Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 02:50 PM EDT

PDB ID	:	5AFJ
Title	:	alpha7-AChBP in complex with lobeline and fragment 1
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	:	2.20 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:

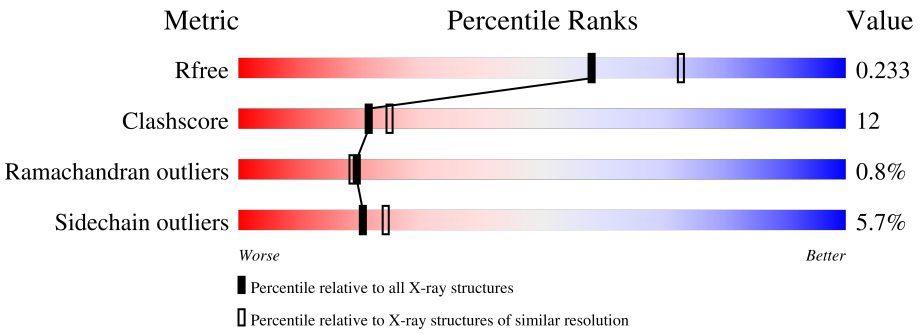
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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)

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%

Mol	Chain	Length	Quality of chain
1	A	205	76% 22% •
1	B	205	72% 27% •
1	C	205	70% 28% •
1	D	205	79% 17% •
1	E	205	82% 15% •

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
3	42R	B	1206	-	-	X	-
4	L0B	B	1207	-	-	X	-

2 Entry composition (i)

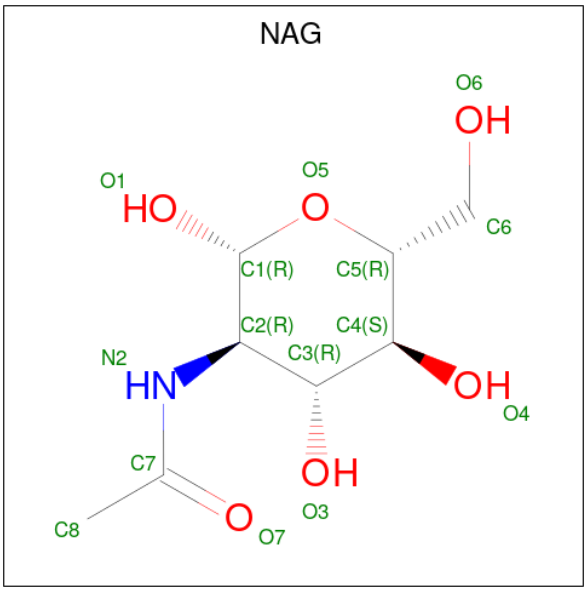
There are 8 unique types of molecules in this entry. The entry contains 9623 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

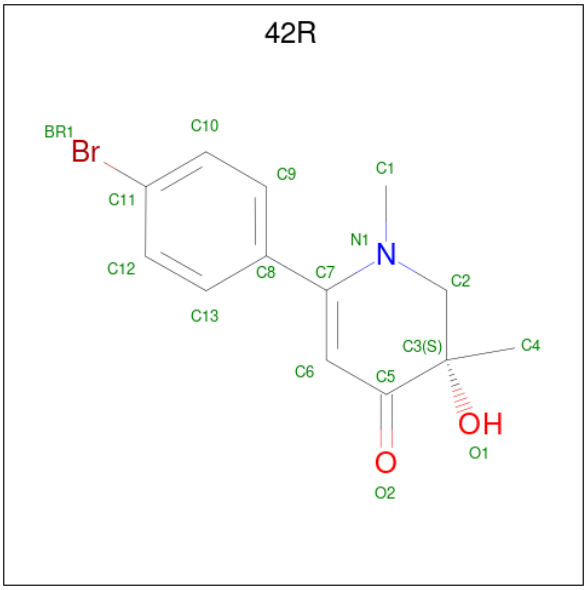
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	204	1703	1093	283	320	7	0	5	0
1	B	205	1694	1088	282	317	7	0	3	0
1	C	205	1698	1090	283	318	7	0	4	0
1	D	205	1703	1096	283	317	7	0	4	0
1	E	205	1687	1083	281	316	7	0	2	0

- 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
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	D	1	14	8	1	5	0	0
2	D	1	14	8	1	5	0	0
2	E	1	14	8	1	5	0	0
2	E	1	14	8	1	5	0	0

- Molecule 3 is (3S)-6-(4-bromophenyl)-3-hydroxy-1,3-dimethyl-2,3-dihydropyridin-4(1H)-one (three-letter code: 42R) (formula: $C_{13}H_{14}BrNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	A	1	17	1	13	1	2	0	0

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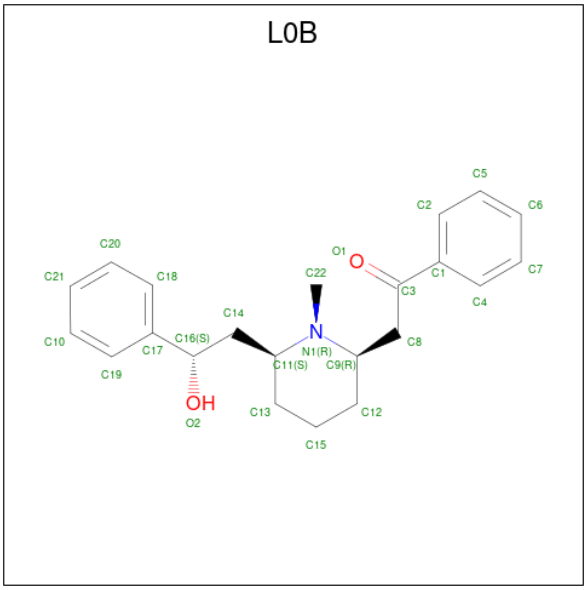
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	A	1	17	1	13	1	2	0	0
3	B	1	17	1	13	1	2	0	0
3	B	1	17	1	13	1	2	0	0
3	C	1	17	1	13	1	2	0	0
3	C	1	17	1	13	1	2	0	0
3	D	1	17	1	13	1	2	0	0
3	D	1	17	1	13	1	2	0	0
3	E	1	17	1	13	1	2	0	0
3	E	1	17	1	13	1	2	0	0

- Molecule 4 is Alpha-Lobeline (three-letter code: L0B) (formula: $C_{22}H_{27}NO_2$).



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

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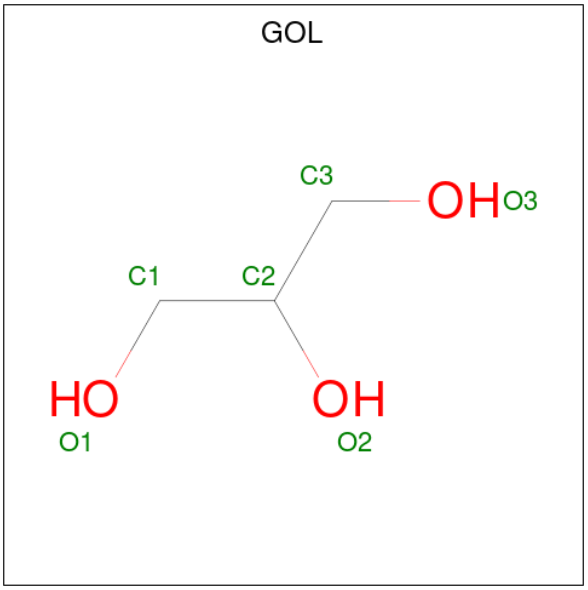
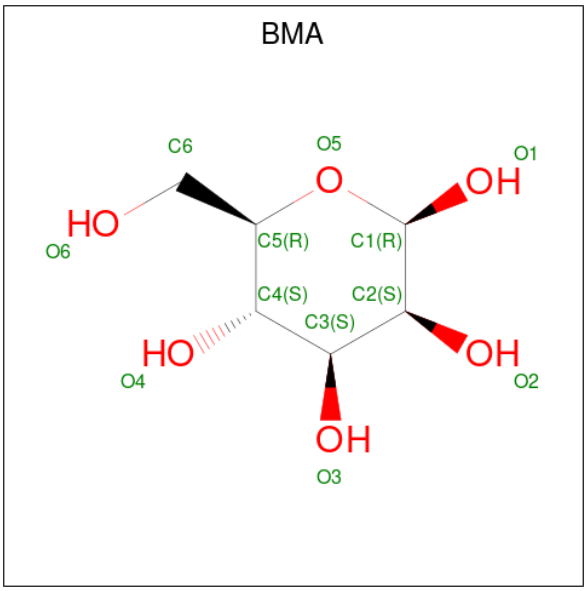
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	25	22	1	2	0	0
			Total	C	N	O		
4	D	1	25	22	1	2	0	0
			Total	C	N	O		
4	E	1	25	22	1	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



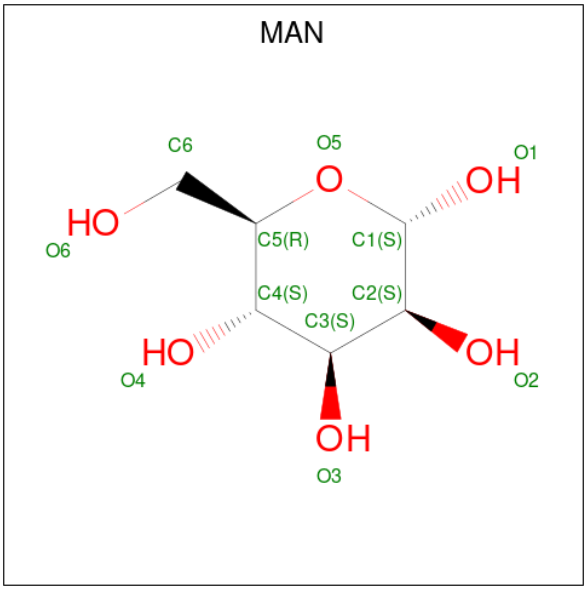
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	D	1	6	3	3		0	0
			Total	C	O			
5	E	1	6	3	3		0	0

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	11	6	5	0	0

- Molecule 8 is water.

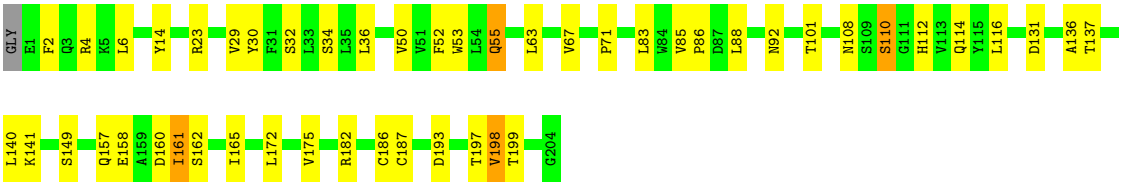
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	137	137	137	0	0
			Total	O		
8	B	126	126	126	0	0
			Total	O		
8	C	135	135	135	0	0
			Total	O		
8	D	155	155	155	0	0
			Total	O		
8	E	110	110	110	0	0

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.

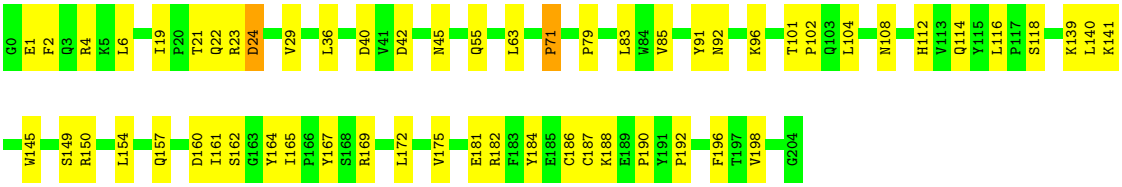
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain A:



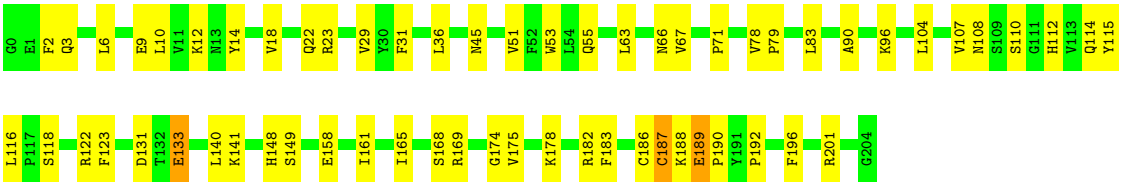
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain B:



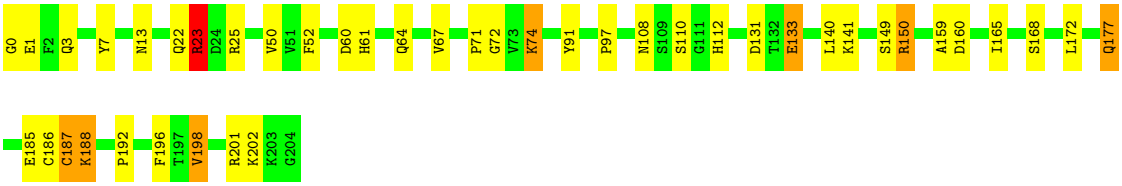
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain C:



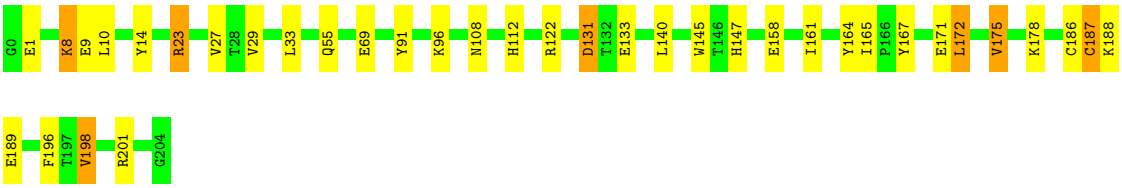
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

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	85.20Å 106.48Å 140.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.20 48.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.4 (48.38-2.20) 91.8 (48.38-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.168 , 0.233 0.171 , 0.233	Depositor DCC
R_{free} test set	3018 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 82.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	9623	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: BMA, 42R, NAG, GOL, 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	0.38	0/1748	0.55	0/2380
1	B	0.40	0/1740	0.56	0/2367
1	C	0.40	0/1743	0.57	0/2373
1	D	0.43	0/1749	0.58	0/2382
1	E	0.39	0/1733	0.56	0/2357
All	All	0.40	0/8713	0.56	0/11859

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 (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	1703	0	1666	33	0
1	B	1694	0	1653	46	2
1	C	1698	0	1664	56	0
1	D	1703	0	1669	36	0
1	E	1687	0	1645	26	2
2	A	28	0	26	3	0
2	B	28	0	26	2	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	5	0
2	E	28	0	26	2	0
3	A	34	0	26	4	0
3	B	34	0	26	9	0
3	C	34	0	26	6	0
3	D	34	0	26	5	0
3	E	34	0	26	6	0
4	A	25	0	27	3	0
4	B	25	0	27	10	0
4	C	25	0	27	3	0
4	D	25	0	27	4	0
4	E	25	0	27	7	0
5	C	6	0	8	0	0
5	D	6	0	8	1	0
5	E	6	0	8	0	0
6	D	11	0	10	1	0
7	D	11	0	10	0	0
8	A	137	0	0	10	0
8	B	126	0	0	12	0
8	C	135	0	0	18	0
8	D	155	0	0	11	0
8	E	110	0	0	9	0
All	All	9623	0	8736	212	2

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 12.

All (212) 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)
3:B:1206:42R:H10	1:C:53:TRP:HH2	1.40	0.85
8:A:2096:HOH:O	1:B:102:PRO:O	1.95	0.84
1:B:141:LYS:NZ	3:B:1206:42R:O1	2.09	0.84
3:B:1206:42R:H10	1:C:53:TRP:CH2	2.14	0.81
1:E:186:CYS:SG	1:E:187:CYS:N	2.56	0.78
1:D:186:CYS:SG	1:D:187:CYS:N	2.56	0.76
1:D:23:ARG:NH1	8:D:2037:HOH:O	2.20	0.75
1:B:150:ARG:NH1	8:B:2097:HOH:O	2.18	0.74
1:C:36:LEU:HD21	1:C:53:TRP:CZ3	2.22	0.73
1:B:139:LYS:NZ	8:B:2089:HOH:O	2.19	0.73
4:B:1207:L0B:O2	4:B:1207:L0B:N1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:GLU:HB2	3:C:1205:42R:H11	1.71	0.70
1:C:115:TYR:OH	8:C:2079:HOH:O	2.08	0.70
1:C:141:LYS:HD3	3:C:1206:42R:H4	1.74	0.70
1:B:184:TYR:CD1	4:B:1207:L0B:H16	2.29	0.67
1:C:161:ILE:HG21	1:C:175:VAL:HG11	1.77	0.67
8:C:2052:HOH:O	1:D:0:GLY:O	2.13	0.67
3:D:1206:42R:H11	4:D:1207:L0B:H20	1.78	0.66
4:B:1207:L0B:H7	1:C:114:GLN:O	1.97	0.65
8:A:2013:HOH:O	1:B:4:ARG:NH1	2.29	0.65
1:A:4:ARG:NH1	8:A:2007:HOH:O	2.30	0.65
1:A:50[B]:VAL:HG12	1:A:52:PHE:HD1	1.62	0.65
1:A:193:ASP:OD2	8:A:2131:HOH:O	2.14	0.64
1:C:45:ASN:OD1	8:C:2038:HOH:O	2.14	0.64
3:E:1206:42R:H11	4:E:1207:L0B:C20	2.28	0.64
1:A:186:CYS:SG	1:A:187:CYS:N	2.71	0.64
1:D:60:ASP:OD1	8:D:2073:HOH:O	2.15	0.63
1:B:145:TRP:CD1	4:B:1207:L0B:H5	2.33	0.63
1:D:108:ASN:HD21	2:D:301:NAG:C1	2.10	0.63
1:B:96:LYS:NZ	8:B:2067:HOH:O	2.32	0.63
2:D:302:NAG:O4	6:D:303:BMA:O6	2.16	0.63
1:C:2:PHE:O	8:C:2001:HOH:O	2.16	0.61
3:D:1206:42R:H13	1:E:165:ILE:HD11	1.82	0.61
3:D:1206:42R:H12	8:D:2091:HOH:O	1.99	0.61
1:E:158:GLU:O	8:E:2029:HOH:O	2.16	0.60
1:B:149:SER:HB3	1:B:192:PRO:HD3	1.83	0.60
1:D:150:ARG:NH1	8:D:2124:HOH:O	2.33	0.60
3:C:1206:42R:H11	4:C:1207:L0B:H20	1.82	0.60
3:E:1206:42R:H11	4:E:1207:L0B:H20	1.84	0.60
1:E:108:ASN:HD21	2:E:301:NAG:C1	2.15	0.59
1:C:112:HIS:CD2	2:C:301:NAG:H62	2.37	0.59
4:C:1207:L0B:N1	4:C:1207:L0B:O2	2.37	0.58
1:B:182:ARG:NE	8:B:2112:HOH:O	2.35	0.58
1:C:133:GLU:O	1:C:201:ARG:NH1	2.36	0.58
1:C:108:ASN:HD21	1:C:112:HIS:HB3	1.69	0.58
1:B:161:ILE:HG21	1:B:175[A]:VAL:HG21	1.86	0.58
1:C:122:ARG:NH1	8:C:2086:HOH:O	2.38	0.57
1:B:186:CYS:SG	4:B:1207:L0B:H81C	2.45	0.57
1:C:6:LEU:N	8:C:2001:HOH:O	2.27	0.57
1:D:159:ALA:HB2	1:D:196[B]:PHE:HE2	1.70	0.57
1:B:181:GLU:HG2	1:B:190:PRO:HB2	1.87	0.57
1:B:108:ASN:ND2	2:B:301:NAG:O6	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TRP:NE1	1:C:118:SER:HB2	2.20	0.57
1:C:169:ARG:HD2	8:C:2114:HOH:O	2.05	0.57
1:D:160:ASP:HA	8:D:2130:HOH:O	2.05	0.56
1:B:91:TYR:O	3:B:1206:42R:H11	2.05	0.56
1:D:50[B]:VAL:HG12	1:D:52:PHE:HD1	1.68	0.56
1:C:18:VAL:HG13	1:D:3:GLN:HG2	1.88	0.55
1:B:161:ILE:CG2	1:B:175[A]:VAL:HG21	2.37	0.55
1:C:66:ASN:HA	8:C:2054:HOH:O	2.07	0.55
1:B:63:LEU:HD11	1:B:83:LEU:HD22	1.89	0.55
1:A:36:LEU:HD13	3:E:1206:42R:H12	1.89	0.55
3:B:1206:42R:BR1	1:C:36:LEU:HB3	2.62	0.54
1:D:188:LYS:HZ2	1:D:188:LYS:HB2	1.72	0.54
1:B:186:CYS:SG	1:B:187:CYS:N	2.79	0.54
1:C:116:LEU:HB3	8:C:2084:HOH:O	2.06	0.54
3:C:1206:42R:H13	1:D:165[A]:ILE:HD11	1.90	0.53
1:C:186:CYS:SG	1:C:187:CYS:N	2.82	0.53
1:A:197:THR:O	8:A:2114:HOH:O	2.19	0.52
1:C:112:HIS:CG	2:C:301:NAG:H62	2.44	0.52
1:D:23:ARG:NH2	8:D:2038:HOH:O	2.27	0.52
1:C:36:LEU:HD11	1:C:53:TRP:CE3	2.45	0.52
1:B:140:LEU:HB2	1:B:196[B]:PHE:HB3	1.92	0.52
3:B:1206:42R:C6	1:C:53:TRP:HH2	2.15	0.52
1:C:55:GLN:HA	1:C:116:LEU:HD22	1.91	0.52
1:C:174:GLY:HA3	8:C:2118:HOH:O	2.09	0.52
4:D:1207:L0B:N1	4:D:1207:L0B:O2	2.43	0.52
1:A:114:GLN:NE2	8:A:2080:HOH:O	2.42	0.51
1:A:92:ASN:HB3	3:A:1206:42R:H1	1.92	0.51
1:D:196[A]:PHE:CE2	1:D:198:VAL:HG22	2.45	0.51
1:D:177:GLN:HB3	1:D:196[B]:PHE:CE2	2.46	0.51
1:E:9:GLU:OE1	3:E:1205:42R:H7	2.11	0.51
1:B:182:ARG:HD3	8:B:2115:HOH:O	2.11	0.50
1:D:22:GLN:O	1:D:25:ARG:HB2	2.12	0.50
1:E:27:VAL:HB	8:E:2089:HOH:O	2.11	0.50
1:B:79:PRO:HA	1:B:104:LEU:HD23	1.94	0.49
1:B:154:LEU:N	8:B:2099:HOH:O	2.45	0.49
1:E:10:LEU:O	1:E:14:TYR:HB3	2.12	0.49
8:A:2078:HOH:O	1:E:96:LYS:NZ	2.44	0.49
1:C:78:VAL:O	8:C:2060:HOH:O	2.20	0.49
1:D:133:GLU:HG2	1:D:201:ARG:NH1	2.27	0.49
1:A:165:ILE:HD11	3:E:1206:42R:H13	1.93	0.49
1:B:40:ASP:OD1	1:B:169:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLN:HB3	1:D:196[B]:PHE:CD2	2.47	0.49
1:D:13:ASN:HB2	8:D:2009:HOH:O	2.13	0.48
1:B:19:ILE:HG12	1:B:21:THR:HG23	1.95	0.48
1:B:165:ILE:HD12	1:B:167:TYR:CE2	2.49	0.48
1:A:114:GLN:OE1	4:E:1207:L0B:H5	2.13	0.48
1:A:160:ASP:OD1	1:A:162:SER:OG	2.27	0.48
1:A:136:ALA:O	1:A:199:THR:HA	2.14	0.48
1:B:101:THR:HG23	1:B:118:SER:HB3	1.94	0.48
1:A:110:SER:OG	2:A:301:NAG:N2	2.46	0.48
1:C:148:HIS:CG	1:C:189:GLU:HG3	2.48	0.48
1:D:97:PRO:HG3	5:D:1208:GOL:H32	1.96	0.48
1:B:45:ASN:OD1	1:C:169:ARG:NH2	2.43	0.48
1:D:188:LYS:HB2	1:D:188:LYS:NZ	2.29	0.48
1:D:91:TYR:OH	4:D:1207:L0B:H131	2.14	0.47
1:D:131:ASP:HB2	8:D:2116:HOH:O	2.14	0.47
1:E:131:ASP:HB2	8:E:2040:HOH:O	2.14	0.47
1:C:14:TYR:O	8:C:2004:HOH:O	2.20	0.47
1:A:30:TYR:HD1	8:A:2025:HOH:O	1.98	0.47
1:C:83:LEU:HD21	8:E:2109:HOH:O	2.13	0.47
1:A:53:TRP:CE2	4:E:1207:L0B:H19	2.50	0.47
1:C:96:LYS:NZ	8:C:2076:HOH:O	2.36	0.47
1:C:115:TYR:C	1:C:116:LEU:HD23	2.35	0.47
1:C:178:LYS:HE3	1:C:178:LYS:HB2	1.77	0.47
3:D:1206:42R:H13	1:E:165:ILE:CD1	2.45	0.47
1:E:112:HIS:HB2	8:E:2043:HOH:O	2.15	0.47
3:A:1206:42R:H11	4:A:1207:L0B:H20	1.97	0.47
1:E:196[B]:PHE:CE2	1:E:198:VAL:HG22	2.50	0.47
1:C:148:HIS:CD2	1:C:189:GLU:HG3	2.50	0.47
1:E:171:GLU:OE2	1:E:201:ARG:NE	2.44	0.47
1:B:157:GLN:OE1	8:B:2030:HOH:O	2.20	0.46
1:C:10:LEU:HA	8:C:2003:HOH:O	2.15	0.46
1:A:101:THR:HG21	1:E:145:TRP:CZ2	2.50	0.46
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.65	0.46
1:C:161:ILE:CG2	1:C:175:VAL:HG11	2.45	0.46
1:A:161:ILE:HG21	1:A:175[A]:VAL:HG11	1.98	0.46
1:C:36:LEU:HA	1:C:36:LEU:HD23	1.61	0.46
1:D:131:ASP:OD2	1:D:202:LYS:HD2	2.16	0.46
1:A:32[A]:SER:OG	1:A:55:GLN:HB2	2.15	0.45
1:C:107:VAL:HG21	8:E:2109:HOH:O	2.15	0.45
1:E:91:TYR:OH	4:E:1207:L0B:H131	2.16	0.45
1:A:2:PHE:HB2	8:A:2002:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1207:L0B:H223	4:A:1207:L0B:H141	1.78	0.45
1:C:149:SER:HB3	1:C:192:PRO:HD3	1.98	0.45
1:D:25:ARG:NH1	8:D:2036:HOH:O	2.48	0.45
1:A:53:TRP:CG	4:E:1207:L0B:H10	2.51	0.45
1:E:178:LYS:HB2	1:E:178:LYS:HE3	1.74	0.45
1:C:36:LEU:HD21	1:C:53:TRP:HZ3	1.76	0.45
1:D:168:SER:HB3	8:D:2134:HOH:O	2.16	0.45
1:C:90:ALA:HB1	1:C:123:PHE:HE2	1.82	0.45
1:A:175[B]:VAL:HG13	8:A:2114:HOH:O	2.16	0.45
1:E:133:GLU:HG2	1:E:201:ARG:NH1	2.31	0.45
1:E:165:ILE:HD12	1:E:167:TYR:CZ	2.52	0.44
1:A:63:LEU:HD11	1:A:83:LEU:HD22	1.97	0.44
1:C:110:SER:OG	2:C:301:NAG:H82	2.17	0.44
1:C:183:PHE:CE1	1:C:190:PRO:HD3	2.51	0.44
1:E:122:ARG:NH1	8:E:2042:HOH:O	2.21	0.44
1:E:188:LYS:HG2	1:E:189:GLU:CD	2.38	0.44
1:B:55:GLN:HG2	1:B:116:LEU:HD22	2.00	0.44
3:C:1206:42R:H11	4:C:1207:L0B:C20	2.46	0.44
1:D:61:HIS:O	1:D:64:GLN:HG2	2.17	0.44
2:B:301:NAG:O4	2:B:302:NAG:N2	2.51	0.44
1:C:182:ARG:HD2	8:C:2042:HOH:O	2.17	0.44
1:B:2:PHE:CD2	1:B:71:PRO:HD2	2.53	0.43
4:B:1207:L0B:H82C	4:B:1207:L0B:H221	1.39	0.43
1:D:141:LYS:NZ	3:D:1206:42R:O1	2.50	0.43
1:E:8:LYS:HE3	1:E:8:LYS:HB3	1.86	0.43
1:B:92:ASN:HA	3:B:1206:42R:C9	2.48	0.43
1:B:182:ARG:NE	8:B:2090:HOH:O	2.51	0.43
1:D:1:GLU:N	8:D:2003:HOH:O	2.48	0.43
1:D:3:GLN:O	1:D:7:TYR:HD1	2.01	0.43
2:D:301:NAG:O4	2:D:302:NAG:O5	2.29	0.43
1:E:23:ARG:H	1:E:23:ARG:HG2	1.52	0.43
2:E:301:NAG:O4	2:E:302:NAG:H3	2.18	0.43
3:B:1206:42R:H13	1:C:165:ILE:HD11	2.00	0.43
1:A:108:ASN:HD21	2:A:301:NAG:C1	2.32	0.43
1:E:161:ILE:HD13	1:E:175:VAL:HG11	1.99	0.43
1:A:137:THR:HA	1:A:198:VAL:O	2.19	0.43
1:C:63:LEU:HD11	1:C:83:LEU:HD22	2.00	0.43
1:B:112:HIS:HB2	8:B:2050:HOH:O	2.19	0.43
1:B:164:TYR:OH	8:B:2036:HOH:O	2.21	0.43
1:C:108:ASN:ND2	2:C:301:NAG:O5	2.52	0.43
1:B:165:ILE:HA	1:B:165:ILE:HD13	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:NZ	8:B:2088:HOH:O	2.53	0.42
1:A:86:PRO:HB2	1:A:88[A]:LEU:HG	2.01	0.42
3:C:1206:42R:O1	8:C:2096:HOH:O	2.21	0.42
1:B:91:TYR:OH	4:B:1207:L0B:H131	2.19	0.42
1:D:112:HIS:CD2	2:D:301:NAG:H62	2.54	0.42
4:A:1207:L0B:H4	4:A:1207:L0B:H81C	1.91	0.42
1:B:145:TRP:O	4:B:1207:L0B:H122	2.19	0.42
1:B:160:ASP:OD2	1:B:162:SER:OG	2.37	0.42
1:E:147:HIS:HE1	8:E:2061:HOH:O	2.02	0.42
1:C:36:LEU:HD12	1:C:51:VAL:HG12	2.01	0.42
3:A:1206:42R:C10	1:B:36:LEU:HD13	2.50	0.41
3:B:1206:42R:H13	1:C:165:ILE:HG12	2.02	0.41
1:D:149:SER:HB3	1:D:192:PRO:HD3	2.01	0.41
1:B:42:ASP:OD2	1:B:45:ASN:ND2	2.53	0.41
1:C:79:PRO:HA	1:C:104:LEU:HD23	2.02	0.41
1:D:110:SER:OG	2:D:301:NAG:N2	2.53	0.41
1:B:6:LEU:HD12	1:B:6:LEU:HA	1.91	0.41
1:D:72:GLY:O	1:D:74:LYS:HD2	2.20	0.41
1:A:32[B]:SER:HB2	1:A:157:GLN:HB2	2.01	0.41
1:B:196[B]:PHE:CE2	1:B:198:VAL:HG22	2.56	0.41
8:B:2015:HOH:O	1:C:3:GLN:NE2	2.53	0.41
1:A:165:ILE:HD11	3:E:1206:42R:C12	2.50	0.41
4:B:1207:L0B:H82C	1:C:116:LEU:HD12	2.03	0.41
1:C:31:PHE:CE2	1:C:196:PHE:HE2	2.39	0.41
8:C:2024:HOH:O	1:D:1:GLU:HB2	2.19	0.41
1:E:33:LEU:HD22	1:E:196[B]:PHE:CD2	2.56	0.41
1:A:112:HIS:ND1	2:A:301:NAG:H61	2.36	0.41
1:A:14:TYR:HA	1:B:4:ARG:NH2	2.36	0.40
1:A:34:SER:OG	1:A:160:ASP:HB3	2.21	0.40
1:A:53:TRP:CZ2	4:E:1207:L0B:H19	2.56	0.40
4:B:1207:L0B:H223	4:B:1207:L0B:H141	1.90	0.40
1:D:91:TYR:CE2	4:D:1207:L0B:H142	2.56	0.40
1:E:164:TYR:CZ	1:E:172:LEU:HD13	2.57	0.40
1:B:22:GLN:O	1:B:24:ASP:N	2.54	0.40
1:A:116:LEU:HD13	8:E:2108:HOH:O	2.20	0.40
1:C:182:ARG:HG2	8:C:2126:HOH:O	2.21	0.40
1:A:141:LYS:HE2	3:A:1206:42R:H4	2.04	0.40

All (2) 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)
1:B:188:LYS:CE	1:E:69:GLU:OE1[3_545]	2.13	0.07
1:B:188:LYS:NZ	1:E:69:GLU:OE1[3_545]	2.19	0.01

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	207/205 (101%)	199 (96%)	7 (3%)	1 (0%)	29	31
1	B	206/205 (100%)	200 (97%)	3 (2%)	3 (2%)	10	8
1	C	207/205 (101%)	200 (97%)	5 (2%)	2 (1%)	15	14
1	D	207/205 (101%)	202 (98%)	3 (1%)	2 (1%)	15	14
1	E	205/205 (100%)	195 (95%)	10 (5%)	0	100	100
All	All	1032/1025 (101%)	996 (96%)	28 (3%)	8 (1%)	19	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	ARG
1	C	71	PRO
1	D	23	ARG
1	B	24	ASP
1	C	22	GLN
1	A	71	PRO
1	D	71	PRO
1	B	71	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	195/190 (103%)	180 (92%)	15 (8%)	13	13
1	B	193/190 (102%)	189 (98%)	4 (2%)	53	67
1	C	194/190 (102%)	182 (94%)	12 (6%)	18	21
1	D	194/190 (102%)	182 (94%)	12 (6%)	18	21
1	E	192/190 (101%)	181 (94%)	11 (6%)	20	24
All	All	968/950 (102%)	914 (94%)	54 (6%)	20	25

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	23	ARG
1	A	29	VAL
1	A	55	GLN
1	A	67	VAL
1	A	85	VAL
1	A	110	SER
1	A	131	ASP
1	A	140	LEU
1	A	149	SER
1	A	158	GLU
1	A	161	ILE
1	A	172	LEU
1	A	182	ARG
1	A	198	VAL
1	B	1	GLU
1	B	29	VAL
1	B	85	VAL
1	B	114	GLN
1	C	12	LYS
1	C	23	ARG
1	C	29	VAL
1	C	67	VAL
1	C	131	ASP
1	C	133	GLU
1	C	140	LEU
1	C	158	GLU
1	C	168	SER

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Mol	Chain	Res	Type
1	C	187	CYS
1	C	188	LYS
1	C	189	GLU
1	D	23	ARG
1	D	67	VAL
1	D	74	LYS
1	D	133	GLU
1	D	140	LEU
1	D	150	ARG
1	D	172	LEU
1	D	177	GLN
1	D	185	GLU
1	D	187	CYS
1	D	188	LYS
1	D	198	VAL
1	E	1	GLU
1	E	8	LYS
1	E	23	ARG
1	E	29	VAL
1	E	55	GLN
1	E	131	ASP
1	E	140	LEU
1	E	172	LEU
1	E	175	VAL
1	E	187	CYS
1	E	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	ASN
1	C	112	HIS
1	E	108	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

30 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	B	302	-	14,14,15	0.53	0	17,19,21	0.77	0
2	NAG	C	302	-	14,14,15	0.49	0	17,19,21	0.98	1 (5%)
3	42R	C	1206	-	15,18,18	2.59	6 (40%)	22,27,27	1.48	3 (13%)
4	L0B	D	1207	-	27,27,27	0.57	0	33,36,36	1.18	2 (6%)
4	L0B	A	1207	-	27,27,27	0.56	0	33,36,36	1.32	3 (9%)
2	NAG	D	301	-	14,14,15	0.53	0	17,19,21	2.04	5 (29%)
3	42R	D	1206	-	15,18,18	2.60	6 (40%)	22,27,27	1.55	3 (13%)
3	42R	B	1205	-	15,18,18	2.49	6 (40%)	22,27,27	1.52	4 (18%)
2	NAG	D	302	-	14,14,15	0.53	0	17,19,21	1.72	4 (23%)
3	42R	C	1205	-	15,18,18	2.59	5 (33%)	22,27,27	1.79	3 (13%)
2	NAG	A	302	-	14,14,15	0.57	0	17,19,21	0.79	0
2	NAG	E	301	-	14,14,15	0.58	0	17,19,21	1.53	3 (17%)
4	L0B	E	1207	-	27,27,27	0.52	0	33,36,36	1.51	6 (18%)
3	42R	E	1206	-	15,18,18	2.58	6 (40%)	22,27,27	1.45	3 (13%)
4	L0B	B	1207	-	27,27,27	0.67	1 (3%)	33,36,36	1.63	9 (27%)
2	NAG	C	301	-	14,14,15	0.46	0	17,19,21	1.29	2 (11%)
3	42R	B	1206	-	15,18,18	2.57	6 (40%)	22,27,27	1.83	5 (22%)
7	MAN	D	304	-	11,11,12	0.56	0	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	42R	A	1206	-	15,18,18	2.54	6 (40%)	22,27,27	1.39	3 (13%)
3	42R	E	1205	-	15,18,18	2.44	5 (33%)	22,27,27	1.85	5 (22%)
5	GOL	C	1208	-	5,5,5	0.28	0	5,5,5	0.39	0
6	BMA	D	303	-	11,11,12	0.43	0	15,15,17	1.71	3 (20%)
3	42R	D	1205	-	15,18,18	2.44	4 (26%)	22,27,27	1.50	4 (18%)
4	L0B	C	1207	-	27,27,27	0.61	0	33,36,36	1.42	4 (12%)
2	NAG	A	301	-	14,14,15	0.56	0	17,19,21	1.45	2 (11%)
3	42R	A	1205	-	15,18,18	2.54	6 (40%)	22,27,27	1.50	3 (13%)
2	NAG	B	301	-	14,14,15	0.54	0	17,19,21	1.51	2 (11%)
5	GOL	E	1208	-	5,5,5	0.41	0	5,5,5	0.29	0
2	NAG	E	302	-	14,14,15	0.50	0	17,19,21	0.92	1 (5%)
5	GOL	D	1208	-	5,5,5	0.35	0	5,5,5	0.33	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	NAG	B	302	-	-	3/6/23/26	0/1/1/1
2	NAG	C	302	-	-	2/6/23/26	0/1/1/1
3	42R	C	1206	-	-	0/4/23/23	0/2/2/2
4	L0B	D	1207	-	-	6/16/30/30	0/3/3/3
4	L0B	A	1207	-	-	2/16/30/30	0/3/3/3
2	NAG	D	301	-	-	0/6/23/26	0/1/1/1
3	42R	D	1206	-	-	2/4/23/23	0/2/2/2
3	42R	B	1205	-	-	2/4/23/23	0/2/2/2
2	NAG	D	302	-	-	2/6/23/26	0/1/1/1
3	42R	C	1205	-	-	2/4/23/23	0/2/2/2
2	NAG	A	302	-	-	2/6/23/26	0/1/1/1
2	NAG	E	301	-	-	0/6/23/26	0/1/1/1
4	L0B	E	1207	-	-	3/16/30/30	0/3/3/3
3	42R	E	1206	-	-	0/4/23/23	0/2/2/2
4	L0B	B	1207	-	-	7/16/30/30	0/3/3/3
2	NAG	C	301	-	-	3/6/23/26	0/1/1/1
3	42R	B	1206	-	-	0/4/23/23	0/2/2/2
7	MAN	D	304	-	-	0/2/19/22	0/1/1/1
3	42R	A	1206	-	-	3/4/23/23	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	42R	E	1205	-	-	4/4/23/23	0/2/2/2
5	GOL	C	1208	-	-	2/4/4/4	-
6	BMA	D	303	-	-	2/2/19/22	0/1/1/1
3	42R	D	1205	-	-	0/4/23/23	0/2/2/2
4	L0B	C	1207	-	-	5/16/30/30	0/3/3/3
2	NAG	A	301	-	-	1/6/23/26	0/1/1/1
3	42R	A	1205	-	-	3/4/23/23	0/2/2/2
2	NAG	B	301	-	-	2/6/23/26	0/1/1/1
5	GOL	E	1208	-	-	1/4/4/4	-
2	NAG	E	302	-	-	3/6/23/26	0/1/1/1
5	GOL	D	1208	-	-	4/4/4/4	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1206	42R	C6-C7	6.54	1.51	1.37
3	E	1206	42R	C6-C7	6.51	1.51	1.37
3	C	1205	42R	C6-C7	6.51	1.51	1.37
3	D	1206	42R	C6-C7	6.50	1.51	1.37
3	B	1206	42R	C6-C7	6.46	1.51	1.37
3	A	1206	42R	C6-C7	6.41	1.51	1.37
3	D	1205	42R	C6-C7	6.36	1.51	1.37
3	A	1205	42R	C6-C7	6.35	1.51	1.37
3	B	1205	42R	C6-C7	6.19	1.51	1.37
3	E	1205	42R	C6-C7	5.78	1.50	1.37
3	B	1206	42R	O1-C3	-4.72	1.35	1.43
3	D	1205	42R	O1-C3	-4.43	1.35	1.43
3	C	1206	42R	O1-C3	-4.31	1.36	1.43
3	E	1205	42R	O1-C3	-4.30	1.36	1.43
3	B	1205	42R	O1-C3	-4.29	1.36	1.43
3	C	1205	42R	O1-C3	-4.24	1.36	1.43
3	E	1206	42R	O1-C3	-4.21	1.36	1.43
3	A	1205	42R	O1-C3	-4.20	1.36	1.43
3	D	1206	42R	O1-C3	-4.13	1.36	1.43
3	A	1206	42R	O1-C3	-4.11	1.36	1.43
3	D	1206	42R	C6-C5	4.02	1.54	1.45
3	C	1205	42R	C6-C5	3.96	1.53	1.45
3	A	1206	42R	C6-C5	3.93	1.53	1.45
3	C	1206	42R	C6-C5	3.93	1.53	1.45
3	E	1206	42R	C6-C5	3.84	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1205	42R	C6-C5	3.77	1.53	1.45
3	B	1205	42R	C6-C5	3.48	1.52	1.45
3	D	1205	42R	C6-C5	3.48	1.52	1.45
3	B	1206	42R	C6-C5	3.44	1.52	1.45
3	E	1205	42R	C4-C3	-3.17	1.47	1.52
3	E	1205	42R	C6-C5	3.03	1.52	1.45
3	C	1205	42R	BR1-C11	2.76	1.95	1.90
3	D	1205	42R	C4-C3	-2.68	1.48	1.52
3	E	1205	42R	C10-C9	-2.67	1.33	1.38
3	A	1205	42R	C4-C3	-2.57	1.48	1.52
3	D	1206	42R	BR1-C11	2.54	1.95	1.90
3	B	1205	42R	C4-C3	-2.53	1.48	1.52
4	B	1207	L0B	C17-C16	-2.48	1.47	1.51
3	C	1205	42R	C4-C3	-2.48	1.48	1.52
3	D	1206	42R	C4-C3	-2.46	1.48	1.52
3	E	1206	42R	C4-C3	-2.46	1.48	1.52
3	A	1206	42R	C4-C3	-2.46	1.48	1.52
3	A	1205	42R	C2-N1	-2.37	1.44	1.46
3	C	1206	42R	C4-C3	-2.35	1.49	1.52
3	C	1206	42R	BR1-C11	2.32	1.95	1.90
3	B	1206	42R	C4-C3	-2.29	1.49	1.52
3	E	1206	42R	C2-N1	-2.27	1.44	1.46
3	B	1206	42R	BR1-C11	2.22	1.94	1.90
3	B	1205	42R	BR1-C11	2.19	1.94	1.90
3	C	1206	42R	C2-N1	-2.19	1.44	1.46
3	D	1206	42R	C2-N1	-2.15	1.44	1.46
3	B	1205	42R	C10-C9	-2.09	1.34	1.38
3	A	1206	42R	C2-N1	-2.09	1.44	1.46
3	E	1206	42R	C10-C9	-2.08	1.35	1.38
3	A	1206	42R	BR1-C11	2.07	1.94	1.90
3	A	1205	42R	BR1-C11	2.05	1.94	1.90
3	B	1206	42R	C2-N1	-2.01	1.44	1.46

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1205	42R	C1-N1-C2	-6.36	108.62	117.31
3	B	1206	42R	C4-C3-C5	4.70	113.20	107.81
4	E	1207	L0B	C22-N1-C11	-4.65	109.40	113.16
3	D	1206	42R	C1-N1-C2	-4.56	111.07	117.31
3	A	1206	42R	C1-N1-C2	-4.46	111.22	117.31
3	C	1206	42R	C1-N1-C2	-4.42	111.27	117.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1207	L0B	C22-N1-C9	-4.38	109.61	113.16
4	C	1207	L0B	C12-C9-C8	4.36	117.97	112.70
2	D	301	NAG	O5-C1-C2	-4.35	104.42	111.29
3	D	1205	42R	C1-N1-C2	-4.31	111.42	117.31
3	E	1206	42R	C1-N1-C2	-4.30	111.43	117.31
3	B	1205	42R	C1-N1-C2	-4.30	111.44	117.31
6	D	303	BMA	C1-O5-C5	4.26	117.97	112.19
2	D	301	NAG	C4-C3-C2	-4.15	104.93	111.02
2	D	302	NAG	C2-N2-C7	-4.11	117.05	122.90
4	D	1207	L0B	C22-N1-C9	-4.10	109.84	113.16
2	B	301	NAG	C1-O5-C5	4.06	117.70	112.19
4	E	1207	L0B	C9-C8-C3	4.06	119.78	112.86
2	D	302	NAG	C1-O5-C5	4.02	117.64	112.19
2	D	301	NAG	C1-O5-C5	-4.01	106.77	112.19
3	E	1205	42R	C1-N1-C2	-3.93	111.94	117.31
2	A	301	NAG	O5-C1-C2	-3.89	105.15	111.29
4	C	1207	L0B	C9-N1-C11	-3.87	103.16	109.94
3	B	1206	42R	C1-N1-C2	-3.81	112.11	117.31
2	E	301	NAG	O5-C1-C2	-3.79	105.31	111.29
4	B	1207	L0B	C22-N1-C11	-3.76	110.12	113.16
4	A	1207	L0B	C22-N1-C11	-3.73	110.14	113.16
3	A	1205	42R	C1-N1-C2	-3.70	112.25	117.31
4	B	1207	L0B	C14-C16-C17	3.68	117.90	111.32
2	B	301	NAG	C3-C4-C5	3.59	116.64	110.24
2	C	301	NAG	C1-O5-C5	3.38	116.78	112.19
4	D	1207	L0B	C22-N1-C11	-3.29	110.50	113.16
3	E	1205	42R	C13-C8-C9	3.26	123.23	118.59
3	A	1205	42R	C4-C3-C5	3.22	111.50	107.81
4	B	1207	L0B	C22-N1-C9	-3.15	110.61	113.16
3	D	1206	42R	C4-C3-C5	3.14	111.40	107.81
4	C	1207	L0B	C9-C8-C3	3.12	118.17	112.86
3	D	1205	42R	C4-C3-C5	3.04	111.29	107.81
4	B	1207	L0B	C15-C13-C11	-3.01	104.83	110.82
6	D	303	BMA	C1-C2-C3	3.01	113.37	109.67
3	E	1205	42R	C12-C13-C8	-2.99	117.29	120.78
3	C	1206	42R	C1-N1-C7	2.87	131.92	120.48
4	E	1207	L0B	O1-C3-C8	2.83	124.05	120.76
2	D	301	NAG	O5-C5-C6	2.82	111.62	107.20
3	E	1205	42R	C4-C3-C5	2.79	111.01	107.81
2	E	301	NAG	C1-O5-C5	-2.78	108.43	112.19
3	B	1205	42R	C4-C3-C5	2.75	110.95	107.81
3	E	1206	42R	C4-C3-C5	2.74	110.95	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1206	42R	C1-N1-C7	2.72	131.30	120.48
6	D	303	BMA	O5-C5-C6	2.71	111.46	107.20
2	A	301	NAG	C4-C3-C2	-2.67	107.10	111.02
3	A	1205	42R	C1-N1-C7	2.67	131.09	120.48
2	D	302	NAG	O5-C5-C6	2.66	111.38	107.20
3	B	1206	42R	C1-N1-C7	2.65	131.03	120.48
2	C	302	NAG	C1-O5-C5	2.65	115.78	112.19
3	B	1206	42R	O1-C3-C5	-2.64	104.38	108.98
4	A	1207	L0B	C9-C8-C3	2.63	117.34	112.86
3	C	1205	42R	C4-C3-C5	2.63	110.82	107.81
7	D	304	MAN	C1-O5-C5	2.63	115.75	112.19
4	E	1207	L0B	C14-C16-C17	-2.57	106.73	111.32
4	C	1207	L0B	C22-N1-C11	-2.56	111.09	113.16
4	B	1207	L0B	C9-C8-C3	2.56	117.22	112.86
3	A	1206	42R	C1-N1-C7	2.50	130.44	120.48
3	C	1205	42R	C1-N1-C7	2.49	130.38	120.48
3	D	1206	42R	C1-N1-C7	2.49	130.38	120.48
3	B	1206	42R	O2-C5-C3	2.47	123.52	119.80
3	C	1206	42R	C4-C3-C5	2.46	110.62	107.81
3	A	1206	42R	C4-C3-C5	2.41	110.56	107.81
3	E	1205	42R	O2-C5-C3	2.36	123.35	119.80
3	D	1205	42R	O1-C3-C5	-2.28	105.00	108.98
4	B	1207	L0B	O2-C16-C17	-2.27	105.92	111.15
3	B	1205	42R	C1-N1-C7	2.25	129.42	120.48
2	E	301	NAG	C3-C4-C5	2.21	114.19	110.24
2	E	302	NAG	O5-C5-C6	2.18	110.62	107.20
2	D	302	NAG	C4-C3-C2	-2.17	107.84	111.02
3	B	1205	42R	O1-C3-C5	-2.17	105.21	108.98
4	B	1207	L0B	C18-C17-C19	2.16	120.99	118.29
4	E	1207	L0B	C8-C3-C1	-2.13	116.41	118.71
4	B	1207	L0B	C14-C11-C13	2.12	116.89	113.03
2	D	301	NAG	C2-N2-C7	-2.12	119.89	122.90
4	E	1207	L0B	C14-C11-C13	-2.08	109.23	113.03
4	B	1207	L0B	C15-C12-C9	2.08	114.95	110.82
3	D	1205	42R	C1-N1-C7	2.06	128.67	120.48
2	C	301	NAG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	302	NAG	O7-C7-N2-C2
2	B	302	NAG	C8-C7-N2-C2
2	B	302	NAG	O7-C7-N2-C2
2	C	301	NAG	C1-C2-N2-C7
2	C	301	NAG	C8-C7-N2-C2
2	C	301	NAG	O7-C7-N2-C2
2	C	302	NAG	C8-C7-N2-C2
2	C	302	NAG	O7-C7-N2-C2
2	E	302	NAG	C8-C7-N2-C2
2	E	302	NAG	O7-C7-N2-C2
4	B	1207	L0B	C2-C1-C3-O1
4	B	1207	L0B	C3-C8-C9-C12
5	C	1208	GOL	C1-C2-C3-O3
4	B	1207	L0B	C4-C1-C3-O1
4	B	1207	L0B	C4-C1-C3-C8
4	B	1207	L0B	C2-C1-C3-C8
4	D	1207	L0B	C2-C1-C3-O1
4	D	1207	L0B	C4-C1-C3-C8
4	D	1207	L0B	C2-C1-C3-C8
4	D	1207	L0B	C4-C1-C3-O1
2	D	302	NAG	C8-C7-N2-C2
2	D	302	NAG	O7-C7-N2-C2
6	D	303	BMA	C4-C5-C6-O6
2	B	301	NAG	C4-C5-C6-O6
5	D	1208	GOL	C1-C2-C3-O3
2	E	302	NAG	O5-C5-C6-O6
5	D	1208	GOL	O2-C2-C3-O3
2	B	301	NAG	O5-C5-C6-O6
6	D	303	BMA	O5-C5-C6-O6
5	C	1208	GOL	O2-C2-C3-O3
4	C	1207	L0B	C2-C1-C3-C8
2	A	301	NAG	O5-C5-C6-O6
4	C	1207	L0B	C2-C1-C3-O1
5	D	1208	GOL	O1-C1-C2-O2
4	D	1207	L0B	C1-C3-C8-C9
4	C	1207	L0B	C4-C1-C3-C8
4	C	1207	L0B	C4-C1-C3-O1
4	D	1207	L0B	O1-C3-C8-C9
4	B	1207	L0B	C1-C3-C8-C9
3	A	1205	42R	C6-C7-C8-C9
3	A	1205	42R	C6-C7-C8-C13
3	C	1205	42R	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	1206	42R	C6-C7-C8-C13
4	B	1207	L0B	O1-C3-C8-C9
3	A	1206	42R	C6-C7-C8-C9
3	C	1205	42R	C6-C7-C8-C13
3	E	1205	42R	C6-C7-C8-C9
3	B	1205	42R	C6-C7-C8-C13
3	D	1206	42R	C6-C7-C8-C9
3	E	1205	42R	C6-C7-C8-C13
4	E	1207	L0B	C2-C1-C3-O1
4	E	1207	L0B	C2-C1-C3-C8
4	A	1207	L0B	O1-C3-C8-C9
5	D	1208	GOL	O1-C1-C2-C3
4	C	1207	L0B	O2-C16-C17-C19
3	D	1206	42R	C6-C7-C8-C13
3	A	1205	42R	N1-C7-C8-C13
3	A	1206	42R	N1-C7-C8-C13
2	B	302	NAG	O5-C5-C6-O6
5	E	1208	GOL	O1-C1-C2-O2
3	E	1205	42R	N1-C7-C8-C9
3	E	1205	42R	N1-C7-C8-C13
4	E	1207	L0B	C4-C1-C3-O1
4	A	1207	L0B	C1-C3-C8-C9
3	B	1205	42R	C6-C7-C8-C9

There are no ring outliers.

22 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	NAG	1	0
3	C	1206	42R	5	0
4	D	1207	L0B	4	0
4	A	1207	L0B	3	0
2	D	301	NAG	4	0
3	D	1206	42R	5	0
2	D	302	NAG	2	0
3	C	1205	42R	1	0
2	E	301	NAG	2	0
4	E	1207	L0B	7	0
3	E	1206	42R	5	0
4	B	1207	L0B	10	0
2	C	301	NAG	4	0
3	B	1206	42R	9	0

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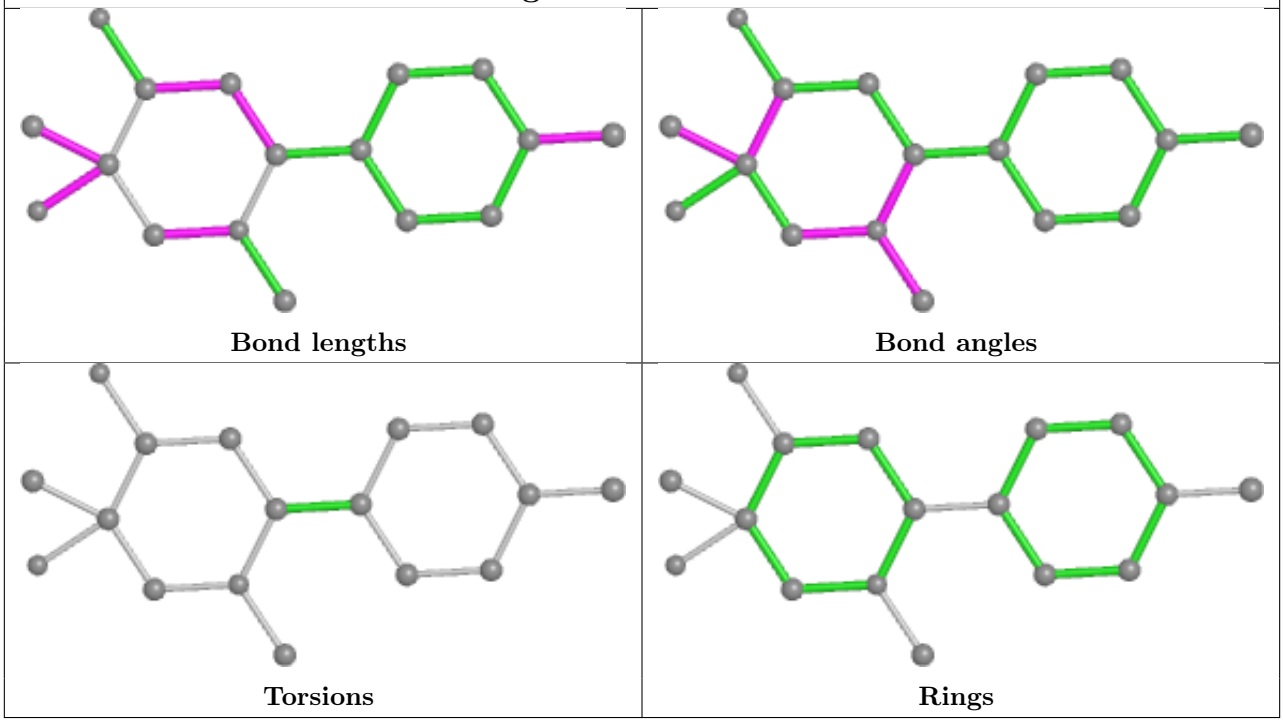
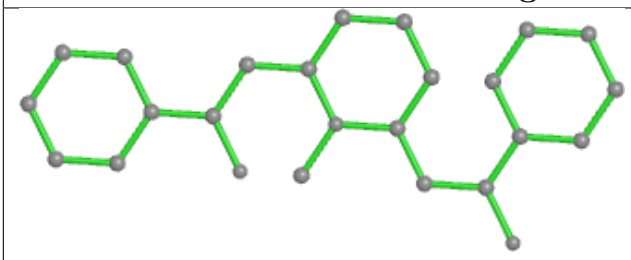
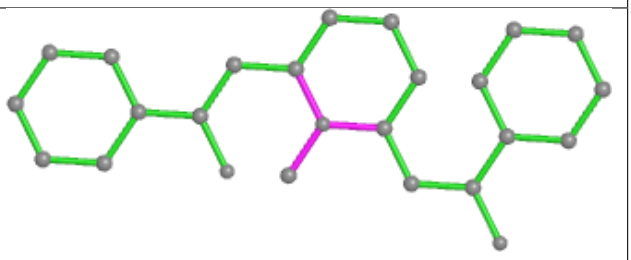
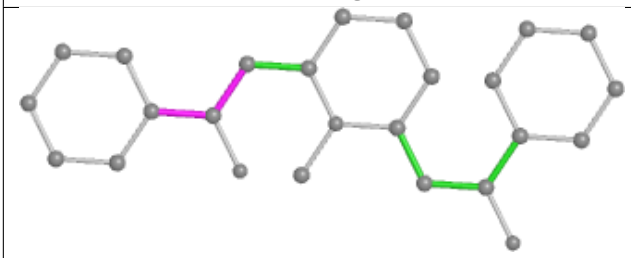
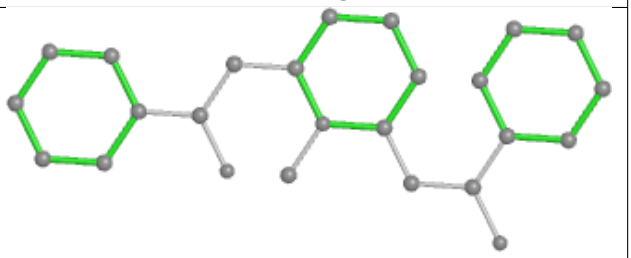
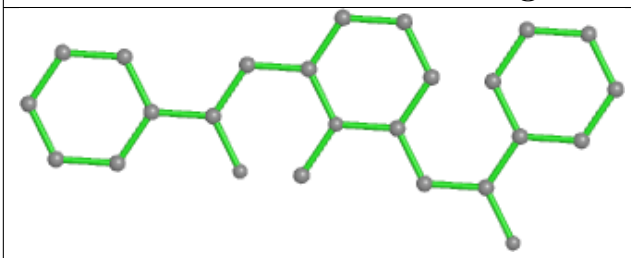
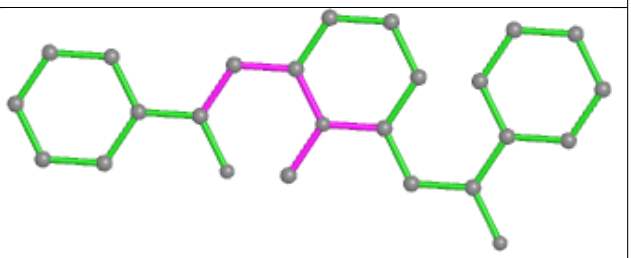
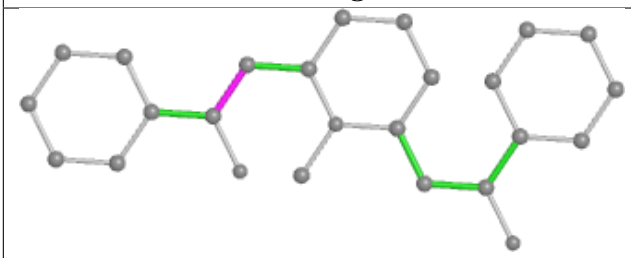
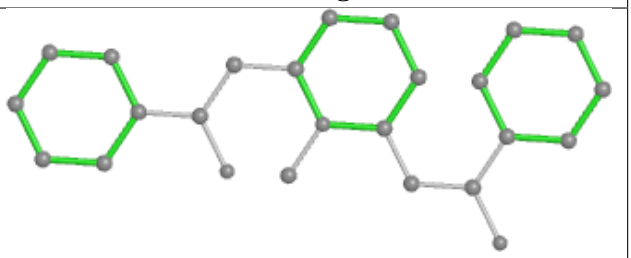
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1206	42R	4	0
3	E	1205	42R	1	0
6	D	303	BMA	1	0
4	C	1207	L0B	3	0
2	A	301	NAG	3	0
2	B	301	NAG	2	0
2	E	302	NAG	1	0
5	D	1208	GOL	1	0

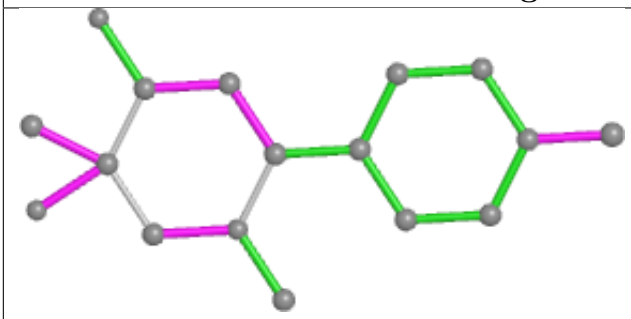
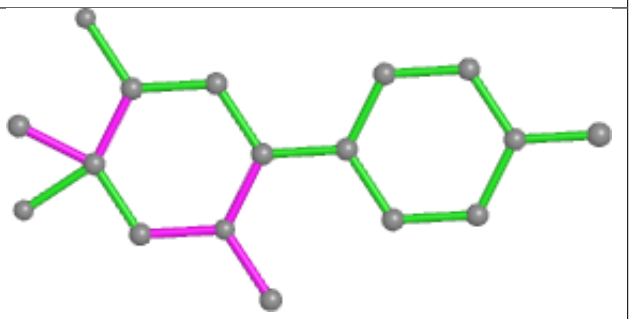
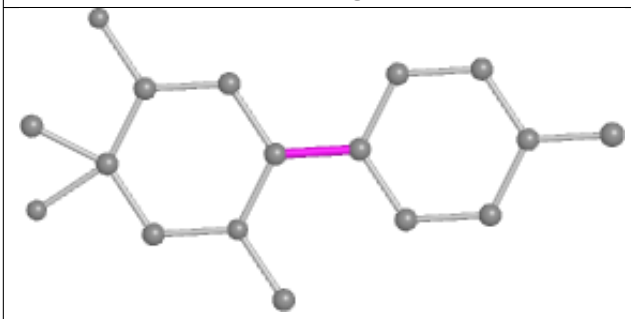
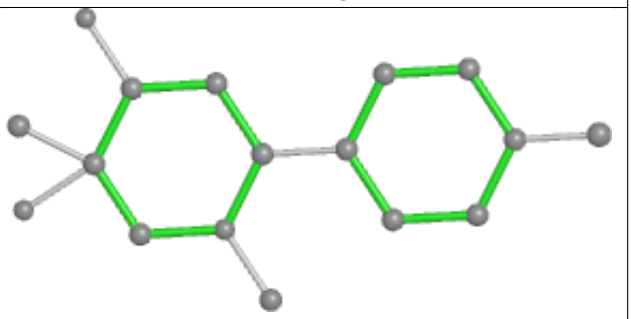
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

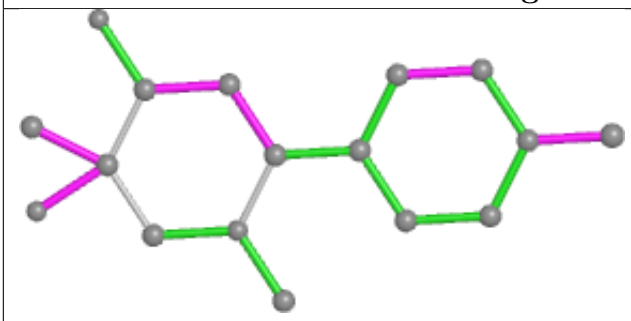
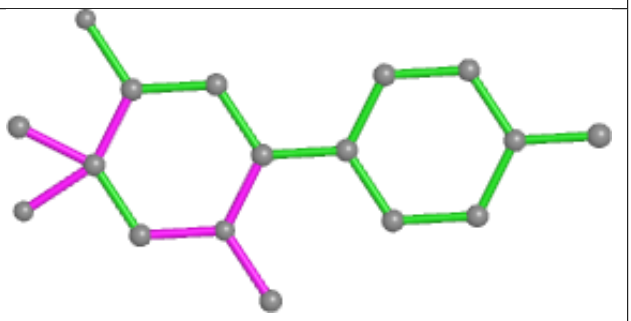
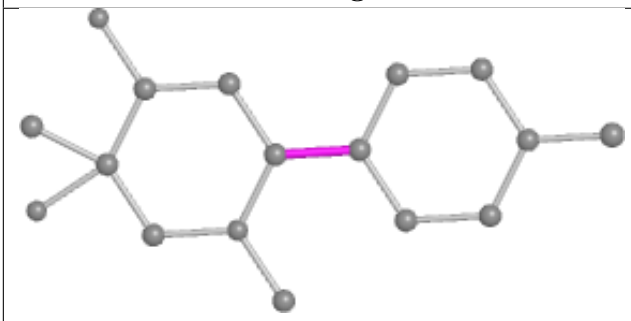
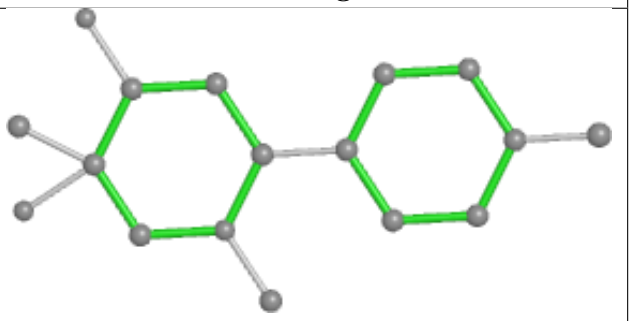
Ligand 42R C 1206



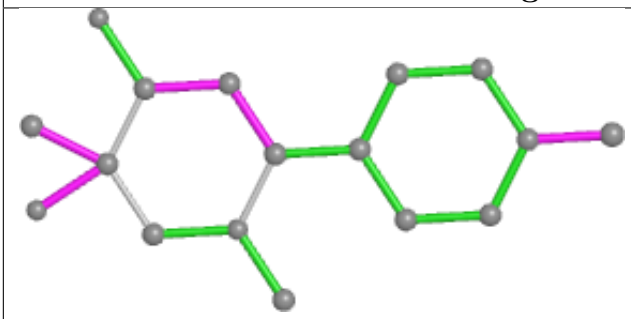
Ligand L0B D 1207	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand L0B A 1207	
 Bond lengths	 Bond angles
 Torsions	 Rings

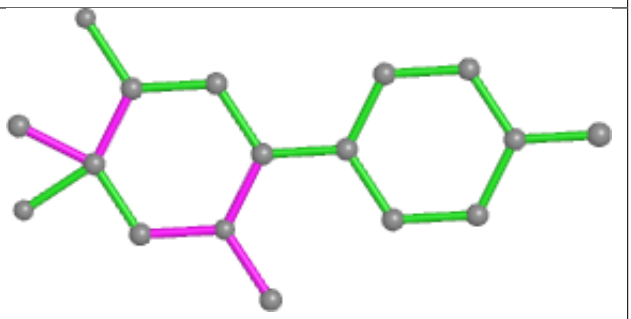
Ligand 42R D 1206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 42R B 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings

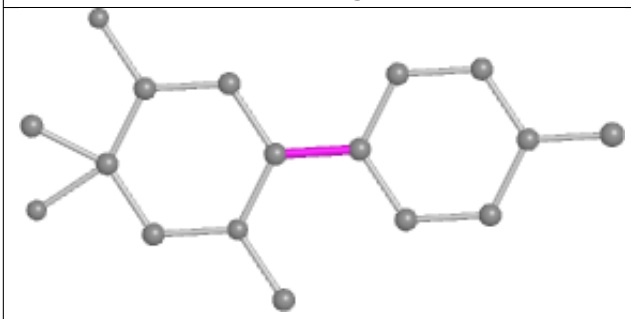
Ligand 42R C 1205



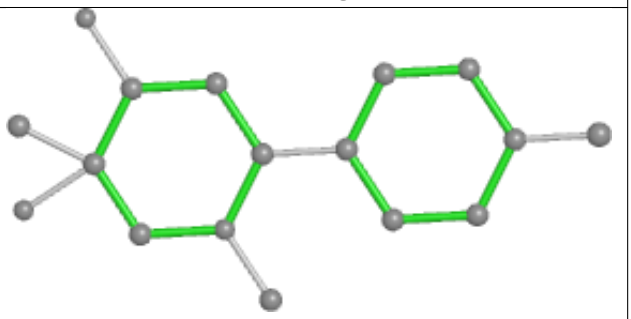
Bond lengths



Bond angles

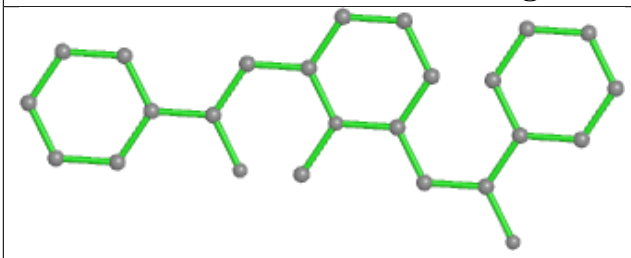


Torsions

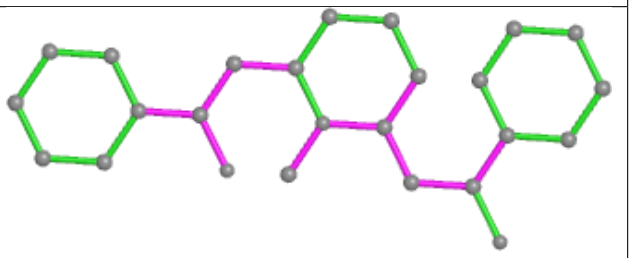


Rings

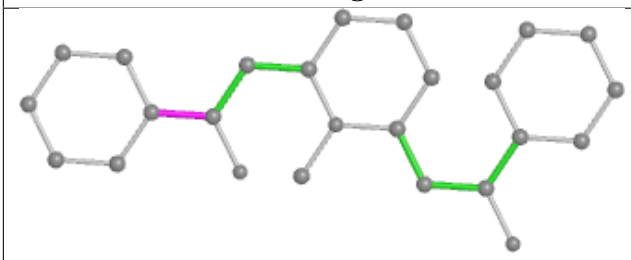
Ligand L0B E 1207



Bond lengths



Bond angles



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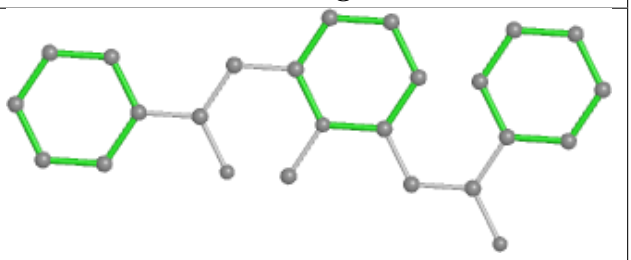
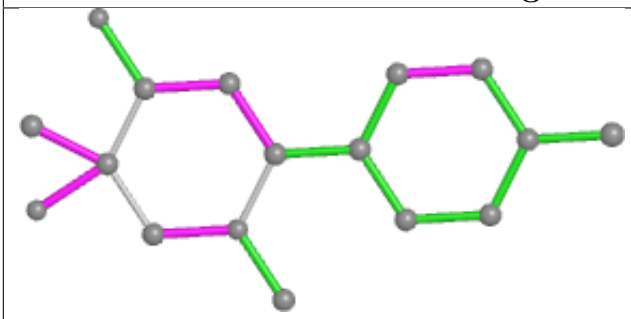
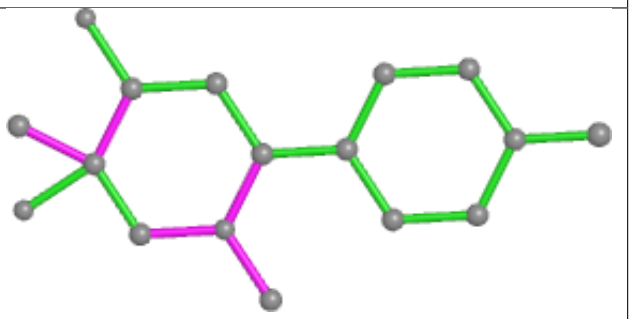


Rings

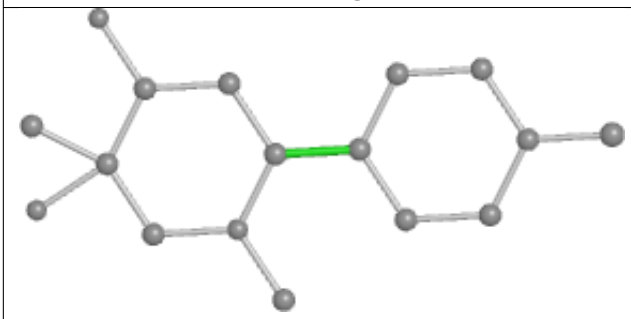
Ligand 42R E 1206



Bond lengths



Bond angles



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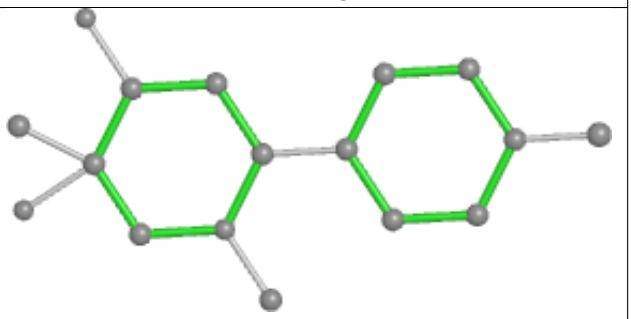
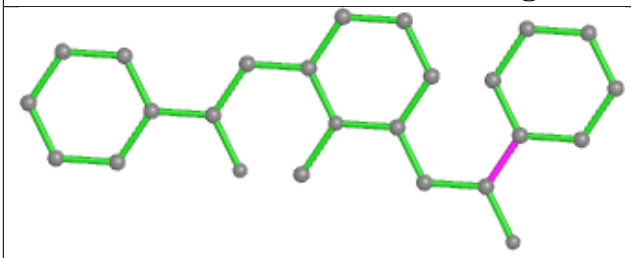
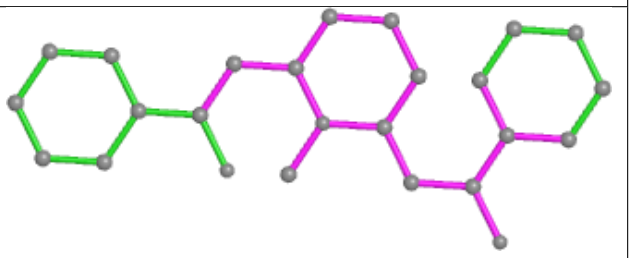


Rings

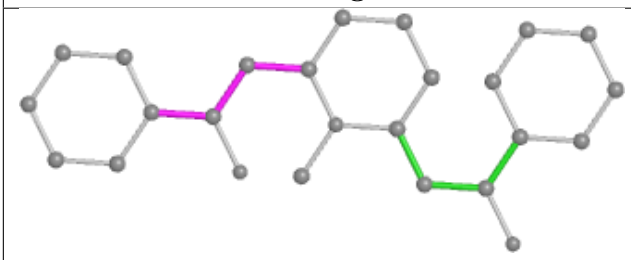
Ligand L0B B 1207



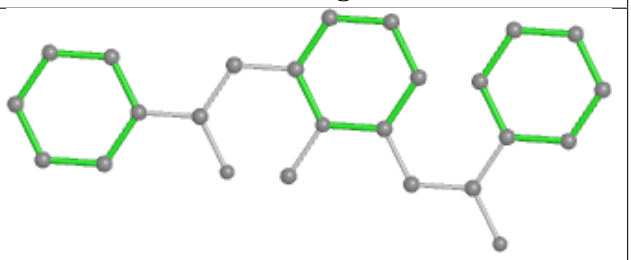
Bond lengths



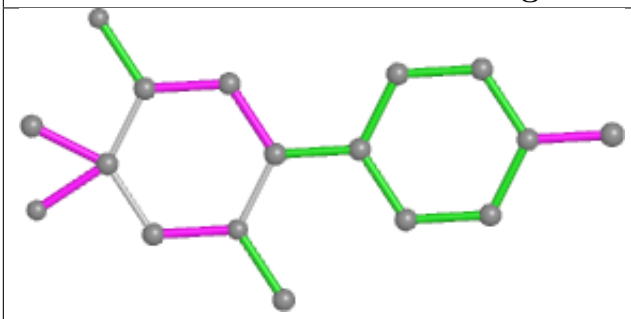
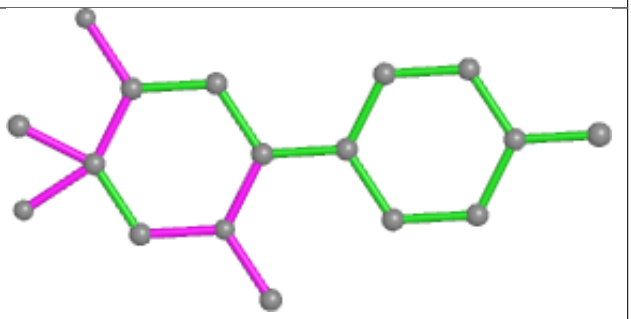
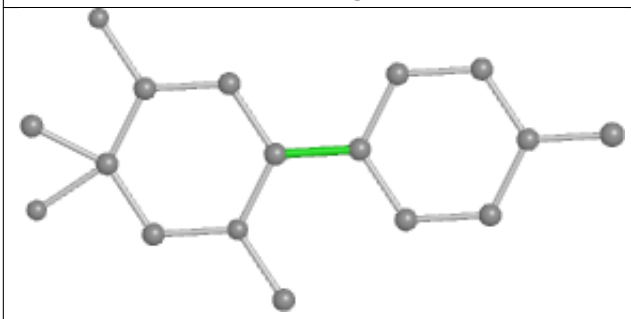
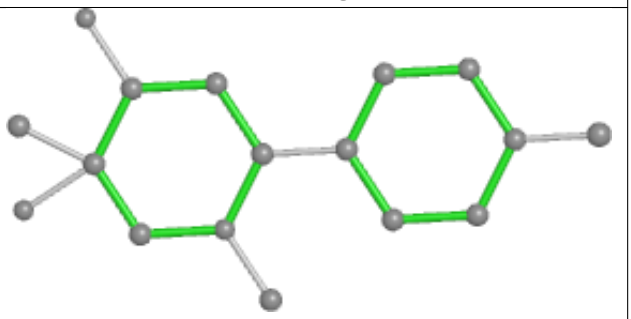
Bond angles

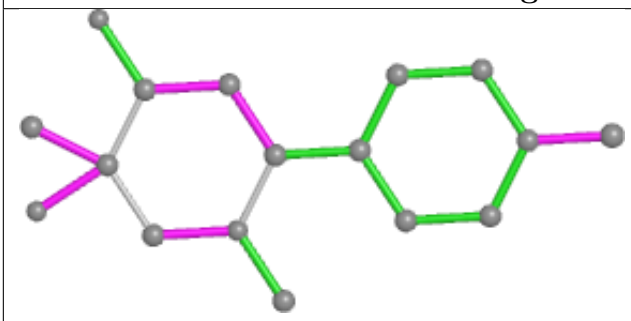
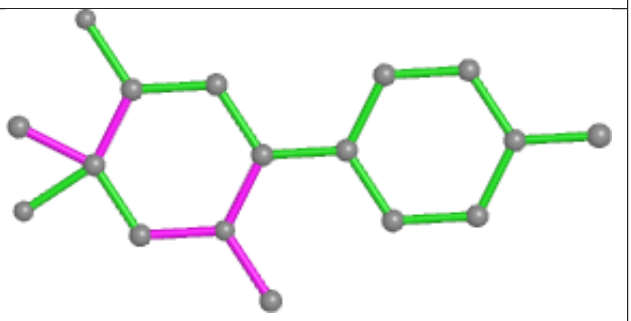
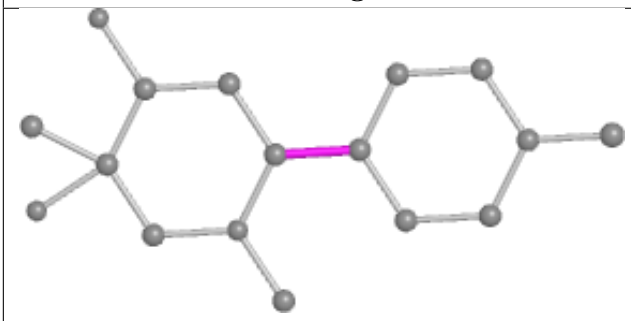
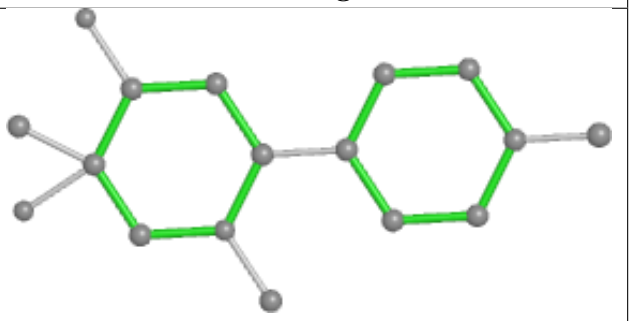


Torsions

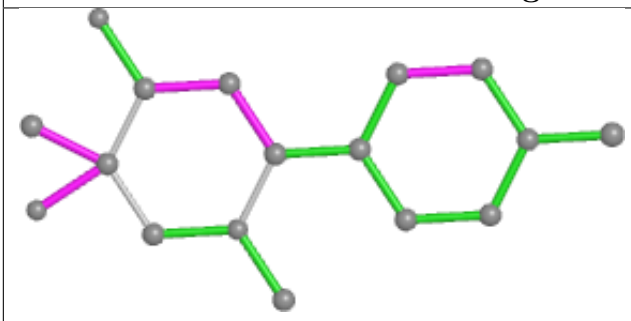


Rings

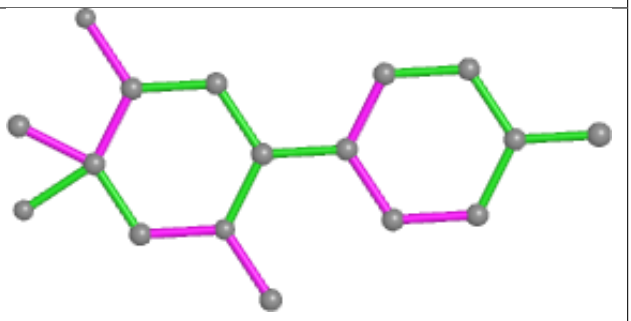
Ligand 42R B 1206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 42R A 1206	
 Bond lengths	 Bond angles
 Torsions	 Rings

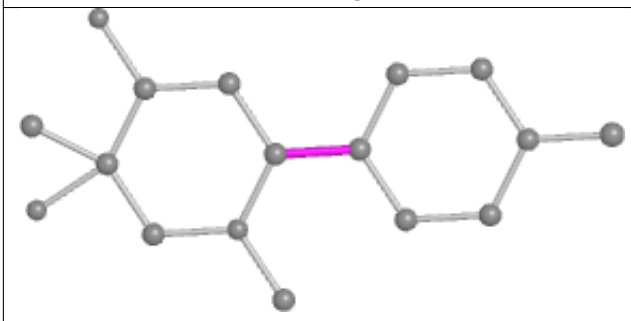
Ligand 42R E 1205



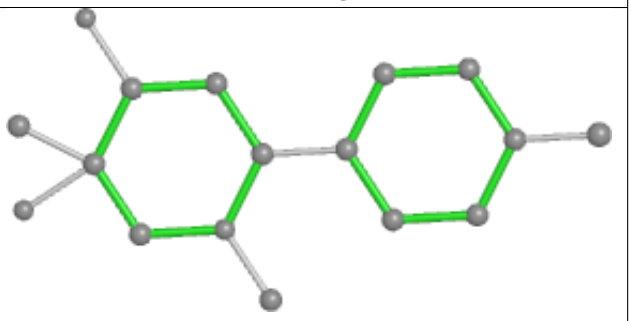
Bond lengths



Bond angles

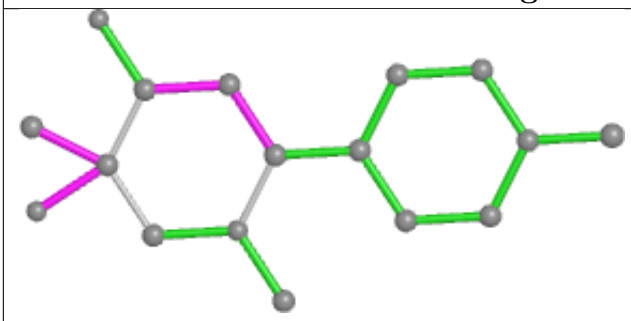


Torsions

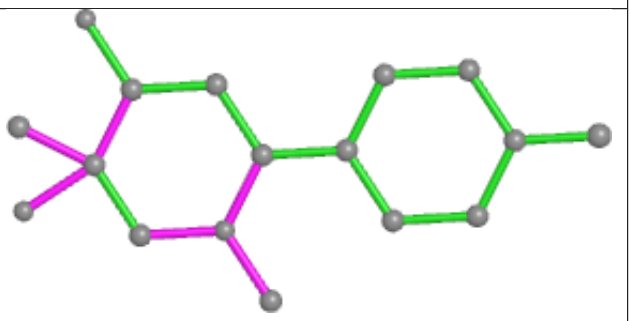


Rings

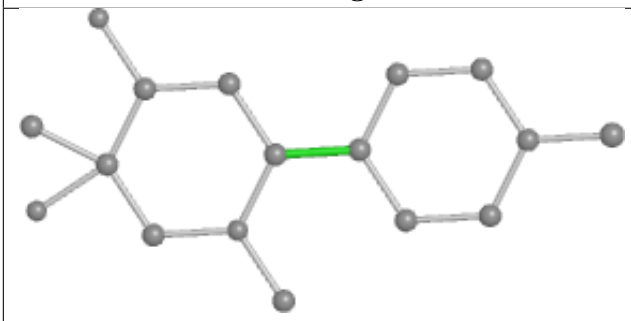
Ligand 42R D 1205



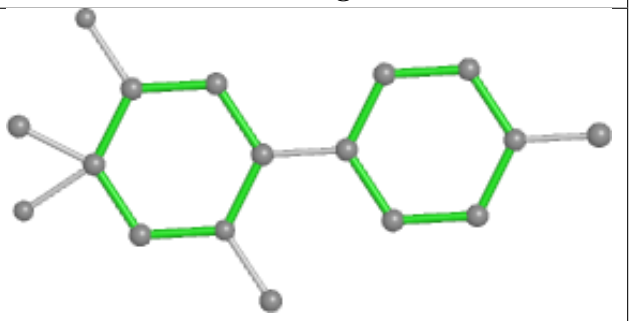
Bond lengths



Bond angles

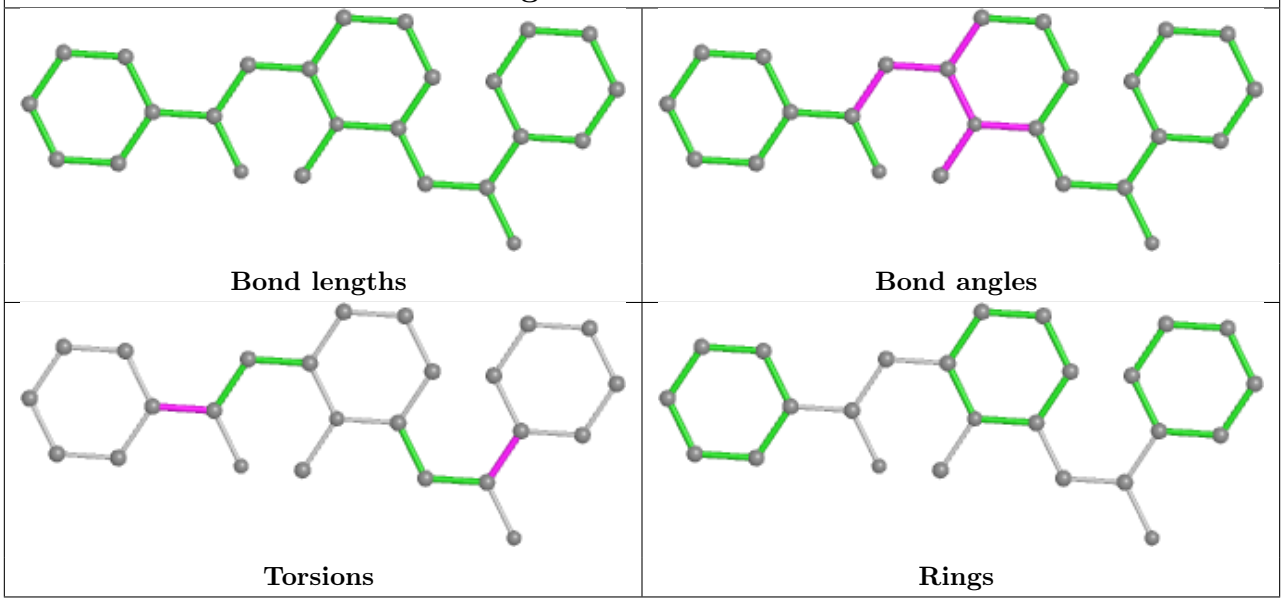


Torsions

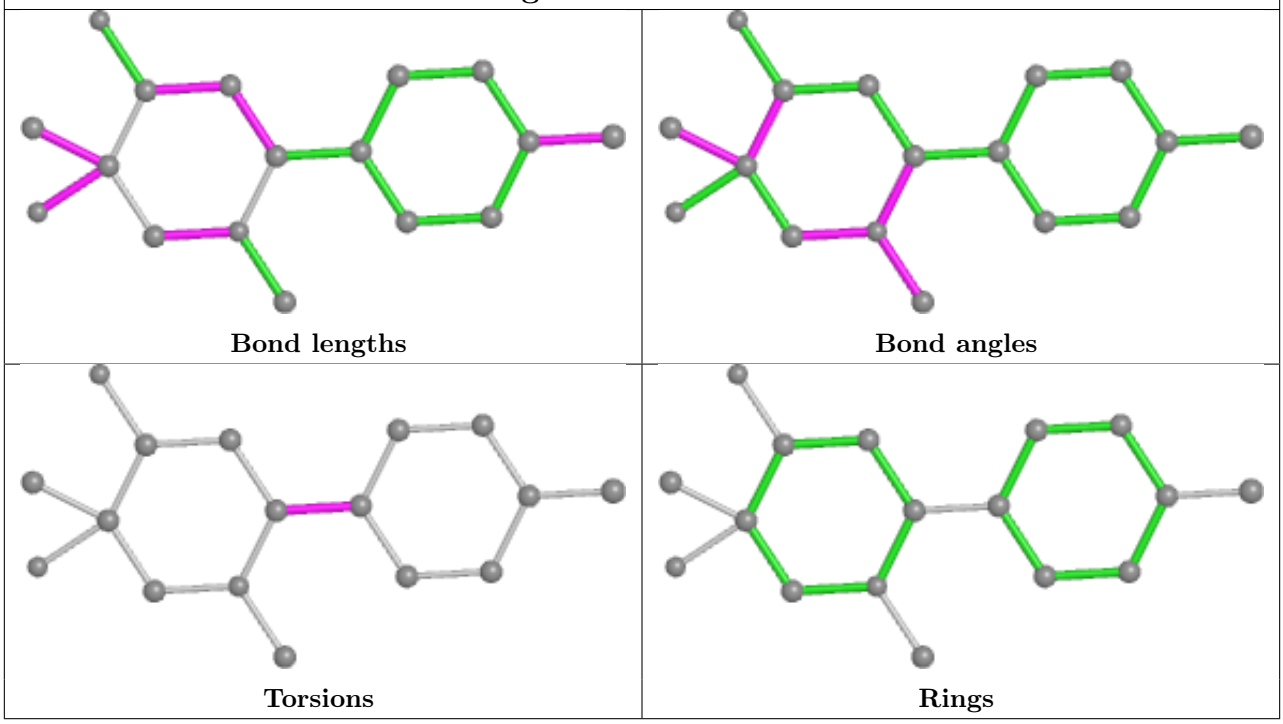


Rings

Ligand L0B C 1207



Ligand 42R A 1205



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)

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

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

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

6.3 Carbohydrates (i)

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

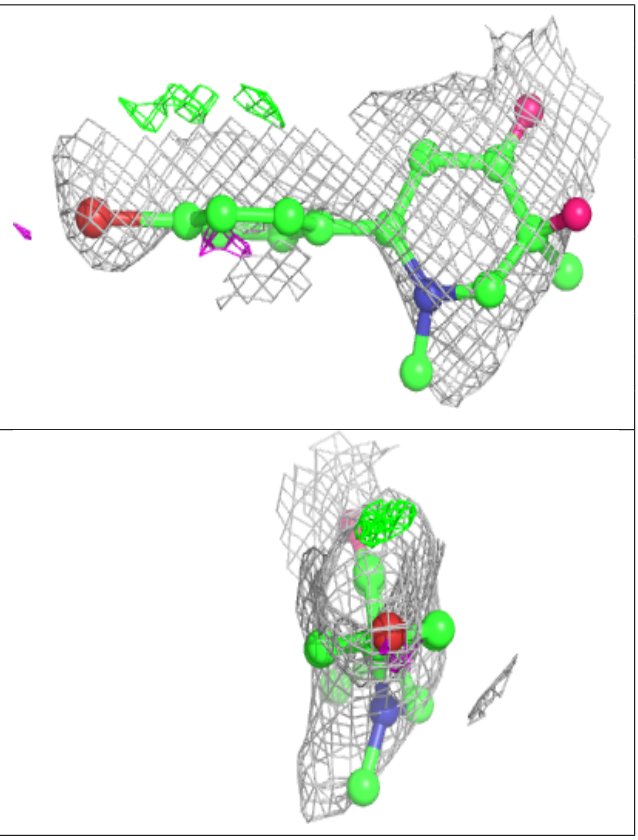
6.4 Ligands (i)

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.

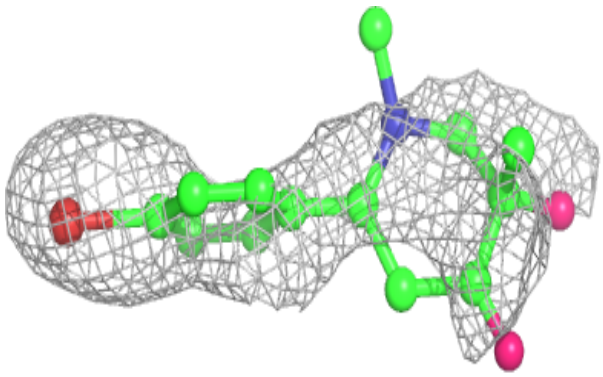
Electron density around 42R A 1205:

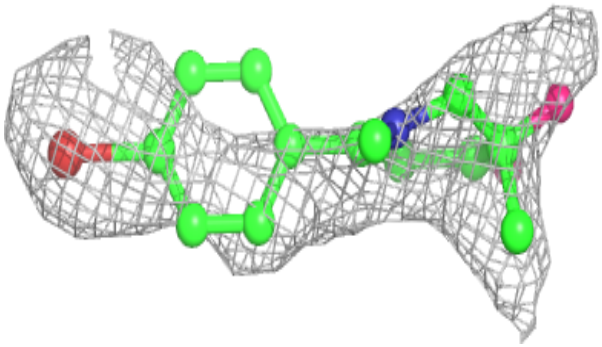
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

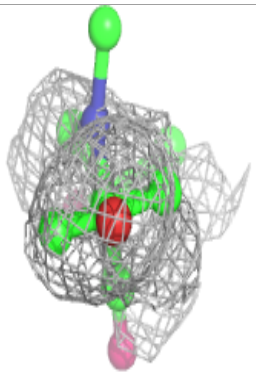


Electron density around 42R A 1206:

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

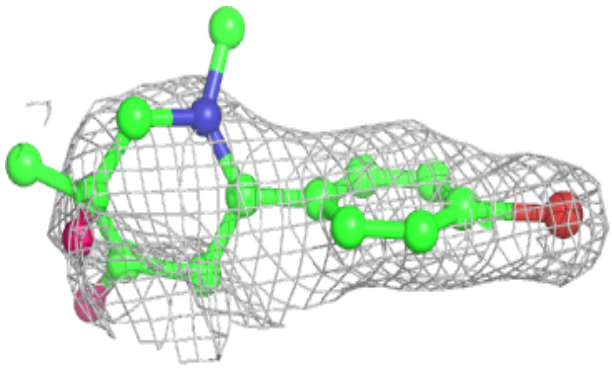


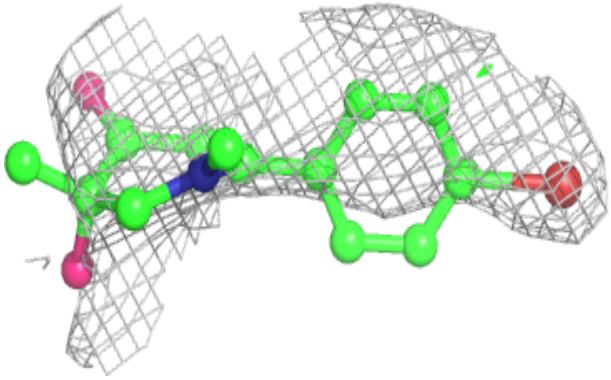


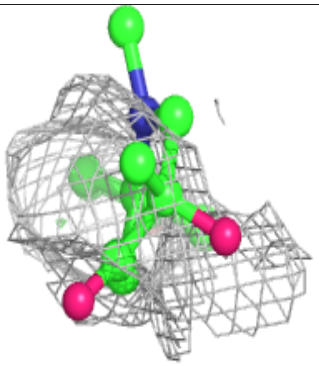


Electron density around 42R B 1205:

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

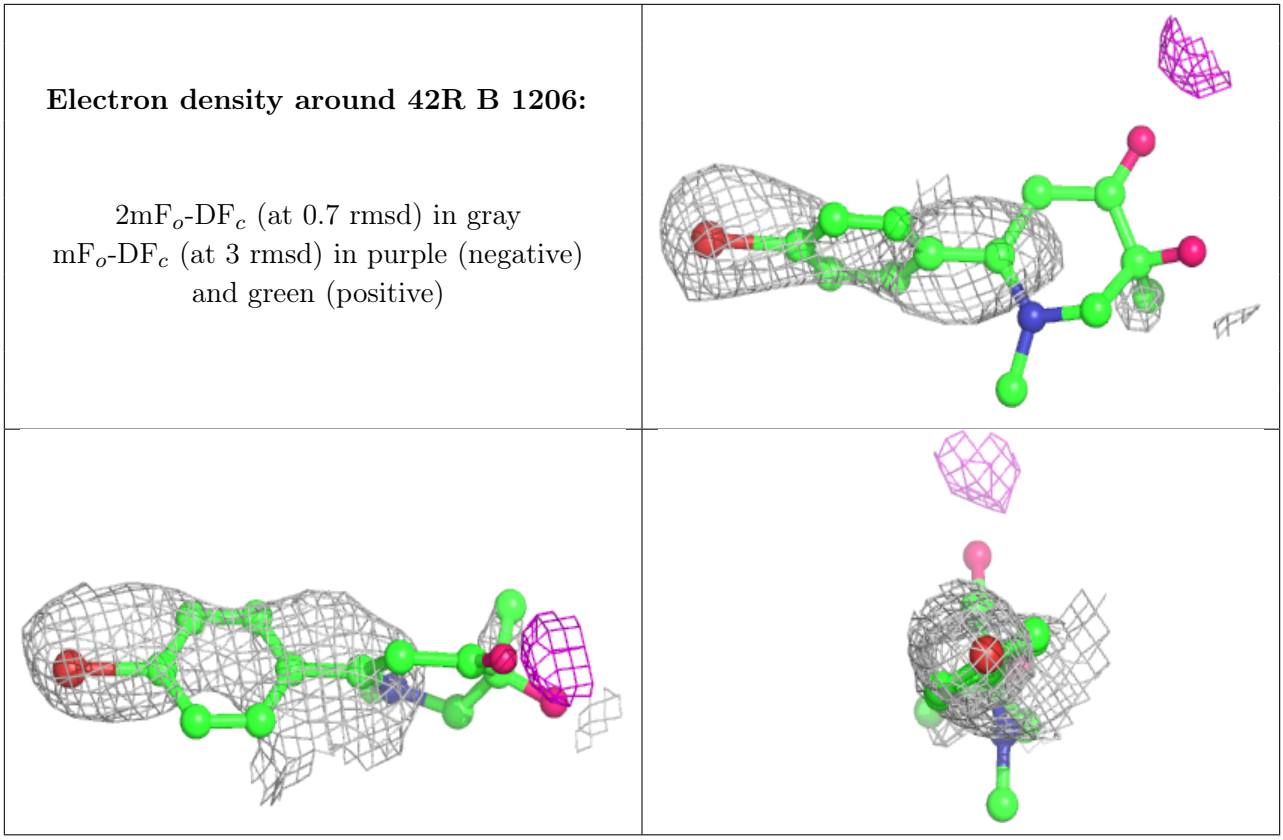






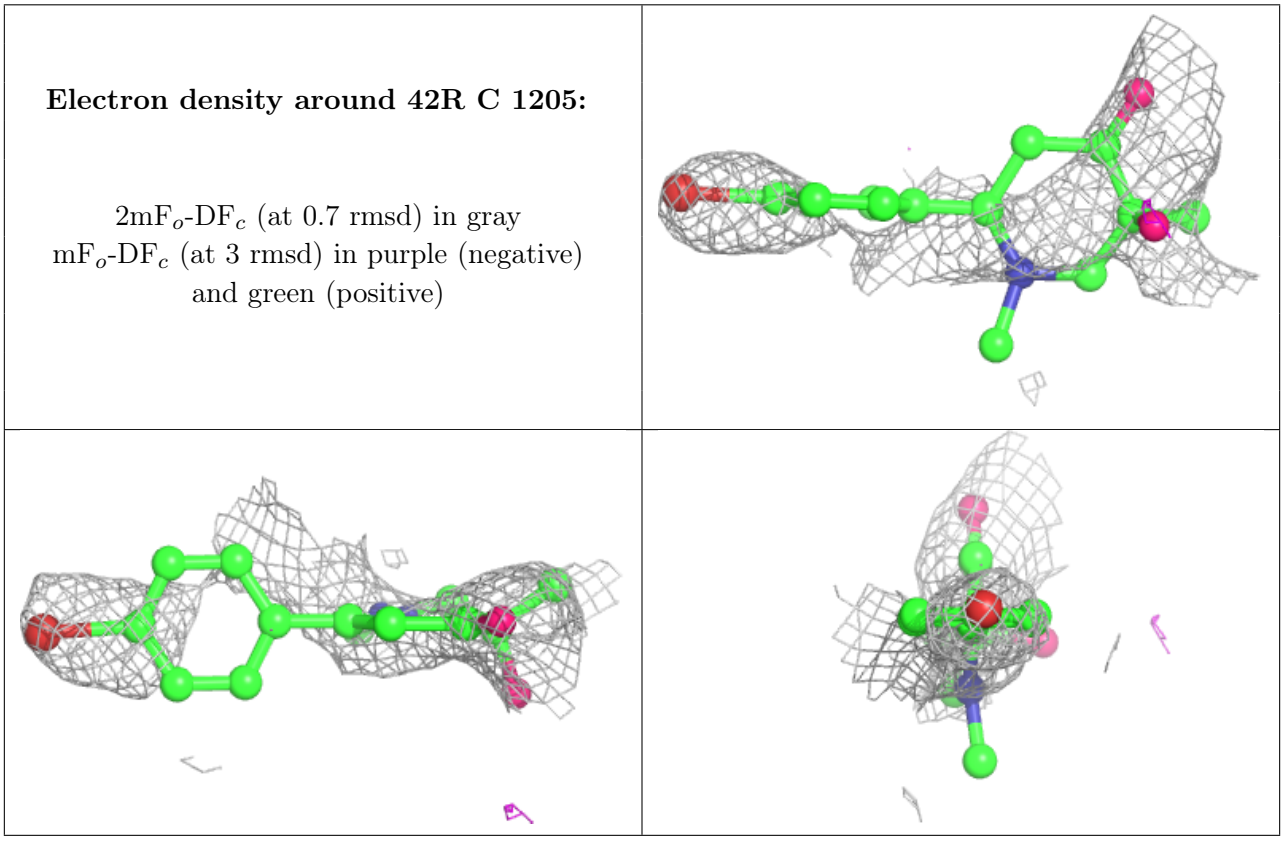
Electron density around 42R B 1206:

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



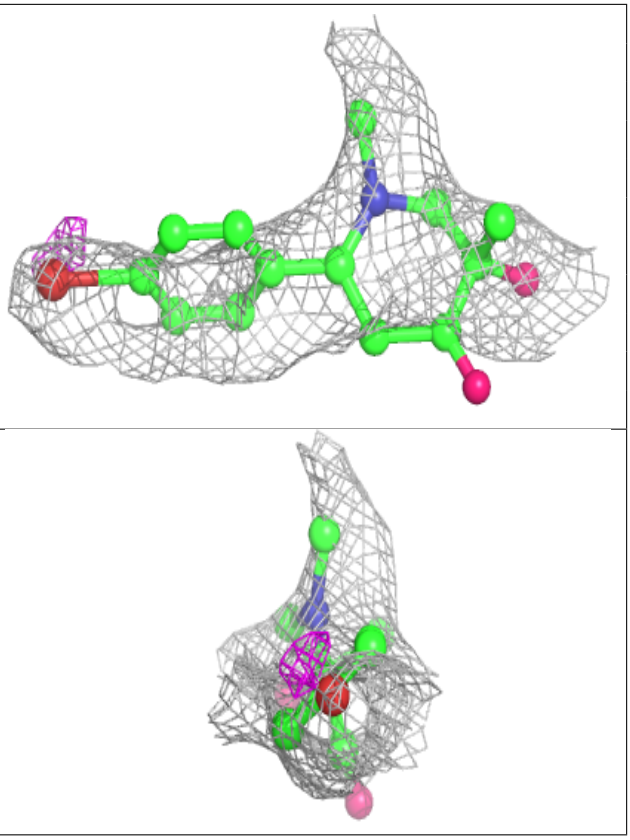
Electron density around 42R C 1205:

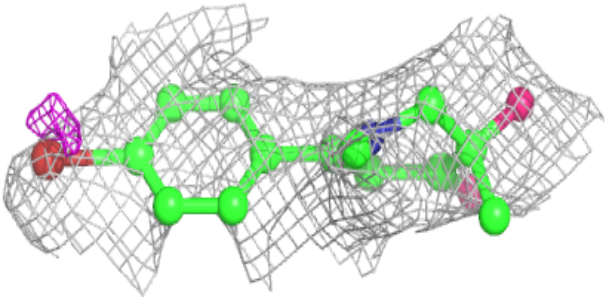
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 42R C 1206:

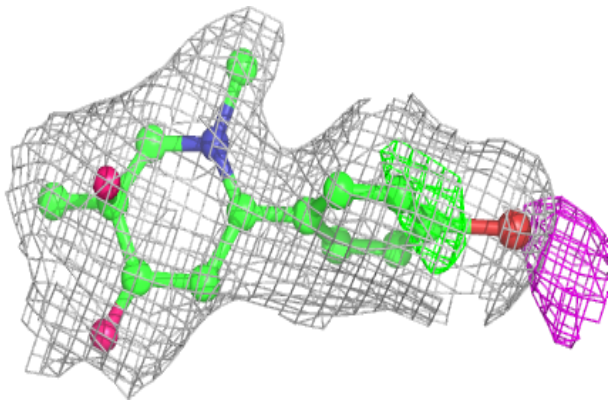
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

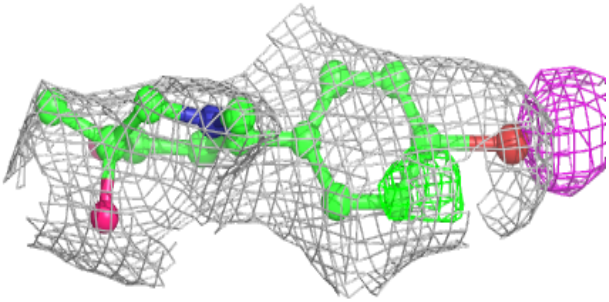


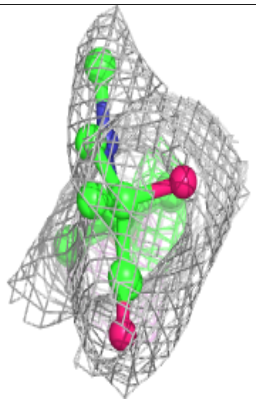


Electron density around 42R D 1205:

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

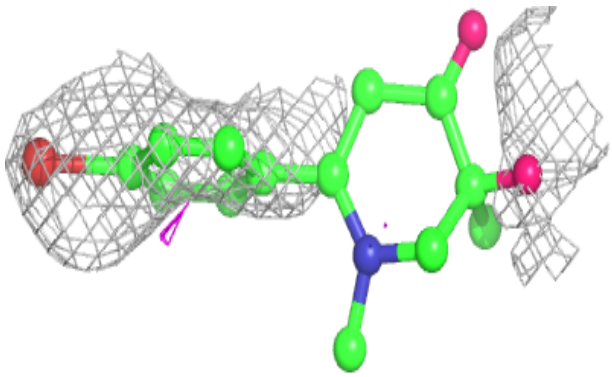


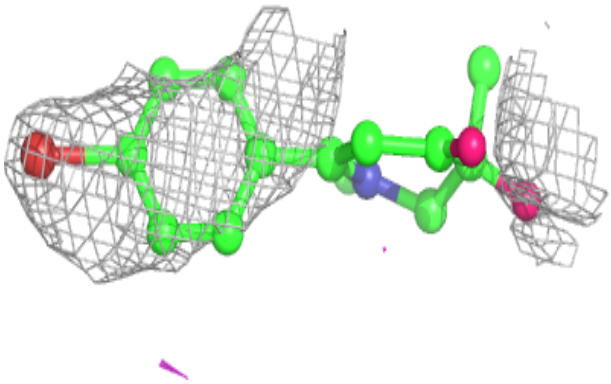


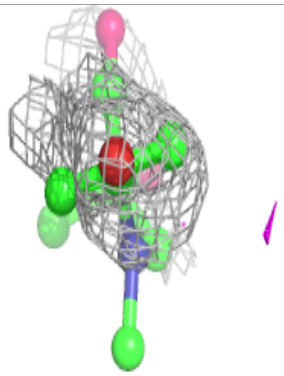


Electron density around 42R D 1206:

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

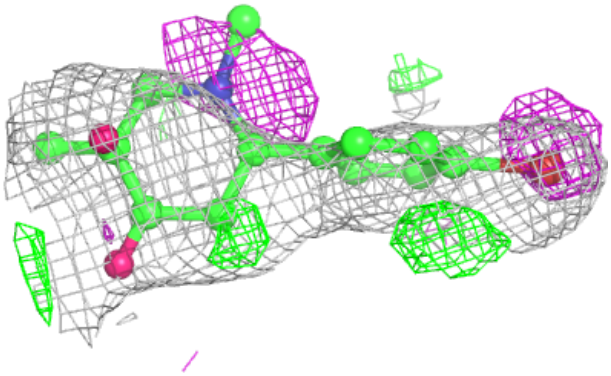


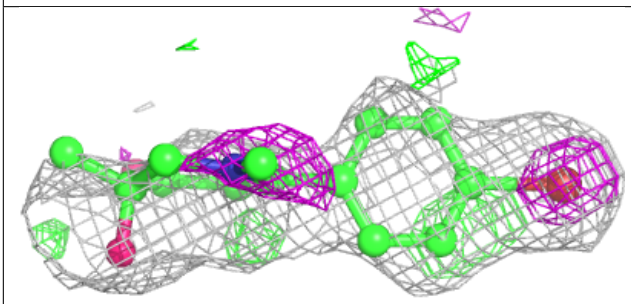


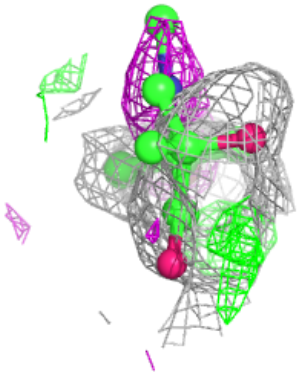


Electron density around 42R E 1205:

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

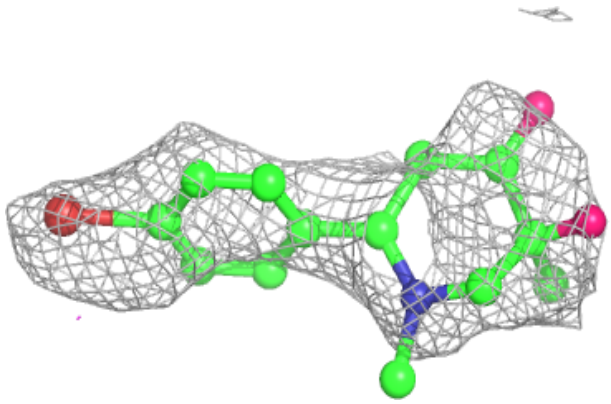


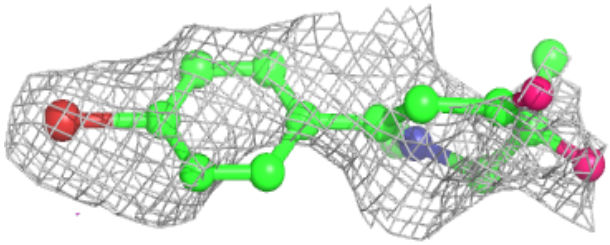


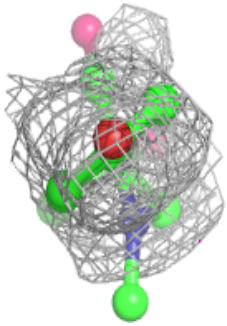


Electron density around 42R E 1206:

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

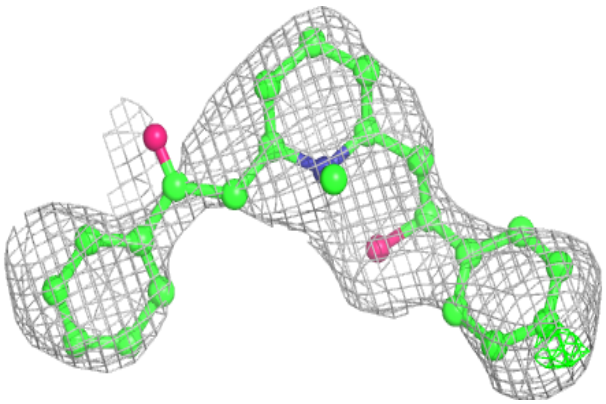


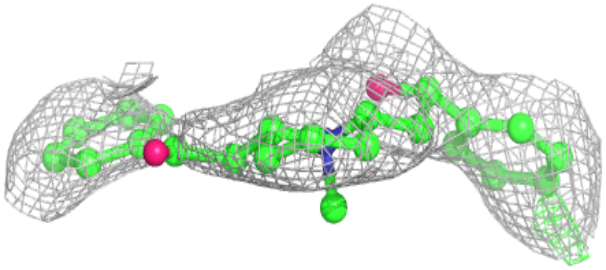


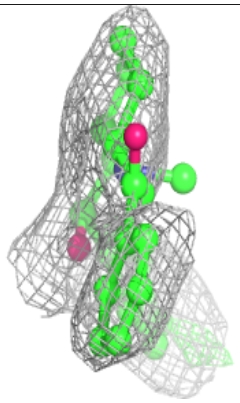


Electron density around L0B A 1207:

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

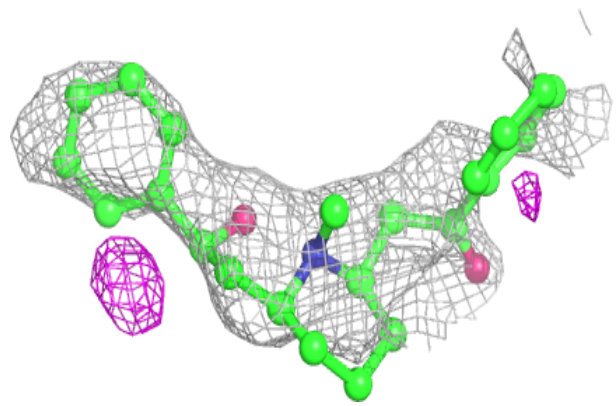


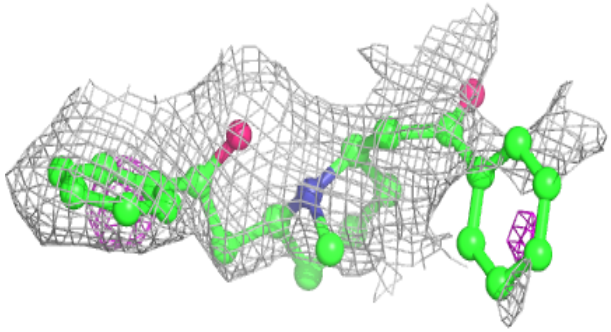


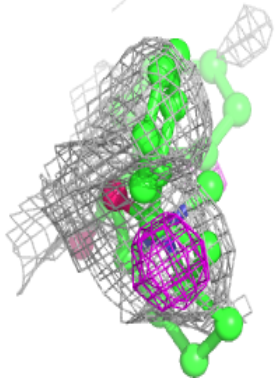


Electron density around L0B B 1207:

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

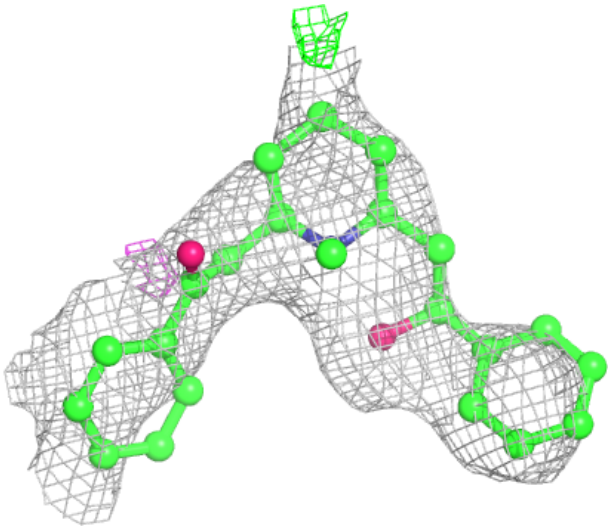


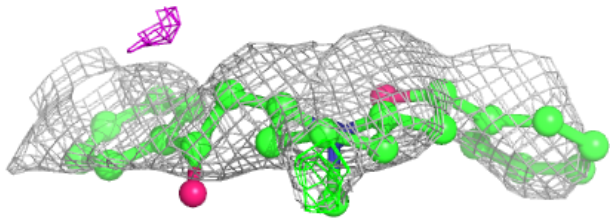


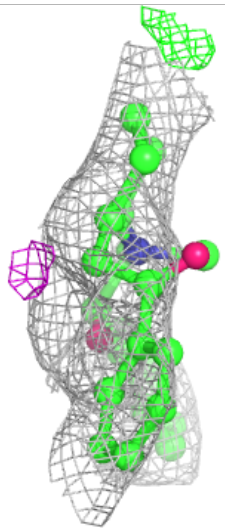


Electron density around L0B C 1207:

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

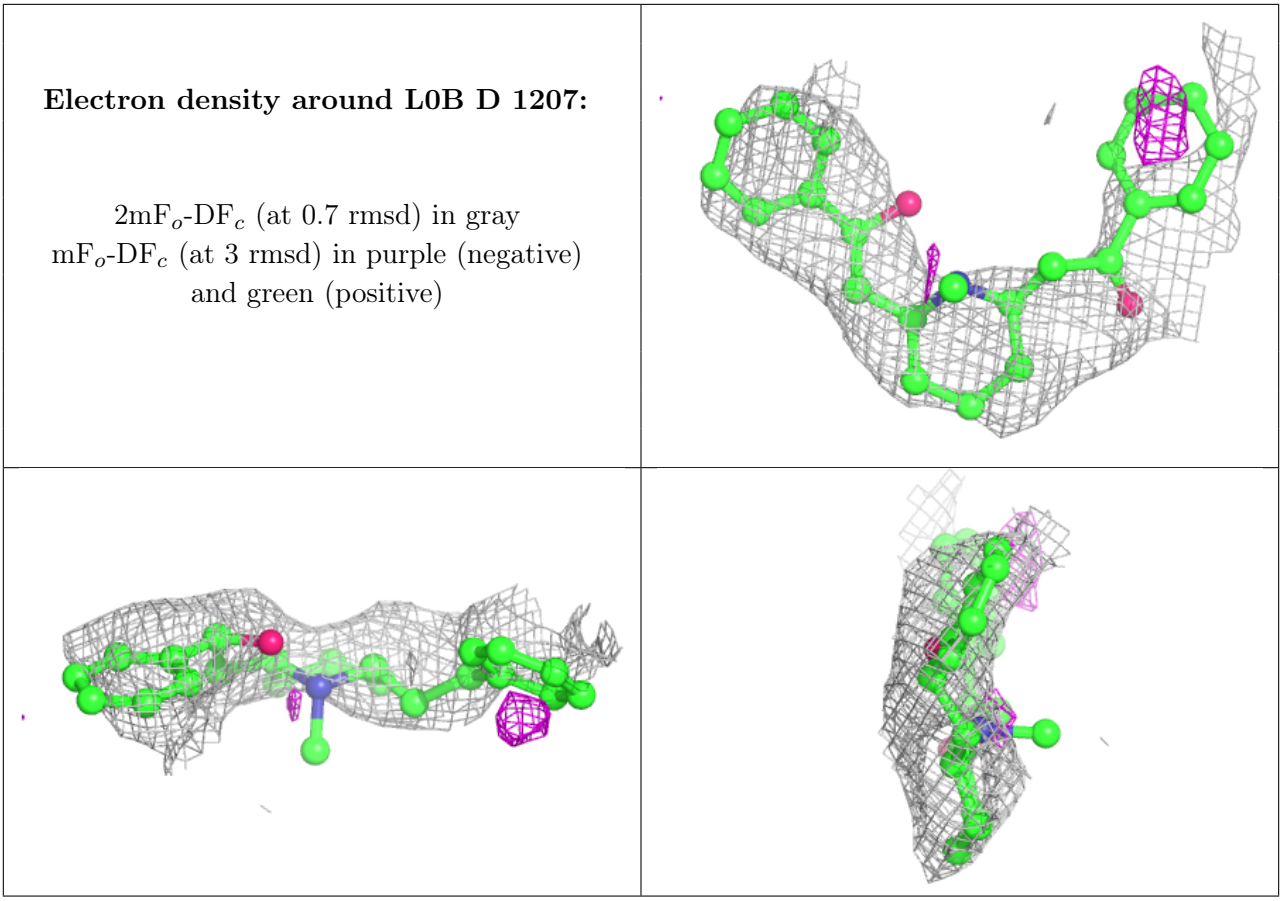






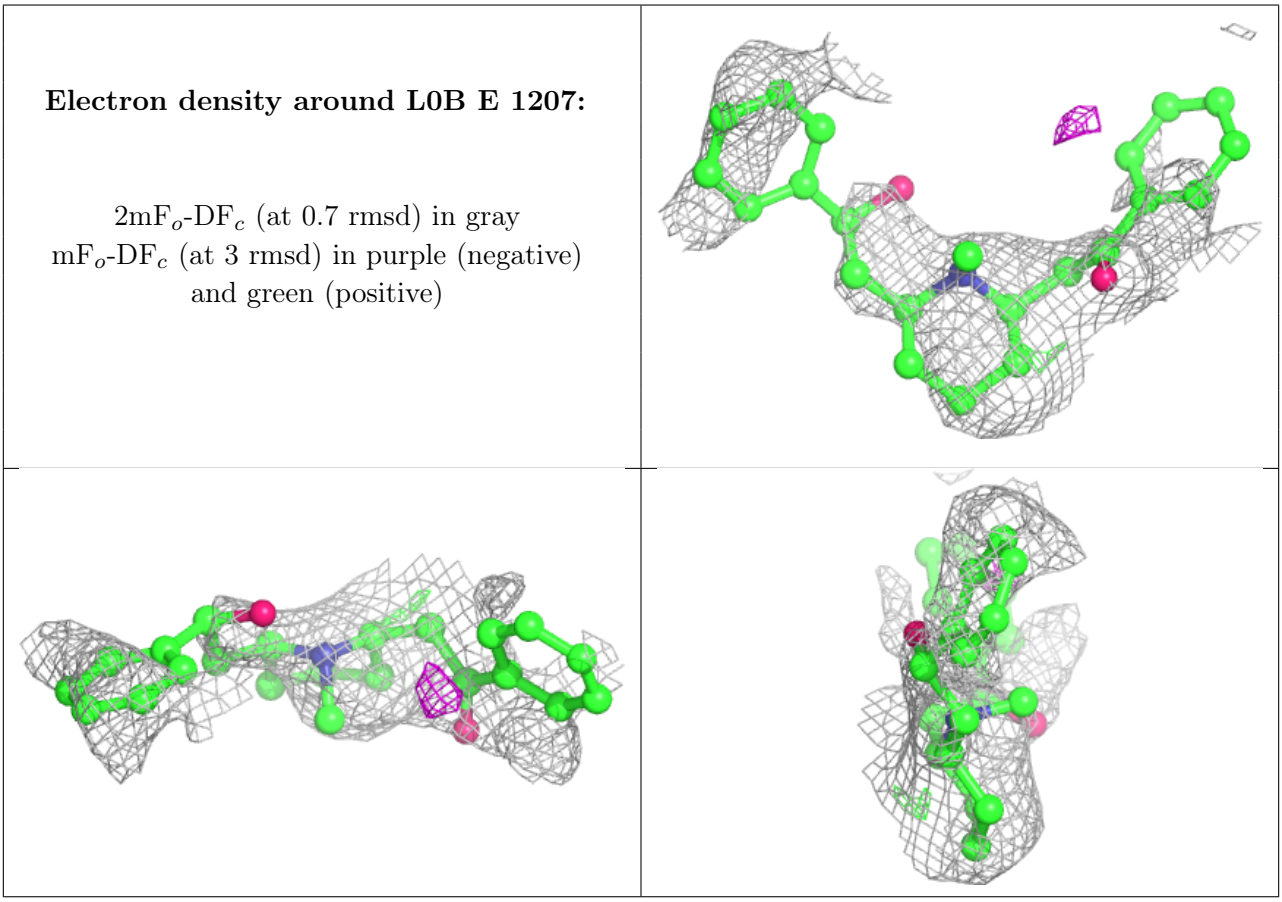
Electron density around L0B D 1207:

$2mF_o$-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 E 1207:

$2mF_o$-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.