Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 06:12 PM EDT

PDB ID	:	5UL5
Title	:	Crystal structure of RPE65 in complex with MB-004 and palmitate
Authors	:	Kiser, P.D.; Palczewski, K.
Deposited on	:	2017-01-24
Resolution	:	2.20 Å(reported)

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

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

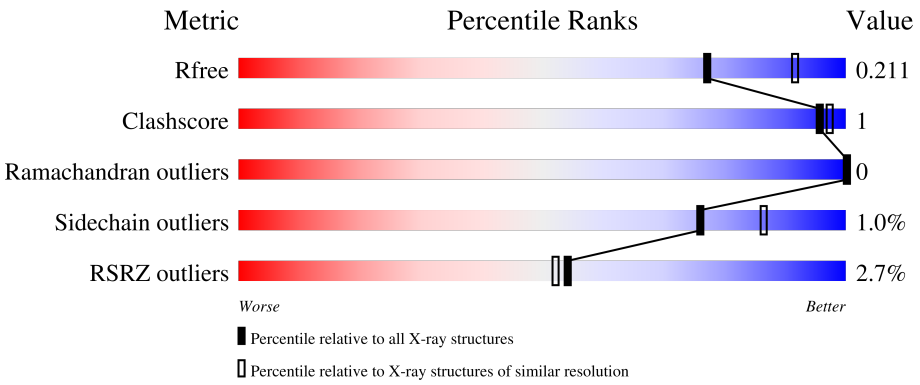
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	533	2% 92%
1	B	533	3% 92%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8894 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 Retinoid isomerohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	4171	2699	686	770	16	0	6	0
1	B	513	4167	2697	685	771	14	0	4	0

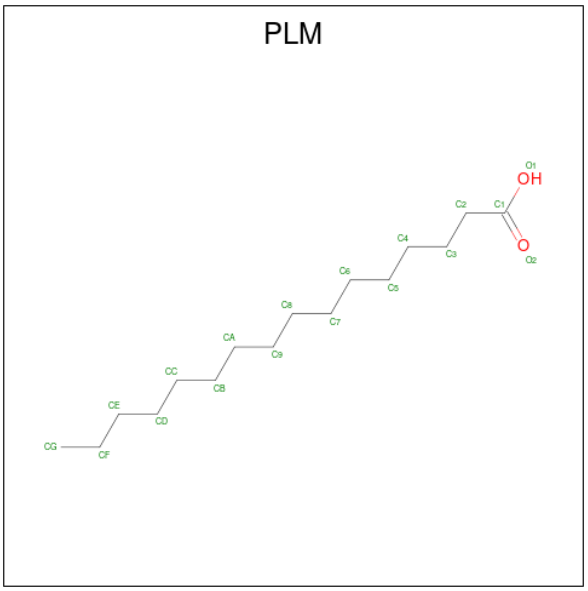
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	LEU	SER	see remark 999	UNP Q28175
B	341	LEU	SER	see remark 999	UNP Q28175

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

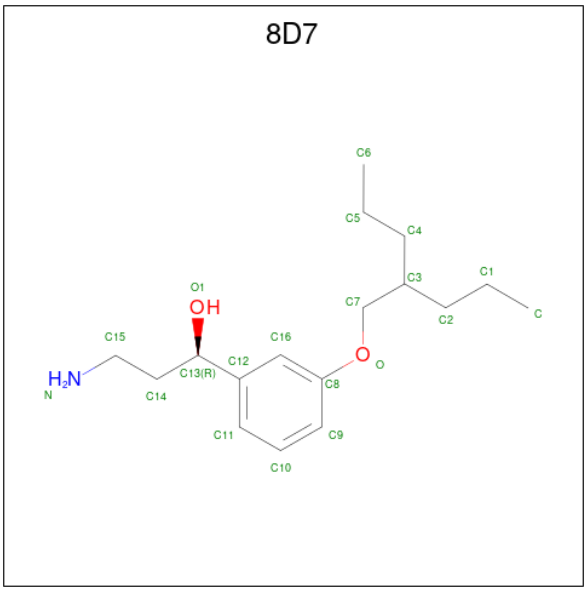
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	18	16	2	0	0
			Total	C	O		
3	B	1	18	16	2	0	0

- Molecule 4 is (1R)-3-amino-1-{3-[(2-propylpentyl)oxy]phenyl}propan-1-ol (three-letter code: 8D7) (formula: $C_{17}H_{29}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	20	17	1	2	0	0

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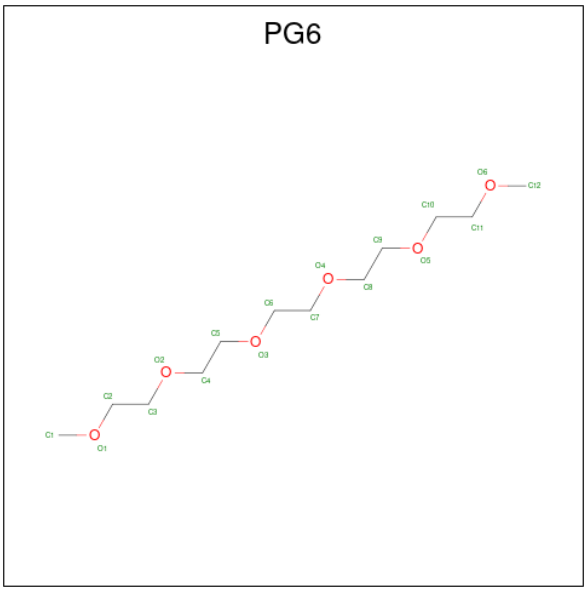
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	20	17	1	2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0
			Total	Na		
5	B	1	1	1	0	0

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	16	10	6	0	0
			Total	C	O		
6	B	1	13	8	5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	228	228	228	0	0

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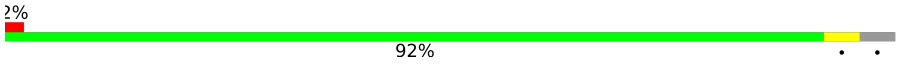
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	219	219	219	0	0

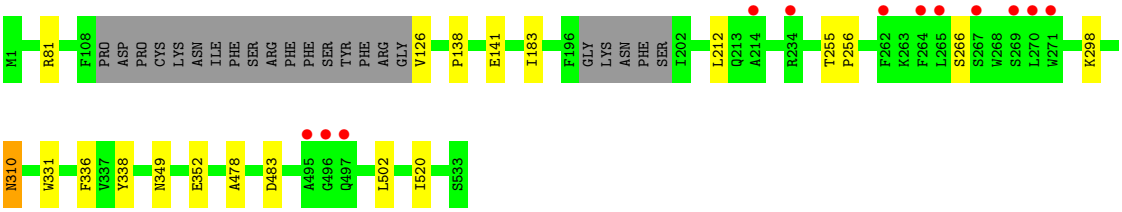
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Retinoid isomerohydrolase

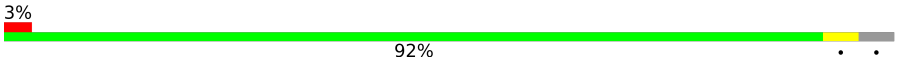
Chain A:

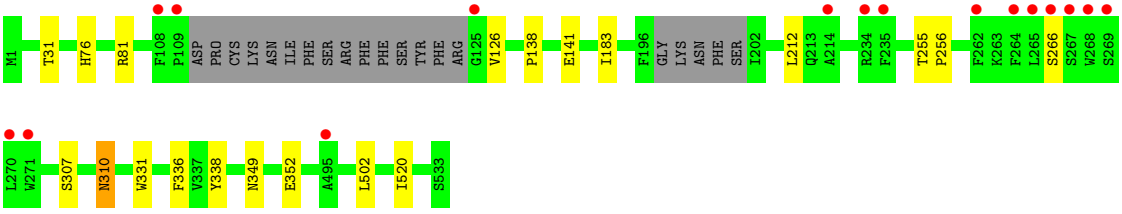




• Molecule 1: Retinoid isomerohydrolase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	175.73Å 175.73Å 86.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.88 – 2.20 47.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.88-2.20) 100.0 (47.88-2.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.170 , 0.209 0.180 , 0.211	Depositor DCC
R_{free} test set	3938 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8894	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, PG6, FE2, 8D7, NA

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	0.64	0/4294	0.75	0/5844
1	B	0.64	1/4291 (0.0%)	0.76	0/5842
All	All	0.64	1/8585 (0.0%)	0.76	0/11686

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	SER	CB-OG	-5.27	1.35	1.42

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	4171	0	4063	9	0
1	B	4167	0	4057	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	31	0	0
3	B	18	0	31	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	16	0	20	0	0
6	B	13	0	16	0	0
7	A	228	0	0	0	0
7	B	219	0	0	2	0
All	All	8894	0	8218	19	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 (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:NH2	1:A:520:ILE:HD12	2.22	0.55
1:B:31:THR:HG23	7:B:716:HOH:O	2.08	0.54
1:B:81:ARG:NH2	1:B:520:ILE:HD12	2.24	0.52
1:A:310:ASN:HB2	1:A:331:TRP:HB2	1.94	0.50
1:B:310:ASN:HB2	1:B:331:TRP:HB2	1.95	0.48
1:B:336:PHE:CZ	1:B:338:TYR:CD2	3.03	0.47
1:A:336:PHE:CZ	1:A:338:TYR:CD2	3.03	0.46
1:A:349:ASN:HB2	1:A:352[A]:GLU:OE1	2.18	0.44
1:B:76:HIS:HD2	7:B:911:HOH:O	2.00	0.44
1:B:138:PRO:HD2	1:B:183:ILE:CD1	2.49	0.43
1:A:138:PRO:HD2	1:A:183:ILE:CD1	2.49	0.43
1:A:255:THR:HB	1:A:256:PRO:HD2	2.01	0.42
1:A:310:ASN:HD22	1:A:310:ASN:N	2.18	0.42
1:B:141:GLU:HG3	1:B:212:LEU:HD22	2.02	0.41
1:B:349:ASN:HB2	1:B:352:GLU:OE1	2.20	0.41
1:A:478:ALA:HB1	1:A:483:ASP:HB3	2.02	0.41
1:A:141:GLU:HG3	1:A:212:LEU:HD22	2.03	0.41
1:B:310:ASN:HD22	1:B:310:ASN:N	2.19	0.41
1:B:255:THR:HB	1:B:256:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/533 (96%)	497 (97%)	14 (3%)	0	100	100
1	B	511/533 (96%)	498 (98%)	13 (2%)	0	100	100
All	All	1022/1066 (96%)	995 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	460/475 (97%)	455 (99%)	5 (1%)	73	85
1	B	459/475 (97%)	455 (99%)	4 (1%)	78	88
All	All	919/950 (97%)	910 (99%)	9 (1%)	76	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	266	SER
1	A	298	LYS
1	A	310	ASN
1	A	502	LEU
1	B	126	VAL
1	B	266	SER
1	B	310	ASN

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Mol	Chain	Res	Type
1	B	502	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	PLM	A	602	2	17,17,17	0.60	0	17,17,17	0.68	0
4	8D7	A	603	-	20,20,20	0.40	0	23,24,24	0.75	1 (4%)
6	PG6	A	605	5	15,15,17	0.50	0	14,14,16	0.44	0
6	PG6	B	604	5	12,12,17	0.49	0	11,11,16	0.56	0
3	PLM	B	602	2	17,17,17	0.46	0	17,17,17	0.88	0
4	8D7	B	603	-	20,20,20	0.39	0	23,24,24	0.73	1 (4%)

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
3	PLM	A	602	2	-	8/15/15/15	-
4	8D7	A	603	-	-	2/18/18/18	0/1/1/1
6	PG6	A	605	5	-	4/13/13/15	-
6	PG6	B	604	5	-	0/10/10/15	-
3	PLM	B	602	2	-	8/15/15/15	-
4	8D7	B	603	-	-	0/18/18/18	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	8D7	C7-O-C8	2.18	122.55	117.93
4	B	603	8D7	C7-O-C8	2.06	122.29	117.93

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	605	PG6	O1-C2-C3-O2
3	B	602	PLM	C9-CA-CB-CC
3	A	602	PLM	C9-CA-CB-CC
6	A	605	PG6	O5-C10-C11-O6
3	B	602	PLM	C2-C3-C4-C5
3	A	602	PLM	C2-C3-C4-C5
6	A	605	PG6	C2-C3-O2-C4
6	A	605	PG6	C5-C4-O2-C3
3	A	602	PLM	C6-C7-C8-C9
3	A	602	PLM	C3-C4-C5-C6
3	B	602	PLM	C3-C4-C5-C6
3	B	602	PLM	CB-CC-CD-CE
3	B	602	PLM	CA-CB-CC-CD
3	A	602	PLM	CA-CB-CC-CD
3	A	602	PLM	CC-CD-CE-CF
4	A	603	8D7	C11-C12-C13-C14
3	A	602	PLM	CB-CC-CD-CE
4	A	603	8D7	C11-C12-C13-O1
3	B	602	PLM	O2-C1-C2-C3
3	B	602	PLM	O1-C1-C2-C3
3	B	602	PLM	CC-CD-CE-CF

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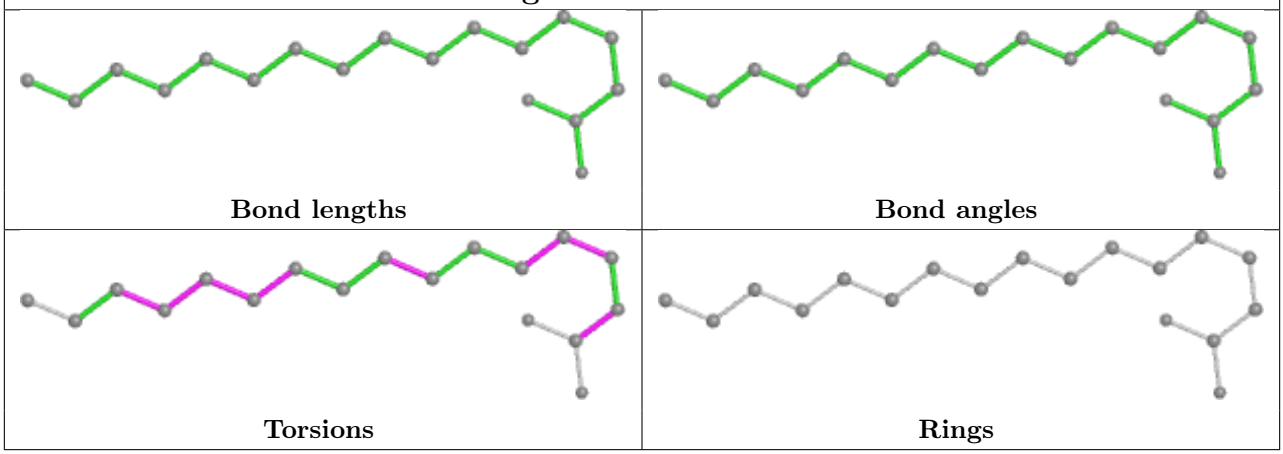
Mol	Chain	Res	Type	Atoms
3	A	602	PLM	O2-C1-C2-C3

There are no ring outliers.

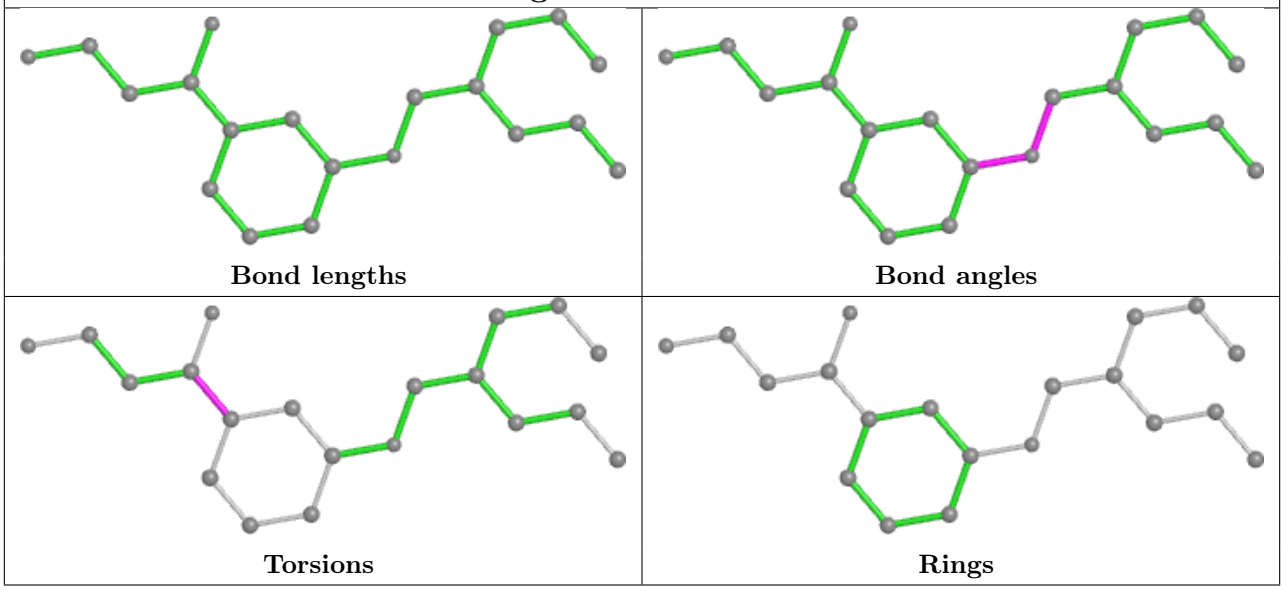
No monomer is involved in short contacts.

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

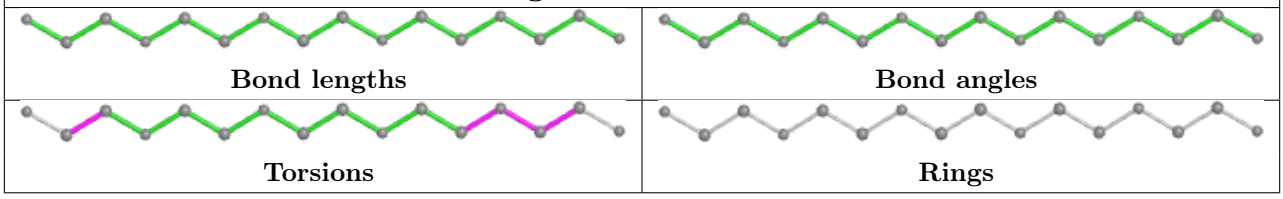
Ligand PLM A 602



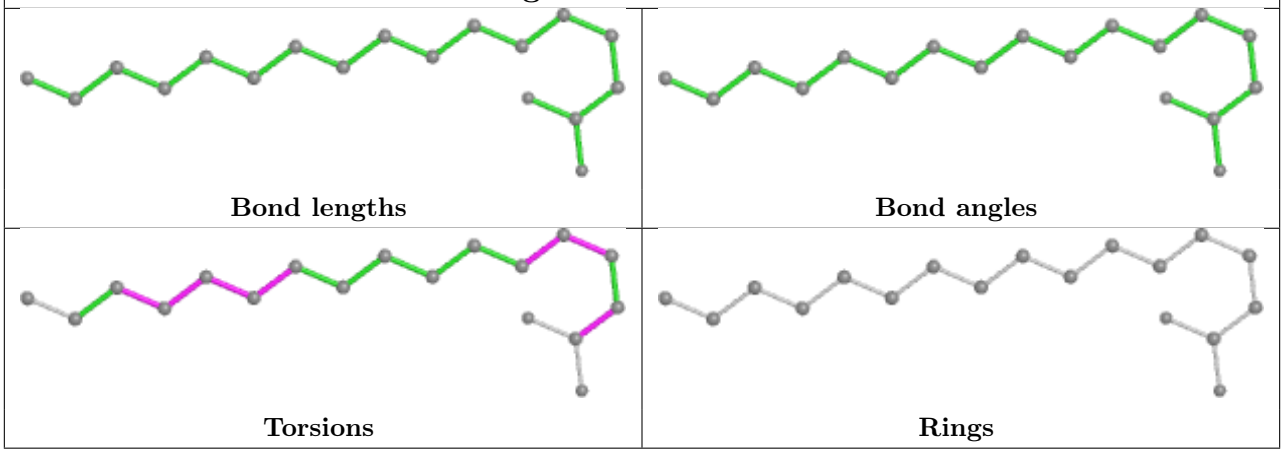
Ligand 8D7 A 603

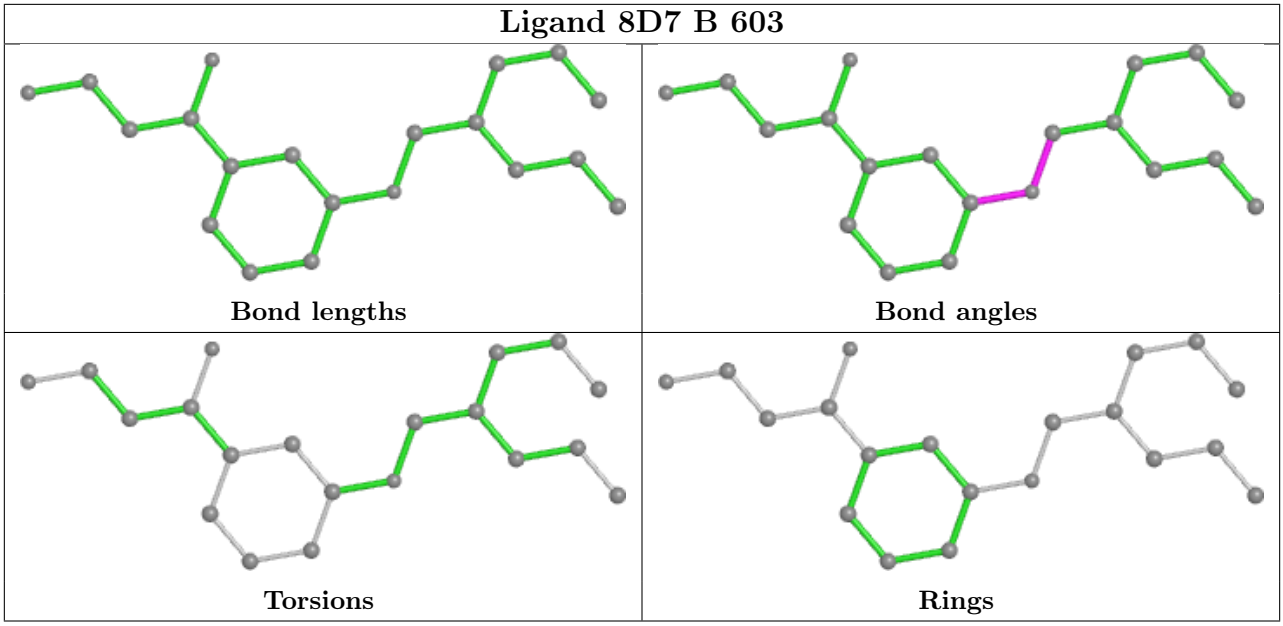


Ligand PG6 A 605



Ligand PLM B 602





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	511/533 (95%)	-0.59	12 (2%)	60	58	29, 41, 70, 126	0
1	B	513/533 (96%)	-0.51	16 (3%)	49	47	28, 40, 66, 121	0
All	All	1024/1066 (96%)	-0.55	28 (2%)	54	52	28, 41, 69, 126	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	TRP	8.1
1	A	271	TRP	7.6
1	A	270	LEU	6.5
1	B	270	LEU	5.8
1	B	265	LEU	5.4
1	A	495	ALA	5.3
1	A	269	SER	4.8
1	A	265	LEU	4.6
1	B	269	SER	4.0
1	A	496	GLY	4.0
1	B	267	SER	3.9
1	B	264	PHE	3.9
1	A	214	ALA	3.6
1	B	266	SER	3.5
1	A	497	GLN	2.9
1	B	234	ARG	2.9
1	A	267	SER	2.8
1	B	125	GLY	2.8
1	B	108	PHE	2.7
1	A	264	PHE	2.7
1	A	262	PHE	2.6
1	B	235	PHE	2.6
1	B	495	ALA	2.6
1	A	234	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	268	TRP	2.2
1	B	214	ALA	2.2
1	B	262	PHE	2.1
1	B	109	PRO	2.1

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)

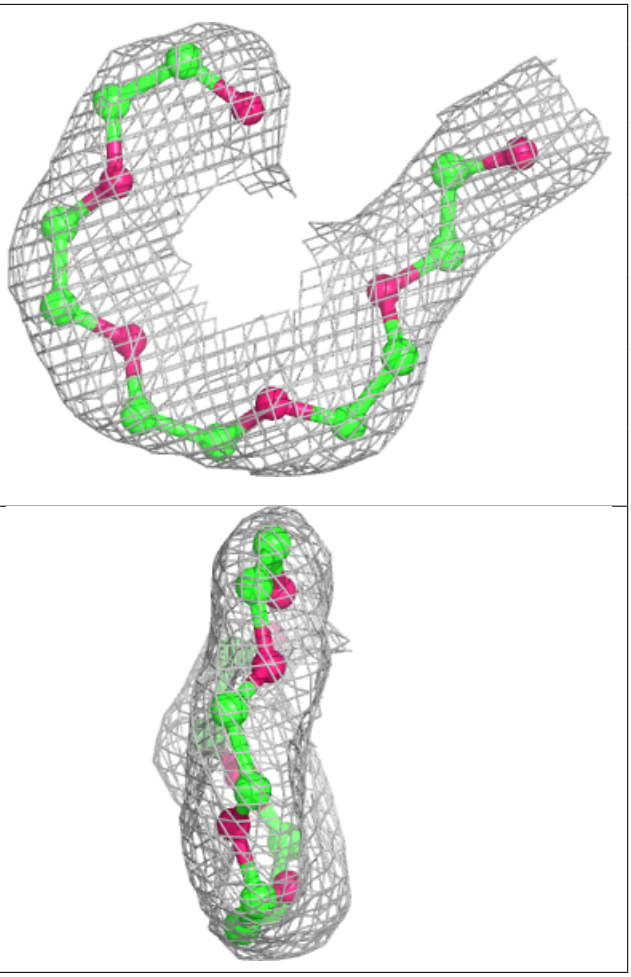
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	A	604	1/1	0.91	0.14	58,58,58,58	0
6	PG6	A	605	16/18	0.93	0.26	52,63,76,77	0
6	PG6	B	604	13/18	0.94	0.11	46,52,64,65	0
3	PLM	A	602	18/18	0.95	0.19	52,56,59,59	0
5	NA	B	605	1/1	0.95	0.17	53,53,53,53	0
3	PLM	B	602	18/18	0.96	0.28	47,49,52,54	0
4	8D7	B	603	20/20	0.96	0.13	35,39,51,52	0
4	8D7	A	603	20/20	0.97	0.11	33,40,49,49	0
2	FE2	A	601	1/1	1.00	0.13	36,36,36,36	0
2	FE2	B	601	1/1	1.00	0.14	33,33,33,33	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.

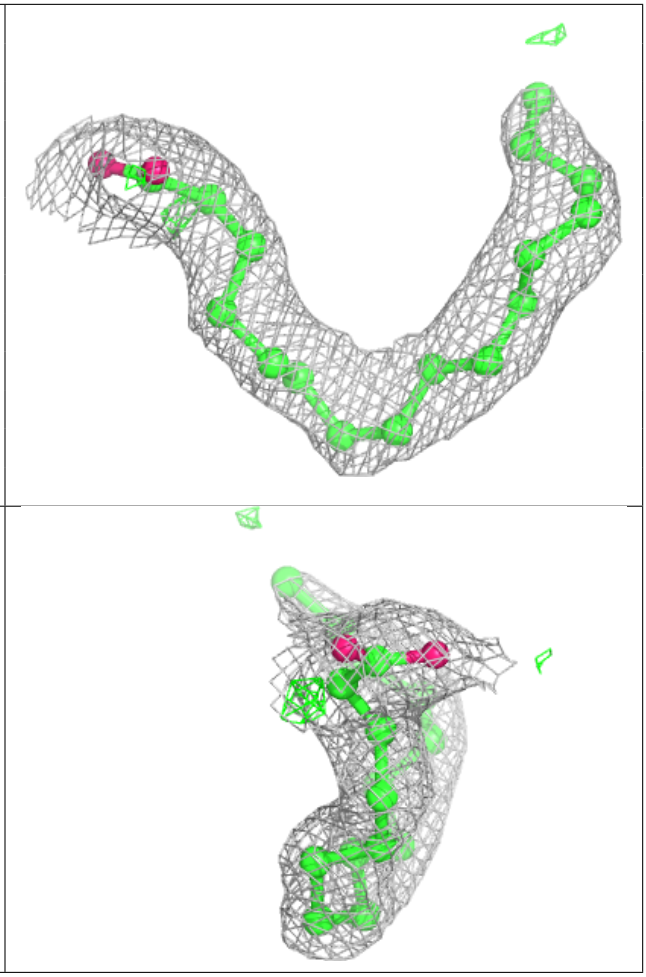
Electron density around PG6 A 605:

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



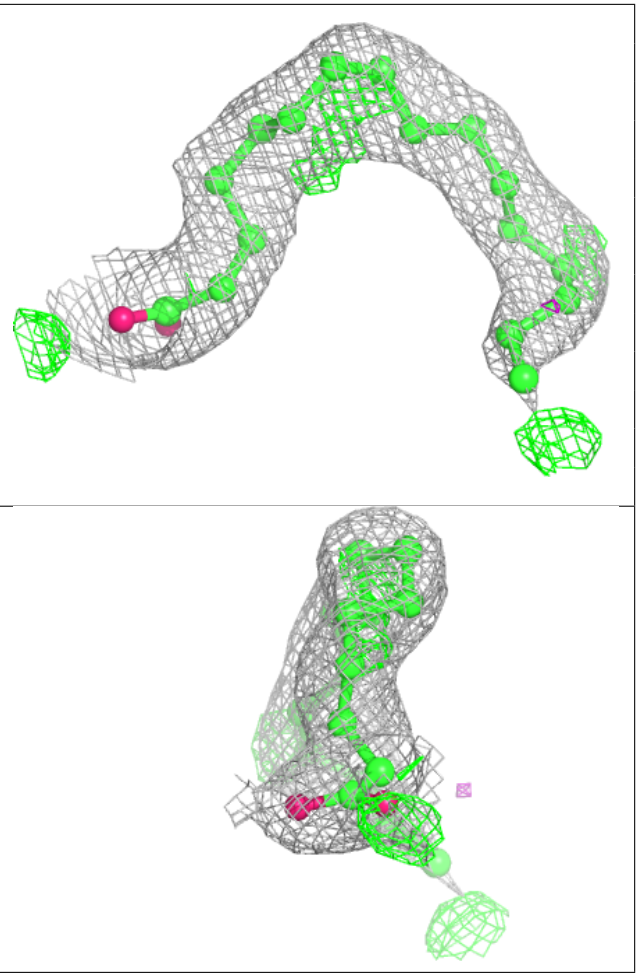
Electron density around PLM A 602:

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



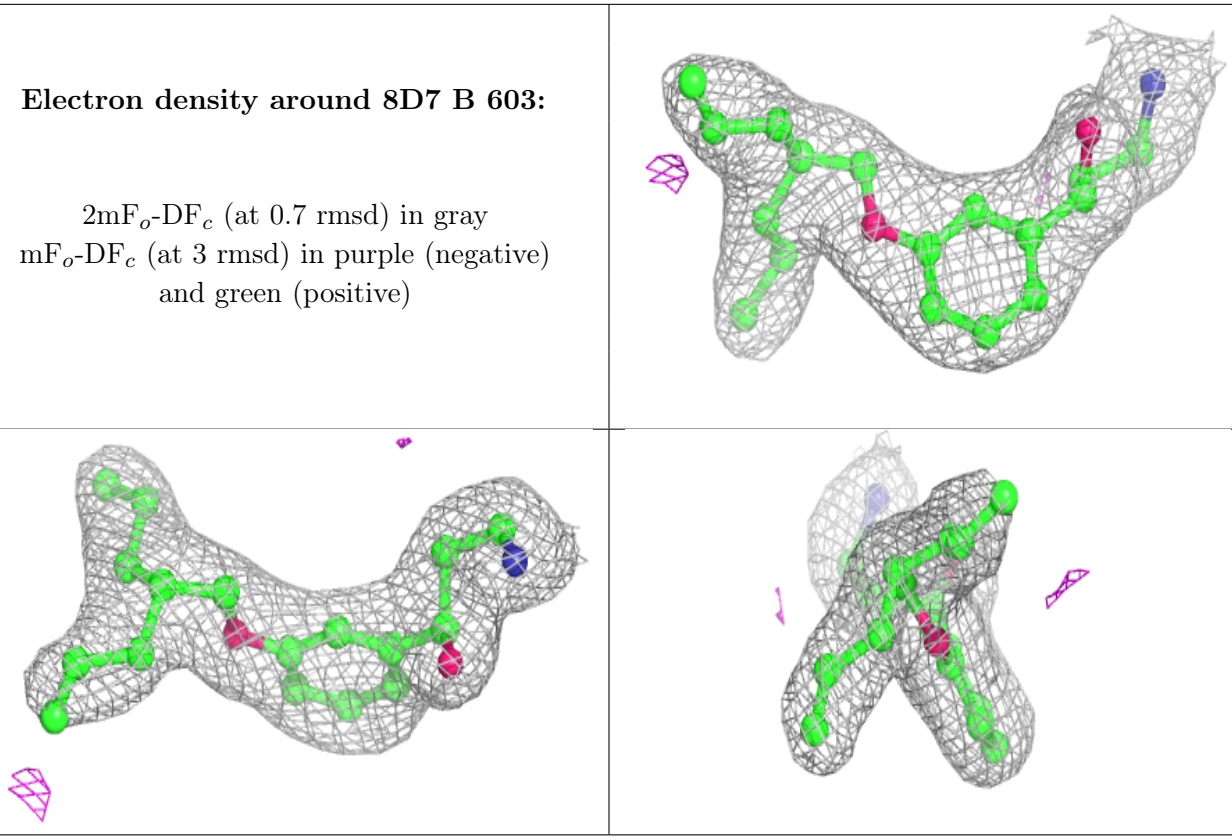
Electron density around PLM B 602:

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



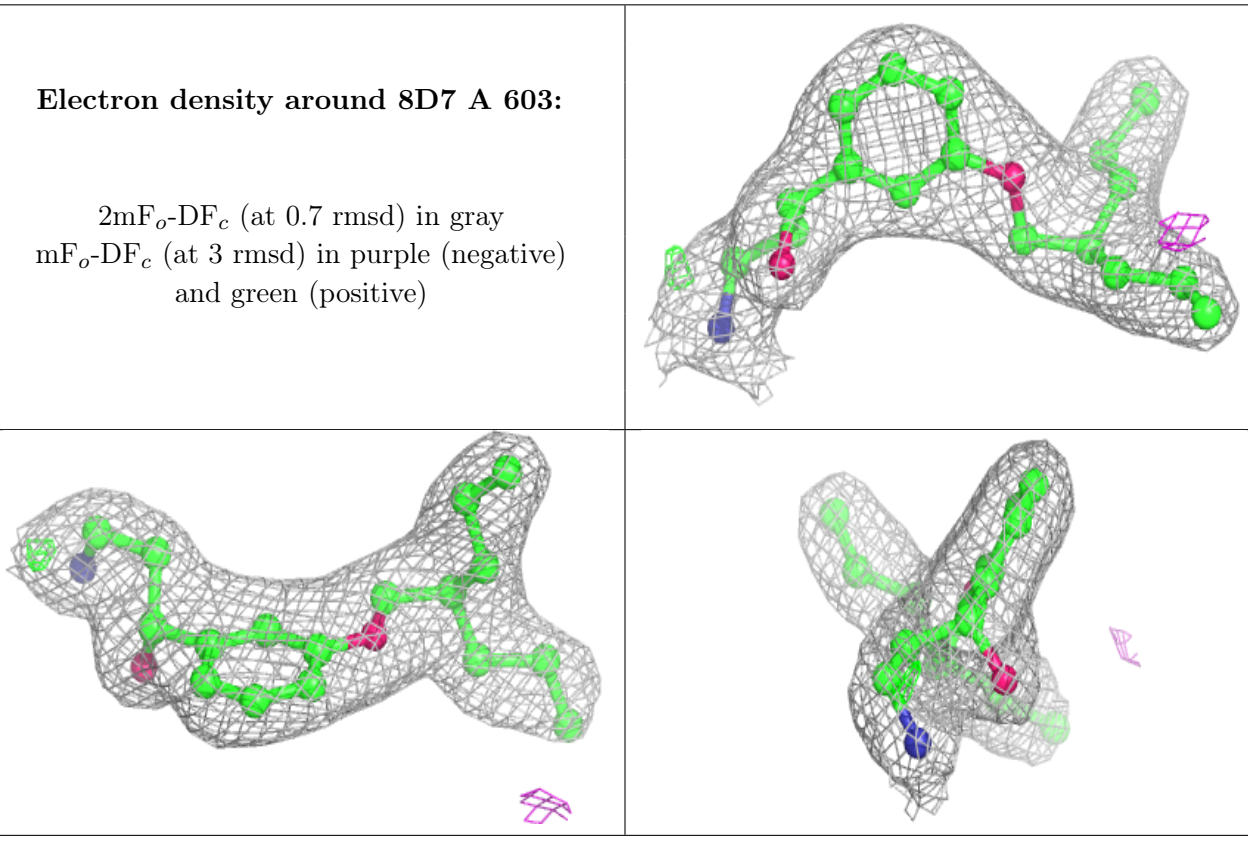
Electron density around 8D7 B 603:

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



Electron density around 8D7 A 603:

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



6.5 Other polymers (i)

There are no such residues in this entry.