Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:49 pm BST

PDB ID	:	4U15
Title	:	M3-mT4L receptor bound to tiotropium
Authors	:	Thorsen, T.S.; Matt, R.; Weis, W.I.; Kobilka, B.
Deposited on	:	2014-07-15
Resolution	:	2.80 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:

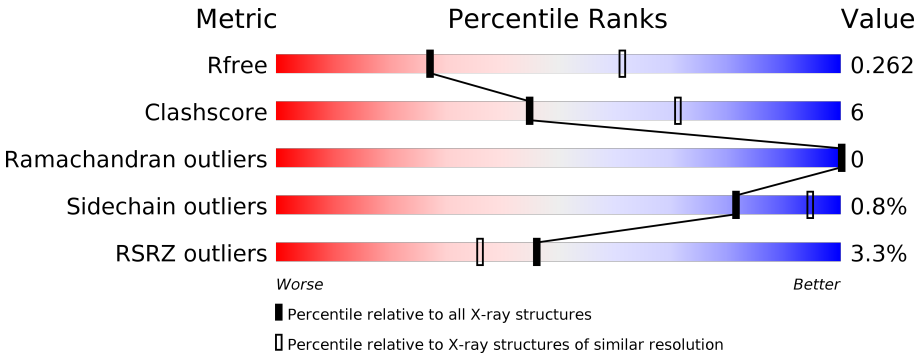
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	418	4% 78% 15% 6%
1	B	418	2% 80% 14% 6%

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
5	OLC	B	1202	-	-	-	X
5	OLC	B	1203	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6342 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 Muscarinic acetylcholine receptor M3,Lysozyme,Muscarinic acetylcholine receptor M3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3048	1997	499	532	20			
1	B	392	Total	C	N	O	S	0	0	0
			3075	2019	503	533	20			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	GLY	-	expression tag	UNP P08483
A	1001	MET	-	linker	UNP P08483
A	1002	ASN	-	linker	UNP P08483
A	1003	ILE	-	linker	UNP P08483
A	1004	PHE	-	linker	UNP P08483
A	1005	GLU	-	linker	UNP P08483
A	1006	MET	-	linker	UNP P08483
A	1007	LEU	-	linker	UNP P08483
A	1008	ARG	-	linker	UNP P08483
A	1009	ILE	-	linker	UNP P08483
A	1010	ASP	-	linker	UNP P08483
A	1011	GLU	-	linker	UNP P08483
A	1012	GLY	-	linker	UNP P08483
A	1013	GLY	-	linker	UNP P08483
A	1014	GLY	-	linker	UNP P08483
A	1015	SER	-	linker	UNP P08483
A	1016	GLY	-	linker	UNP P08483
A	1017	GLY	-	linker	UNP P08483
A	1054	ALA	CYS	conflict	UNP D9IEF7
A	564	LYS	-	expression tag	UNP P08483
A	565	ARG	-	expression tag	UNP P08483
A	566	LYS	-	expression tag	UNP P08483
A	567	ARG	-	expression tag	UNP P08483
A	568	ARG	-	expression tag	UNP P08483

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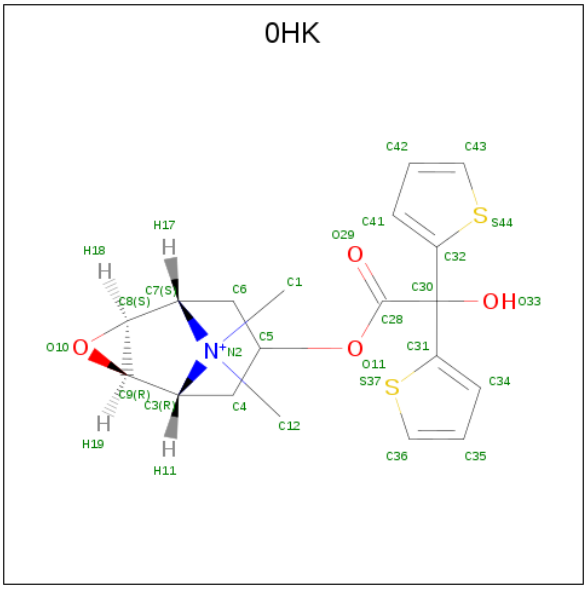
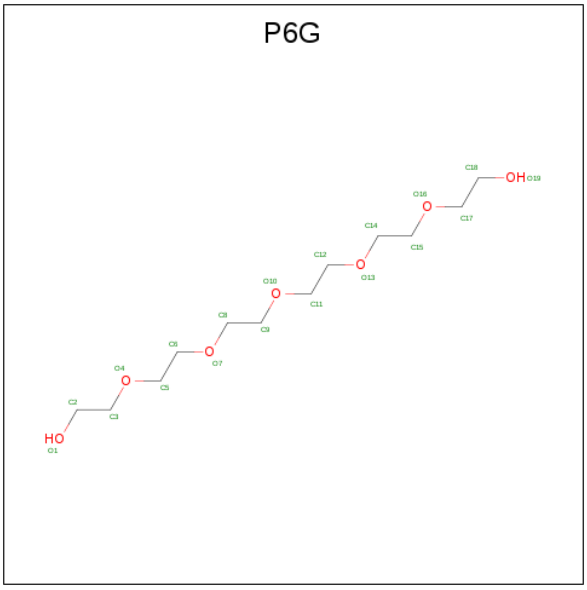
Chain	Residue	Modelled	Actual	Comment	Reference
A	569	LYS	-	expression tag	UNP P08483
A	570	HIS	-	expression tag	UNP P08483
A	571	HIS	-	expression tag	UNP P08483
A	572	HIS	-	expression tag	UNP P08483
A	573	HIS	-	expression tag	UNP P08483
A	574	HIS	-	expression tag	UNP P08483
A	575	HIS	-	expression tag	UNP P08483
A	576	HIS	-	expression tag	UNP P08483
A	577	HIS	-	expression tag	UNP P08483
B	56	GLY	-	expression tag	UNP P08483
B	1001	MET	-	linker	UNP P08483
B	1002	ASN	-	linker	UNP P08483
B	1003	ILE	-	linker	UNP P08483
B	1004	PHE	-	linker	UNP P08483
B	1005	GLU	-	linker	UNP P08483
B	1006	MET	-	linker	UNP P08483
B	1007	LEU	-	linker	UNP P08483
B	1008	ARG	-	linker	UNP P08483
B	1009	ILE	-	linker	UNP P08483
B	1010	ASP	-	linker	UNP P08483
B	1011	GLU	-	linker	UNP P08483
B	1012	GLY	-	linker	UNP P08483
B	1013	GLY	-	linker	UNP P08483
B	1014	GLY	-	linker	UNP P08483
B	1015	SER	-	linker	UNP P08483
B	1016	GLY	-	linker	UNP P08483
B	1017	GLY	-	linker	UNP P08483
B	1054	ALA	CYS	conflict	UNP D9IEF7
B	564	LYS	-	expression tag	UNP P08483
B	565	ARG	-	expression tag	UNP P08483
B	566	LYS	-	expression tag	UNP P08483
B	567	ARG	-	expression tag	UNP P08483
B	568	ARG	-	expression tag	UNP P08483
B	569	LYS	-	expression tag	UNP P08483
B	570	HIS	-	expression tag	UNP P08483
B	571	HIS	-	expression tag	UNP P08483
B	572	HIS	-	expression tag	UNP P08483
B	573	HIS	-	expression tag	UNP P08483
B	574	HIS	-	expression tag	UNP P08483
B	575	HIS	-	expression tag	UNP P08483
B	576	HIS	-	expression tag	UNP P08483
B	577	HIS	-	expression tag	UNP P08483

- Molecule 2 is (1R,2R,4S,5S,7S)-7-{[hydroxy(dithiophen-2-yl)acetyl]oxy}-9,9-dimethyl-3-oxa-9-azoniatricyclo[3.3.1.0 2,4]nonane (three-letter code: 0HK) (formula: $C_{19}H_{22}NO_4S_2$).



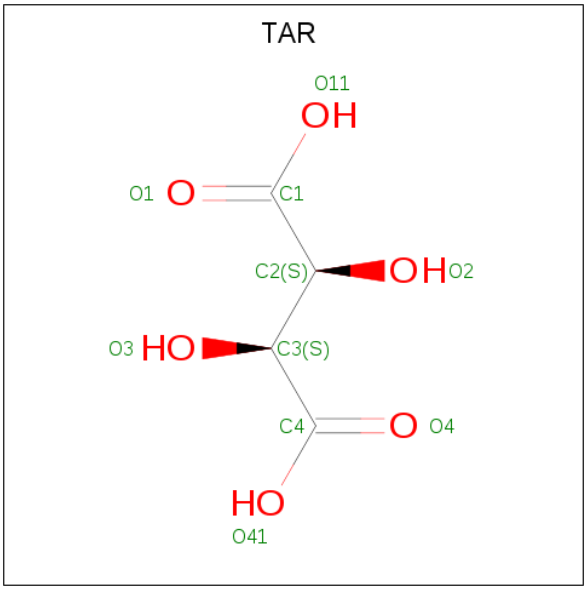
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	19	1	4	2		
2	B	1	Total	C	N	O	S	0	0
			26	19	1	4	2		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



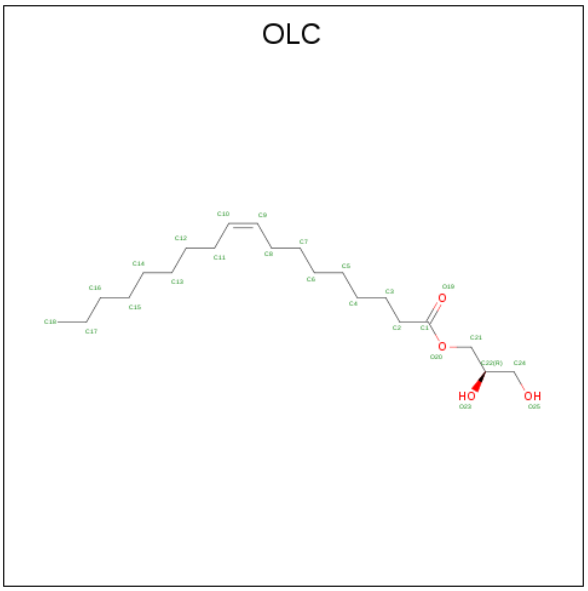
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0
3	A	1	Total C O 19 12 7	0	0
3	A	1	Total C O 19 12 7	0	0
3	B	1	Total C O 19 12 7	0	0

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



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

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 25 21 4	0	0
5	B	1	Total C O 25 21 4	0	0

- Molecule 6 is water.

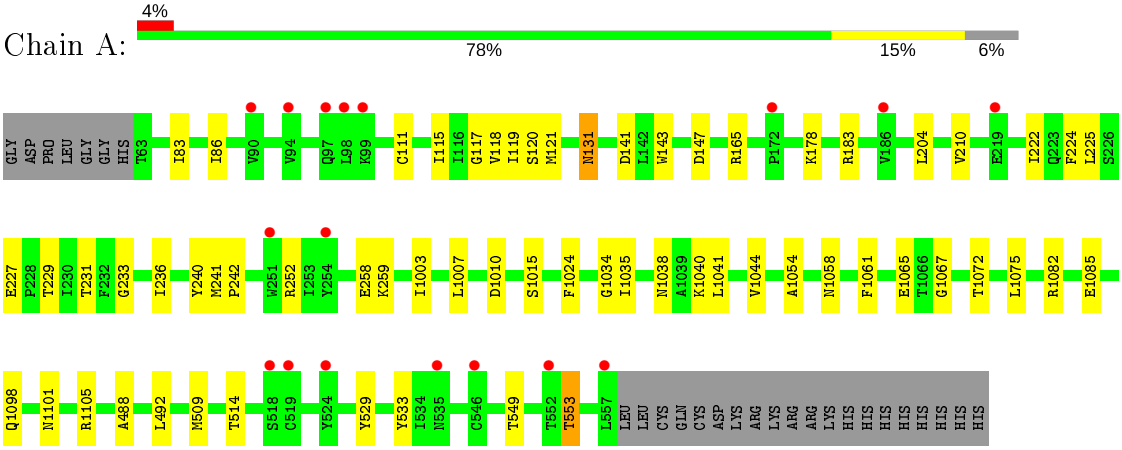
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0

3 Residue-property plots

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.

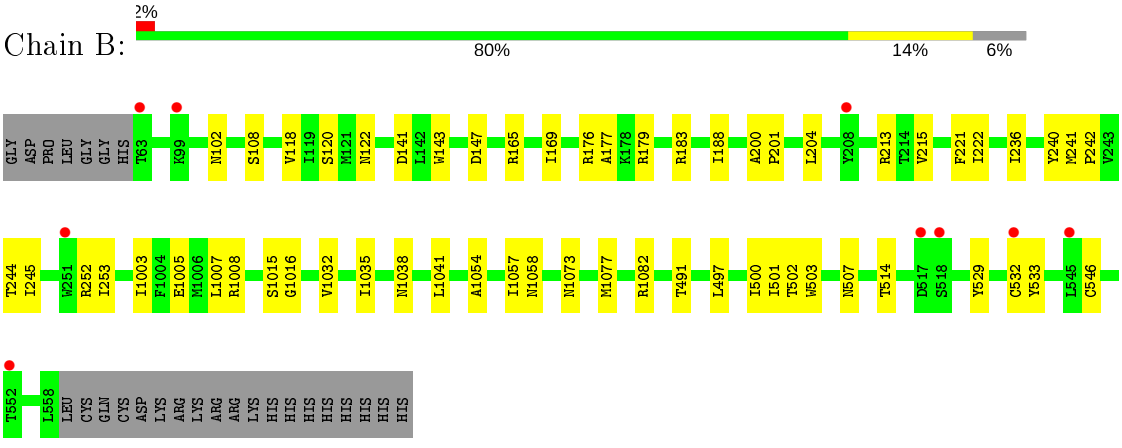
• Molecule 1: Muscarinic acetylcholine receptor M3,Lysozyme,Muscarinic acetylcholine receptor M3

Chain A:



• Molecule 1: Muscarinic acetylcholine receptor M3,Lysozyme,Muscarinic acetylcholine receptor M3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.31Å 184.56Å 52.61Å 90.00° 98.54° 90.00°	Depositor
Resolution (Å)	28.48 – 2.80 28.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (28.48-2.80) 90.5 (28.48-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.230 , 0.261 0.236 , 0.262	Depositor DCC
R_{free} test set	1704 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6342	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0HK, OLC, P6G, TAR

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	0.23	0/3125	0.37	0/4272
1	B	0.22	0/3150	0.37	0/4303
All	All	0.22	0/6275	0.37	0/8575

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3048	0	2983	42	0
1	B	3075	0	3065	37	0
2	A	26	0	22	4	0
2	B	26	0	22	3	0
3	A	57	0	78	6	0
3	B	19	0	26	4	0
4	A	20	0	8	1	0
4	B	20	0	8	2	0
5	B	50	0	80	1	0
6	A	1	0	0	0	0
All	All	6342	0	6292	82	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 6.

All (82) 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:1040:LYS:HZ1	1:A:1072:THR:HA	1.48	0.78
1:A:233:GLY:HA3	1:B:245:ILE:HD11	1.73	0.70
1:A:1101:ASN:ND2	4:A:2005:TAR:O3	2.31	0.64
1:B:1077:MET:HG2	1:B:1082:ARG:HH21	1.62	0.64
1:A:118:VAL:HG13	1:A:119:ILE:HG13	1.81	0.62
1:B:1005:GLU:OE2	1:B:1008:ARG:NE	2.24	0.58
1:B:503:TRP:O	1:B:507:ASN:ND2	2.32	0.57
1:A:1024:PHE:HD1	3:A:2002:P6G:H31	1.70	0.57
1:A:1024:PHE:HE1	3:A:2002:P6G:H82	1.69	0.57
1:B:118:VAL:O	1:B:122:ASN:ND2	2.37	0.57
1:A:514:THR:O	1:B:252:ARG:NH2	2.38	0.57
1:A:222:ILE:HD12	1:A:225:LEU:HD12	1.86	0.56
1:A:147:ASP:OD2	1:A:533:TYR:OH	2.22	0.56
1:A:165:ARG:NH1	1:A:488:ALA:HB1	2.21	0.56
1:B:491:THR:HG22	1:B:546:CYS:HB3	1.88	0.56
1:B:102:ASN:OD1	1:B:179:ARG:NH1	2.39	0.55
1:B:222:ILE:H	3:B:1204:P6G:H62	1.70	0.55
2:A:2001:0HK:H12	2:A:2001:0HK:H1	1.89	0.55
1:A:165:ARG:HD2	1:A:492:LEU:HD22	1.89	0.54
1:A:83:ILE:HA	1:A:86:ILE:HG22	1.90	0.53
1:B:108:SER:HB2	1:B:188:ILE:HD13	1.91	0.53
1:A:120:SER:HA	1:A:143:TRP:HE1	1.74	0.53
1:B:1035:ILE:HG23	1:B:1041:LEU:HB3	1.92	0.52
1:B:147:ASP:OD2	1:B:533:TYR:OH	2.23	0.52
1:A:178:LYS:O	1:A:183:ARG:NH1	2.43	0.52
1:A:236:ILE:HA	1:A:240:TYR:HB2	1.91	0.52
1:B:1073:ASN:HB2	4:B:1205:TAR:H2	1.91	0.51
1:A:529:TYR:CZ	2:A:2001:0HK:H22	2.46	0.51
1:A:227:GLU:HG3	1:A:229:THR:H	1.75	0.51
1:B:244:THR:HG22	5:B:1202:OLC:H6	1.94	0.49
1:B:213:ARG:NH1	1:B:215:VAL:O	2.45	0.49
1:B:497:LEU:HA	1:B:500:ILE:HG22	1.94	0.49
1:B:1003:ILE:HD13	1:B:1054:ALA:HB1	1.94	0.48
1:A:1040:LYS:NZ	1:A:1072:THR:HA	2.24	0.48
1:A:1067:GLY:HA2	3:A:2004:P6G:H51	1.95	0.48
1:A:549:THR:O	1:A:553:THR:OG1	2.33	0.47
1:A:258:GLU:HA	1:A:259:LYS:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ALA:HB3	1:B:201:PRO:HD3	1.98	0.46
1:B:532:CYS:SG	2:B:1201:0HK:H16	2.56	0.46
1:B:241:MET:HB3	1:B:242:PRO:HD3	1.98	0.46
1:A:141:ASP:HB3	1:A:204:LEU:HD23	1.96	0.46
3:A:2002:P6G:H141	3:A:2002:P6G:H112	1.64	0.45
2:A:2001:0HK:H20	2:A:2001:0HK:O10	2.17	0.45
1:B:1038:ASN:HB3	1:B:1041:LEU:HB2	1.97	0.45
1:A:231:THR:HG23	2:A:2001:0HK:H3	1.97	0.45
1:B:141:ASP:HB3	1:B:204:LEU:HD23	1.98	0.45
1:A:210:VAL:O	1:B:183:ARG:NH2	2.50	0.45
1:B:1032:VAL:HG22	1:B:1057:ILE:HD13	1.99	0.44
1:A:1035:ILE:HG23	1:A:1041:LEU:HB3	2.00	0.44
1:B:120:SER:HA	1:B:143:TRP:HE1	1.82	0.44
1:A:1038:ASN:HB3	1:A:1041:LEU:HB2	2.00	0.44
1:B:177:ALA:HB2	1:B:1015:SER:HB2	1.98	0.44
1:A:252:ARG:NH2	1:B:514:THR:O	2.37	0.44
1:A:241:MET:HB3	1:A:242:PRO:HD3	1.98	0.44
1:A:165:ARG:HH11	1:A:488:ALA:HB1	1.83	0.44
1:B:236:ILE:HA	1:B:240:TYR:HB2	2.01	0.43
1:A:1082:ARG:NH2	1:A:1085:GLU:OE1	2.35	0.43
1:B:176:ARG:HA	1:B:179:ARG:HG3	2.00	0.43
1:B:1015:SER:HA	1:B:1016:GLY:HA3	1.78	0.43
3:A:2004:P6G:H52	3:A:2004:P6G:H81	1.74	0.43
1:A:1098:GLN:NE2	3:A:2004:P6G:O19	2.51	0.43
1:A:1003:ILE:HD13	1:A:1054:ALA:HB1	2.00	0.42
1:B:165:ARG:HB3	1:B:253:ILE:HD13	2.02	0.42
1:A:1007:LEU:HD21	1:A:1058:ASN:HA	2.01	0.42
1:A:1034:GLY:HA3	1:A:1065:GLU:OE2	2.20	0.42
1:A:1044:VAL:HG21	1:A:1075:LEU:HB3	2.01	0.42
1:A:509:MET:HE2	1:A:509:MET:HB3	1.93	0.42
1:B:169:ILE:HD12	1:B:253:ILE:HG23	2.02	0.42
1:A:1040:LYS:HZ1	1:A:1072:THR:HG23	1.85	0.42
2:B:1201:0HK:H20	2:B:1201:0HK:O10	2.19	0.42
1:B:221:PHE:HB2	3:B:1204:P6G:H32	2.02	0.42
1:A:117:GLY:HA2	1:A:121:MET:SD	2.60	0.41
1:A:1010:ASP:HA	1:A:1105:ARG:HH21	1.85	0.41
1:B:176:ARG:NH2	4:B:1206:TAR:O1	2.49	0.41
1:A:111:CYS:O	1:A:115:ILE:HG13	2.21	0.41
1:B:529:TYR:CE2	3:B:1204:P6G:H91	2.56	0.41
1:A:1040:LYS:HZ1	1:A:1072:THR:CA	2.26	0.41
1:B:501:ILE:HG23	1:B:502:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:LEU:HD21	1:B:1058:ASN:HA	2.03	0.40
3:B:1204:P6G:H122	3:B:1204:P6G:H92	1.78	0.40
1:A:131:ASN:ND2	1:A:131:ASN:O	2.44	0.40
2:B:1201:0HK:H1	2:B:1201:0HK:H12	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	389/418 (93%)	377 (97%)	12 (3%)	0	100	100
1	B	390/418 (93%)	376 (96%)	14 (4%)	0	100	100
All	All	779/836 (93%)	753 (97%)	26 (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	310/360 (86%)	305 (98%)	5 (2%)	62	88
1	B	319/360 (89%)	319 (100%)	0	100	100
All	All	629/720 (87%)	624 (99%)	5 (1%)	81	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	224	PHE
1	A	1015	SER
1	A	1061	PHE
1	A	553	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	1026	GLN
1	A	1089	ASN
1	A	1098	GLN
1	A	1101	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)

12 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	$\#\|Z\|>2$
3	P6G	A	2002	-	18,18,18	0.63	0	17,17,17	0.50	0
2	0HK	A	2001	-	28,30,30	1.67	6 (21%)	38,48,48	5.16	17 (44%)
5	OLC	B	1202	-	24,24,24	0.94	1 (4%)	25,25,25	0.78	0
2	0HK	B	1201	-	28,30,30	1.66	7 (25%)	38,48,48	5.16	18 (47%)
4	TAR	A	2006	-	3,9,9	0.35	0	6,12,12	1.09	0
3	P6G	A	2004	-	18,18,18	0.59	0	17,17,17	0.46	0
4	TAR	B	1206	-	3,9,9	0.39	0	6,12,12	0.89	0
3	P6G	B	1204	-	18,18,18	0.60	0	17,17,17	0.50	0
4	TAR	A	2005	-	3,9,9	0.25	0	6,12,12	0.94	0
3	P6G	A	2003	-	18,18,18	0.58	0	17,17,17	0.55	0
5	OLC	B	1203	-	24,24,24	0.95	1 (4%)	25,25,25	0.90	0
4	TAR	B	1205	-	3,9,9	0.39	0	6,12,12	1.07	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
3	P6G	A	2002	-	-	3/16/16/16	-
2	0HK	A	2001	-	-	6/10/55/55	0/6/5/5
5	OLC	B	1202	-	-	1/24/24/24	-
2	0HK	B	1201	-	-	1/10/55/55	0/6/5/5
4	TAR	A	2006	-	-	0/4/12/12	-
3	P6G	A	2004	-	-	7/16/16/16	-
4	TAR	B	1206	-	-	0/4/12/12	-
3	P6G	B	1204	-	-	6/16/16/16	-
4	TAR	A	2005	-	-	0/4/12/12	-
3	P6G	A	2003	-	-	3/16/16/16	-
5	OLC	B	1203	-	-	1/24/24/24	-
4	TAR	B	1205	-	-	0/4/12/12	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	0HK	O11-C28	3.98	1.41	1.34
5	B	1202	OLC	C9-C10	3.80	1.53	1.31
2	B	1201	0HK	O11-C28	3.74	1.41	1.34
5	B	1203	OLC	C9-C10	3.73	1.53	1.31
2	A	2001	0HK	C1-N2	-3.25	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	0HK	C1-N2	-3.25	1.44	1.51
2	A	2001	0HK	O33-C30	-2.51	1.38	1.43
2	B	1201	0HK	C31-S37	2.46	1.78	1.74
2	A	2001	0HK	C31-S37	2.42	1.78	1.74
2	B	1201	0HK	C32-S44	2.41	1.78	1.74
2	B	1201	0HK	O33-C30	-2.40	1.38	1.43
2	A	2001	0HK	C12-N2	-2.38	1.46	1.51
2	B	1201	0HK	C12-N2	-2.38	1.46	1.51
2	A	2001	0HK	C32-S44	2.25	1.78	1.74
2	B	1201	0HK	O11-C5	-2.10	1.41	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	0HK	C42-C43-S44	-13.80	101.78	112.98
2	B	1201	0HK	C35-C36-S37	-13.73	101.83	112.98
2	A	2001	0HK	C42-C43-S44	-13.43	102.07	112.98
2	A	2001	0HK	C35-C36-S37	-13.36	102.14	112.98
2	A	2001	0HK	C4-C3-N2	11.76	116.21	108.82
2	B	1201	0HK	C6-C7-N2	10.31	115.30	108.82
2	A	2001	0HK	C6-C7-N2	10.22	115.25	108.82
2	B	1201	0HK	C4-C3-N2	10.17	115.22	108.82
2	A	2001	0HK	C3-C9-C8	-8.06	102.52	107.46
2	B	1201	0HK	C3-C9-C8	-7.96	102.58	107.46
2	B	1201	0HK	O10-C9-C3	7.51	124.13	117.11
2	A	2001	0HK	O10-C9-C3	7.49	124.11	117.11
2	B	1201	0HK	C7-C8-C9	-7.45	102.89	107.46
2	A	2001	0HK	C7-C8-C9	-7.16	103.07	107.46
2	B	1201	0HK	C8-C7-N2	6.74	107.73	103.54
2	B	1201	0HK	O10-C8-C7	6.38	123.07	117.11
2	A	2001	0HK	O10-C8-C7	6.36	123.06	117.11
2	A	2001	0HK	C8-C7-N2	6.14	107.36	103.54
2	B	1201	0HK	C9-C3-N2	6.02	107.28	103.54
2	A	2001	0HK	C9-C3-N2	5.56	107.00	103.54
2	A	2001	0HK	C4-C3-C9	-4.58	103.26	107.04
2	B	1201	0HK	C6-C7-C8	-4.25	103.53	107.04
2	B	1201	0HK	C34-C31-S37	-4.24	101.44	111.36
2	A	2001	0HK	O11-C28-C30	4.14	117.21	110.82
2	B	1201	0HK	C41-C32-S44	-4.06	101.86	111.36
2	A	2001	0HK	C34-C31-S37	-3.99	102.03	111.36
2	A	2001	0HK	C41-C32-S44	-3.93	102.18	111.36
2	A	2001	0HK	C6-C7-C8	-3.57	104.09	107.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	0HK	C4-C3-C9	-3.25	104.36	107.04
2	B	1201	0HK	O11-C28-O29	-3.03	118.51	123.97
2	B	1201	0HK	C9-O10-C8	2.78	63.34	60.78
2	A	2001	0HK	C5-O11-C28	2.77	122.07	117.66
2	B	1201	0HK	C5-O11-C28	2.72	121.99	117.66
2	B	1201	0HK	O11-C28-C30	2.72	115.01	110.82
2	A	2001	0HK	C9-O10-C8	2.71	63.28	60.78

There are no chirality outliers.

All (28) torsion outliers are listed below:

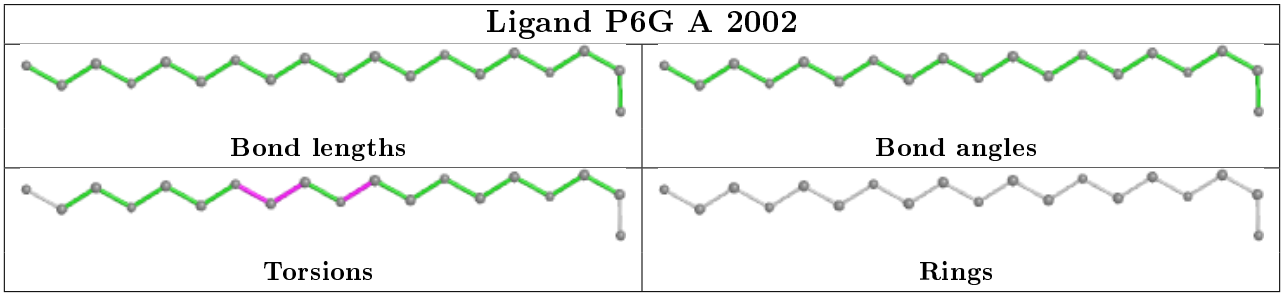
Mol	Chain	Res	Type	Atoms
2	A	2001	0HK	O29-C28-C30-O33
2	A	2001	0HK	O11-C28-C30-O33
2	B	1201	0HK	O29-C28-O11-C5
2	A	2001	0HK	C30-C28-O11-C5
2	A	2001	0HK	O29-C28-C30-C32
3	A	2002	P6G	C11-C12-O13-C14
2	A	2001	0HK	O11-C28-C30-C32
3	B	1204	P6G	C6-C5-O4-C3
3	B	1204	P6G	C12-C11-O10-C9
3	B	1204	P6G	C5-C6-O7-C8
3	A	2003	P6G	C2-C3-O4-C5
2	A	2001	0HK	O29-C28-C30-C31
3	A	2004	P6G	C12-C11-O10-C9
3	A	2004	P6G	C15-C14-O13-C12
3	A	2004	P6G	O4-C5-C6-O7
3	B	1204	P6G	O4-C5-C6-O7
3	B	1204	P6G	O7-C8-C9-O10
3	A	2004	P6G	O7-C8-C9-O10
3	A	2004	P6G	O13-C14-C15-O16
3	A	2003	P6G	O4-C5-C6-O7
5	B	1202	OLC	C7-C8-C9-C10
3	A	2004	P6G	C5-C6-O7-C8
3	A	2002	P6G	O10-C11-C12-O13
3	B	1204	P6G	C18-C17-O16-C15
5	B	1203	OLC	C7-C8-C9-C10
3	A	2002	P6G	C8-C9-O10-C11
3	A	2004	P6G	C2-C3-O4-C5
3	A	2003	P6G	C12-C11-O10-C9

There are no ring outliers.

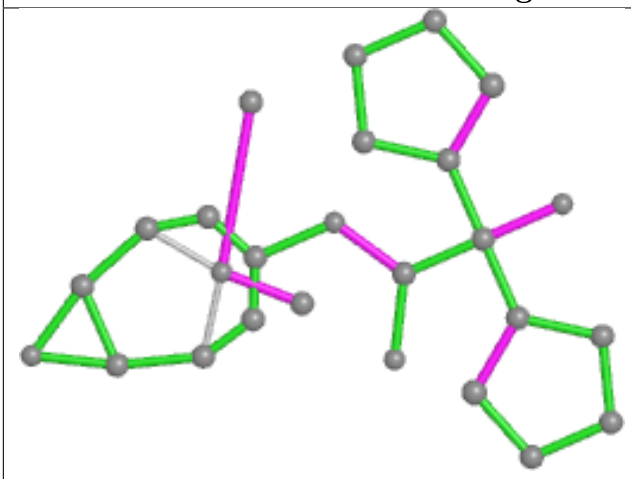
9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2002	P6G	3	0
2	A	2001	0HK	4	0
5	B	1202	OLC	1	0
2	B	1201	0HK	3	0
3	A	2004	P6G	3	0
4	B	1206	TAR	1	0
3	B	1204	P6G	4	0
4	A	2005	TAR	1	0
4	B	1205	TAR	1	0

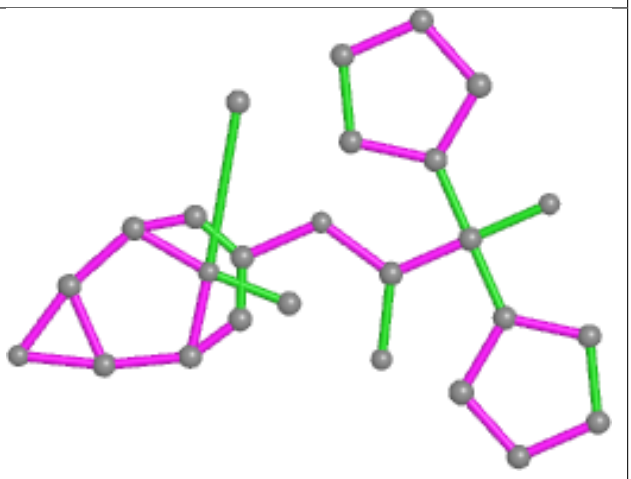
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



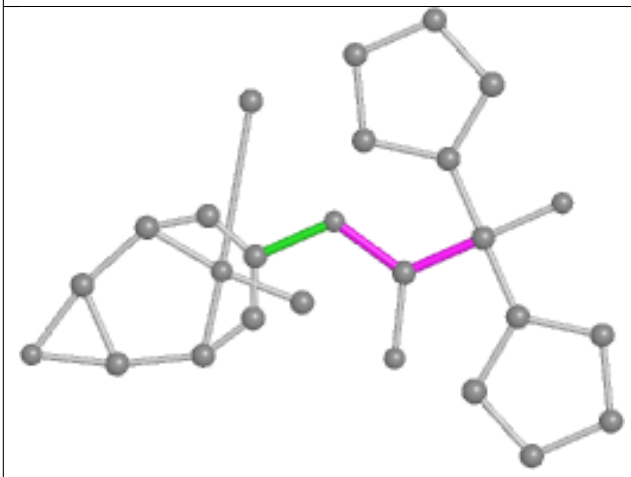
Ligand 0HK A 2001



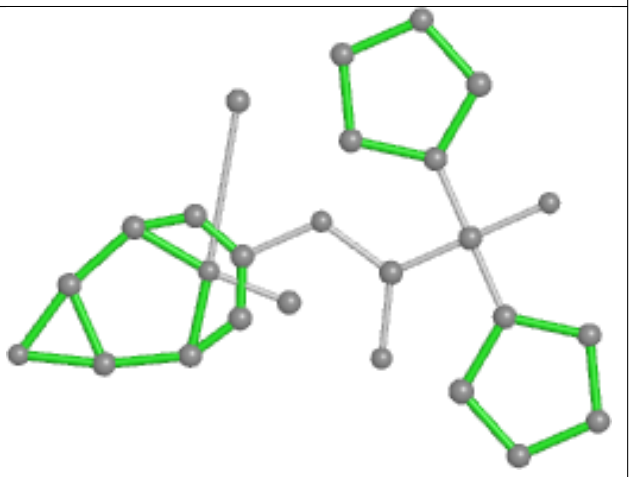
Bond lengths



Bond angles

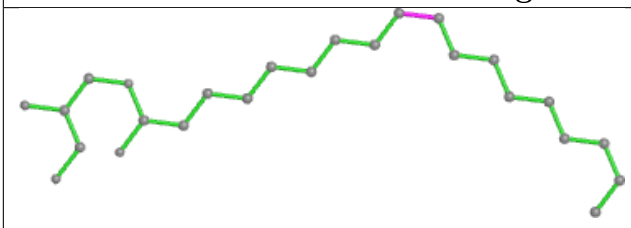


Torsions



Rings

Ligand OLC B 1202



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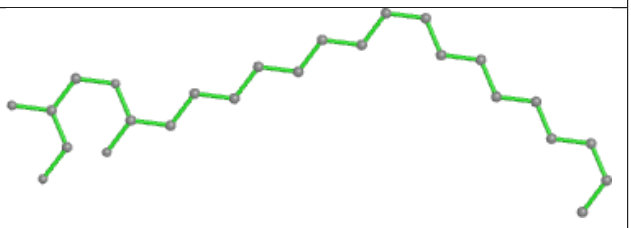
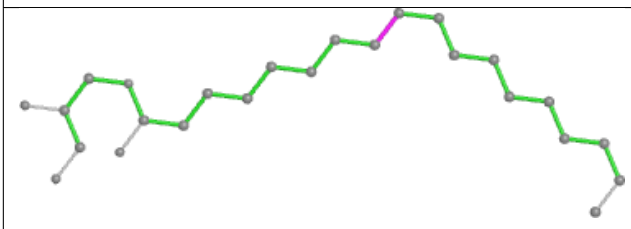
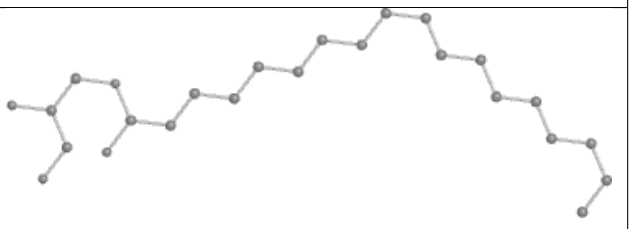


Bond angles

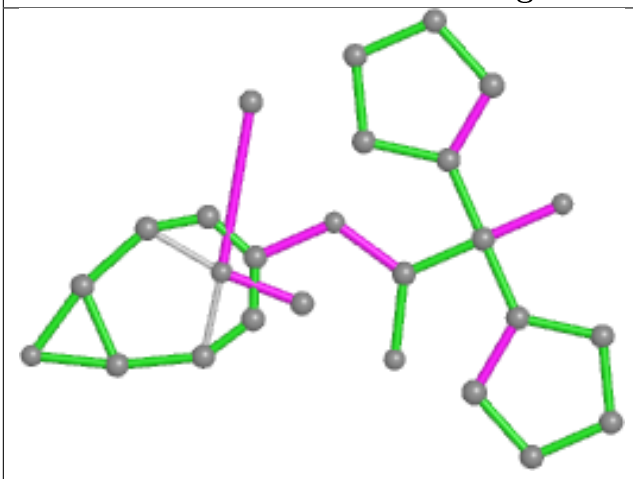


Torsions

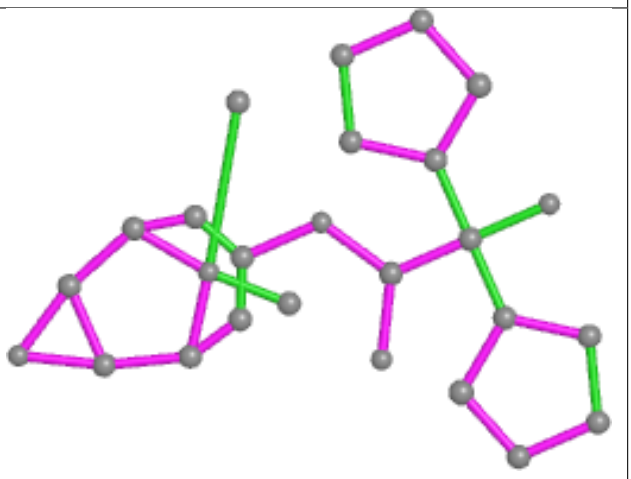


Rings

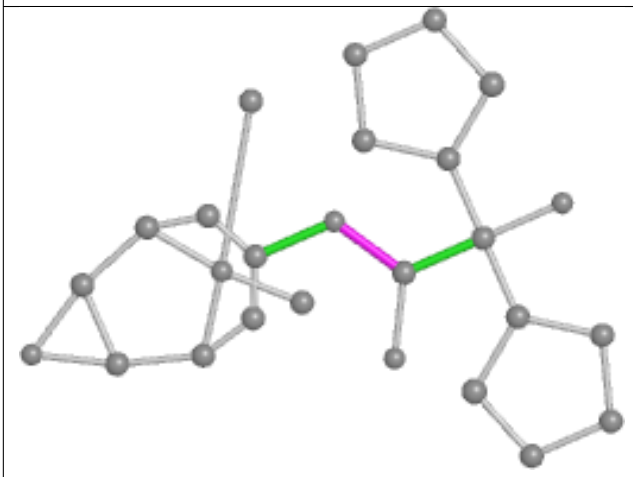
Ligand 0HK B 1201



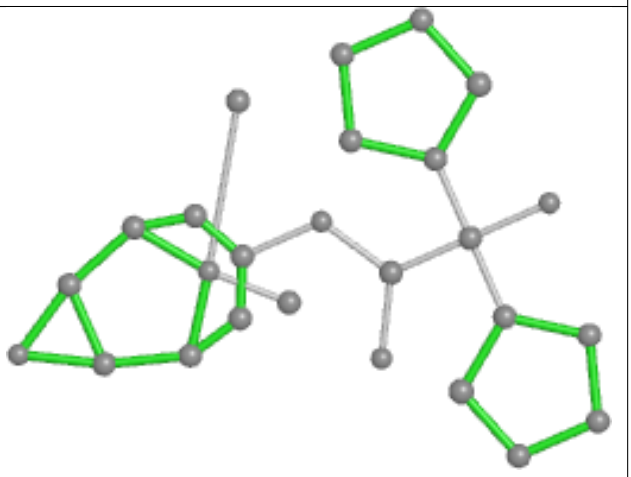
Bond lengths



Bond angles

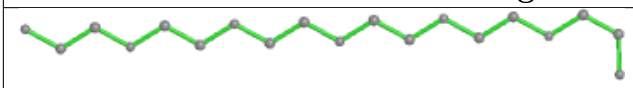


Torsions

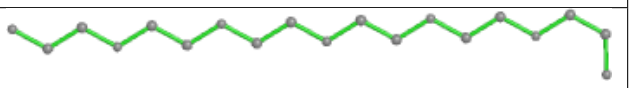


Rings

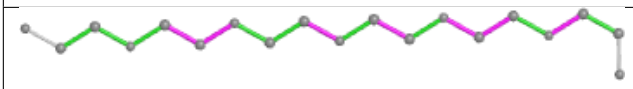
Ligand P6G A 2004



Bond lengths



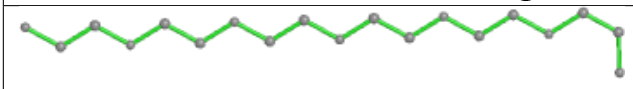
Bond angles



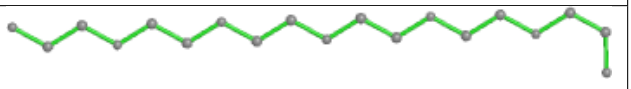
Torsions

Rings

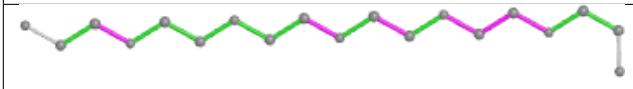
Ligand P6G B 1204



Bond lengths

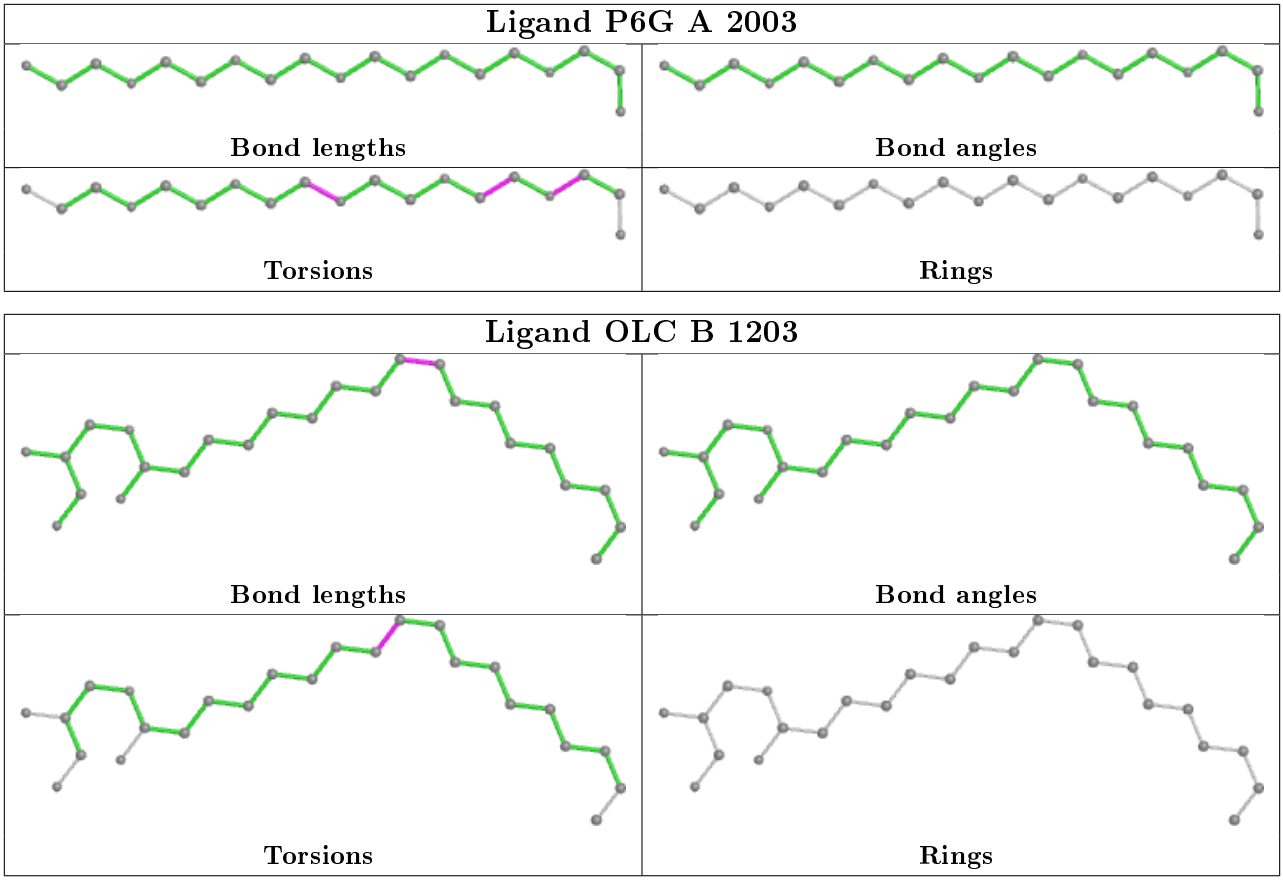


Bond angles



Torsions

Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	391/418 (93%)	0.17	17 (4%) 35 25	53, 91, 142, 165	0
1	B	392/418 (93%)	0.05	9 (2%) 60 51	54, 85, 121, 144	0
All	All	783/836 (93%)	0.11	26 (3%) 46 36	53, 88, 131, 165	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	5.4
1	A	519	CYS	4.3
1	A	518	SER	3.9
1	A	251	TRP	2.9
1	A	557	LEU	2.9
1	B	517	ASP	2.9
1	B	63	THR	2.9
1	A	98	LEU	2.9
1	B	518	SER	2.6
1	A	546	CYS	2.6
1	B	251	TRP	2.5
1	B	545	LEU	2.5
1	A	172	PRO	2.5
1	A	94	VAL	2.5
1	A	97	GLN	2.3
1	B	99	LYS	2.3
1	A	186	VAL	2.3
1	A	552	THR	2.3
1	B	208	TYR	2.3
1	B	552	THR	2.2
1	A	254	TYR	2.2
1	B	532	CYS	2.2
1	A	535	ASN	2.0
1	A	219	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	99	LYS	2.0
1	A	524	TYR	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)

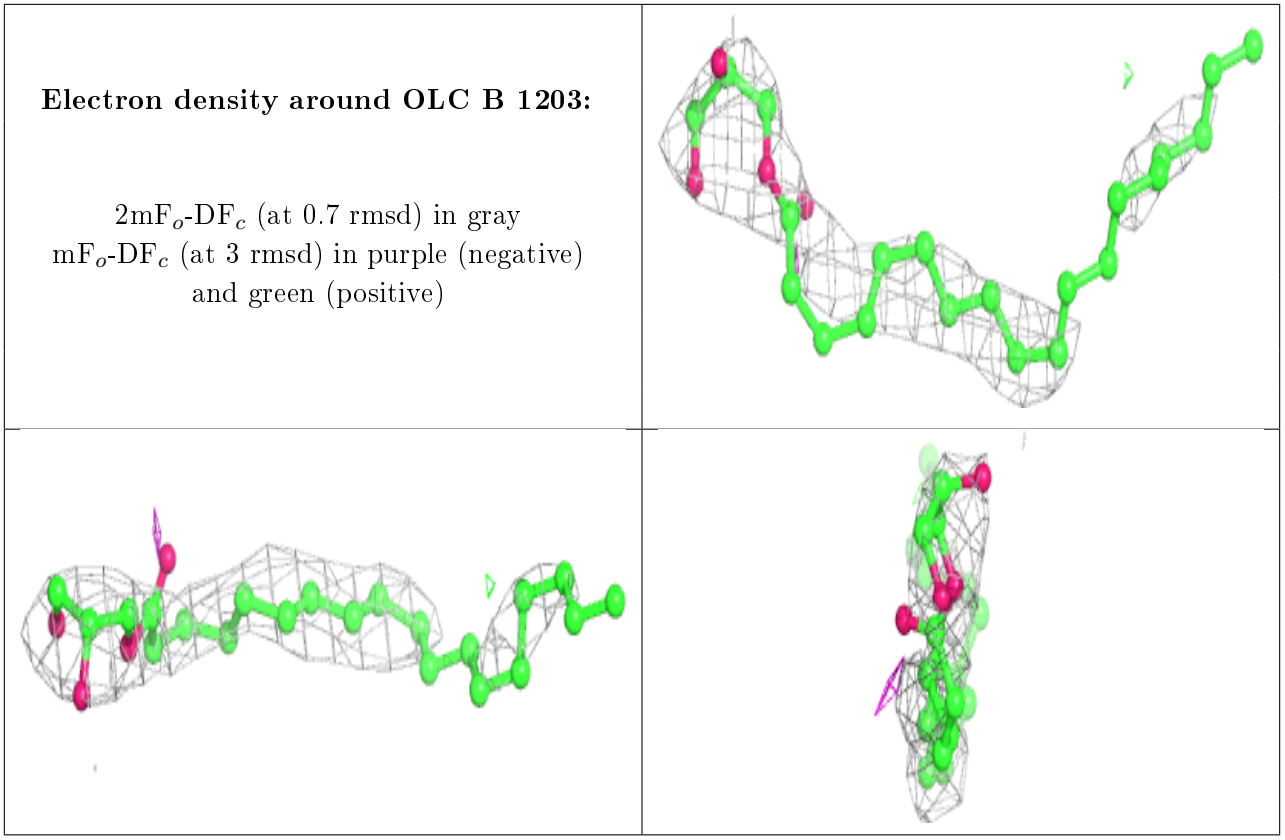
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	OLC	B	1203	25/25	0.76	0.65	90,118,133,148	0
3	P6G	A	2004	19/19	0.77	0.38	86,100,116,122	0
3	P6G	A	2002	19/19	0.78	0.38	82,102,117,122	0
5	OLC	B	1202	25/25	0.78	0.53	92,106,124,126	0
4	TAR	B	1206	10/10	0.81	0.28	109,132,134,142	0
3	P6G	A	2003	19/19	0.82	0.32	68,82,99,108	0
3	P6G	B	1204	19/19	0.82	0.32	92,111,125,131	0
4	TAR	A	2006	10/10	0.86	0.24	79,94,123,124	0
4	TAR	B	1205	10/10	0.89	0.33	84,92,122,127	0
4	TAR	A	2005	10/10	0.90	0.25	78,91,97,100	0
2	0HK	B	1201	26/26	0.92	0.27	64,80,96,101	0
2	0HK	A	2001	26/26	0.94	0.25	71,82,99,102	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.

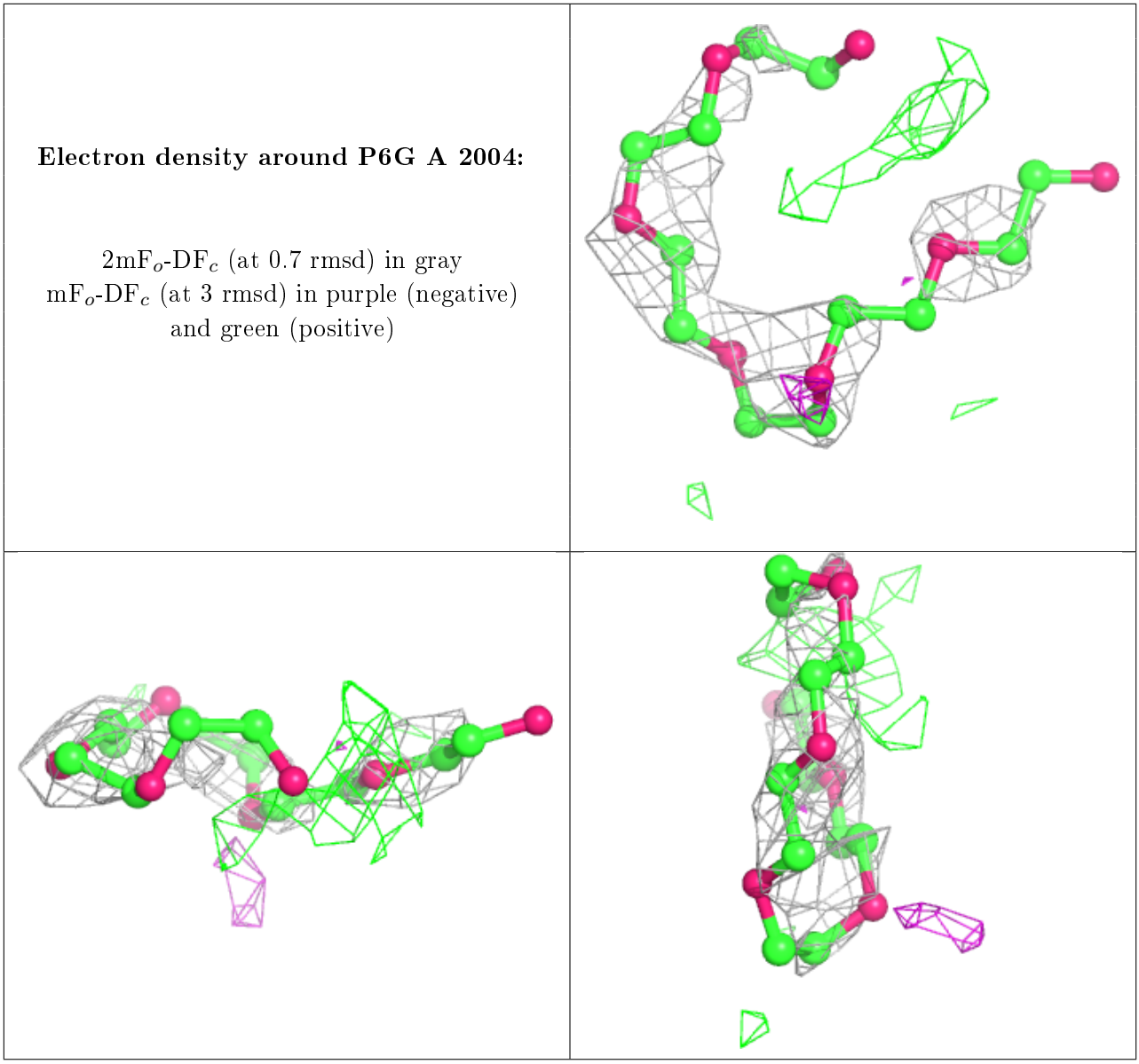
Electron density around OLC B 1203:

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



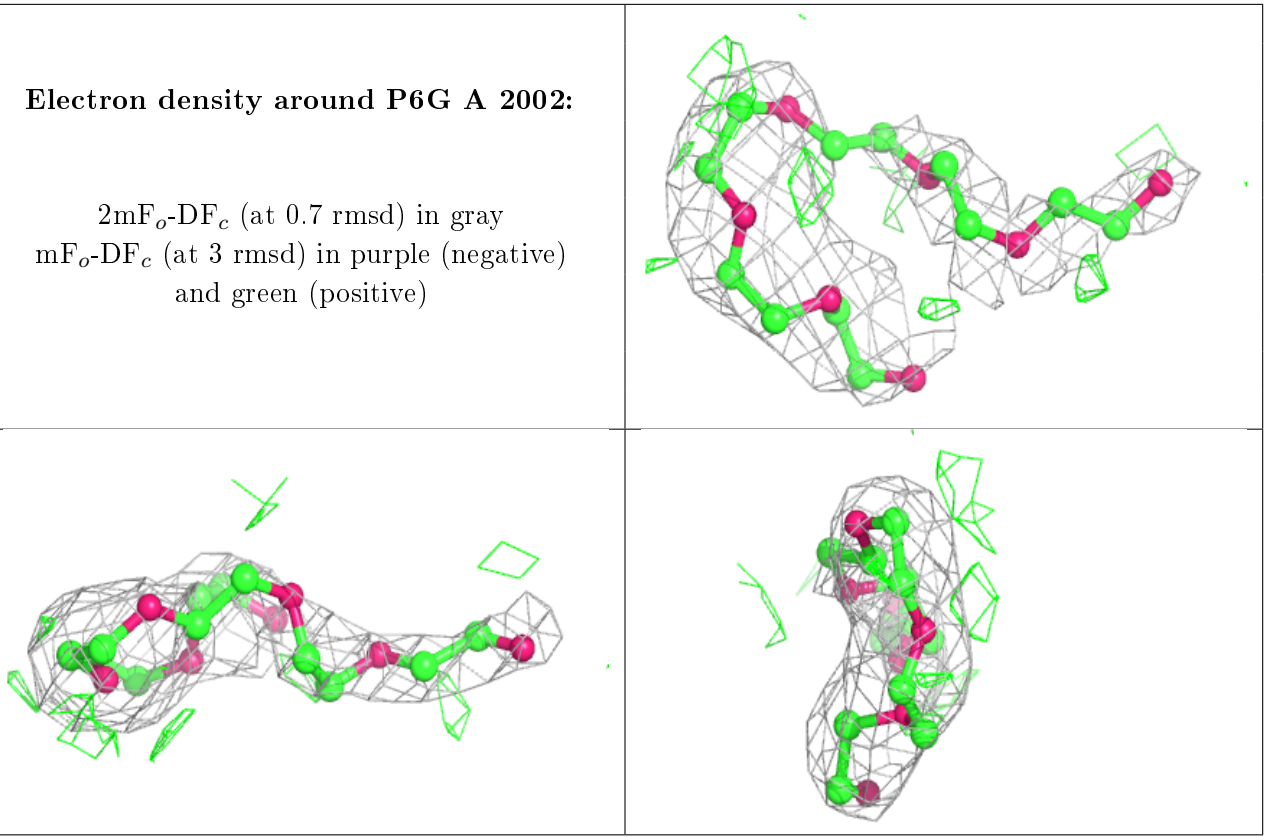
Electron density around P6G A 2004:

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



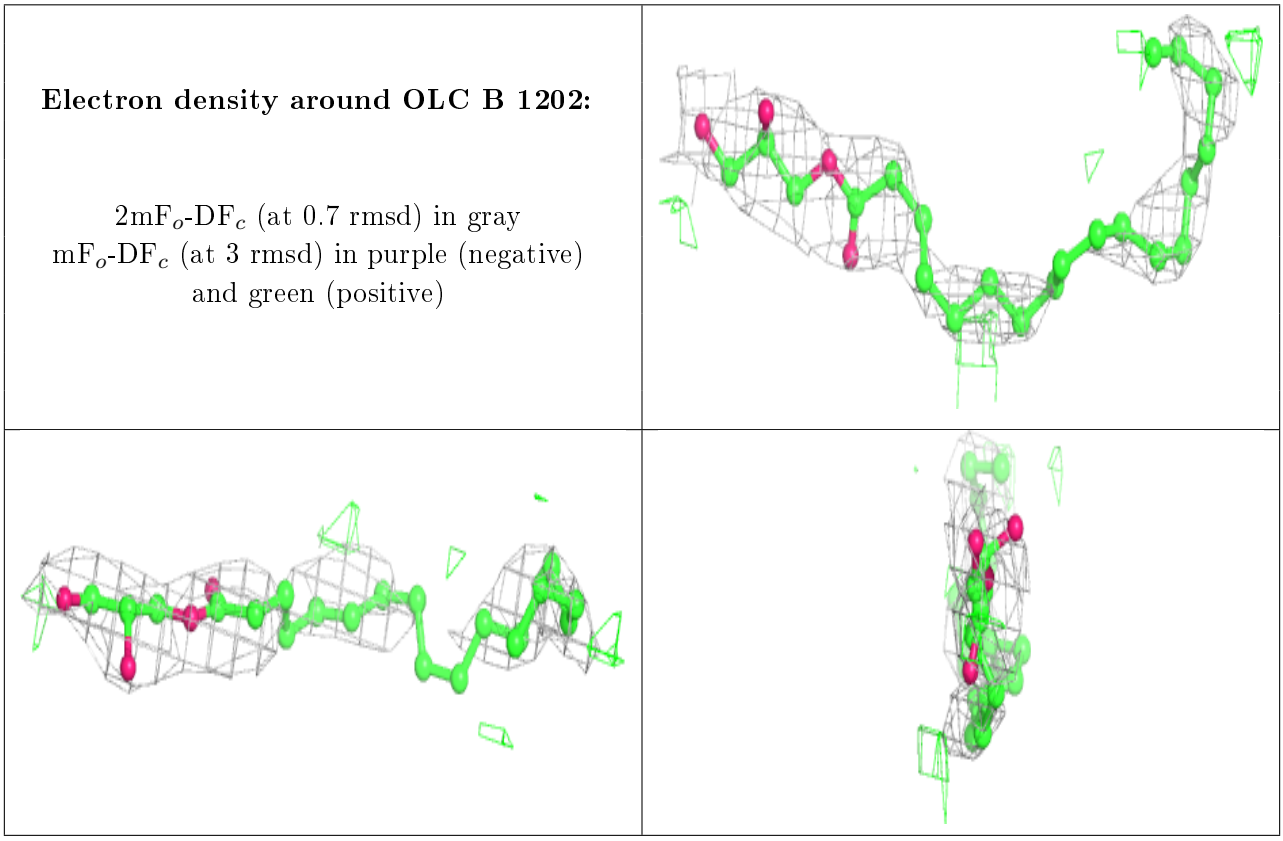
Electron density around P6G A 2002:

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



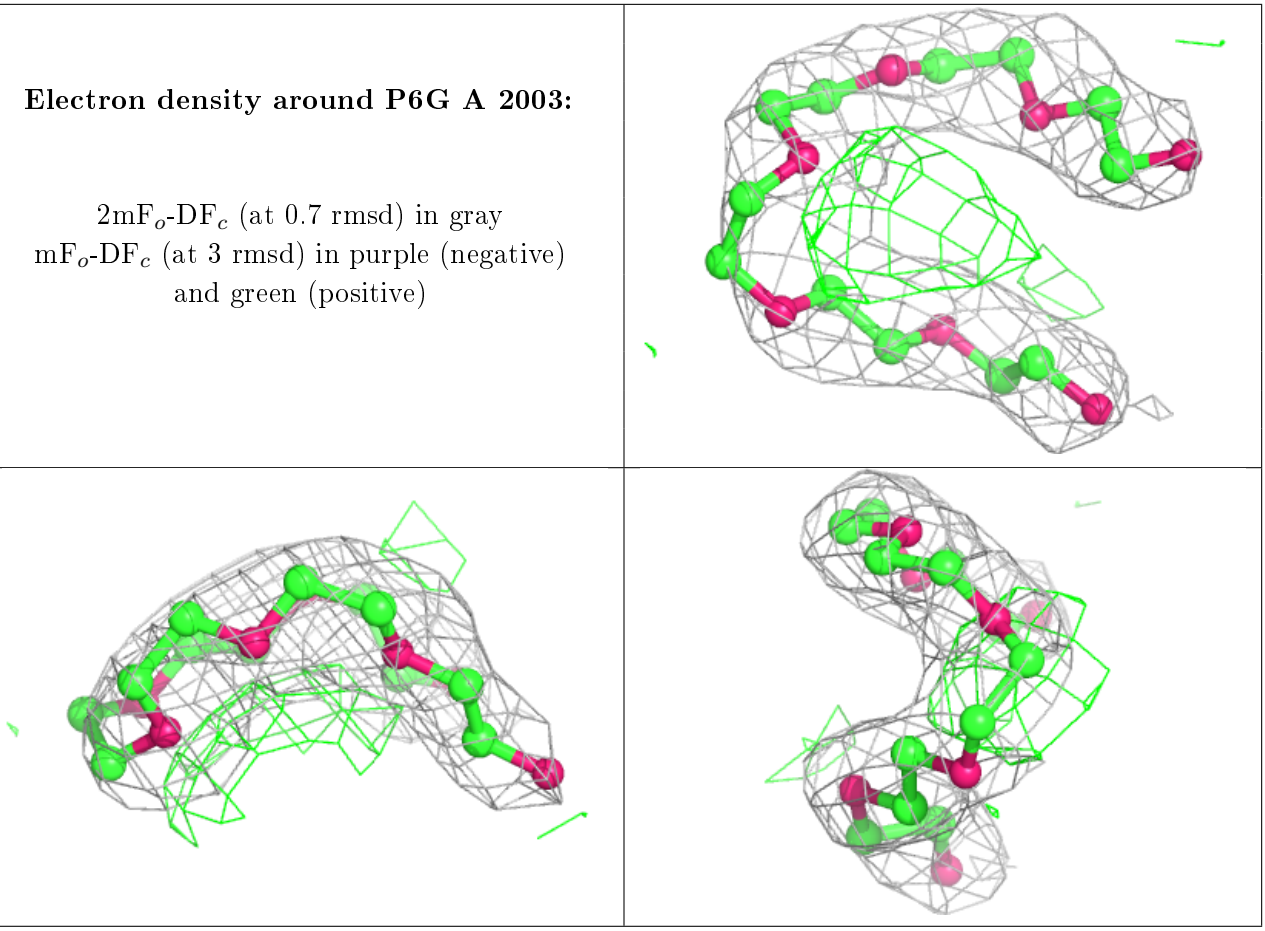
Electron density around OLC B 1202:

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



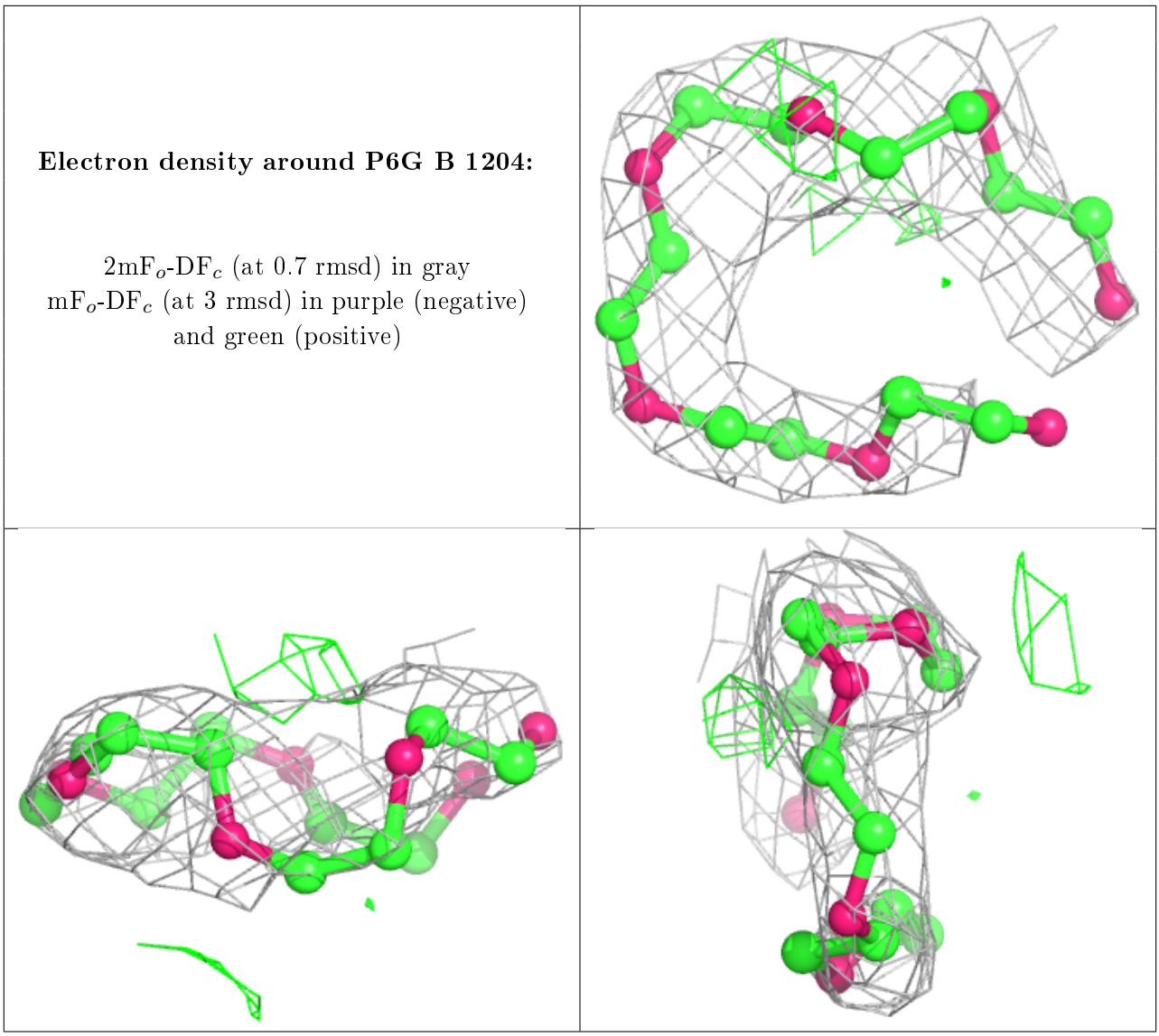
Electron density around P6G A 2003:

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



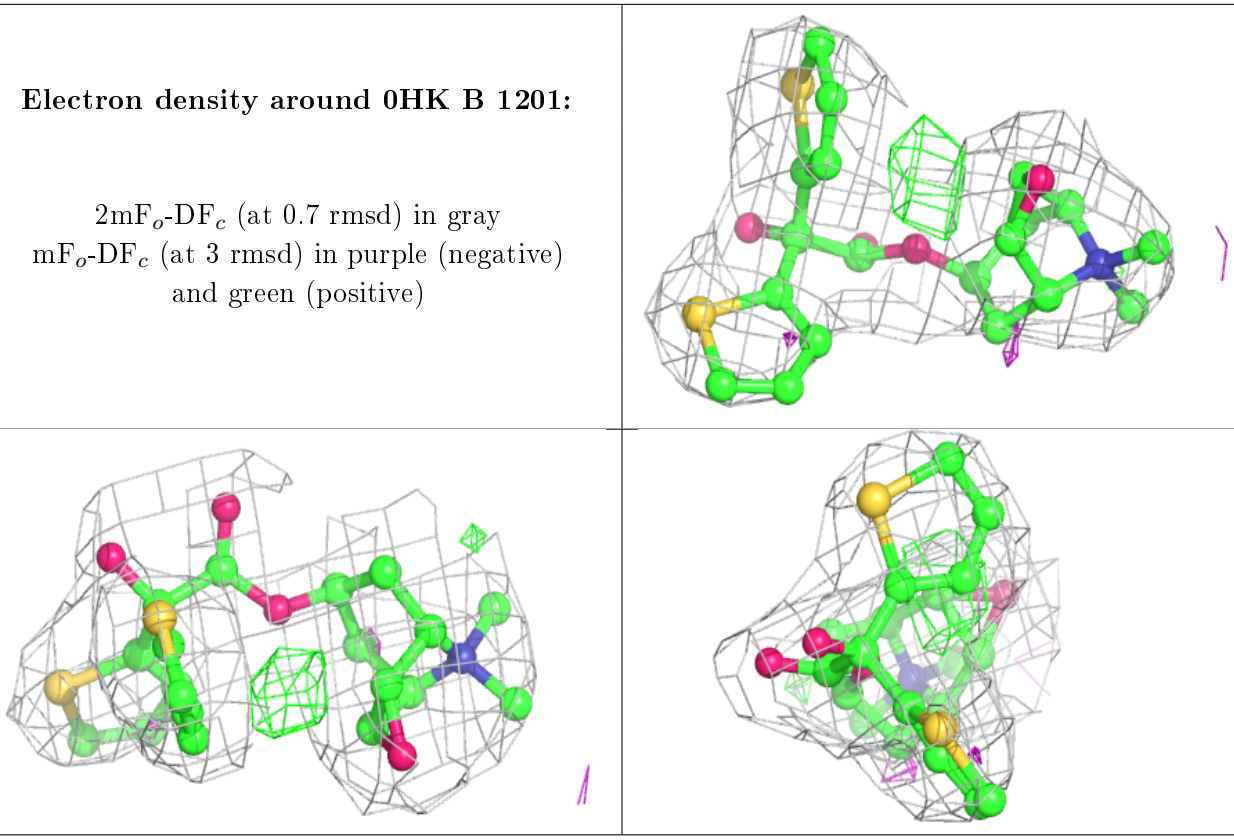
Electron density around P6G B 1204:

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



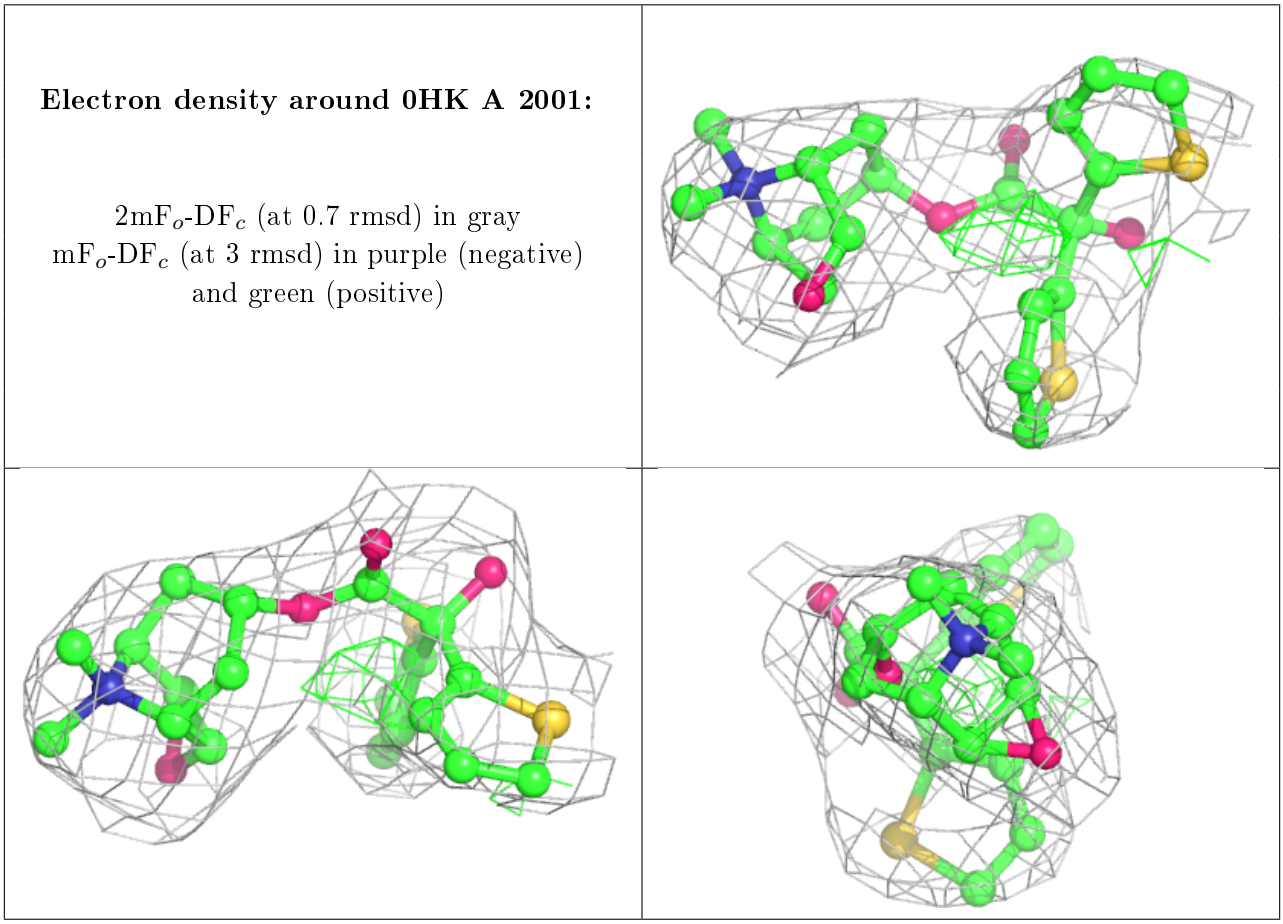
Electron density around 0HK B 1201:

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



Electron density around 0HK A 2001:

$2mF_o$-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.