



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:47 AM UTC

PDB ID : 5AFN / pdb_00005afn
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

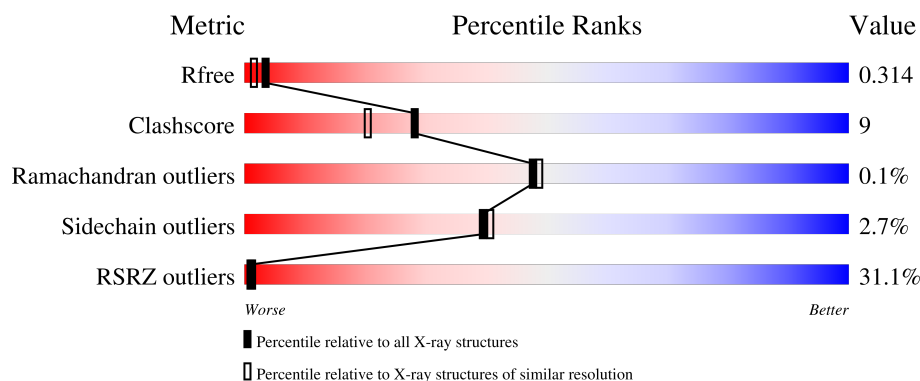
1 Overall quality at a glance

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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	207	36% 84% 15% .
1	B	207	29% 81% 17% .
1	C	207	20% 81% 18% .
1	D	207	29% 80% 18% ..
1	E	207	40% 85% 14% .

2 Entry composition [i](#)

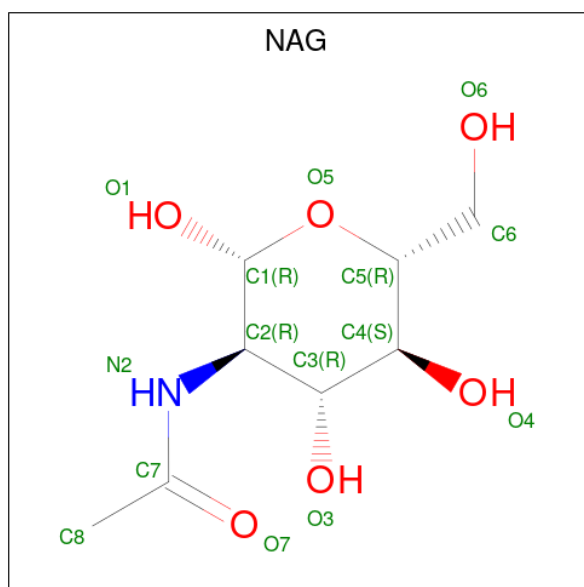
There are 8 unique types of molecules in this entry. The entry contains 9647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

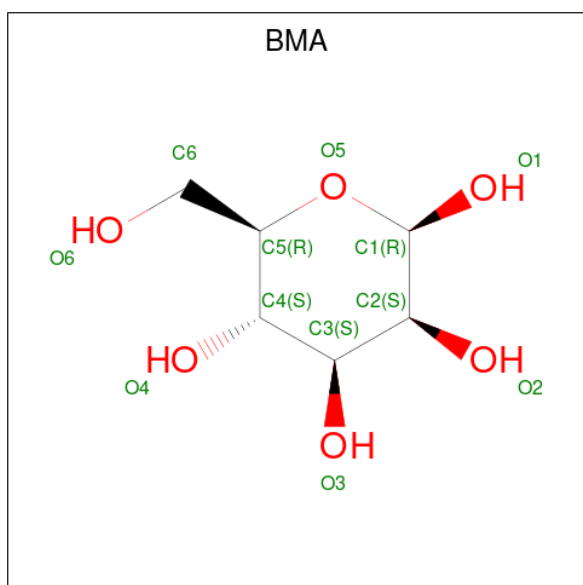
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	1	0
			1678	1077	280	314	7			
1	B	207	Total	C	N	O	S	0	1	0
			1699	1089	285	318	7			
1	C	205	Total	C	N	O	S	0	0	0
			1670	1071	279	313	7			
1	D	205	Total	C	N	O	S	0	5	0
			1707	1095	284	321	7			
1	E	205	Total	C	N	O	S	0	1	0
			1678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

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



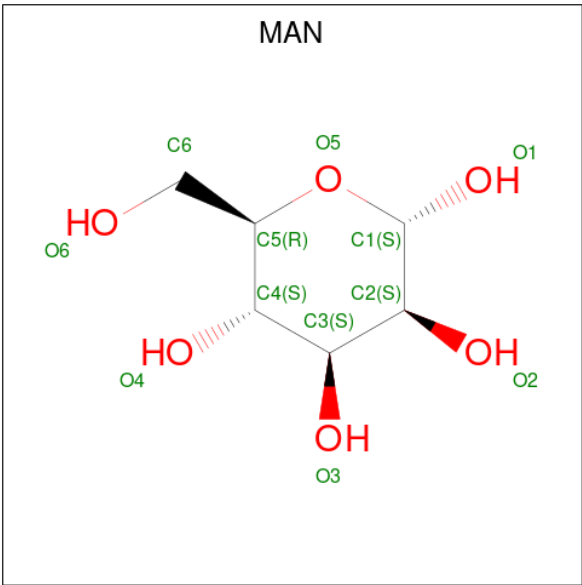
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1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

- Molecule 3 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



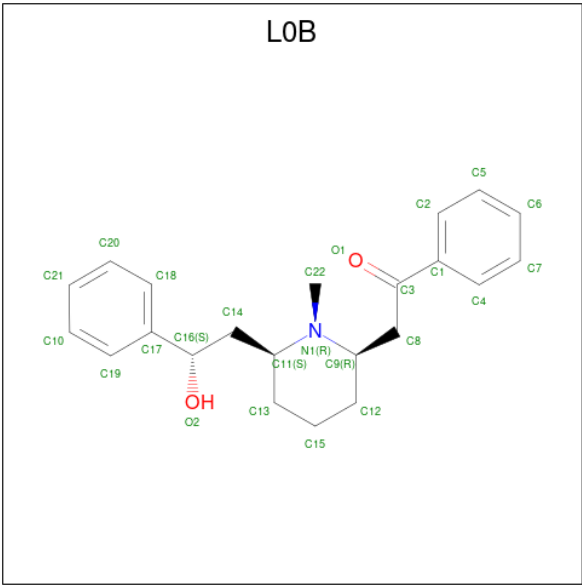
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 is Alpha-Lobeline (CCD ID: L0B) (formula: C₂₂H₂₇NO₂).



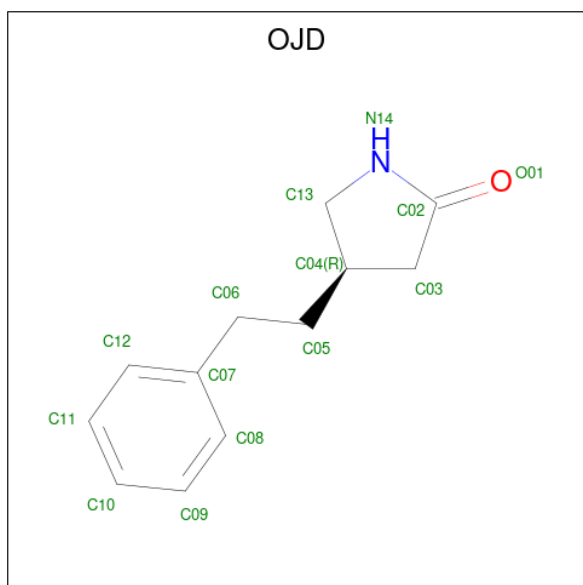
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	22	1	2		
5	B	1	Total	C	N	O	0	0
			25	22	1	2		
5	C	1	Total	C	N	O	0	0
			25	22	1	2		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is (4R)-4-(2-phenylethyl)pyrrolidin-2-one (CCD ID: OJD) (formula: C₁₂H₁₅NO).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

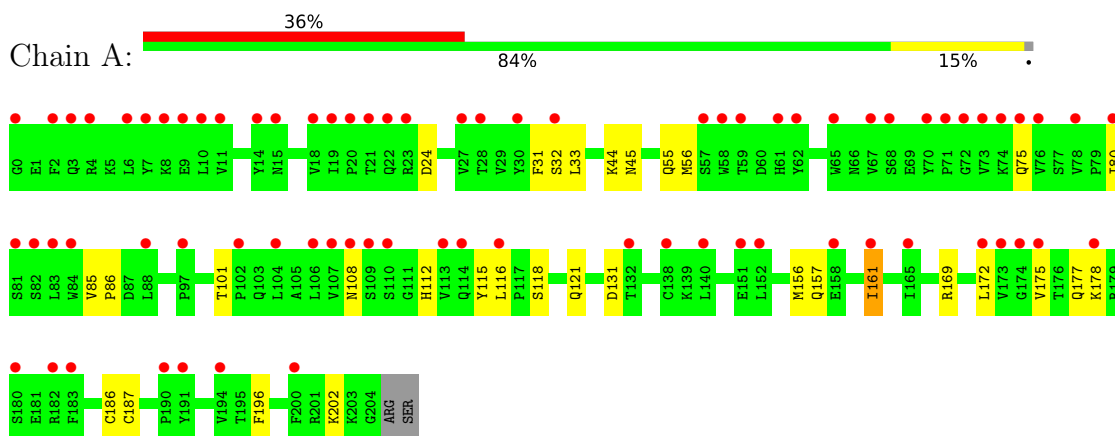
- Molecule 8 is water.

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

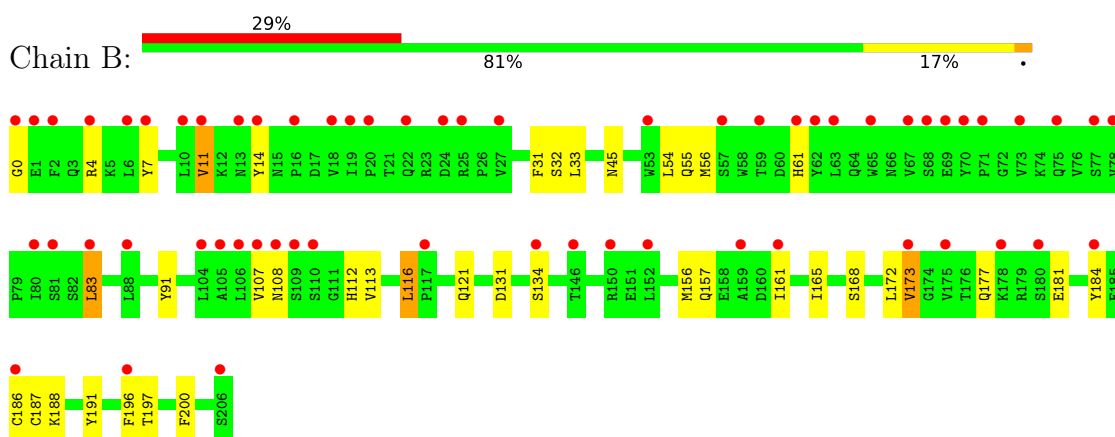
3 Residue-property plots [i](#)

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

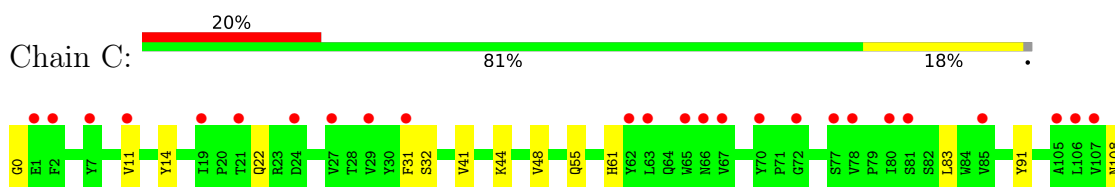
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

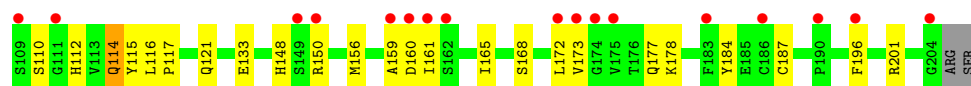


• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

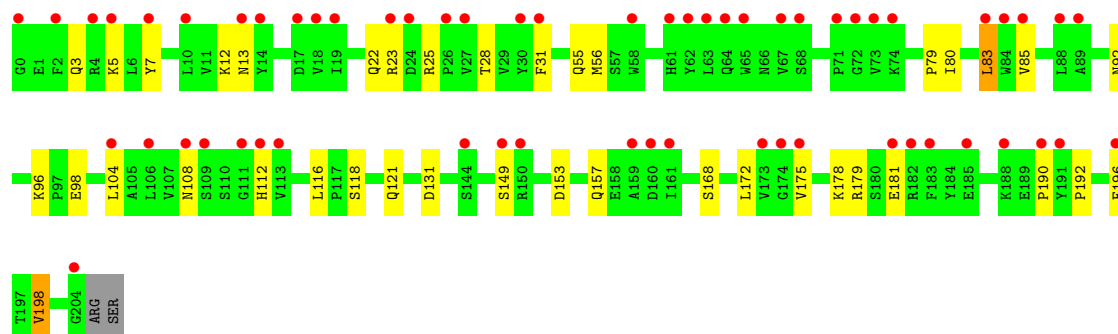
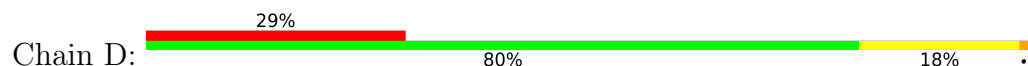


• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

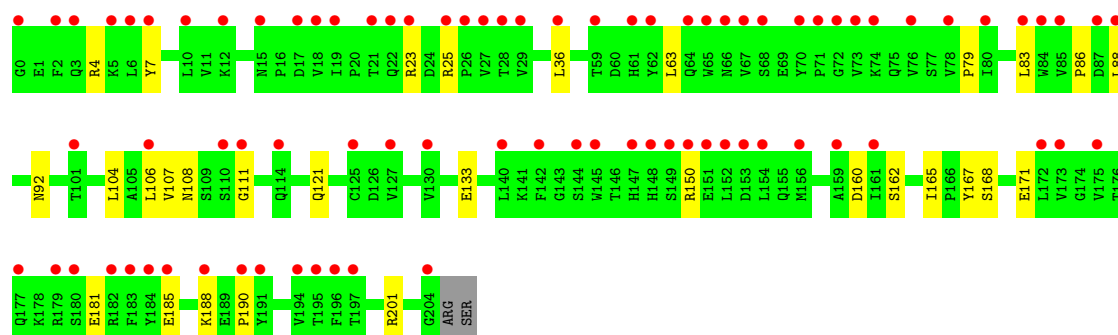
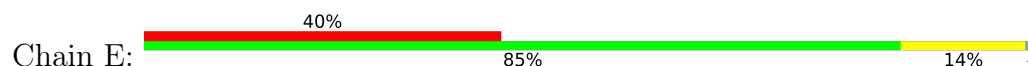




- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7



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



4 Data and refinement statistics

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 46.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.90-2.15) 99.3 (46.90-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.167 , 0.223 0.284 , 0.314	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)	0.34 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, L0B, MAN, NAG, GOL, OJD

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	0.48	0/1723	0.79	1/2344 (0.0%)
1	B	0.47	0/1745	0.77	0/2373
1	C	0.42	0/1715	0.78	0/2333
1	D	0.43	0/1753	0.77	0/2384
1	E	0.50	0/1723	0.78	0/2344
All	All	0.46	0/8659	0.78	1/11778 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ILE	N-CA-CB	-5.03	106.68	112.21

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	1678	0	1643	30	0
1	B	1699	0	1659	26	1
1	C	1670	0	1633	35	0
1	D	1707	0	1663	27	1
1	E	1678	0	1643	23	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	26	1	0
2	B	28	0	26	3	0
2	C	28	0	26	4	0
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	5	0
6	B	14	0	15	3	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	14	0
8	D	154	0	0	5	4
8	E	161	0	0	7	1
All	All	9647	0	8633	155	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 9.

All (155) 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:56:MET:SD	8:A:2081:HOH:O	2.43	0.77
1:B:181:GLU:OE2	8:B:2126:HOH:O	2.04	0.76
1:E:121:GLN:OE1	6:E:1215:OJD:H11	1.86	0.75
1:C:115:TYR:OH	8:C:2094:HOH:O	2.02	0.75
1:D:157:GLN:NE2	8:D:2039:HOH:O	2.18	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:GLN:HE22	6:D:1215:OJD:H10	1.52	0.74
1:C:110:SER:HB3	2:C:301:NAG:H82	1.68	0.74
1:C:121:GLN:OE1	6:C:1215:OJD:H11	1.89	0.73
1:E:121:GLN:HE22	6:E:1215:OJD:H10	1.52	0.72
8:B:2023:HOH:O	1:C:0:GLY:N	2.24	0.71
1:D:96:LYS:NZ	8:D:2097:HOH:O	2.25	0.69
2:E:301:NAG:H61	2:E:302:NAG:H3	1.73	0.69
1:D:121:GLN:OE1	6:D:1215:OJD:H11	1.94	0.68
1:D:56:MET:O	8:D:2065:HOH:O	2.11	0.68
1:D:23:ARG:O	8:D:2033:HOH:O	2.12	0.68
1:C:117:PRO:O	8:C:2057:HOH:O	2.12	0.67
1:B:184:TYR:OH	8:B:2155:HOH:O	2.12	0.67
1:A:44:LYS:NZ	8:A:2068:HOH:O	2.29	0.66
1:C:114:GLN:NE2	8:C:2097:HOH:O	2.28	0.66
1:D:22:GLN:HG2	1:D:25:ARG:HB2	1.75	0.66
1:D:108:ASN:HD21	2:D:301:NAG:C1	2.10	0.65
5:B:1207:L0B:O1	8:B:3002:HOH:O	2.15	0.64
1:A:56:MET:HE1	6:A:1215:OJD:H04	1.82	0.62
1:A:121:GLN:HE22	6:A:1215:OJD:H10	1.65	0.61
1:D:80[B]:ILE:HG13	1:D:85:VAL:HG21	1.81	0.61
1:A:75:GLN:OE1	8:A:2100:HOH:O	2.17	0.61
1:D:92:ASN:HA	7:D:1206:GOL:H32	1.82	0.60
1:E:160:ASP:OD2	1:E:162:SER:OG	2.19	0.60
1:D:181:GLU:HG2	1:D:190:PRO:HB2	1.83	0.59
1:C:108:ASN:ND2	2:C:301:NAG:O5	2.36	0.59
1:D:80[B]:ILE:HD12	1:D:83:LEU:HD11	1.84	0.59
1:B:31:PHE:HE2	1:B:196:PHE:HE2	1.51	0.58
1:B:121:GLN:OE1	6:B:1217:OJD:H11	2.04	0.58
1:B:91:TYR:OH	8:B:2085:HOH:O	2.15	0.57
1:B:191:TYR:OH	8:B:2121:HOH:O	2.15	0.57
8:C:2088:HOH:O	1:D:98:GLU:OE2	2.18	0.56
1:A:80[B]:ILE:HD12	1:A:115:TYR:CZ	2.40	0.56
1:B:56:MET:HE1	6:B:1217:OJD:H132	1.87	0.56
8:A:2026:HOH:O	1:B:0:GLY:N	2.38	0.56
1:E:181:GLU:CD	8:E:2148:HOH:O	2.43	0.55
1:A:161:ILE:HD12	1:A:172:LEU:HD21	1.89	0.55
5:E:1205:L0B:H2	8:E:2157:HOH:O	2.05	0.55
1:B:55:GLN:HA	1:B:116:LEU:HD12	1.88	0.55
1:B:112:HIS:CG	2:B:301:NAG:H62	2.41	0.55
1:A:80[A]:ILE:HG21	1:A:115:TYR:CE1	2.41	0.55
1:E:171:GLU:OE2	1:E:201:ARG:NH1	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:GLU:HG2	1:E:190:PRO:HB2	1.88	0.54
1:C:112:HIS:CD2	2:C:301:NAG:H61	2.43	0.54
1:C:133:GLU:HG3	1:C:201:ARG:NH1	2.23	0.54
1:A:45:ASN:OD1	8:A:2070:HOH:O	2.19	0.53
2:E:301:NAG:O4	2:E:302:NAG:O5	2.26	0.53
1:D:55:GLN:HG2	1:D:116:LEU:HD22	1.90	0.53
1:A:112:HIS:CD2	2:A:301:NAG:H62	2.43	0.53
1:C:184:TYR:OH	8:C:2084:HOH:O	2.18	0.53
1:E:165:ILE:HD13	1:E:167:TYR:CE1	2.43	0.53
8:D:2012:HOH:O	1:E:4:ARG:NH2	2.43	0.52
1:C:160:ASP:OD2	8:C:2043:HOH:O	2.18	0.52
1:A:31:PHE:HE2	1:A:196:PHE:HE2	1.56	0.52
1:A:157:GLN:O	1:A:177:GLN:NE2	2.43	0.52
1:A:108:ASN:ND2	1:A:112:HIS:HB3	2.17	0.51
1:C:55:GLN:HG3	8:C:2039:HOH:O	2.09	0.51
1:C:161:ILE:HD12	1:C:172:LEU:HD21	1.92	0.51
1:B:31:PHE:CE2	1:B:196:PHE:HE2	2.27	0.51
1:A:31:PHE:HE2	1:A:196:PHE:CE2	2.28	0.51
1:C:32:SER:HB2	8:C:2040:HOH:O	2.10	0.51
1:E:107:VAL:N	8:E:2081:HOH:O	2.39	0.50
1:B:61:HIS:ND1	8:B:2026:HOH:O	2.33	0.50
1:E:92:ASN:HA	7:E:1207:GOL:H31	1.93	0.50
1:C:44:LYS:NZ	8:C:2053:HOH:O	2.45	0.49
1:A:202:LYS:NZ	8:A:2190:HOH:O	2.36	0.49
1:E:7:TYR:CD2	7:E:1206:GOL:H11	2.47	0.49
1:B:45:ASN:OD1	8:B:2050:HOH:O	2.19	0.49
1:A:32:SER:HB3	1:A:55:GLN:HB2	1.95	0.49
1:A:55:GLN:HG2	1:A:116:LEU:HD22	1.95	0.49
1:A:202:LYS:NZ	8:A:2064:HOH:O	2.45	0.48
2:B:301:NAG:O4	2:B:302:NAG:H2	2.13	0.48
1:A:169:ARG:NE	8:A:2056:HOH:O	2.31	0.47
1:B:14:TYR:HE2	1:B:83:LEU:HA	1.79	0.47
1:C:112:HIS:HD2	8:C:2096:HOH:O	1.97	0.47
1:E:63:LEU:HD11	1:E:83:LEU:HD22	1.97	0.47
5:E:1205:L0B:H223	5:E:1205:L0B:H141	1.68	0.47
1:E:86:PRO:HB2	1:E:88[A]:LEU:HG	1.97	0.46
1:E:121:GLN:HE22	6:E:1215:OJD:C10	2.25	0.46
1:B:32:SER:HB3	1:B:157:GLN:HG3	1.97	0.46
1:D:31:PHE:HE1	1:D:196[A]:PHE:HE1	1.64	0.46
5:D:1205:L0B:H223	5:D:1205:L0B:H141	1.78	0.46
1:D:196[B]:PHE:CE2	1:D:198:VAL:HG22	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:THR:HG23	1:A:118:SER:HB3	1.98	0.46
1:C:148:HIS:CE1	1:C:150:ARG:HB2	2.51	0.45
1:D:13:ASN:O	1:E:4:ARG:NH1	2.50	0.45
1:D:112:HIS:ND1	2:D:301:NAG:H62	2.31	0.45
1:B:177:GLN:OE1	8:B:2135:HOH:O	2.21	0.45
5:B:1207:L0B:H6	1:C:114:GLN:NE2	2.32	0.45
1:A:161:ILE:HD11	1:A:175:VAL:HB	1.98	0.45
1:C:41:VAL:HG12	1:C:48:VAL:HG23	1.97	0.45
1:B:131:ASP:HB2	8:B:2110:HOH:O	2.16	0.44
1:C:150:ARG:NH1	8:C:2112:HOH:O	2.49	0.44
2:C:301:NAG:O4	2:C:302:NAG:N2	2.51	0.44
1:C:31:PHE:CE2	1:C:196:PHE:HE2	2.35	0.44
1:B:156:MET:HB2	8:B:2135:HOH:O	2.17	0.44
1:B:161:ILE:HD12	1:B:172:LEU:HD21	1.99	0.44
1:B:186:CYS:SG	1:B:187:CYS:N	2.91	0.43
1:B:161:ILE:HD13	1:B:161:ILE:HA	1.84	0.43
6:B:1217:OJD:H131	6:B:1217:OJD:H062	1.46	0.43
1:D:5:LYS:HD2	1:D:5:LYS:HA	1.86	0.43
1:D:172:LEU:HD12	1:D:172:LEU:HA	1.90	0.43
1:A:33:LEU:C	1:A:33:LEU:HD23	2.43	0.43
1:D:31:PHE:HE1	1:D:196[A]:PHE:CE1	2.37	0.43
1:B:7[B]:TYR:CE1	1:B:11:VAL:HG21	2.54	0.43
1:E:111:GLY:N	8:E:2108:HOH:O	2.51	0.43
1:D:79:PRO:HA	1:D:104:LEU:HD23	2.00	0.43
2:D:301:NAG:O4	2:D:302:NAG:N2	2.52	0.43
1:E:23:ARG:C	1:E:25:ARG:H	2.27	0.43
1:A:121:GLN:HE22	6:A:1215:OJD:C10	2.29	0.43
1:C:22:GLN:HB3	1:C:61:HIS:CE1	2.54	0.43
1:C:156:MET:HE1	1:C:178:LYS:HA	1.99	0.43
7:D:1206:GOL:H31	1:E:36:LEU:HD13	2.00	0.43
1:E:79:PRO:HA	1:E:104:LEU:HD23	2.01	0.42
1:A:156:MET:HE1	1:A:178:LYS:HA	2.00	0.42
1:C:161:ILE:HD13	1:C:161:ILE:HA	1.88	0.42
1:C:177:GLN:HB3	1:C:196:PHE:CE1	2.54	0.42
1:A:186:CYS:SG	1:A:187:CYS:N	2.92	0.42
1:C:116:LEU:HD22	8:C:2058:HOH:O	2.19	0.42
6:D:1215:OJD:H131	6:D:1215:OJD:H062	1.64	0.42
1:C:178:LYS:HE3	1:C:178:LYS:HB2	1.91	0.42
1:E:106:LEU:HD12	8:E:2111:HOH:O	2.19	0.42
1:A:161:ILE:HA	1:A:161:ILE:HD13	1.81	0.42
1:D:28:THR:HA	1:D:153:ASP:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:2020:HOH:O	1:D:7:TYR:HD2	2.02	0.42
1:A:80[B]:ILE:CD1	1:A:85:VAL:HG11	2.50	0.41
6:A:1215:OJD:H09	8:B:2093:HOH:O	2.19	0.41
1:C:115:TYR:HE2	6:C:1215:OJD:H032	1.85	0.41
1:B:173:VAL:HG13	1:B:200:PHE:HA	2.02	0.41
5:B:1207:L0B:H141	5:B:1207:L0B:H223	1.78	0.41
1:A:86:PRO:HG2	8:A:2081:HOH:O	2.20	0.41
1:B:33:LEU:HD12	1:B:54:LEU:HD21	2.02	0.41
1:B:108:ASN:ND2	2:B:301:NAG:O5	2.53	0.41
1:D:178:LYS:HE3	1:D:178:LYS:HB2	1.88	0.41
1:C:14:TYR:HE2	1:C:83:LEU:HA	1.84	0.41
1:D:149:SER:OG	1:D:192:PRO:HD3	2.21	0.41
5:E:1205:L0B:H81C	5:E:1205:L0B:H221	1.72	0.41
1:C:121:GLN:HE22	6:C:1215:OJD:C10	2.33	0.41
1:C:159:ALA:HA	8:C:2040:HOH:O	2.21	0.41
1:C:91:TYR:OH	5:C:1205:L0B:H131	2.21	0.40
1:C:121:GLN:HE22	6:C:1215:OJD:H10	1.87	0.40
1:E:7:TYR:HB3	7:E:1206:GOL:H32	2.02	0.40
1:B:107:VAL:HG22	1:B:113:VAL:HG22	2.04	0.40
1:C:115:TYR:C	1:C:116:LEU:HD23	2.46	0.40
1:C:31:PHE:HE2	1:C:196:PHE:HE2	1.69	0.40
1:D:12:LYS:HE3	1:D:12:LYS:HB2	1.85	0.40
3:A:303:BMA:H2	4:A:304:MAN:O2	2.22	0.40

All (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
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
4:A:304:MAN:C5	8:D:2132:HOH:O[3_645]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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%)	24	19
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%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ASP

5.3.2 Protein sidechains

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%)	190 (100%)	1 (0%)	81	86
1	B	193/192 (100%)	184 (95%)	9 (5%)	23	19
1	C	190/192 (99%)	184 (97%)	6 (3%)	34	35
1	D	195/192 (102%)	188 (96%)	7 (4%)	31	30
1	E	191/192 (100%)	188 (98%)	3 (2%)	55	61
All	All	960/960 (100%)	934 (97%)	26 (3%)	39	41

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ASP
1	B	4	ARG
1	B	11	VAL
1	B	83	LEU
1	B	116	LEU
1	B	134	SER
1	B	165	ILE
1	B	168	SER
1	B	173	VAL
1	B	188	LYS
1	C	11	VAL
1	C	114	GLN
1	C	165	ILE
1	C	168	SER
1	C	173	VAL
1	C	187	CYS
1	D	3	GLN
1	D	83	LEU
1	D	118	SER
1	D	131	ASP
1	D	168	SER
1	D	175	VAL
1	D	198	VAL
1	E	133	GLU
1	E	168	SER
1	E	188	LYS

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

Mol	Chain	Res	Type
1	A	108	ASN
1	B	55	GLN
1	C	112	HIS
1	D	55	GLN
1	D	108	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
4	MAN	A	304	-	11,11,12	0.74	0	15,15,17	1.53	2 (13%)
2	NAG	E	301	-	14,14,15	0.87	1 (7%)	17,19,21	1.69	4 (23%)
5	L0B	C	1205	-	27,27,27	0.54	0	33,36,36	1.25	4 (12%)
6	OJD	C	1215	-	14,15,15	1.69	5 (35%)	17,19,19	1.90	5 (29%)
5	L0B	B	1207	-	27,27,27	0.54	0	33,36,36	1.50	4 (12%)
7	GOL	E	1208	-	5,5,5	0.35	0	5,5,5	0.29	0
5	L0B	E	1205	-	27,27,27	0.66	0	33,36,36	1.45	5 (15%)
6	OJD	E	1215	-	14,15,15	1.83	5 (35%)	17,19,19	2.16	6 (35%)
2	NAG	A	301	-	14,14,15	0.60	0	17,19,21	1.78	4 (23%)
6	OJD	A	1215	-	14,15,15	1.75	5 (35%)	17,19,19	2.05	5 (29%)
5	L0B	D	1205	-	27,27,27	0.56	0	33,36,36	1.26	5 (15%)
2	NAG	B	301	-	14,14,15	0.63	0	17,19,21	1.07	2 (11%)
7	GOL	E	1206	-	5,5,5	0.37	0	5,5,5	0.24	0
2	NAG	A	302	-	14,14,15	0.73	0	17,19,21	2.05	2 (11%)
2	NAG	D	301	-	14,14,15	0.62	0	17,19,21	1.77	3 (17%)
2	NAG	C	301	-	14,14,15	0.57	0	17,19,21	1.38	3 (17%)
2	NAG	D	302	-	14,14,15	0.41	0	17,19,21	0.90	1 (5%)
2	NAG	B	302	-	14,14,15	0.45	0	17,19,21	0.81	0
2	NAG	C	302	-	14,14,15	0.45	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	A	303	-	11,11,12	0.50	0	15,15,17	2.26	4 (26%)
6	OJD	D	1215	-	14,15,15	1.73	4 (28%)	17,19,19	2.02	4 (23%)
5	L0B	A	1205	-	27,27,27	0.59	0	33,36,36	1.35	3 (9%)
7	GOL	D	1206	-	5,5,5	0.38	0	5,5,5	0.21	0
6	OJD	B	1217	-	14,15,15	1.71	5 (35%)	17,19,19	1.95	3 (17%)
7	GOL	E	1207	-	5,5,5	0.33	0	5,5,5	0.82	0
2	NAG	E	302	-	14,14,15	0.48	0	17,19,21	1.67	3 (17%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	E	1207	-	-	2/4/4/4	-
2	NAG	E	302	-	-	3/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1215	OJD	C02-N14	3.65	1.45	1.33
6	D	1215	OJD	C02-N14	3.63	1.45	1.33
6	C	1215	OJD	C02-N14	3.55	1.45	1.33
6	B	1217	OJD	C02-N14	3.51	1.44	1.33
6	A	1215	OJD	C02-N14	3.49	1.44	1.33
6	E	1215	OJD	C03-C04	-2.83	1.45	1.53
6	A	1215	OJD	C03-C04	-2.81	1.45	1.53
6	C	1215	OJD	C03-C04	-2.76	1.45	1.53
6	E	1215	OJD	C11-C10	2.68	1.44	1.38
6	A	1215	OJD	C12-C07	2.64	1.44	1.38
6	D	1215	OJD	C03-C04	-2.62	1.46	1.53
6	D	1215	OJD	C12-C07	2.59	1.44	1.38
6	A	1215	OJD	C11-C10	2.59	1.43	1.38
6	B	1217	OJD	C03-C04	-2.59	1.46	1.53
6	E	1215	OJD	C12-C07	2.55	1.44	1.38
6	E	1215	OJD	C11-C12	-2.49	1.34	1.38
6	C	1215	OJD	C12-C07	2.36	1.43	1.38
6	B	1217	OJD	C11-C10	2.35	1.43	1.38
6	B	1217	OJD	C12-C07	2.35	1.43	1.38
6	D	1215	OJD	C11-C10	2.23	1.43	1.38
6	B	1217	OJD	C11-C12	-2.21	1.35	1.38
6	C	1215	OJD	C11-C10	2.09	1.42	1.38
6	A	1215	OJD	C11-C12	-2.09	1.35	1.38
2	E	301	NAG	O5-C1	-2.07	1.40	1.43
6	C	1215	OJD	C11-C12	-2.01	1.35	1.38

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	NAG	O5-C1-C2	-7.01	100.45	111.29
6	E	1215	OJD	C13-N14-C02	-6.55	107.78	114.13
3	A	303	BMA	C1-O5-C5	6.19	120.48	112.19
6	A	1215	OJD	C13-N14-C02	-5.59	108.71	114.13
6	C	1215	OJD	C13-N14-C02	-5.55	108.75	114.13
2	D	301	NAG	O5-C1-C2	-5.54	102.72	111.29
6	D	1215	OJD	C04-C13-N14	5.43	106.95	103.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1217	OJD	C04-C13-N14	4.95	106.61	103.16
2	A	301	NAG	O5-C1-C2	4.94	118.93	111.29
6	D	1215	OJD	C13-N14-C02	-4.76	109.52	114.13
6	B	1217	OJD	C13-N14-C02	-4.75	109.53	114.13
5	A	1205	L0B	C22-N1-C9	-4.69	109.36	113.16
2	E	301	NAG	C1-O5-C5	-4.55	106.08	112.19
2	E	302	NAG	C2-N2-C7	4.45	128.86	122.90
5	B	1207	L0B	C22-N1-C9	-4.37	109.62	113.16
4	A	304	MAN	C1-C2-C3	4.28	115.88	109.64
5	E	1205	L0B	C22-N1-C9	-4.12	109.83	113.16
5	B	1207	L0B	C12-C9-C8	-4.07	107.75	112.77
3	A	303	BMA	C1-C2-C3	-3.92	103.93	109.64
5	E	1205	L0B	C12-C9-C8	-3.89	107.96	112.77
5	D	1205	L0B	C22-N1-C9	-3.75	110.12	113.16
5	B	1207	L0B	C22-N1-C11	-3.71	110.15	113.16
5	C	1205	L0B	C22-N1-C9	-3.66	110.20	113.16
5	A	1205	L0B	C12-C9-C8	-3.59	108.34	112.77
5	C	1205	L0B	C12-C9-C8	-3.55	108.38	112.77
2	E	302	NAG	C1-C2-N2	3.52	115.98	110.43
2	A	302	NAG	C3-C4-C5	3.36	116.32	110.23
6	A	1215	OJD	C11-C12-C07	-3.28	116.00	120.61
6	A	1215	OJD	C10-C11-C12	3.16	124.14	120.24
3	A	303	BMA	C3-C4-C5	3.15	115.94	110.23
5	E	1205	L0B	C14-C11-C13	-3.09	107.60	112.94
2	E	301	NAG	C3-C4-C5	3.04	115.75	110.23
2	A	301	NAG	C2-N2-C7	-3.01	118.86	122.90
5	E	1205	L0B	C22-N1-C11	-3.00	110.73	113.16
2	C	301	NAG	C2-N2-C7	-2.88	119.04	122.90
5	A	1205	L0B	C14-C11-C13	-2.81	108.08	112.94
2	C	302	NAG	C1-O5-C5	2.80	115.94	112.19
5	D	1205	L0B	C12-C9-C8	-2.76	109.36	112.77
2	A	301	NAG	C1-O5-C5	2.74	115.86	112.19
2	D	302	NAG	C1-O5-C5	2.73	115.84	112.19
6	E	1215	OJD	C11-C12-C07	-2.67	116.86	120.61
2	D	301	NAG	C3-C4-C5	2.66	115.06	110.23
2	C	301	NAG	C4-C3-C2	-2.61	107.19	111.02
6	C	1215	OJD	C10-C11-C12	2.55	123.39	120.24
5	B	1207	L0B	C14-C11-C13	-2.54	108.54	112.94
3	A	303	BMA	O5-C5-C4	2.52	116.95	110.83
2	B	301	NAG	C1-O5-C5	-2.50	108.84	112.19
5	C	1205	L0B	C22-N1-C11	-2.49	111.14	113.16
6	E	1215	OJD	C12-C07-C08	2.47	121.91	118.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1215	OJD	C11-C12-C07	-2.47	117.14	120.61
5	D	1205	L0B	C14-C11-C13	-2.46	108.68	112.94
5	D	1205	L0B	C22-N1-C11	-2.44	111.19	113.16
5	E	1205	L0B	C14-C16-C17	-2.39	106.54	111.63
2	C	301	NAG	C3-C4-C5	2.36	114.52	110.23
6	A	1215	OJD	C12-C07-C08	2.36	121.74	118.23
6	E	1215	OJD	C04-C13-N14	2.33	104.79	103.16
6	E	1215	OJD	C05-C04-C03	-2.24	108.53	115.42
4	A	304	MAN	O5-C5-C4	-2.23	105.40	110.83
2	B	301	NAG	C3-C4-C5	2.21	114.24	110.23
2	E	301	NAG	C1-C2-N2	-2.21	106.96	110.43
6	E	1215	OJD	C10-C11-C12	2.17	122.92	120.24
6	D	1215	OJD	C05-C04-C03	-2.16	108.76	115.42
5	C	1205	L0B	C14-C11-C13	-2.16	109.20	112.94
6	A	1215	OJD	C04-C13-N14	2.12	104.64	103.16
2	A	301	NAG	O4-C4-C3	-2.10	105.42	110.38
2	D	301	NAG	C1-O5-C5	-2.09	109.38	112.19
2	E	301	NAG	O5-C1-C2	-2.08	108.07	111.29
6	C	1215	OJD	C05-C04-C03	-2.08	109.02	115.42
6	D	1215	OJD	C06-C05-C04	2.08	117.82	114.16
6	B	1217	OJD	C06-C05-C04	2.05	117.77	114.16
2	E	302	NAG	C1-O5-C5	2.02	114.89	112.19
6	C	1215	OJD	C12-C07-C08	2.01	121.22	118.23
5	D	1205	L0B	C14-C16-C17	-2.01	107.36	111.63

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAG	C1-C2-N2-C7
2	B	301	NAG	C8-C7-N2-C2
2	B	301	NAG	O7-C7-N2-C2
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	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
5	E	1205	L0B	N1-C11-C14-C16
6	B	1217	OJD	C13-C04-C05-C06

Continued on next page...

Continued from previous page...

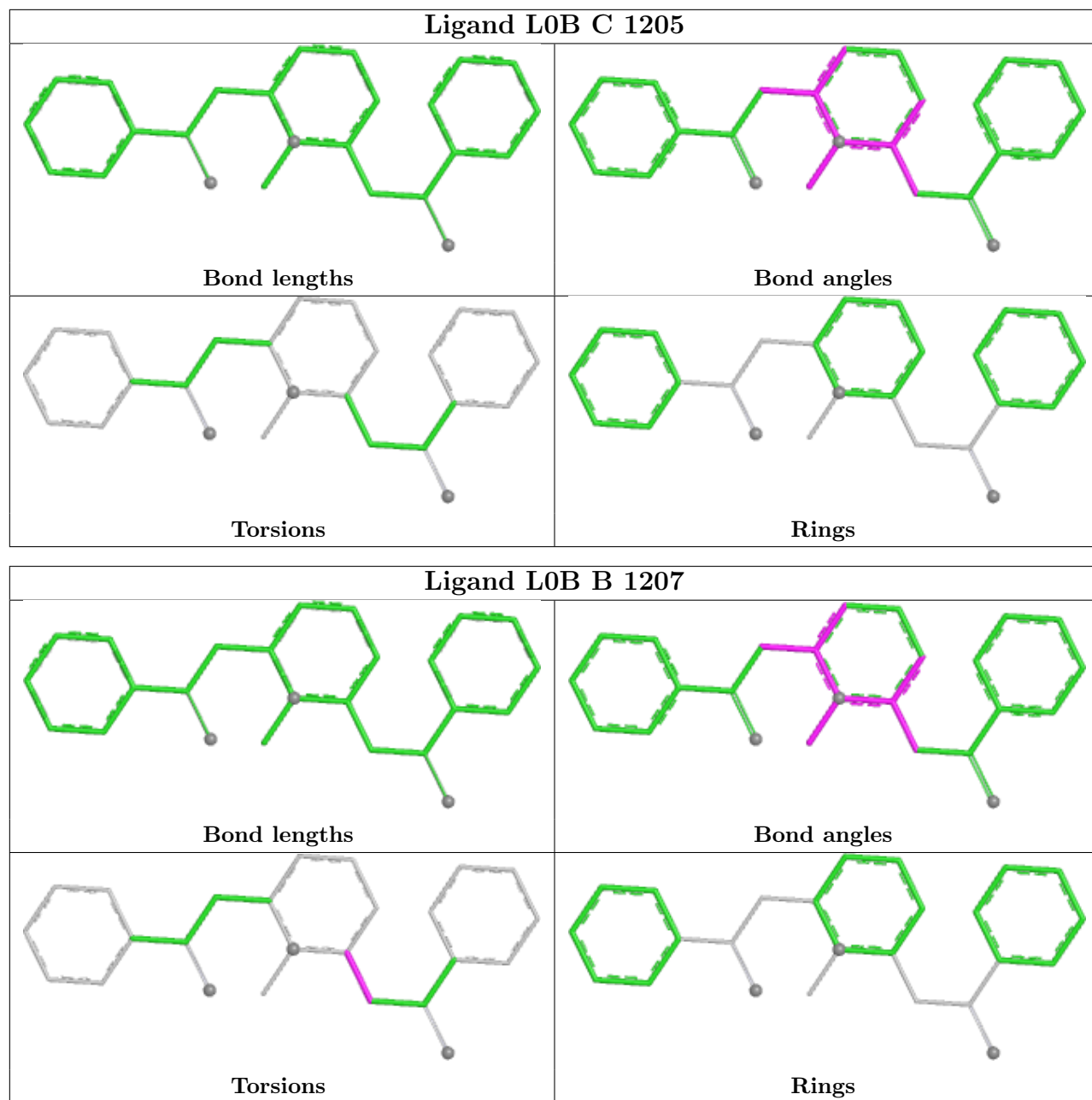
Mol	Chain	Res	Type	Atoms
6	B	1217	OJD	C04-C05-C06-C07
6	D	1215	OJD	C04-C05-C06-C07
7	D	1206	GOL	C1-C2-C3-O3
7	E	1206	GOL	O1-C1-C2-C3
7	E	1208	GOL	O1-C1-C2-C3
2	E	302	NAG	C8-C7-N2-C2
2	C	302	NAG	O5-C5-C6-O6
3	A	303	BMA	C4-C5-C6-O6
7	E	1207	GOL	O1-C1-C2-O2
2	C	302	NAG	C4-C5-C6-O6
3	A	303	BMA	O5-C5-C6-O6
7	E	1206	GOL	C1-C2-C3-O3
7	E	1207	GOL	O1-C1-C2-C3
7	E	1206	GOL	O1-C1-C2-O2
6	B	1217	OJD	C03-C04-C05-C06
6	E	1215	OJD	C03-C04-C05-C06
2	C	301	NAG	O5-C5-C6-O6
7	D	1206	GOL	O2-C2-C3-O3
7	E	1208	GOL	O1-C1-C2-O2
2	A	302	NAG	O5-C5-C6-O6
2	C	301	NAG	C3-C2-N2-C7
4	A	304	MAN	O5-C5-C6-O6
6	E	1215	OJD	C13-C04-C05-C06
6	C	1215	OJD	C04-C05-C06-C07
2	C	301	NAG	C1-C2-N2-C7
6	D	1215	OJD	C13-C04-C05-C06
5	D	1205	L0B	N1-C11-C14-C16
5	E	1205	L0B	C13-C11-C14-C16
6	A	1215	OJD	C13-C04-C05-C06
6	A	1215	OJD	C03-C04-C05-C06
6	D	1215	OJD	C03-C04-C05-C06
7	E	1206	GOL	O2-C2-C3-O3
6	C	1215	OJD	C05-C06-C07-C08
2	E	301	NAG	C4-C5-C6-O6
6	C	1215	OJD	C05-C06-C07-C12
5	B	1207	L0B	N1-C11-C14-C16
6	C	1215	OJD	C13-C04-C05-C06

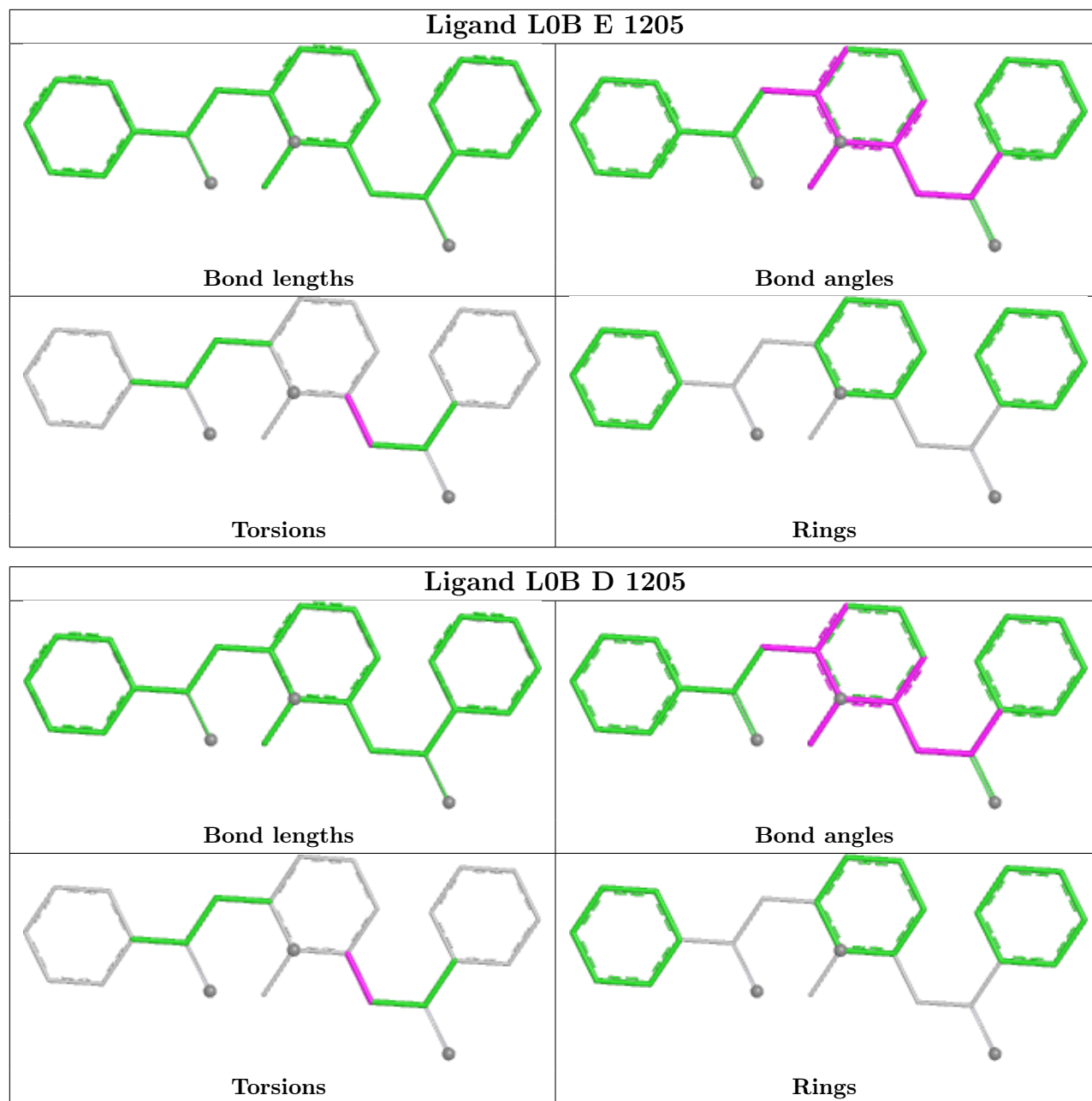
There are no ring outliers.

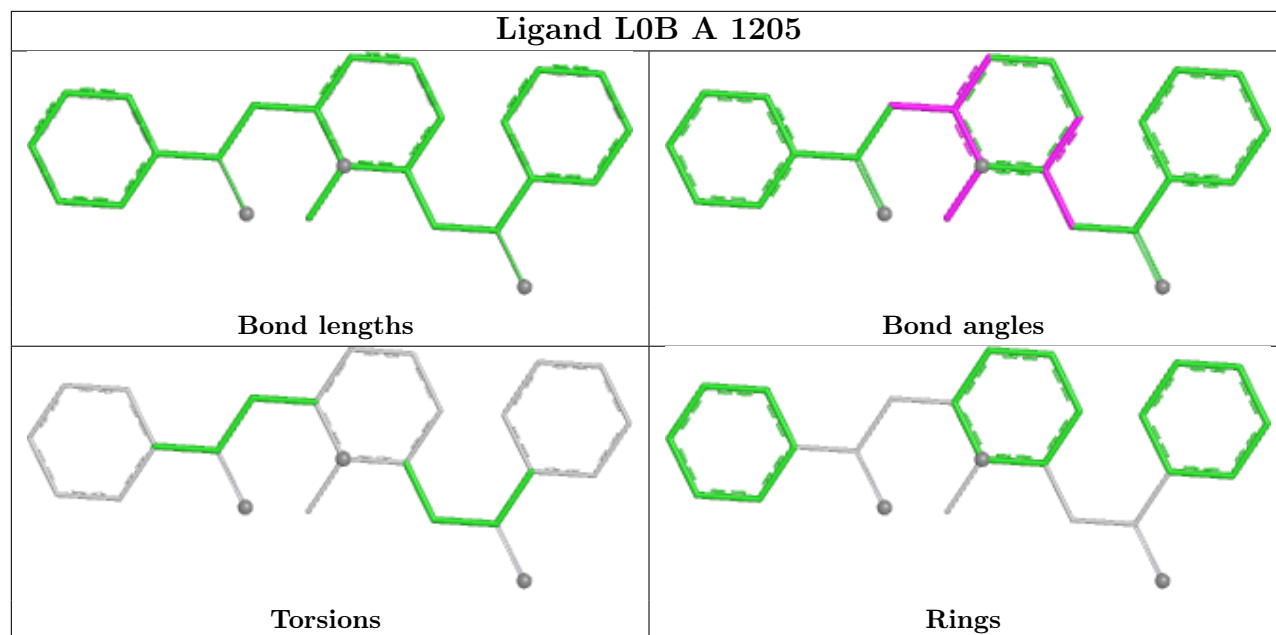
23 monomers are involved in 47 short contacts:

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	205/207 (99%)	1.82	75 (36%) 1 1	19, 42, 80, 115	1 (0%)
1	B	207/207 (100%)	1.49	60 (28%) 1 1	26, 44, 93, 115	1 (0%)
1	C	205/207 (99%)	1.30	42 (20%) 2 3	31, 56, 93, 123	0
1	D	205/207 (99%)	1.58	59 (28%) 1 1	17, 48, 87, 125	5 (2%)
1	E	205/207 (99%)	1.85	83 (40%) 0 1	19, 40, 68, 130	1 (0%)
All	All	1027/1035 (99%)	1.61	319 (31%) 1 1	17, 45, 88, 130	8 (0%)

All (319) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7[A]	TYR	6.8
1	A	71	PRO	5.1
1	E	2	PHE	4.9
1	A	6	LEU	4.7
1	A	67	VAL	4.6
1	B	62	TYR	4.6
1	A	175	VAL	4.5
1	C	7	TYR	4.5
1	D	183	PHE	4.4
1	E	70	TYR	4.4
1	B	105	ALA	4.4
1	A	27	VAL	4.4
1	C	196	PHE	4.3
1	B	0	GLY	4.3
1	B	70	TYR	4.3
1	A	10	LEU	4.2
1	A	59	THR	4.2
1	E	67	VAL	4.2
1	A	80[A]	ILE	4.2
1	D	161	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	73	VAL	4.2
1	A	62	TYR	4.1
1	E	183	PHE	4.0
1	A	84	TRP	3.9
1	E	6	LEU	3.9
1	E	84	TRP	3.9
1	E	156	MET	3.9
1	E	173	VAL	3.9
1	A	70	TYR	3.9
1	D	174	GLY	3.9
1	E	62	TYR	3.9
1	A	20	PRO	3.9
1	D	196[A]	PHE	3.8
1	E	0	GLY	3.8
1	B	186	CYS	3.8
1	A	173	VAL	3.8
1	E	71	PRO	3.7
1	E	190	PRO	3.7
1	A	78	VAL	3.7
1	B	67	VAL	3.7
1	B	109	SER	3.7
1	A	161	ILE	3.7
1	A	88	LEU	3.6
1	B	27	VAL	3.6
1	B	10	LEU	3.6
1	B	2	PHE	3.6
1	B	61	HIS	3.6
1	A	7	TYR	3.5
1	D	58	TRP	3.5
1	B	83	LEU	3.5
1	B	175	VAL	3.5
1	E	73	VAL	3.5
1	E	204	GLY	3.5
1	A	28	THR	3.5
1	A	0	GLY	3.4
1	E	68	SER	3.4
1	A	107	VAL	3.4
1	B	11	VAL	3.4
1	D	159	ALA	3.4
1	A	174	GLY	3.3
1	A	83	LEU	3.3
1	A	11	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	183	PHE	3.3
1	B	68	SER	3.2
1	A	191	TYR	3.2
1	E	185	GLU	3.2
1	D	106	LEU	3.2
1	D	24	ASP	3.2
1	E	72	GLY	3.2
1	E	80	ILE	3.2
1	E	3	GLN	3.2
1	A	82	SER	3.2
1	A	73	VAL	3.1
1	E	88[A]	LEU	3.1
1	E	191	TYR	3.1
1	A	2	PHE	3.1
1	A	116	LEU	3.1
1	A	65	TRP	3.0
1	B	65	TRP	3.0
1	B	159	ALA	3.0
1	B	106	LEU	3.0
1	D	83	LEU	3.0
1	E	172	LEU	3.0
1	A	19	ILE	3.0
1	E	188	LYS	3.0
1	A	113	VAL	3.0
1	E	194	VAL	3.0
1	E	161	ILE	3.0
1	D	111	GLY	3.0
1	B	20	PRO	3.0
1	E	159	ALA	3.0
1	E	18	VAL	3.0
1	A	74	LYS	3.0
1	A	75	GLN	2.9
1	D	109	SER	2.9
1	A	110	SER	2.9
1	E	65	TRP	2.9
1	A	61	HIS	2.9
1	E	7	TYR	2.9
1	D	65	TRP	2.9
1	D	27	VAL	2.8
1	D	19	ILE	2.8
1	D	13	ASN	2.8
1	E	148	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	140	LEU	2.8
1	E	23	ARG	2.8
1	D	72	GLY	2.8
1	D	30	TYR	2.8
1	A	18	VAL	2.8
1	B	173	VAL	2.8
1	B	13	ASN	2.7
1	D	5	LYS	2.7
1	E	12	LYS	2.7
1	B	184	TYR	2.7
1	D	14	TYR	2.7
1	A	194	VAL	2.7
1	E	19	ILE	2.7
1	B	69	GLU	2.7
1	E	145	TRP	2.7
1	B	107	VAL	2.7
1	C	175	VAL	2.7
1	E	127	VAL	2.7
1	E	28	THR	2.7
1	D	191	TYR	2.7
1	E	78	VAL	2.7
1	D	23	ARG	2.7
1	E	147	HIS	2.6
1	C	81	SER	2.6
1	D	18	VAL	2.6
1	E	130	VAL	2.6
1	E	179	ARG	2.6
1	D	61	HIS	2.6
1	A	106	LEU	2.6
1	B	196	PHE	2.6
1	C	2	PHE	2.6
1	E	106	LEU	2.6
1	C	149	SER	2.6
1	B	150	ARG	2.6
1	E	59	THR	2.6
1	A	152	LEU	2.6
1	D	10	LEU	2.6
1	A	68	SER	2.6
1	E	180	SER	2.6
1	B	161	ILE	2.6
1	A	8	LYS	2.6
1	C	159	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	26	PRO	2.6
1	A	140	LEU	2.6
1	E	149	SER	2.6
1	E	152	LEU	2.6
1	E	154	LEU	2.6
1	A	165	ILE	2.5
1	C	11	VAL	2.5
1	C	70	TYR	2.5
1	D	62	TYR	2.5
1	D	89	ALA	2.5
1	B	63	LEU	2.5
1	B	88	LEU	2.5
1	B	152	LEU	2.5
1	D	63	LEU	2.5
1	E	64	GLN	2.5
1	D	7	TYR	2.5
1	E	125	CYS	2.5
1	E	182	ARG	2.5
1	B	24	ASP	2.5
1	A	97	PRO	2.5
1	C	77	SER	2.5
1	A	172	LEU	2.5
1	B	108	ASN	2.5
1	E	66	ASN	2.5
1	D	160	ASP	2.5
1	D	188	LYS	2.5
1	D	84	TRP	2.5
1	C	27	VAL	2.4
1	D	64	GLN	2.4
1	C	62	TYR	2.4
1	A	109	SER	2.4
1	B	71	PRO	2.4
1	D	26	PRO	2.4
1	B	6	LEU	2.4
1	B	78	VAL	2.4
1	B	110	SER	2.4
1	E	197	THR	2.4
1	E	15	ASN	2.4
1	D	31	PHE	2.4
1	D	185	GLU	2.4
1	D	144	SER	2.4
1	E	150	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	151	GLU	2.4
1	C	174	GLY	2.4
1	D	2	PHE	2.4
1	A	4	ARG	2.4
1	A	23	ARG	2.4
1	C	173	VAL	2.4
1	D	67	VAL	2.4
1	D	73	VAL	2.4
1	E	76	VAL	2.4
1	B	206	SER	2.4
1	E	110	SER	2.4
1	D	190	PRO	2.4
1	E	177	GLN	2.3
1	A	72	GLY	2.3
1	D	0	GLY	2.3
1	A	182	ARG	2.3
1	A	57	SER	2.3
1	B	134	SER	2.3
1	C	19	ILE	2.3
1	C	67	VAL	2.3
1	D	175	VAL	2.3
1	A	102	PRO	2.3
1	E	151	GLU	2.3
1	A	58	TRP	2.3
1	B	53	TRP	2.3
1	E	184	TYR	2.3
1	C	72	GLY	2.3
1	C	150	ARG	2.3
1	A	200	PHE	2.3
1	B	57	SER	2.3
1	C	162	SER	2.3
1	A	158	GLU	2.3
1	D	181	GLU	2.3
1	A	190	PRO	2.3
1	E	101	THR	2.3
1	E	114	GLN	2.3
1	E	195	THR	2.3
1	C	172	LEU	2.3
1	D	4	ARG	2.3
1	D	150	ARG	2.3
1	E	111	GLY	2.3
1	A	81	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	81	SER	2.3
1	A	22	GLN	2.3
1	E	22	GLN	2.3
1	A	76	VAL	2.3
1	E	29	VAL	2.3
1	C	63	LEU	2.3
1	B	14	TYR	2.3
1	C	65	TRP	2.3
1	A	3	GLN	2.2
1	B	19	ILE	2.2
1	D	88	LEU	2.2
1	B	1	GLU	2.2
1	B	4	ARG	2.2
1	A	21	THR	2.2
1	B	80	ILE	2.2
1	E	87	ASP	2.2
1	C	106	LEU	2.2
1	B	22	GLN	2.2
1	C	109	SER	2.2
1	A	178	LYS	2.2
1	B	16	PRO	2.2
1	C	161	ILE	2.2
1	D	17	ASP	2.2
1	C	78	VAL	2.2
1	E	85	VAL	2.2
1	A	104	LEU	2.2
1	B	104	LEU	2.2
1	E	10	LEU	2.2
1	A	32	SER	2.2
1	D	68	SER	2.2
1	E	25	ARG	2.2
1	E	144	SER	2.2
1	A	15	ASN	2.2
1	C	66	ASN	2.2
1	D	108	ASN	2.2
1	C	190	PRO	2.1
1	D	71	PRO	2.1
1	D	85	VAL	2.1
1	D	113	VAL	2.1
1	D	173	VAL	2.1
1	C	204	GLY	2.1
1	E	36	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	5	LYS	2.1
1	A	30	TYR	2.1
1	C	160	ASP	2.1
1	E	153	ASP	2.1
1	C	85	VAL	2.1
1	D	112	HIS	2.1
1	B	25	ARG	2.1
1	C	105	ALA	2.1
1	D	104	LEU	2.1
1	E	74	LYS	2.1
1	E	83	LEU	2.1
1	A	138	CYS	2.1
1	A	180	SER	2.1
1	E	17	ASP	2.1
1	C	111	GLY	2.1
1	A	183	PHE	2.1
1	B	18	VAL	2.1
1	E	27	VAL	2.1
1	E	175	VAL	2.1
1	B	180	SER	2.1
1	D	149	SER	2.1
1	C	24	ASP	2.1
1	A	114	GLN	2.1
1	A	132	THR	2.1
1	B	59	THR	2.1
1	B	117	PRO	2.1
1	E	21	THR	2.1
1	E	61	HIS	2.1
1	B	178	LYS	2.1
1	E	142	PHE	2.1
1	C	1	GLU	2.0
1	A	108	ASN	2.0
1	B	75	GLN	2.0
1	B	146	THR	2.0
1	D	74	LYS	2.0
1	D	204	GLY	2.0
1	C	80	ILE	2.0
1	A	9	GLU	2.0
1	C	29	VAL	2.0
1	C	31	PHE	2.0
1	C	107	VAL	2.0
1	E	196	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	77	SER	2.0
1	D	182	ARG	2.0
1	C	186	CYS	2.0
1	C	21	THR	2.0
1	A	14	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

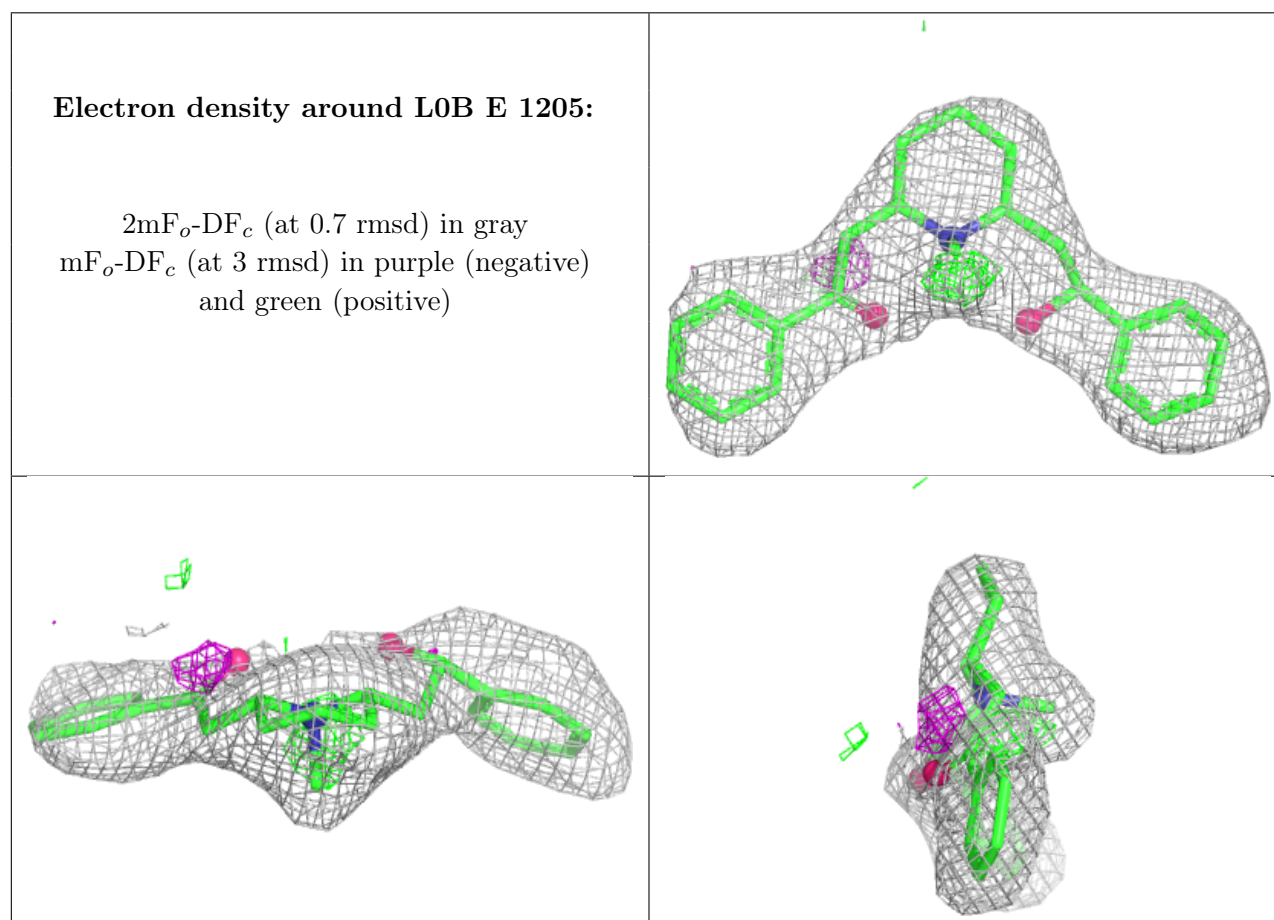
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	302	14/15	0.42	0.17	79,126,133,135	0
2	NAG	E	302	14/15	0.45	0.22	85,117,125,126	0
2	NAG	C	302	14/15	0.51	0.21	122,142,149,151	0
2	NAG	B	302	14/15	0.52	0.17	85,112,125,130	0
4	MAN	A	304	11/12	0.63	0.19	72,96,105,107	0
7	GOL	E	1206	6/6	0.63	0.28	87,91,93,100	0
3	BMA	A	303	11/12	0.66	0.20	64,74,89,92	0
2	NAG	A	302	14/15	0.66	0.21	48,55,65,72	0
2	NAG	B	301	14/15	0.66	0.17	64,82,93,94	0
7	GOL	E	1208	6/6	0.72	0.37	85,85,89,92	0
2	NAG	A	301	14/15	0.73	0.18	39,52,61,66	0
2	NAG	D	301	14/15	0.73	0.15	68,78,89,95	0
2	NAG	E	301	14/15	0.74	0.17	46,54,72,78	0
6	OJD	D	1215	14/14	0.74	0.23	34,64,101,101	0
7	GOL	E	1207	6/6	0.79	0.24	53,55,61,67	0
7	GOL	D	1206	6/6	0.80	0.21	60,70,75,78	0
6	OJD	C	1215	14/14	0.81	0.23	45,75,93,101	0
2	NAG	C	301	14/15	0.81	0.13	71,87,97,99	0

Continued on next page...

Continued from previous page...

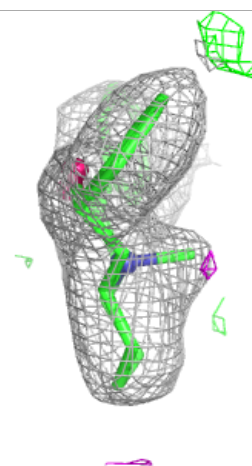
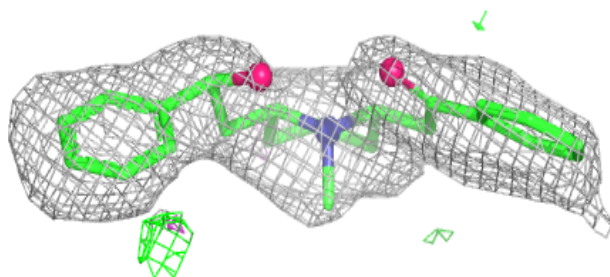
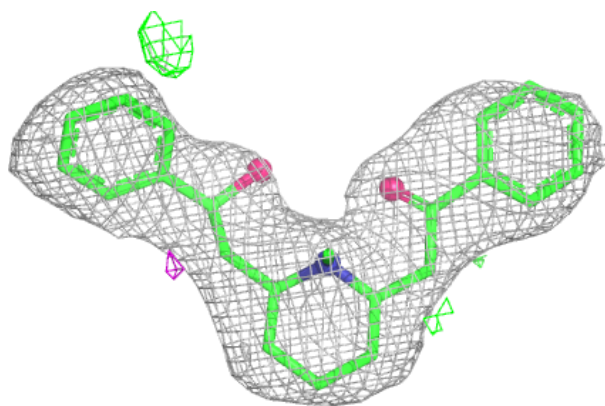
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	L0B	E	1205	25/25	0.81	0.18	34,41,57,65	0
6	OJD	A	1215	14/14	0.83	0.20	31,57,84,97	0
6	OJD	E	1215	14/14	0.83	0.22	33,54,79,90	0
5	L0B	D	1205	25/25	0.84	0.14	37,46,55,58	0
6	OJD	B	1217	14/14	0.84	0.19	42,62,111,112	0
5	L0B	C	1205	25/25	0.84	0.16	45,57,65,69	0
5	L0B	A	1205	25/25	0.86	0.13	39,48,59,60	0
5	L0B	B	1207	25/25	0.86	0.15	46,57,64,72	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



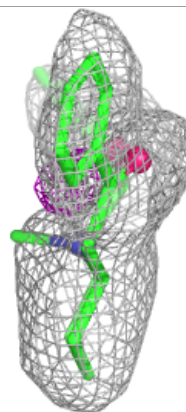
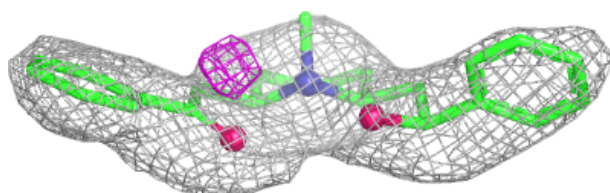
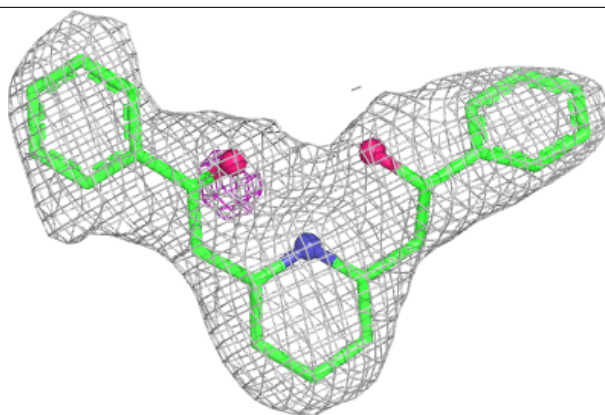
Electron density around L0B D 1205:

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

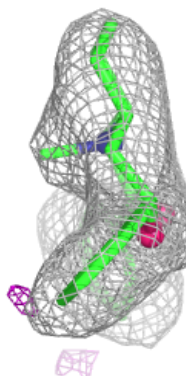
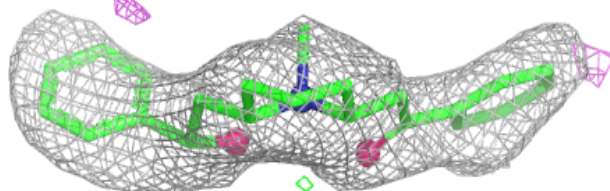
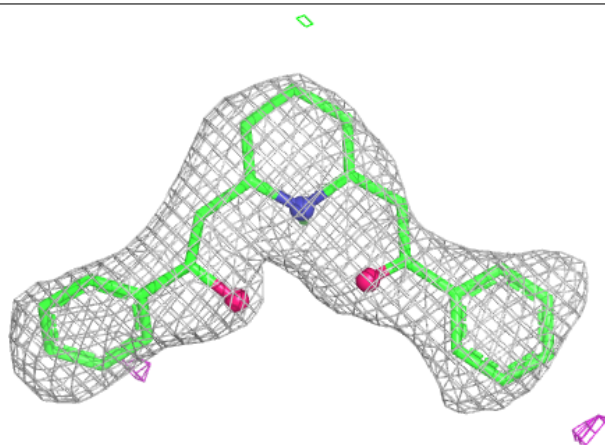


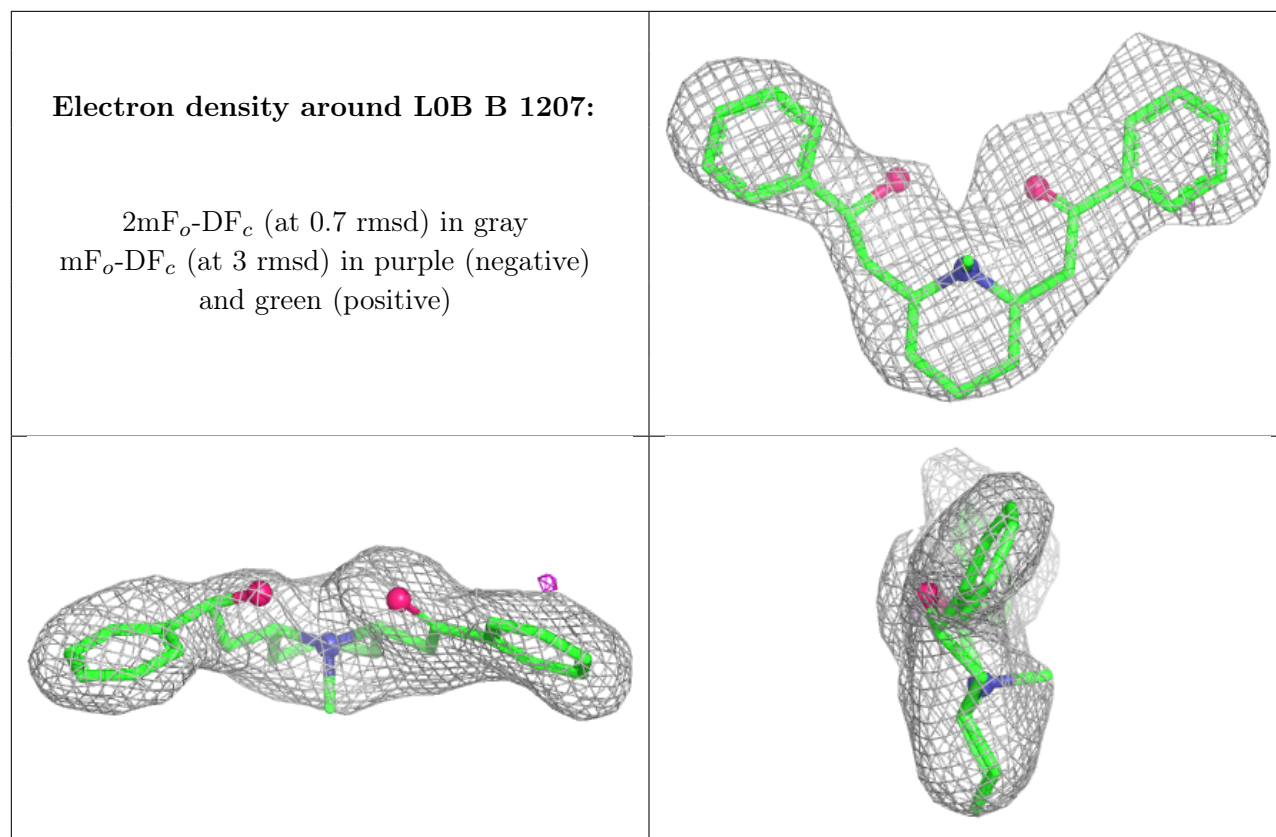
Electron density around L0B C 1205:

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

**Electron density around L0B 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](#)

There are no such residues in this entry.