wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2020 – 02:31 PM BST

PDB ID	:	5AFN
Title	:	alpha7-AChBP in complex with lobeline and fragment 5
Authors	:	Spurny, R.; Debaveye, S.; Farinha, A.; Veys, K.; Gossas, T.; Atack, J.; Bertrand, D.; Kemp, J.; Vos, A.; Danielson, U.H.; Tresadern, G.; Ulens, C.
Deposited on	:	2015-01-22
Resolution	:	2.15 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

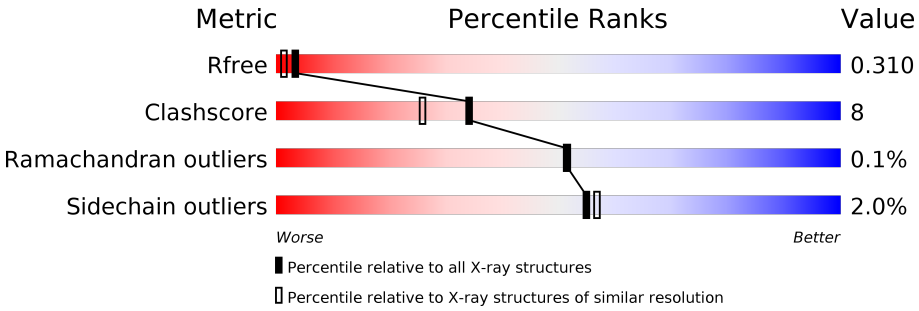
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.15 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)

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%

Mol	Chain	Length	Quality of chain
1	A	207	86% 13%
1	B	207	82% 16%
1	C	207	83% 16%
1	D	207	81% 18%
1	E	207	86% 14%

2 Entry composition

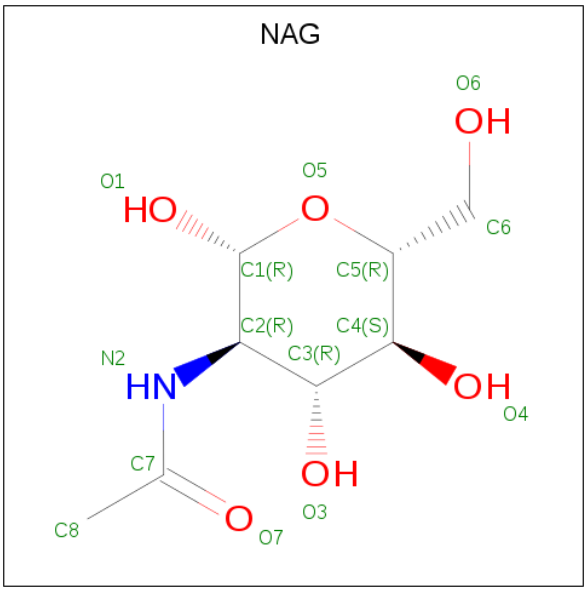
There are 8 unique types of molecules in this entry. The entry contains 9647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7.

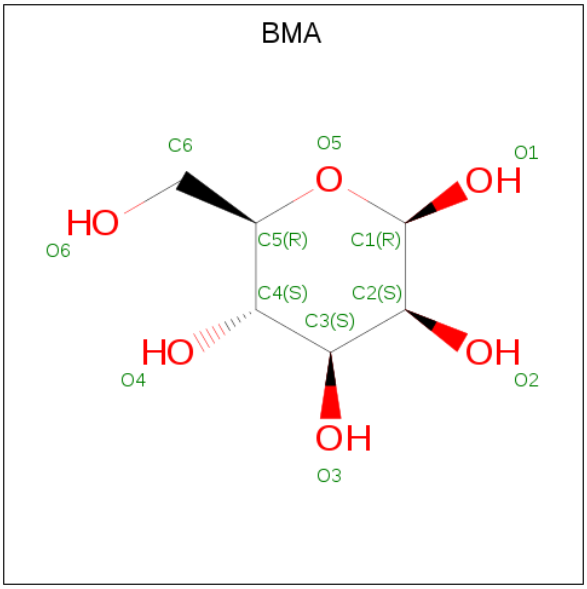
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	1	0
			1678	1077	280	314	7			
1	B	207	Total	C	N	O	S	0	1	0
			1699	1089	285	318	7			
1	C	205	Total	C	N	O	S	0	0	0
			1670	1071	279	313	7			
1	D	205	Total	C	N	O	S	0	5	0
			1707	1095	284	321	7			
1	E	205	Total	C	N	O	S	0	1	0
			1678	1077	280	314	7			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



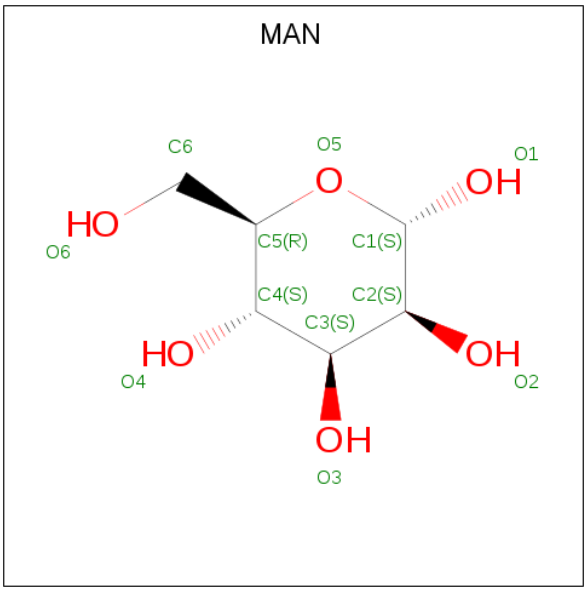
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



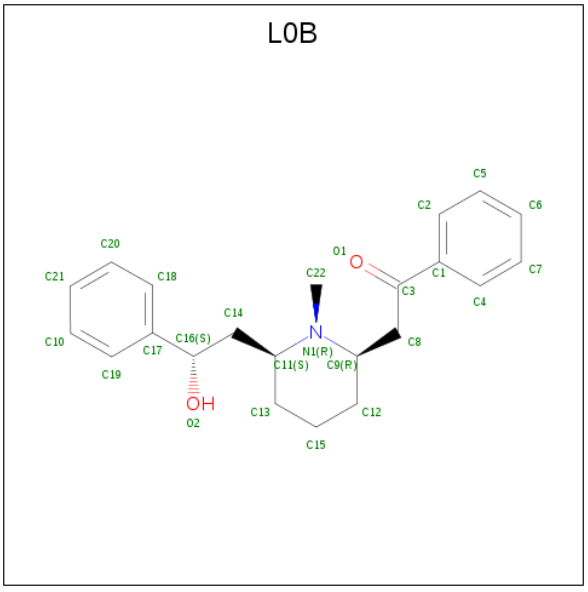
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0

- Molecule 5 is Alpha-Lobeline (three-letter code: L0B) (formula: $C_{22}H_{27}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 25 22 1 2	0	0
5	B	1	Total C N O 25 22 1 2	0	0
5	C	1	Total C N O 25 22 1 2	0	0

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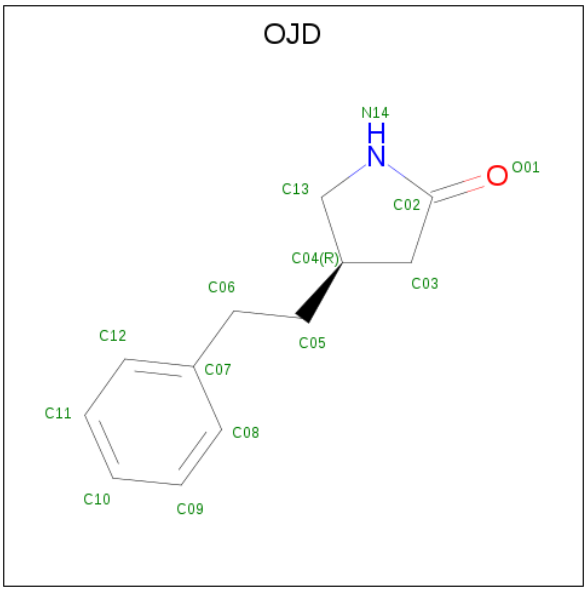
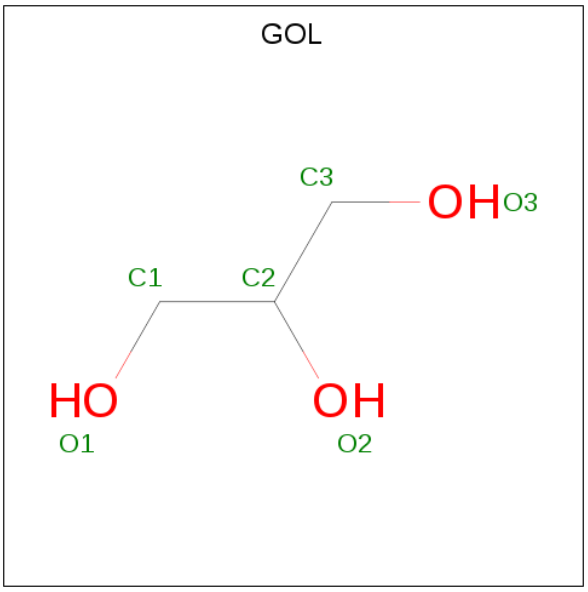
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N O 25 22 1 2	0	0
5	E	1	Total C N O 25 22 1 2	0	0

- Molecule 6 is (4R)-4-(2-phenylethyl)pyrrolidin-2-one (three-letter code: OJD) (formula: $C_{12}H_{15}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 12 1 1	0	0
6	B	1	Total C N O 14 12 1 1	0	0
6	C	1	Total C N O 14 12 1 1	0	0
6	D	1	Total C N O 14 12 1 1	0	0
6	E	1	Total C N O 14 12 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

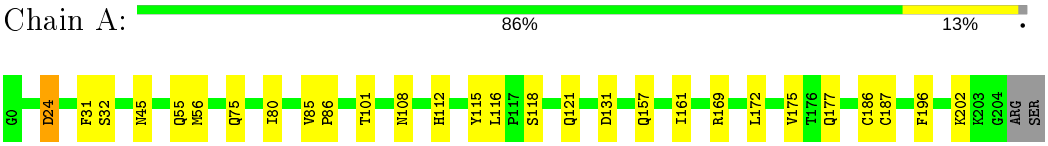
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	214	Total O 214 214	0	0
8	B	173	Total O 173 173	0	0
8	C	132	Total O 132 132	0	0
8	D	154	Total O 154 154	0	0
8	E	161	Total O 161 161	0	0

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. 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. 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.

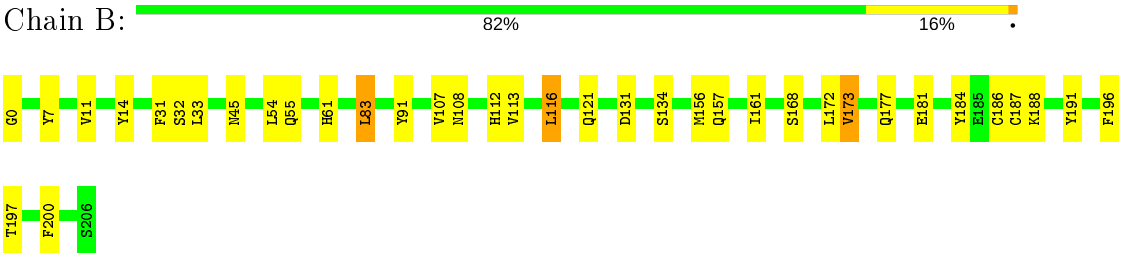
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain A:



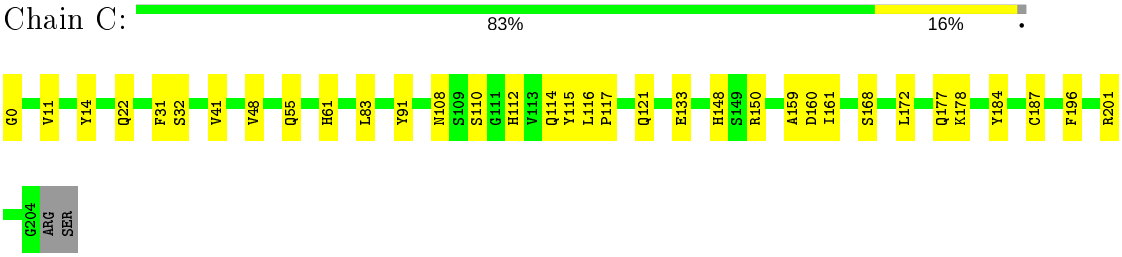
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain B:



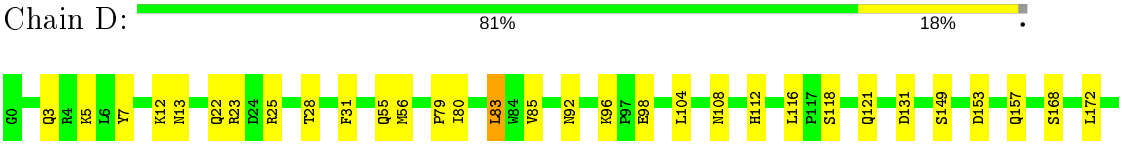
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

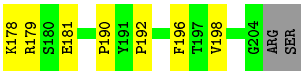
Chain C:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

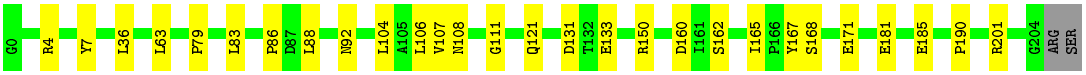
Chain D:





• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.52Å 112.50Å 143.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 2.15 47.00 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.90-2.15) 97.4 (47.00-2.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.167 , 0.223 0.281 , 0.310	Depositor DCC
R_{free} test set	3812 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.4	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	0.93	EDS
Total number of atoms	9647	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: GOL, BMA, NAG, OJD, L0B, MAN

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	0.40	0/1723	0.53	0/2344
1	B	0.38	0/1745	0.55	0/2373
1	C	0.34	0/1715	0.50	0/2333
1	D	0.37	0/1753	0.52	0/2384
1	E	0.42	0/1723	0.56	0/2344
All	All	0.38	0/8659	0.53	0/11778

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	1678	0	1643	27	0
1	B	1699	0	1659	25	1
1	C	1670	0	1633	32	0
1	D	1707	0	1663	27	1
1	E	1678	0	1643	22	2
2	A	28	0	26	1	0
2	B	28	0	26	3	0
2	C	28	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	26	3	0
2	E	28	0	26	2	0
3	A	11	0	10	1	0
4	A	11	0	10	1	2
5	A	25	0	27	0	0
5	B	25	0	27	3	0
5	C	25	0	27	1	0
5	D	25	0	27	1	0
5	E	25	0	27	3	0
6	A	14	0	15	4	0
6	B	14	0	15	2	0
6	C	14	0	15	4	0
6	D	14	0	15	3	0
6	E	14	0	15	3	0
7	D	6	0	8	2	0
7	E	18	0	24	3	0
8	A	214	0	0	9	1
8	B	173	0	0	12	0
8	C	132	0	0	13	0
8	D	154	0	0	5	4
8	E	161	0	0	7	1
All	All	9647	0	8633	147	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 147 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:E:181:GLU:OE1	8:E:2148:HOH:O	1.88	0.92
1:A:121:GLN:OE1	6:A:1215:OJD:H11	1.71	0.91
1:E:108:ASN:OD1	8:E:2108:HOH:O	1.87	0.91
1:A:108:ASN:HD21	1:A:112:HIS:HB3	1.37	0.90
1:A:115:TYR:OH	8:A:2143:HOH:O	1.98	0.81

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2192:HOH:O	8:E:2071:HOH:O[3_645]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ARG:NH2	8:D:2071:HOH:O[3_645]	1.69	0.51
1:B:197:THR:OG1	8:D:2148:HOH:O[2_554]	1.98	0.22
1:D:179:ARG:NH1	4:A:304:MAN:O6[3_655]	2.00	0.20
1:E:185:GLU:OE2	8:D:2030:HOH:O[3_645]	2.01	0.19

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	204/207 (99%)	200 (98%)	3 (2%)	1 (0%)	29 22
1	B	206/207 (100%)	202 (98%)	4 (2%)	0	100 100
1	C	203/207 (98%)	199 (98%)	4 (2%)	0	100 100
1	D	208/207 (100%)	207 (100%)	1 (0%)	0	100 100
1	E	204/207 (99%)	200 (98%)	4 (2%)	0	100 100
All	All	1025/1035 (99%)	1008 (98%)	16 (2%)	1 (0%)	51 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ASP

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	191/192 (100%)	189 (99%)	2 (1%)	76	79
1	B	193/192 (100%)	187 (97%)	6 (3%)	40	38
1	C	190/192 (99%)	187 (98%)	3 (2%)	62	65
1	D	195/192 (102%)	190 (97%)	5 (3%)	46	45
1	E	191/192 (100%)	188 (98%)	3 (2%)	62	65
All	All	960/960 (100%)	941 (98%)	19 (2%)	55	57

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	11	VAL
1	C	187	CYS
1	D	168	SER
1	B	188	LYS
1	E	131	ASP

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

Mol	Chain	Res	Type
1	A	108	ASN
1	D	3	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

26 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	NAG	A	302	-	14,14,15	0.73	0	17,19,21	2.02	2 (11%)
5	L0B	E	1205	-	27,27,27	0.63	0	33,36,36	1.45	5 (15%)
5	L0B	C	1205	-	27,27,27	0.52	0	33,36,36	1.23	4 (12%)
6	OJD	E	1215	-	14,15,15	1.76	5 (35%)	14,19,19	1.38	3 (21%)
2	NAG	B	302	-	14,14,15	0.46	0	17,19,21	0.85	0
2	NAG	D	302	-	14,14,15	0.42	0	17,19,21	0.93	1 (5%)
5	L0B	B	1207	-	27,27,27	0.52	0	33,36,36	1.49	4 (12%)
2	NAG	E	302	-	14,14,15	0.49	0	17,19,21	1.61	2 (11%)
2	NAG	C	301	-	14,14,15	0.58	0	17,19,21	1.37	3 (17%)
2	NAG	D	301	-	14,14,15	0.65	0	17,19,21	1.77	3 (17%)
7	GOL	E	1208	-	5,5,5	0.35	0	5,5,5	0.27	0
7	GOL	E	1206	-	5,5,5	0.36	0	5,5,5	0.21	0
7	GOL	D	1206	-	5,5,5	0.37	0	5,5,5	0.19	0
6	OJD	C	1215	-	14,15,15	1.64	3 (21%)	14,19,19	1.25	3 (21%)
6	OJD	A	1215	-	14,15,15	1.69	4 (28%)	14,19,19	1.45	3 (21%)
5	L0B	D	1205	-	27,27,27	0.54	0	33,36,36	1.25	5 (15%)
6	OJD	B	1217	-	14,15,15	1.66	4 (28%)	14,19,19	1.13	1 (7%)
4	MAN	A	304	-	11,11,12	0.75	0	15,15,17	1.79	3 (20%)
2	NAG	B	301	-	14,14,15	0.64	0	17,19,21	1.09	2 (11%)
2	NAG	E	301	-	14,14,15	0.87	1 (7%)	17,19,21	1.67	4 (23%)
7	GOL	E	1207	-	5,5,5	0.33	0	5,5,5	0.76	0
5	L0B	A	1205	-	27,27,27	0.56	0	33,36,36	1.32	3 (9%)
2	NAG	A	301	-	14,14,15	0.62	0	17,19,21	1.76	4 (23%)
6	OJD	D	1215	-	14,15,15	1.68	3 (21%)	14,19,19	1.12	2 (14%)
2	NAG	C	302	-	14,14,15	0.47	0	17,19,21	0.94	1 (5%)
3	BMA	A	303	-	11,11,12	0.51	0	15,15,17	2.37	4 (26%)

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	NAG	A	302	-	-	1/6/23/26	0/1/1/1
5	L0B	E	1205	-	-	2/16/30/30	0/3/3/3
5	L0B	C	1205	-	-	0/16/30/30	0/3/3/3
6	OJD	E	1215	-	-	2/5/14/14	0/2/2/2
2	NAG	B	302	-	-	0/6/23/26	0/1/1/1
2	NAG	D	302	-	-	2/6/23/26	0/1/1/1
5	L0B	B	1207	-	-	0/16/30/30	0/3/3/3
2	NAG	E	302	-	-	3/6/23/26	0/1/1/1
2	NAG	C	301	-	-	4/6/23/26	0/1/1/1
2	NAG	D	301	-	-	0/6/23/26	0/1/1/1
7	GOL	E	1208	-	-	2/4/4/4	-
7	GOL	E	1206	-	-	4/4/4/4	-
7	GOL	D	1206	-	-	2/4/4/4	-
6	OJD	C	1215	-	-	4/5/14/14	0/2/2/2
6	OJD	A	1215	-	-	2/5/14/14	0/2/2/2
5	L0B	D	1205	-	-	1/16/30/30	0/3/3/3
6	OJD	B	1217	-	-	3/5/14/14	0/2/2/2
4	MAN	A	304	-	-	1/2/19/22	0/1/1/1
2	NAG	B	301	-	-	3/6/23/26	0/1/1/1
2	NAG	E	301	-	-	1/6/23/26	0/1/1/1
7	GOL	E	1207	-	-	2/4/4/4	-
5	L0B	A	1205	-	-	0/16/30/30	0/3/3/3
2	NAG	A	301	-	-	0/6/23/26	0/1/1/1
6	OJD	D	1215	-	-	3/5/14/14	0/2/2/2
2	NAG	C	302	-	-	4/6/23/26	0/1/1/1
3	BMA	A	303	-	-	2/2/19/22	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1215	OJD	C02-N14	3.86	1.45	1.33
6	D	1215	OJD	C02-N14	3.83	1.45	1.33
6	C	1215	OJD	C02-N14	3.75	1.45	1.33
6	B	1217	OJD	C02-N14	3.70	1.44	1.33
6	A	1215	OJD	C02-N14	3.69	1.44	1.33

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	NAG	O5-C1-C2	-6.86	100.45	111.29
3	A	303	BMA	C1-O5-C5	6.12	120.48	112.19
2	D	301	NAG	O5-C1-C2	-5.42	102.72	111.29
4	A	304	MAN	C1-C2-C3	5.05	115.88	109.67
2	A	301	NAG	O5-C1-C2	4.84	118.93	111.29

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1205	L0B	N1-C11-C14-C16
2	D	302	NAG	C8-C7-N2-C2
2	D	302	NAG	O7-C7-N2-C2
2	E	302	NAG	C1-C2-N2-C7
2	E	302	NAG	O7-C7-N2-C2

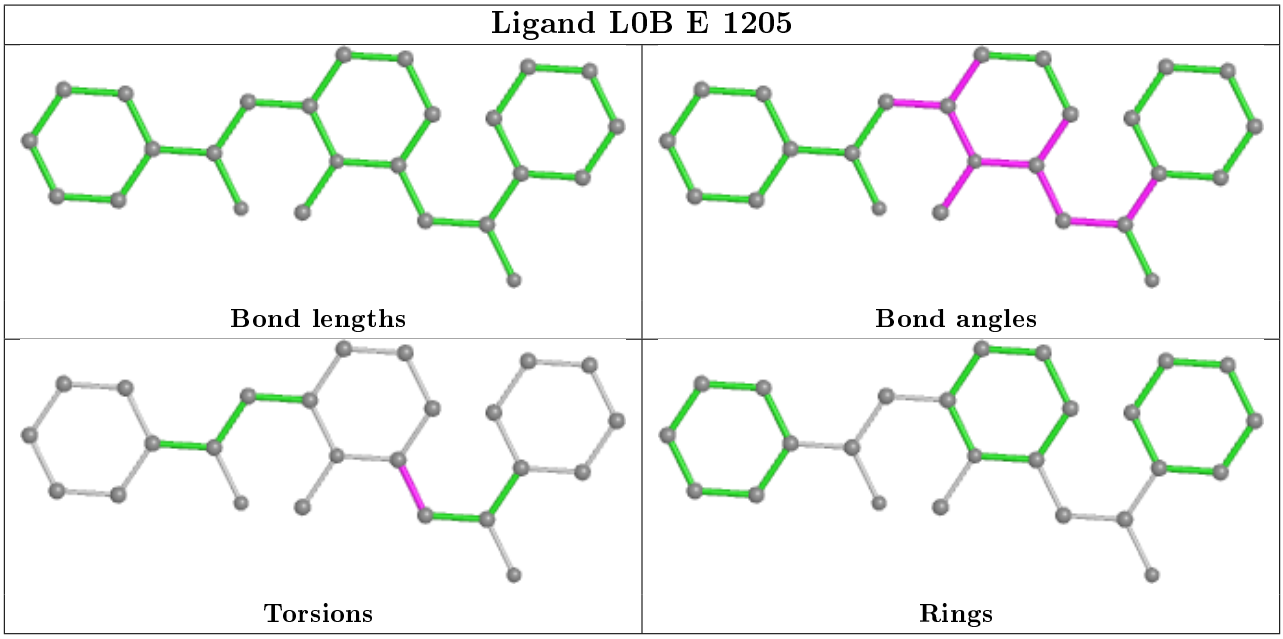
There are no ring outliers.

23 monomers are involved in 45 short contacts:

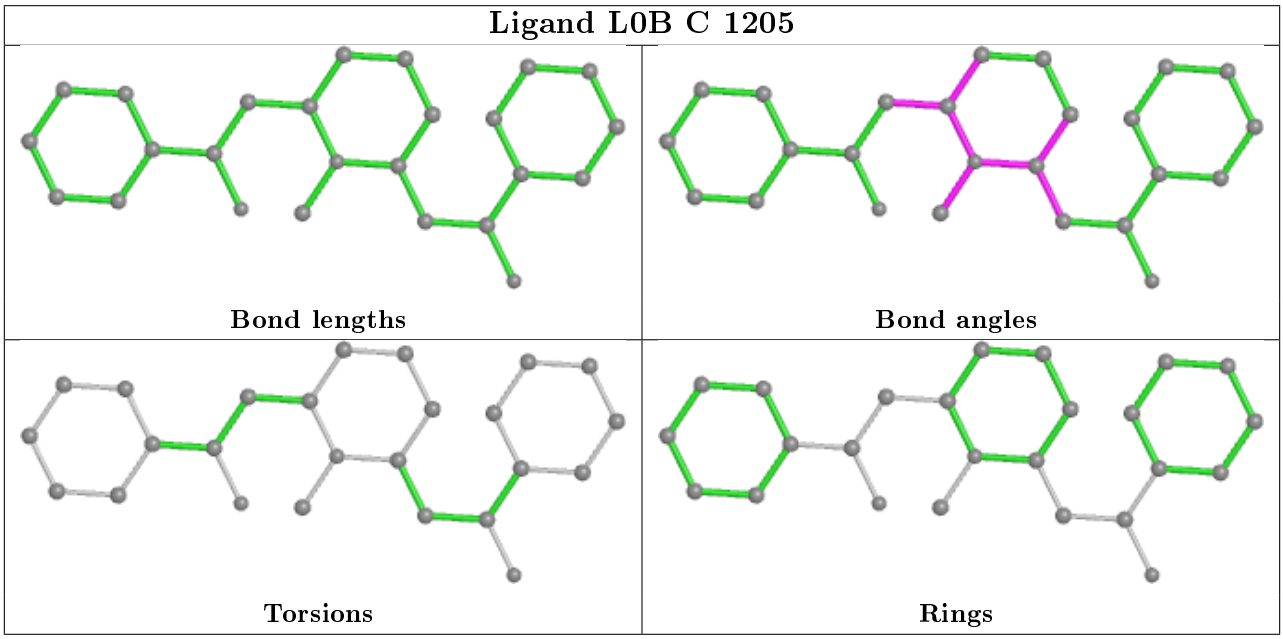
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1205	L0B	3	0
5	C	1205	L0B	1	0
6	E	1215	OJD	3	0
2	B	302	NAG	1	0
2	D	302	NAG	1	0
5	B	1207	L0B	3	0
2	E	302	NAG	2	0
2	C	301	NAG	4	0
2	D	301	NAG	3	0
7	E	1206	GOL	2	0
7	D	1206	GOL	2	0
6	C	1215	OJD	4	0
6	A	1215	OJD	4	0
5	D	1205	L0B	1	0
6	B	1217	OJD	2	0
4	A	304	MAN	1	2
2	B	301	NAG	3	0
2	E	301	NAG	2	0
7	E	1207	GOL	1	0
2	A	301	NAG	1	0
6	D	1215	OJD	3	0
2	C	302	NAG	1	0
3	A	303	BMA	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.

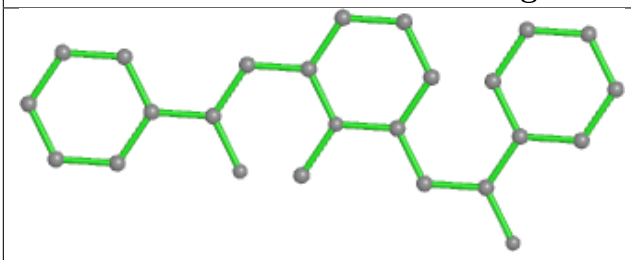
Ligand L0B E 1205



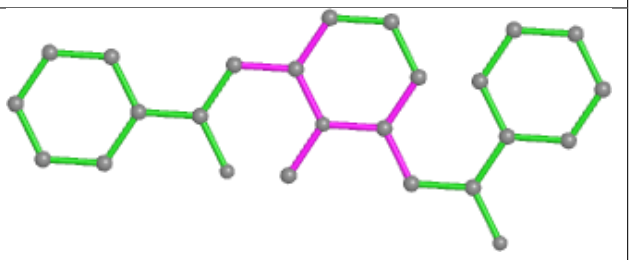
Ligand L0B C 1205



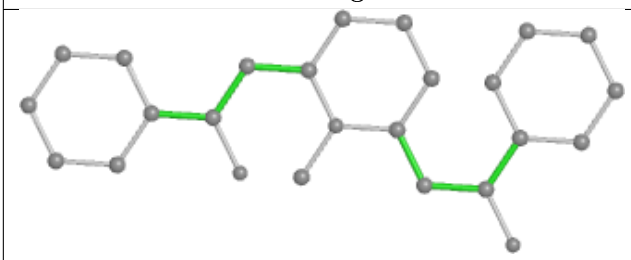
Ligand L0B B 1207



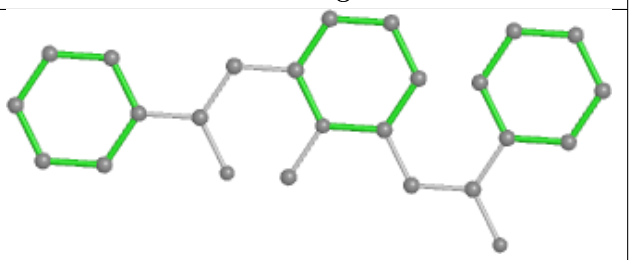
Bond lengths



Bond angles

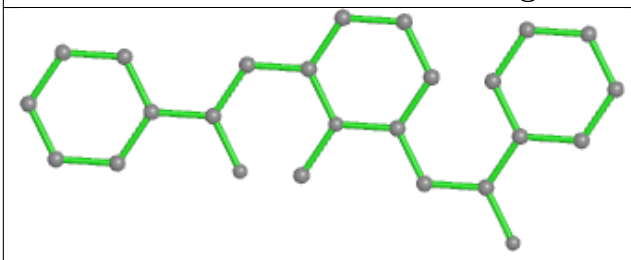


Torsions

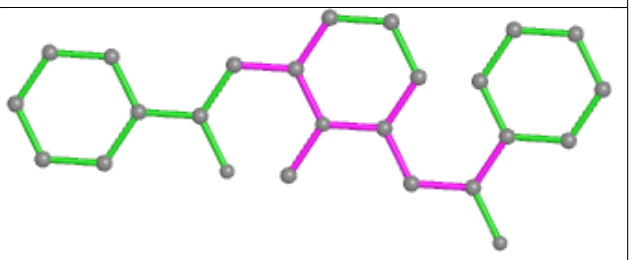


Rings

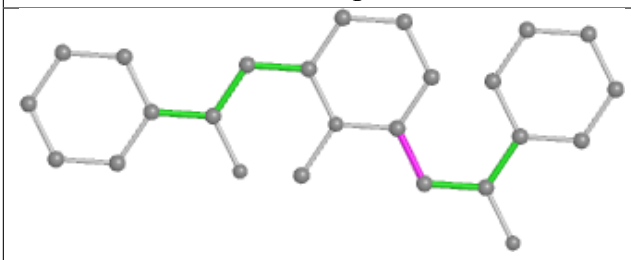
Ligand L0B D 1205



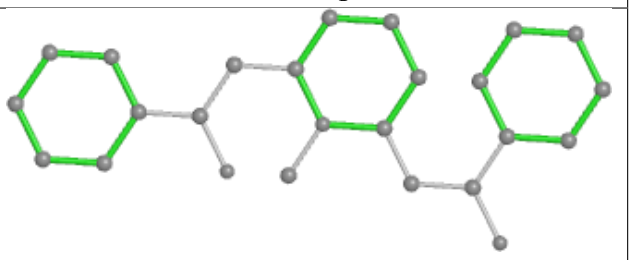
Bond lengths



Bond angles

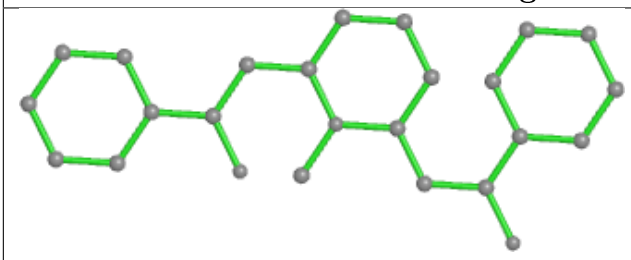


Torsions

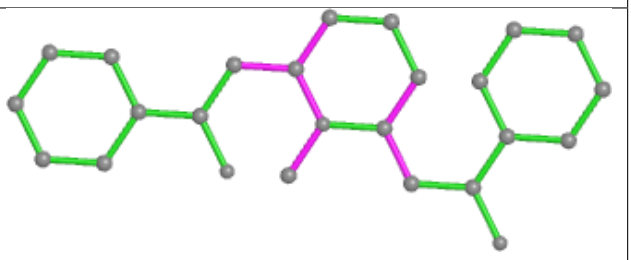


Rings

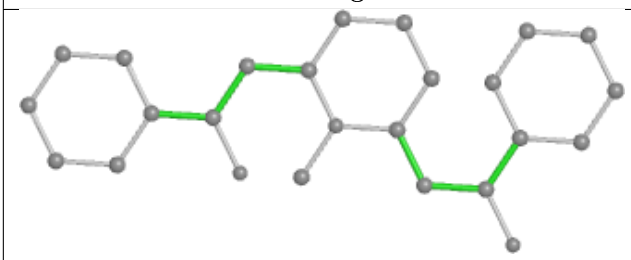
Ligand L0B A 1205



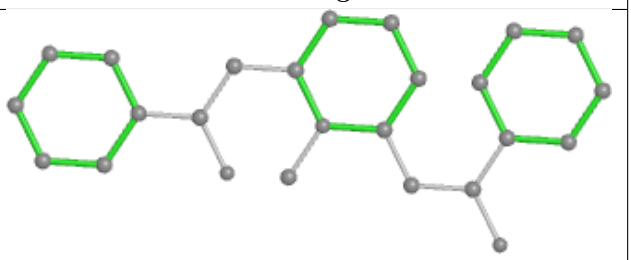
Bond lengths



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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

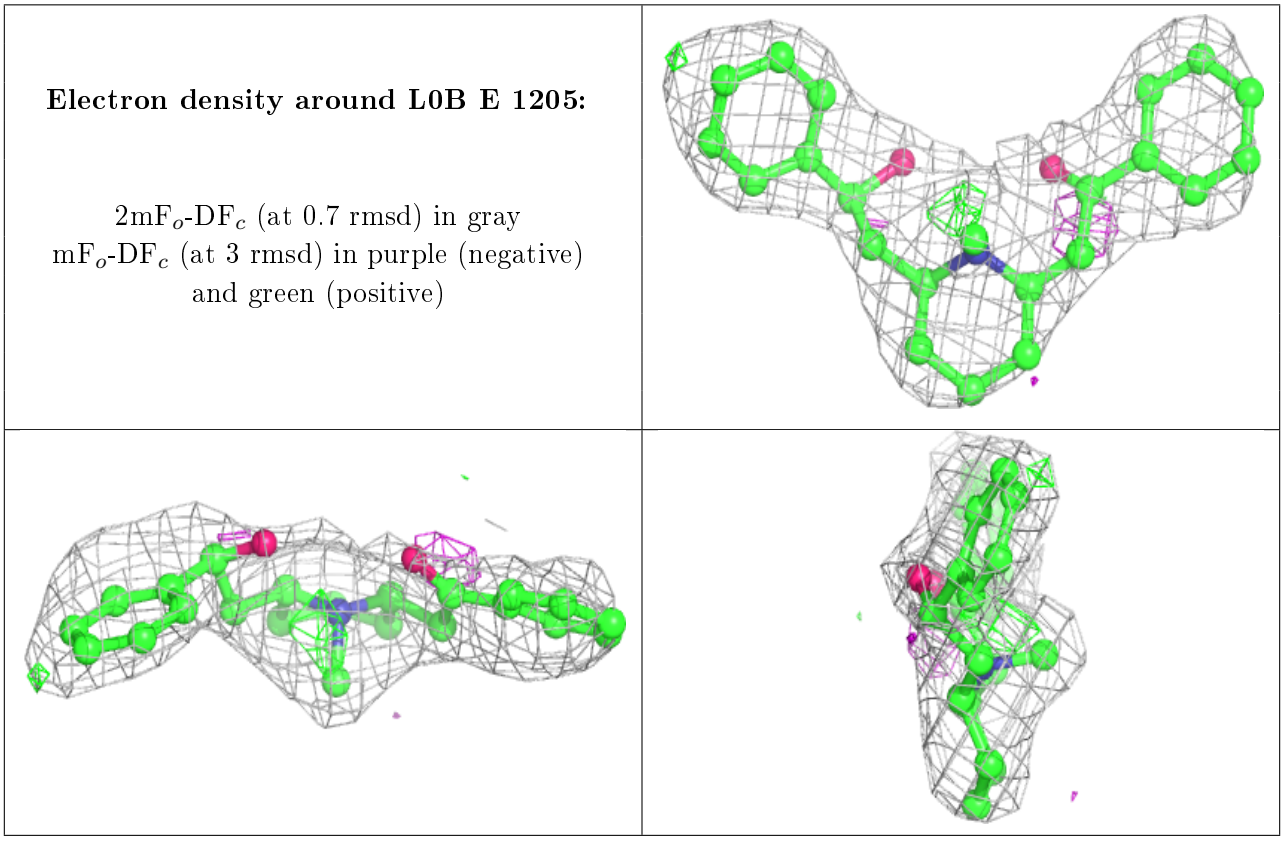
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

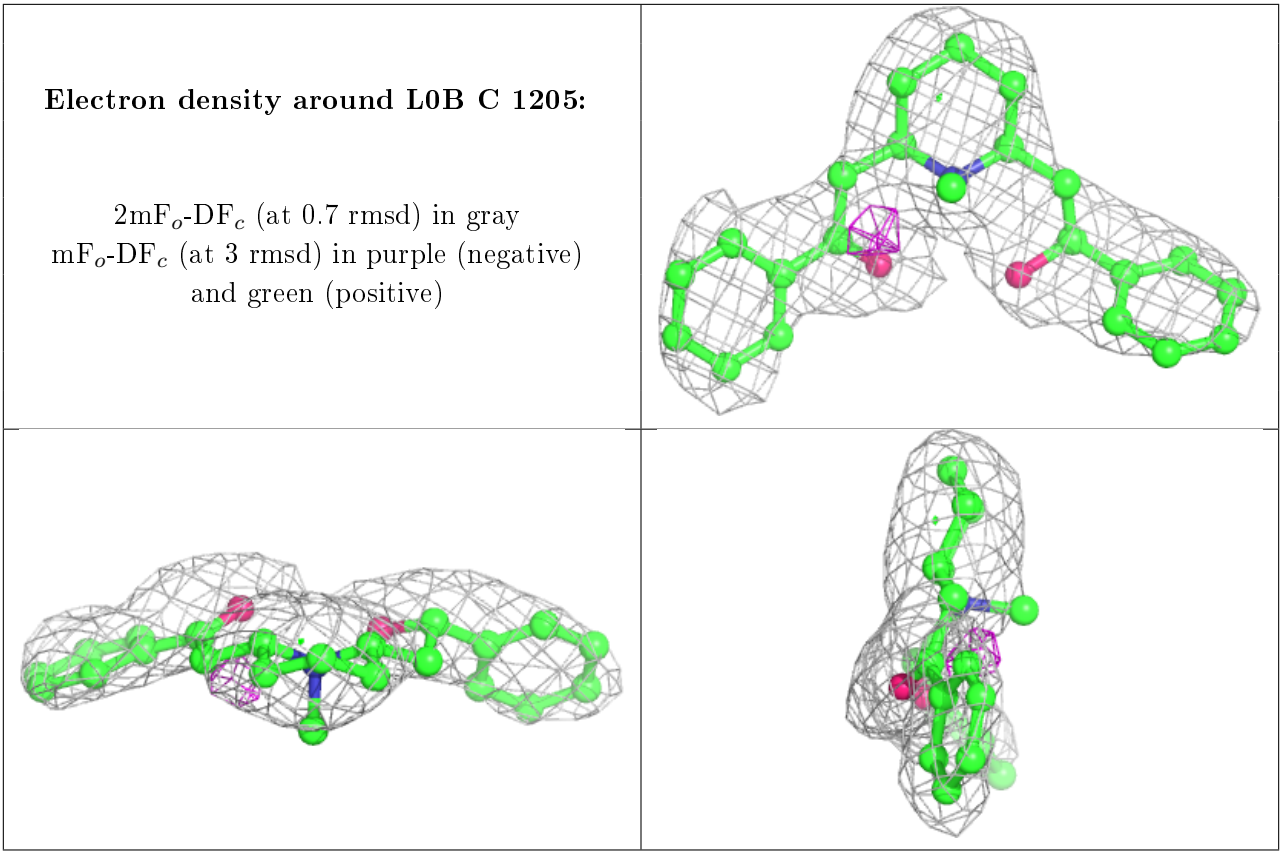
Electron density around L0B E 1205:

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



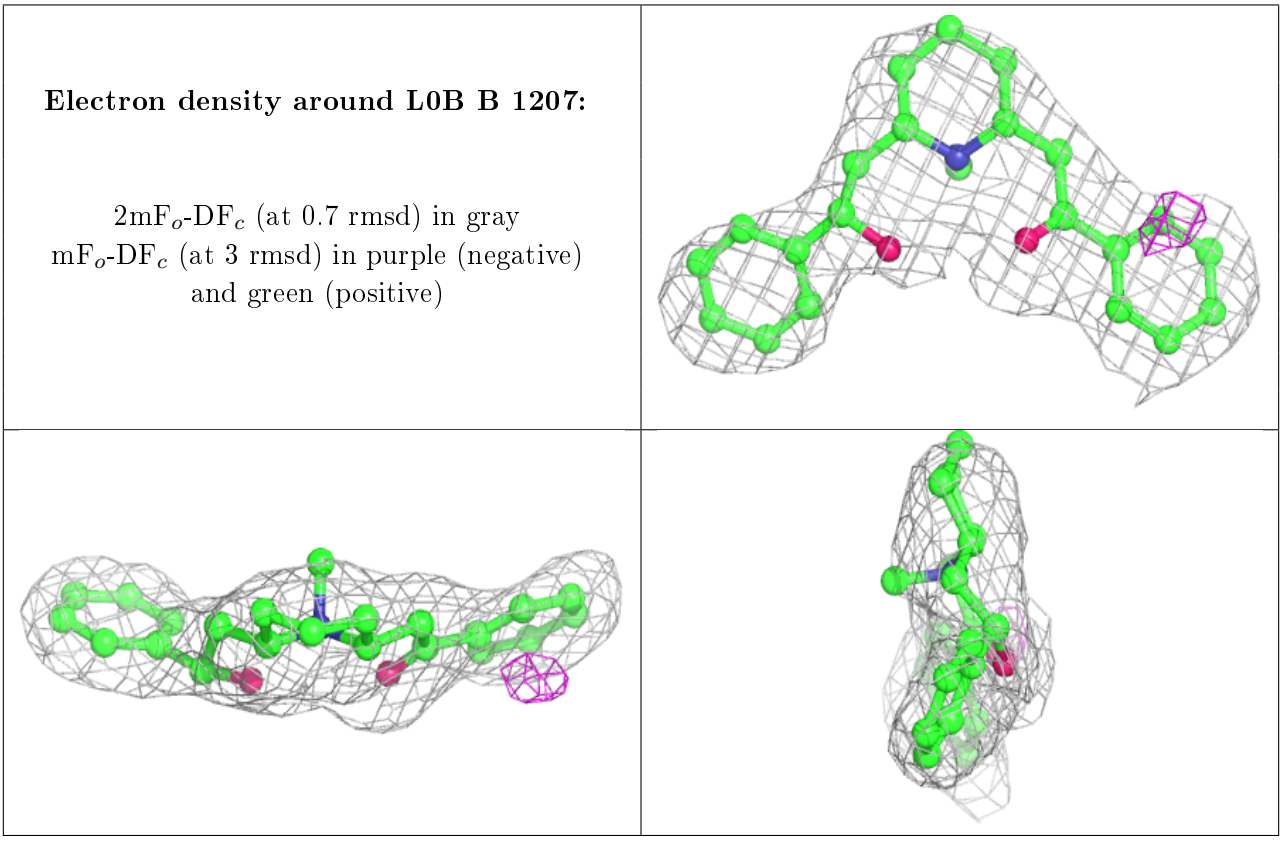
Electron density around L0B C 1205:

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



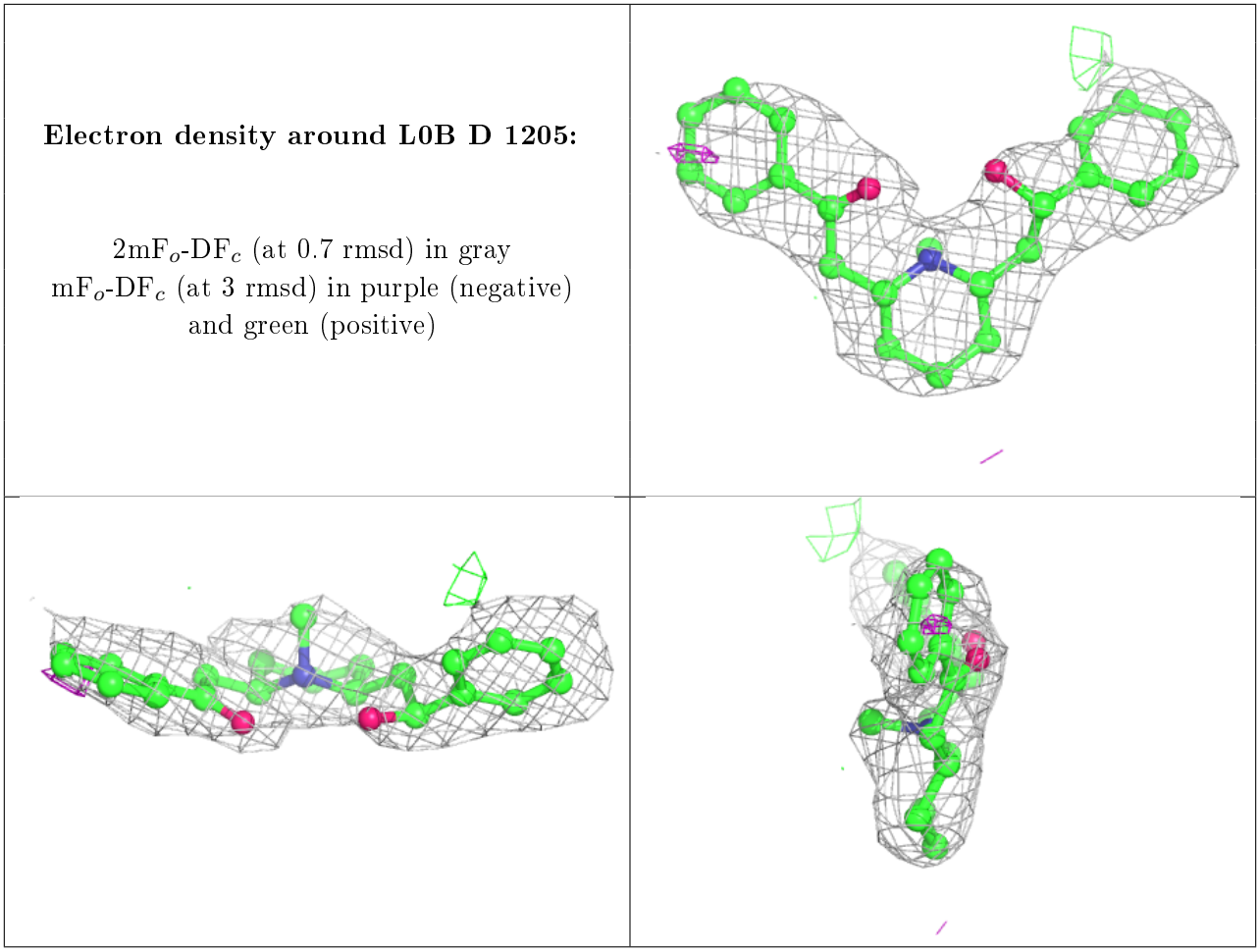
Electron density around L0B B 1207:

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



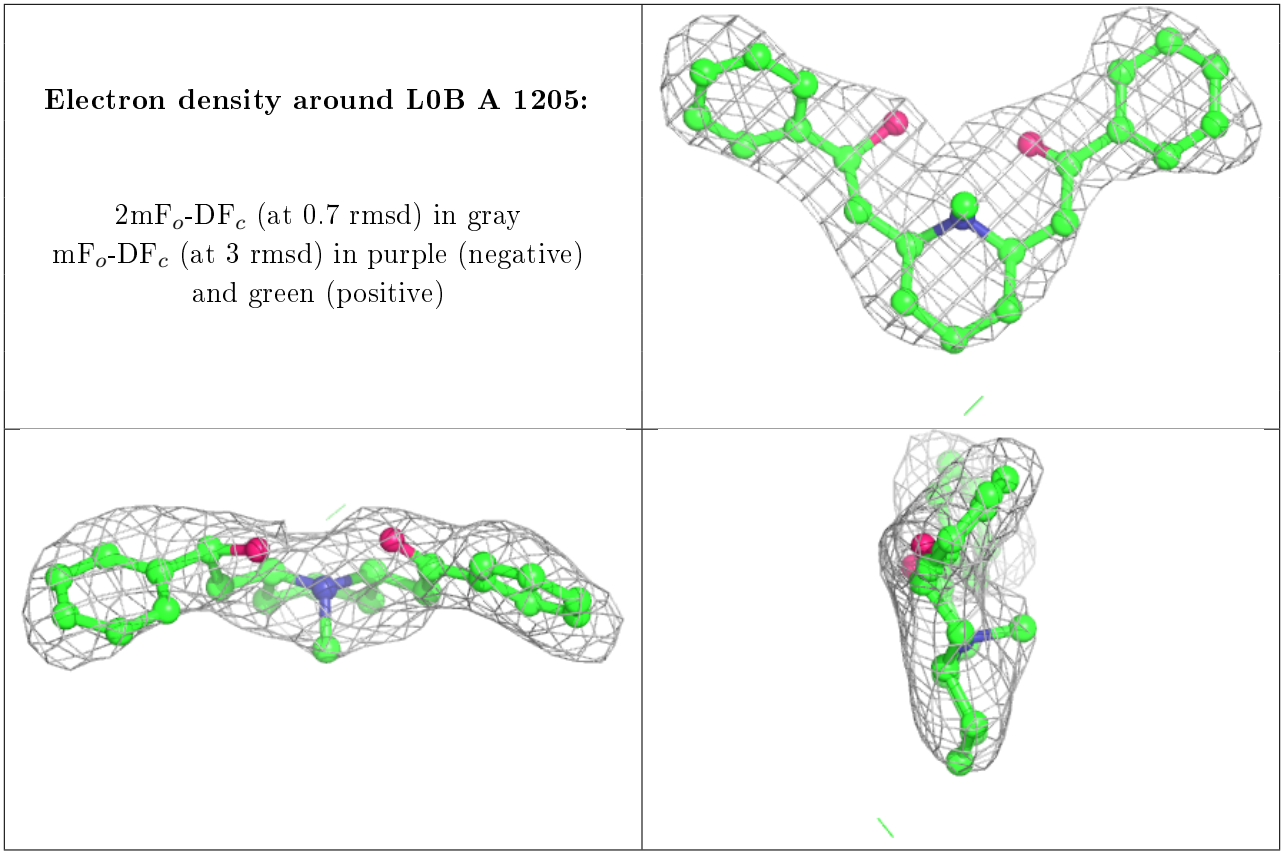
Electron density around L0B D 1205:

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



Electron density around L0B A 1205:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.