A	363	ILE	2.3
1	A	366	ASN	2.2
1	B	246	PRO	2.2
1	B	379	PRO	2.2
1	A	506	HIS	2.2
1	A	430	VAL	2.2
1	B	376	LYS	2.1
1	A	379	PRO	2.1
1	A	333	GLY	2.0
1	B	378	ASN	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](#)

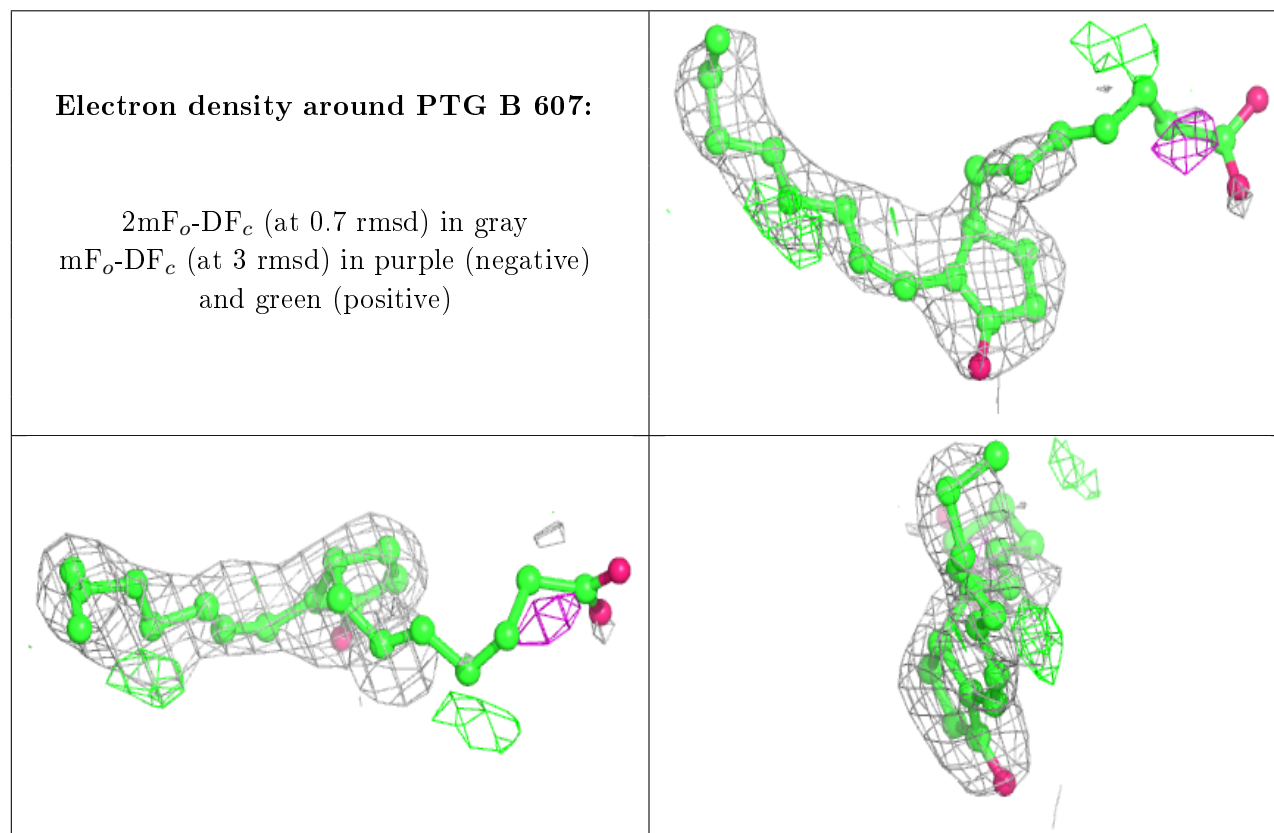
There are no carbohydrates in this entry.

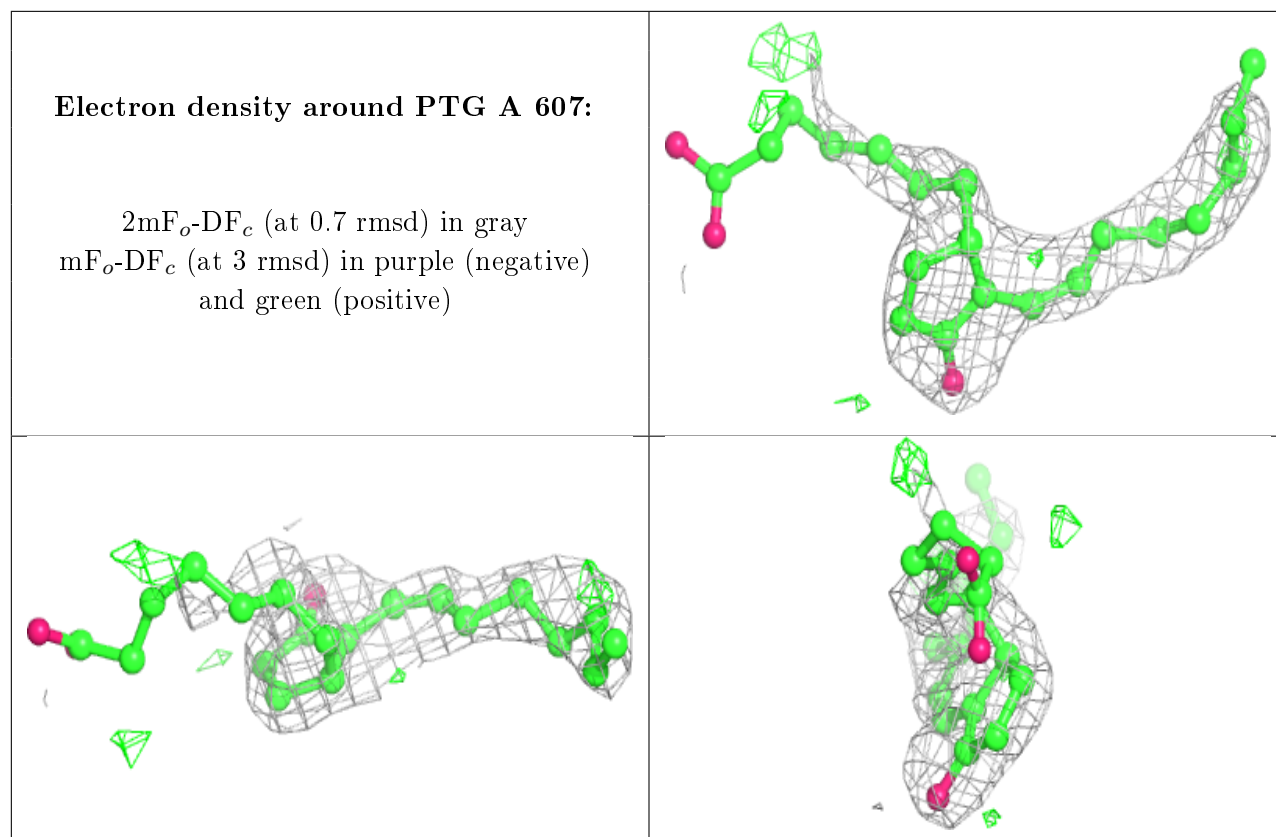
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	PTG	B	607	23/23	0.68	0.30	45,58,84,89	0
3	PTG	A	607	23/23	0.75	0.29	43,58,104,108	0
2	EDO	A	606	4/4	0.82	0.24	38,45,50,51	0
2	EDO	A	605	4/4	0.83	0.35	41,43,49,52	0
2	EDO	B	603	4/4	0.87	0.40	39,41,49,51	0
2	EDO	B	605	4/4	0.89	0.18	40,42,43,51	0
2	EDO	B	604	4/4	0.90	0.26	34,38,42,50	0
2	EDO	A	603	4/4	0.91	0.42	36,40,42,46	0
2	EDO	B	601	4/4	0.93	0.14	26,31,32,35	0
2	EDO	A	602	4/4	0.93	0.24	32,43,46,50	0
2	EDO	A	604	4/4	0.94	0.26	40,44,44,48	0
2	EDO	B	602	4/4	0.95	0.16	37,40,40,41	0
2	EDO	A	601	4/4	0.95	0.18	34,40,47,48	0
2	EDO	B	606	4/4	0.95	0.23	42,42,46,47	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.