



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:55 AM UTC

PDB ID : 5AFM / pdb_00005afm
Title : alpha7-AChBP in complex with lobeline and fragment 4
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 : 2.85 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

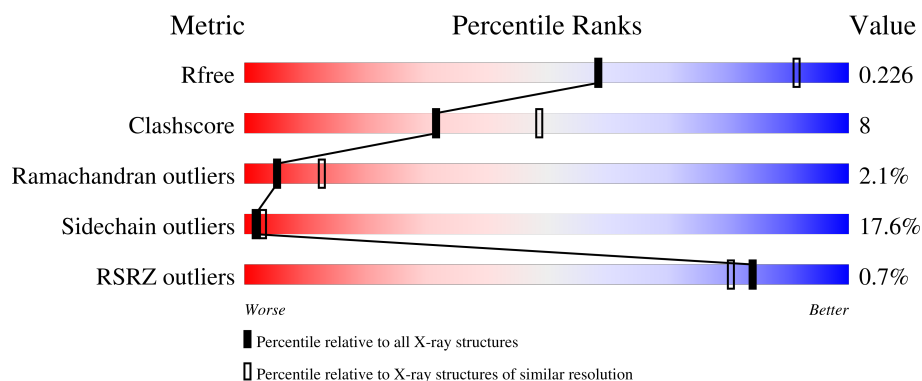
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	205	 70% 21% 7% .
1	C	205	 71% 21% 6% .
1	D	205	 69% 22% 8% .
1	E	205	 72% 21% 6%
2	B	207	 69% 21% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	C	1206	-	X	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9054 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	0	0
			1670	1071	279	313	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	0	0
			1670	1071	279	313	7			
1	E	205	Total	C	N	O	S	0	0	0
			1670	1071	279	313	7			

- Molecule 2 is a protein called ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7.

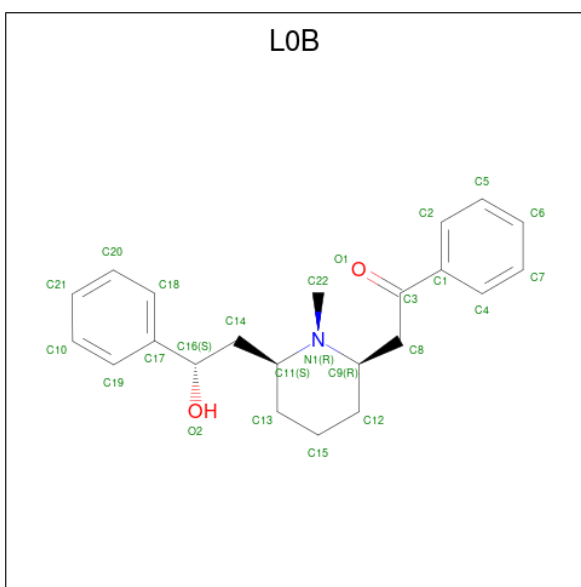
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1687	1080	284	316	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



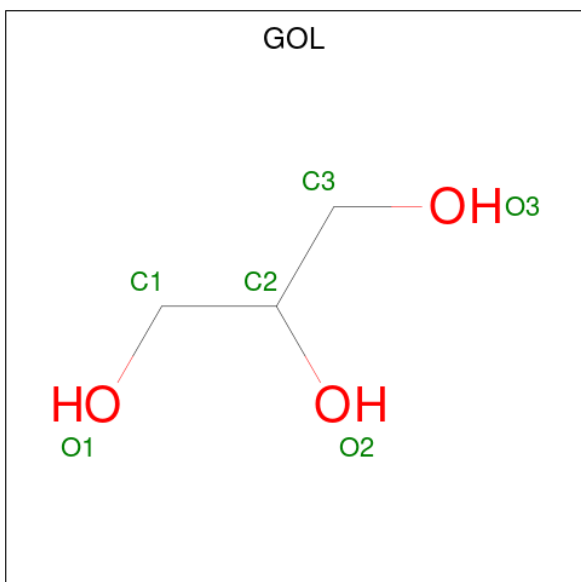
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

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



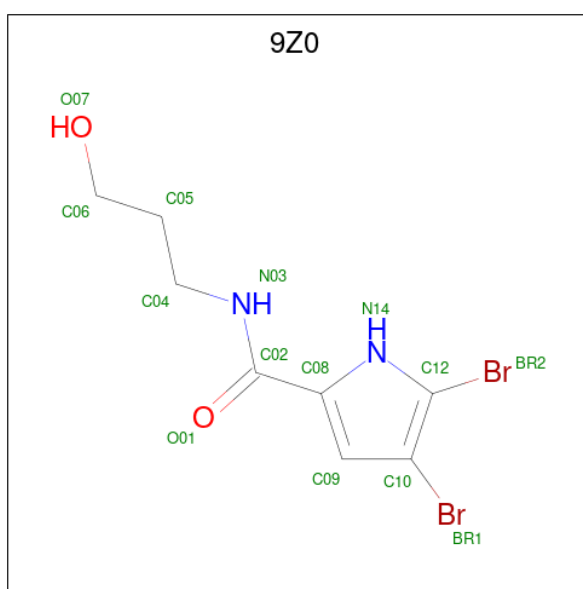
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	22	1	2		
4	B	1	Total	C	N	O	0	0
			25	22	1	2		
4	C	1	Total	C	N	O	0	0
			25	22	1	2		
4	D	1	Total	C	N	O	0	0
			25	22	1	2		
4	E	1	Total	C	N	O	0	0
			25	22	1	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is 4,5-dibromo-N-(3-hydroxypropyl)-1H-pyrrole-2-carboxamide (CCD ID: 9Z0) (formula: $C_8H_{10}Br_2N_2O_2$).



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

- Molecule 7 is water.

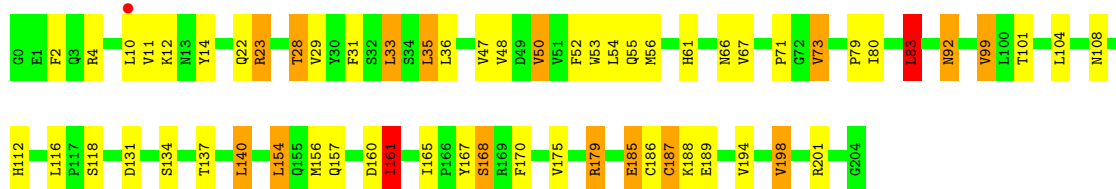
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	73	Total 73	O 73	0	0
7	B	40	Total 40	O 40	0	0
7	C	73	Total 73	O 73	0	0
7	D	75	Total 75	O 75	0	0
7	E	67	Total 67	O 67	0	0

3 Residue-property plots [i](#)

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

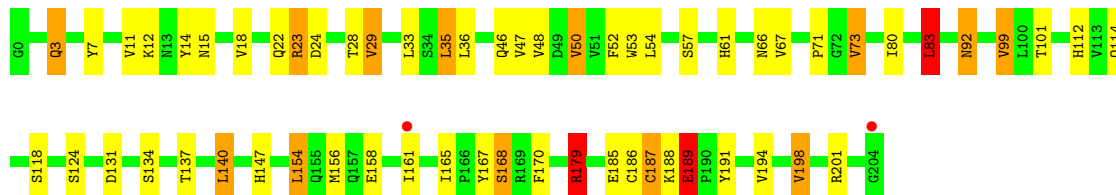
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain A: 



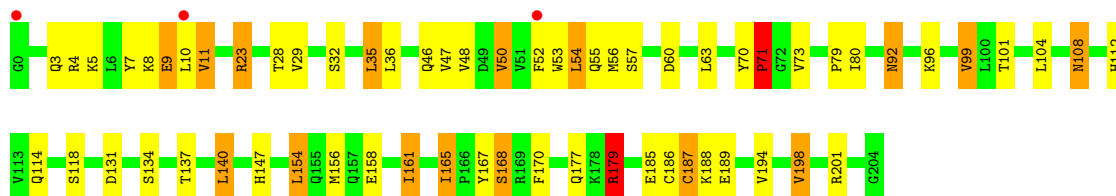
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain C: 



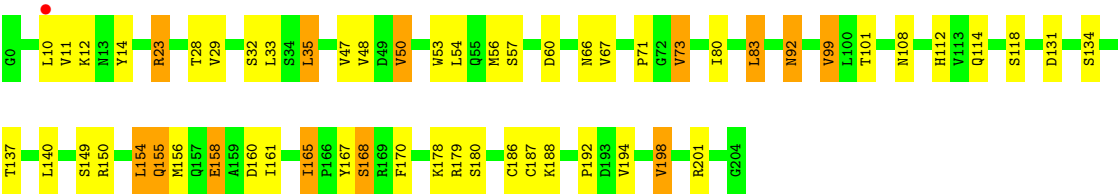
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain D: 

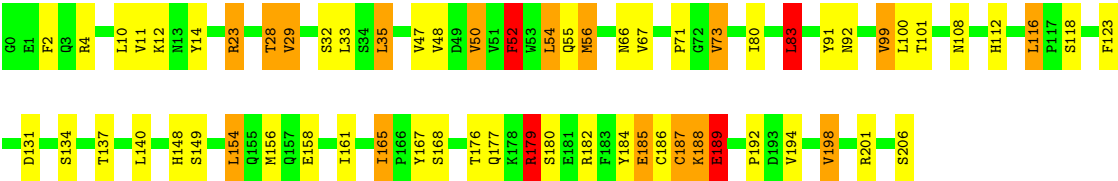


- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain E: 



● Molecule 2: 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	75.70Å 119.60Å 143.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.85 47.72 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.72-2.85) 99.8 (47.72-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.161 , 0.217 0.168 , 0.226	Depositor DCC
R_{free} test set	1553 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 80.8	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	0.96	EDS
Total number of atoms	9054	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, L0B, 9Z0

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	0.84	1/1715 (0.1%)	1.29	12/2333 (0.5%)
1	C	0.84	1/1715 (0.1%)	1.27	10/2333 (0.4%)
1	D	0.88	1/1715 (0.1%)	1.29	13/2333 (0.6%)
1	E	0.85	0/1715	1.27	6/2333 (0.3%)
2	B	0.81	0/1732	1.30	16/2355 (0.7%)
All	All	0.84	3/8592 (0.0%)	1.28	57/11687 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	ILE	CG1-CD1	9.30	1.88	1.51
1	D	10	LEU	CB-CG	5.30	1.64	1.53
1	C	189	GLU	CA-C	5.08	1.59	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	CYS	N-CA-C	10.08	126.87	113.97
1	D	187	CYS	N-CA-C	8.22	123.86	112.93
2	B	185	GLU	CA-C-N	8.03	131.03	120.28
2	B	185	GLU	C-N-CA	8.03	131.03	120.28
1	C	99	VAL	N-CA-CB	7.74	119.82	111.00
2	B	188	LYS	N-CA-C	-7.73	100.56	110.53
1	A	99	VAL	N-CA-CB	7.68	119.75	111.00
1	D	99	VAL	N-CA-CB	7.39	119.43	111.00
1	D	10	LEU	CA-C-N	6.94	134.46	121.97
1	D	10	LEU	C-N-CA	6.94	134.46	121.97
1	E	99	VAL	N-CA-CB	6.63	119.46	111.31
1	D	10	LEU	CB-CA-C	6.35	119.03	111.22
2	B	187	CYS	N-CA-C	6.24	118.55	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	VAL	CB-CA-C	6.22	118.48	110.96
2	B	99	VAL	N-CA-CB	6.19	118.92	111.31
1	C	185	GLU	CA-C-N	5.96	128.19	120.44
1	C	185	GLU	C-N-CA	5.96	128.19	120.44
1	A	185	GLU	CA-C-N	5.95	128.18	120.44
1	A	185	GLU	C-N-CA	5.95	128.18	120.44
1	D	161	ILE	CB-CA-C	5.91	118.98	112.19
2	B	184	TYR	CA-C-N	5.88	128.44	120.38
2	B	184	TYR	C-N-CA	5.88	128.44	120.38
1	A	99	VAL	CB-CA-C	5.85	118.04	110.96
1	D	185	GLU	CA-C-N	5.72	128.42	120.29
1	D	185	GLU	C-N-CA	5.72	128.42	120.29
1	C	99	VAL	CB-CA-C	5.72	117.88	110.96
1	E	99	VAL	CB-CA-C	5.71	118.50	111.25
1	A	187	CYS	N-CA-C	5.62	118.06	108.90
1	E	158	GLU	N-CA-C	5.61	118.72	110.30
1	C	29	VAL	N-CA-CB	5.51	118.40	111.46
2	B	29	VAL	N-CA-CB	5.49	118.72	111.25
1	A	157	GLN	N-CA-C	-5.48	100.47	109.40
2	B	83	LEU	N-CA-C	5.48	118.01	109.52
2	B	2	PHE	CA-C-N	5.47	127.55	120.44
2	B	2	PHE	C-N-CA	5.47	127.55	120.44
2	B	28	THR	CB-CA-C	5.41	119.25	110.22
1	D	189	GLU	N-CA-C	-5.41	101.78	109.62
1	D	179	ARG	CB-CA-C	5.39	118.54	109.48
2	B	99	VAL	CB-CA-C	5.29	117.97	111.25
1	A	160	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	71	PRO	N-CA-C	5.20	123.17	112.47
1	C	83	LEU	N-CA-C	5.17	117.53	109.52
1	E	155	GLN	CA-C-N	-5.15	113.88	122.64
1	E	155	GLN	C-N-CA	-5.15	113.88	122.64
2	B	52	PHE	N-CA-C	5.15	117.02	109.24
1	A	28	THR	CB-CA-C	5.14	118.80	110.22
1	A	2	PHE	CA-C-N	5.13	127.11	120.44
1	A	2	PHE	C-N-CA	5.13	127.11	120.44
2	B	179	ARG	CB-CA-C	5.10	118.05	109.48
1	A	83	LEU	N-CA-C	5.09	117.41	109.52
1	E	170	PHE	N-CA-C	5.09	117.53	109.24
1	D	170	PHE	N-CA-C	5.07	117.50	109.24
1	C	179	ARG	CB-CA-C	5.07	117.99	109.48
1	C	170	PHE	N-CA-C	5.02	117.42	109.24
1	A	170	PHE	N-CA-C	5.01	117.41	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ASP	CA-CB-CG	5.01	117.61	112.60
2	B	52	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1633	19	0
1	C	1670	0	1633	26	0
1	D	1670	0	1633	35	0
1	E	1670	0	1633	26	0
2	B	1687	0	1651	25	0
3	A	28	0	26	4	0
3	B	28	0	26	3	0
3	C	28	0	26	2	0
3	D	28	0	26	6	0
3	E	28	0	26	6	0
4	A	25	0	27	0	0
4	B	25	0	27	1	0
4	C	25	0	27	4	0
4	D	25	0	27	4	0
4	E	25	0	27	0	0
5	A	6	0	8	2	0
5	C	6	0	7	4	0
5	D	6	0	8	3	0
5	E	6	0	8	1	0
6	A	14	0	10	1	0
6	B	14	0	10	3	0
6	C	14	0	10	0	0
6	D	14	0	10	1	0
6	E	14	0	10	0	0
7	A	73	0	0	0	0
7	B	40	0	0	1	0
7	C	73	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	75	0	0	5	0
7	E	67	0	0	2	0
All	All	9054	0	8529	140	0

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

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:CD1	1:A:161:ILE:CG1	1.88	1.47
2:B:52:PHE:CE1	6:B:1208:9Z0:BR2	2.73	0.97
1:E:160:ASP:HB2	7:E:2019:HOH:O	1.67	0.94
2:B:52:PHE:CZ	6:B:1208:9Z0:BR2	2.77	0.93
2:B:33:LEU:HD21	2:B:52:PHE:CD2	2.10	0.85
3:C:301:NAG:H61	3:C:302:NAG:H82	1.66	0.77
1:D:147:HIS:HE1	7:D:2035:HOH:O	1.67	0.77
3:A:301:NAG:H61	3:A:302:NAG:H82	1.68	0.74
4:C:1205:L0B:H10	1:D:53:TRP:CD2	2.23	0.73
3:B:301:NAG:H61	3:B:302:NAG:H82	1.71	0.72
3:E:301:NAG:H61	3:E:302:NAG:H82	1.69	0.71
1:D:54:LEU:HD13	1:D:56:MET:HE2	1.73	0.71
2:B:156:MET:SD	2:B:177:GLN:HG2	2.31	0.71
2:B:55:GLN:HA	2:B:116:LEU:HD12	1.73	0.70
3:D:301:NAG:H61	3:D:302:NAG:H82	1.74	0.70
1:D:54:LEU:CD1	1:D:56:MET:HE2	2.23	0.67
1:C:101:THR:HG23	1:C:118:SER:HB2	1.78	0.65
2:B:33:LEU:HD21	2:B:52:PHE:HD2	1.62	0.65
1:C:92:ASN:HA	5:C:1206:GOL:H12	1.79	0.64
5:C:1206:GOL:H32	1:D:165:ILE:HD13	1.78	0.64
1:D:4:ARG:HH11	1:D:4:ARG:HG2	1.63	0.64
1:E:101:THR:HG23	1:E:118:SER:HB2	1.81	0.63
1:A:92:ASN:HA	5:A:1206:GOL:H31	1.81	0.63
1:D:101:THR:HG23	1:D:118:SER:HB2	1.80	0.63
2:B:101:THR:HG23	2:B:118:SER:HB2	1.81	0.62
1:D:46:GLN:HE21	1:E:167:TYR:HB2	1.65	0.61
1:D:154:LEU:HD13	1:D:194:VAL:HG23	1.84	0.60
1:A:101:THR:HG23	1:A:118:SER:HB2	1.84	0.58
2:B:154:LEU:HD13	2:B:194:VAL:HG23	1.84	0.58
5:C:1206:GOL:H32	1:D:165:ILE:CD1	2.34	0.58
1:A:186:CYS:SG	1:A:187:CYS:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:SER:HB2	1:C:112:HIS:CE1	2.39	0.57
1:A:154:LEU:HD13	1:A:194:VAL:HG23	1.86	0.57
5:D:1206:GOL:H11	1:E:165:ILE:HD11	1.87	0.57
1:E:154:LEU:HD13	1:E:194:VAL:HG23	1.87	0.56
5:D:1206:GOL:H11	1:E:165:ILE:CD1	2.37	0.55
5:A:1206:GOL:H12	2:B:165:ILE:HD11	1.89	0.54
1:D:92:ASN:HA	5:D:1206:GOL:H32	1.90	0.54
1:C:156:MET:HG3	1:C:179:ARG:HB3	1.90	0.54
1:E:156:MET:HB2	7:E:2053:HOH:O	2.06	0.54
1:D:11:VAL:N	7:D:2003:HOH:O	2.40	0.53
4:D:1205:L0B:H5	1:E:114:GLN:NE2	2.24	0.53
1:A:112:HIS:CD2	3:A:301:NAG:H62	2.44	0.52
1:C:14:TYR:HE2	1:C:83:LEU:HA	1.74	0.52
1:D:112:HIS:CD2	3:D:301:NAG:H62	2.44	0.52
1:C:191:TYR:CE2	4:C:1205:L0B:H121	2.45	0.52
1:A:22:GLN:HB3	1:A:61:HIS:CE1	2.44	0.52
6:D:1207:9Z0:H041	7:D:2039:HOH:O	2.09	0.52
1:C:187:CYS:C	1:C:189:GLU:H	2.18	0.51
1:D:156:MET:HG3	1:D:179:ARG:HB3	1.93	0.51
1:A:156:MET:HG3	1:A:179:ARG:HB3	1.93	0.50
1:C:154:LEU:HD13	1:C:194:VAL:HG23	1.92	0.50
1:E:14:TYR:HE2	1:E:83:LEU:HA	1.77	0.50
1:A:14:TYR:HE2	1:A:83:LEU:HA	1.76	0.50
2:B:32:SER:HB3	2:B:55:GLN:HB2	1.93	0.50
2:B:54:LEU:HD13	2:B:56:MET:HE2	1.94	0.50
1:E:108:ASN:CG	3:E:301:NAG:C1	2.85	0.50
2:B:156:MET:HG3	2:B:179:ARG:HB3	1.94	0.49
2:B:52:PHE:HZ	2:B:123:PHE:HZ	1.59	0.49
1:C:35:LEU:HD21	1:C:50:VAL:HG22	1.95	0.49
1:E:108:ASN:ND2	3:E:301:NAG:O5	2.46	0.49
1:C:114:GLN:HG2	7:C:2022:HOH:O	2.12	0.49
2:B:176:THR:HA	7:B:2029:HOH:O	2.11	0.49
1:C:46:GLN:HE21	1:D:167:TYR:HB2	1.78	0.49
1:A:31:PHE:CZ	1:A:33:LEU:HD22	2.48	0.48
4:D:1205:L0B:H10	1:E:53:TRP:CG	2.47	0.48
1:E:108:ASN:HD22	1:E:112:HIS:HB3	1.78	0.48
2:B:14:TYR:HE2	2:B:83:LEU:HA	1.76	0.48
4:C:1205:L0B:H5	1:D:114:GLN:NE2	2.29	0.48
6:A:1207:9Z0:H062	2:B:100:LEU:O	2.13	0.48
1:E:112:HIS:CD2	3:E:301:NAG:H62	2.48	0.48
1:A:108:ASN:CG	3:A:301:NAG:C1	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1205:L0B:H10	1:D:53:TRP:CE3	2.48	0.47
1:C:186:CYS:SG	1:C:187:CYS:N	2.88	0.47
1:D:54:LEU:HD11	1:D:56:MET:HE2	1.97	0.47
1:D:108:ASN:ND2	3:D:301:NAG:O5	2.48	0.47
1:E:186:CYS:SG	1:E:187:CYS:N	2.88	0.47
1:D:35:LEU:HD21	1:D:50:VAL:HG22	1.97	0.47
1:A:52:PHE:HZ	1:A:140:LEU:HD23	1.81	0.46
1:D:96:LYS:NZ	7:D:2041:HOH:O	2.48	0.46
2:B:52:PHE:HZ	2:B:123:PHE:CZ	2.33	0.46
2:B:112:HIS:CD2	3:B:301:NAG:H62	2.51	0.46
1:D:186:CYS:SG	1:D:187:CYS:N	2.88	0.46
2:B:35:LEU:HD21	2:B:50:VAL:HG22	1.98	0.46
1:E:35:LEU:HD21	1:E:50:VAL:HG22	1.98	0.46
1:A:55:GLN:HG2	1:A:116:LEU:HD22	1.98	0.45
1:C:57:SER:HB2	1:C:112:HIS:HE1	1.79	0.45
1:E:92:ASN:HA	5:E:1206:GOL:H32	1.98	0.45
1:C:147:HIS:HE1	7:C:2029:HOH:O	1.99	0.45
1:D:177:GLN:HB2	7:D:2065:HOH:O	2.16	0.45
2:B:148:HIS:ND1	2:B:189:GLU:HG2	2.32	0.45
2:B:54:LEU:CD1	2:B:56:MET:HE2	2.47	0.45
1:E:57:SER:HB2	1:E:112:HIS:NE2	2.32	0.45
1:A:35:LEU:HD21	1:A:50:VAL:HG22	1.98	0.45
1:D:9:GLU:HG3	1:D:70:TYR:OH	2.17	0.44
1:D:108:ASN:CG	3:D:301:NAG:C1	2.90	0.44
1:D:60:ASP:HB3	1:D:63:LEU:HD12	2.00	0.44
1:C:3:GLN:HE21	1:C:7:TYR:HE1	1.64	0.44
1:D:52:PHE:HZ	1:D:140:LEU:HD23	1.82	0.44
1:E:155:GLN:NE2	1:E:155:GLN:HA	2.33	0.44
1:A:137:THR:HA	1:A:198:VAL:O	2.18	0.44
3:D:301:NAG:O4	3:D:302:NAG:O5	2.31	0.44
4:D:1205:L0B:H10	1:E:53:TRP:CD1	2.53	0.44
3:E:301:NAG:O4	3:E:302:NAG:O5	2.29	0.43
1:A:167:TYR:O	1:A:168:SER:CB	2.66	0.43
1:A:36:LEU:HD11	1:A:53:TRP:HB2	2.01	0.43
6:B:1208:9Z0:H061	1:C:101:THR:C	2.44	0.43
1:D:167:TYR:O	1:D:168:SER:CB	2.66	0.43
1:C:22:GLN:HG3	1:C:61:HIS:CE1	2.53	0.43
1:E:156:MET:HE1	1:E:178:LYS:HA	2.01	0.42
2:B:137:THR:HA	2:B:198:VAL:O	2.19	0.42
1:C:15:ASN:H	1:D:4:ARG:HH12	1.66	0.42
1:E:167:TYR:O	1:E:168:SER:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:TYR:CD2	4:B:1207:L0B:H18	2.54	0.42
1:C:18:VAL:HG22	1:D:7:TYR:CD2	2.54	0.42
1:D:137:THR:HA	1:D:198:VAL:O	2.19	0.42
3:E:301:NAG:HO4	3:E:302:NAG:C5	2.33	0.42
3:D:301:NAG:HO4	3:D:302:NAG:C5	2.33	0.41
1:C:137:THR:HA	1:C:198:VAL:O	2.20	0.41
2:B:180:SER:O	2:B:192:PRO:HA	2.20	0.41
3:B:301:NAG:O4	3:B:302:NAG:O5	2.31	0.41
3:C:301:NAG:O4	3:C:302:NAG:O5	2.32	0.41
1:C:167:TYR:O	1:C:168:SER:CB	2.68	0.41
1:D:5:LYS:O	1:D:9:GLU:HG2	2.19	0.41
1:E:180:SER:O	1:E:192:PRO:HA	2.20	0.41
1:D:79:PRO:HA	1:D:104:LEU:HD23	2.02	0.41
4:D:1205:L0B:H132	4:D:1205:L0B:H222	1.79	0.41
2:B:167:TYR:O	2:B:168:SER:CB	2.67	0.41
1:E:137:THR:HA	1:E:198:VAL:O	2.20	0.41
1:C:187:CYS:O	1:C:188:LYS:HB2	2.20	0.41
1:A:79:PRO:HA	1:A:104:LEU:HD23	2.02	0.41
3:A:301:NAG:HO4	3:A:302:NAG:C5	2.34	0.41
1:C:52:PHE:HZ	1:C:140:LEU:HD23	1.85	0.41
1:E:14:TYR:OH	1:E:60:ASP:OD2	2.32	0.41
1:E:57:SER:HB2	1:E:112:HIS:HE2	1.86	0.40
1:C:36:LEU:HD11	1:C:53:TRP:HB2	2.03	0.40
1:C:124:SER:CB	5:C:1206:GOL:H31	2.51	0.40
1:D:36:LEU:HD11	1:D:53:TRP:HB2	2.03	0.40
1:A:175:VAL:HG22	1:A:198:VAL:HG13	2.04	0.40
1:C:15:ASN:H	1:D:4:ARG:NH1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/205 (99%)	193 (95%)	6 (3%)	4 (2%)	6	13
1	C	203/205 (99%)	193 (95%)	6 (3%)	4 (2%)	6	13
1	D	203/205 (99%)	193 (95%)	7 (3%)	3 (2%)	8	18
1	E	203/205 (99%)	193 (95%)	6 (3%)	4 (2%)	6	13
2	B	205/207 (99%)	193 (94%)	6 (3%)	6 (3%)	3	8
All	All	1017/1027 (99%)	965 (95%)	31 (3%)	21 (2%)	5	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	ARG
1	D	23	ARG
1	A	23	ARG
2	B	23	ARG
2	B	149	SER
1	D	73	VAL
1	E	12	LYS
1	E	23	ARG
2	B	12	LYS
2	B	71	PRO
1	C	12	LYS
1	C	71	PRO
1	D	71	PRO
1	A	12	LYS
1	A	71	PRO
2	B	189	GLU
1	E	71	PRO
1	A	73	VAL
2	B	73	VAL
1	E	73	VAL
1	C	73	VAL

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	190/190 (100%)	157 (83%)	33 (17%)	2	3
1	C	190/190 (100%)	160 (84%)	30 (16%)	2	4
1	D	190/190 (100%)	158 (83%)	32 (17%)	2	3
1	E	190/190 (100%)	156 (82%)	34 (18%)	2	3
2	B	192/192 (100%)	153 (80%)	39 (20%)	1	2
All	All	952/952 (100%)	784 (82%)	168 (18%)	2	3

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	10	LEU
1	A	11	VAL
1	A	23	ARG
1	A	28	THR
1	A	29	VAL
1	A	33	LEU
1	A	35	LEU
1	A	47	VAL
1	A	48	VAL
1	A	50	VAL
1	A	54	LEU
1	A	56	MET
1	A	66	ASN
1	A	67	VAL
1	A	73	VAL
1	A	80	ILE
1	A	83	LEU
1	A	92	ASN
1	A	99	VAL
1	A	131	ASP
1	A	134	SER
1	A	140	LEU
1	A	154	LEU
1	A	161	ILE
1	A	165	ILE
1	A	168	SER
1	A	179	ARG
1	A	185	GLU
1	A	188	LYS
1	A	189	GLU

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Mol	Chain	Res	Type
1	A	198	VAL
1	A	201	ARG
2	B	4	ARG
2	B	10	LEU
2	B	11	VAL
2	B	23	ARG
2	B	28	THR
2	B	29	VAL
2	B	35	LEU
2	B	47	VAL
2	B	48	VAL
2	B	50	VAL
2	B	52	PHE
2	B	54	LEU
2	B	56	MET
2	B	66	ASN
2	B	67	VAL
2	B	73	VAL
2	B	80	ILE
2	B	83	LEU
2	B	92	ASN
2	B	99	VAL
2	B	108	ASN
2	B	116	LEU
2	B	131	ASP
2	B	134	SER
2	B	140	LEU
2	B	154	LEU
2	B	158	GLU
2	B	161	ILE
2	B	165	ILE
2	B	179	ARG
2	B	182	ARG
2	B	185	GLU
2	B	186	CYS
2	B	187	CYS
2	B	188	LYS
2	B	189	GLU
2	B	198	VAL
2	B	201	ARG
2	B	206	SER
1	C	3	GLN

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Mol	Chain	Res	Type
1	C	11	VAL
1	C	23	ARG
1	C	28	THR
1	C	29	VAL
1	C	33	LEU
1	C	35	LEU
1	C	47	VAL
1	C	48	VAL
1	C	50	VAL
1	C	54	LEU
1	C	66	ASN
1	C	67	VAL
1	C	73	VAL
1	C	80	ILE
1	C	83	LEU
1	C	92	ASN
1	C	99	VAL
1	C	131	ASP
1	C	134	SER
1	C	140	LEU
1	C	154	LEU
1	C	158	GLU
1	C	161	ILE
1	C	165	ILE
1	C	168	SER
1	C	179	ARG
1	C	189	GLU
1	C	198	VAL
1	C	201	ARG
1	D	3	GLN
1	D	8	LYS
1	D	9	GLU
1	D	11	VAL
1	D	23	ARG
1	D	28	THR
1	D	29	VAL
1	D	32	SER
1	D	35	LEU
1	D	47	VAL
1	D	48	VAL
1	D	50	VAL
1	D	54	LEU

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Mol	Chain	Res	Type
1	D	55	GLN
1	D	57	SER
1	D	71	PRO
1	D	80	ILE
1	D	92	ASN
1	D	99	VAL
1	D	108	ASN
1	D	131	ASP
1	D	134	SER
1	D	140	LEU
1	D	154	LEU
1	D	158	GLU
1	D	161	ILE
1	D	165	ILE
1	D	168	SER
1	D	179	ARG
1	D	188	LYS
1	D	198	VAL
1	D	201	ARG
1	E	10	LEU
1	E	11	VAL
1	E	23	ARG
1	E	28	THR
1	E	29	VAL
1	E	32	SER
1	E	33	LEU
1	E	35	LEU
1	E	47	VAL
1	E	48	VAL
1	E	50	VAL
1	E	54	LEU
1	E	56	MET
1	E	66	ASN
1	E	67	VAL
1	E	73	VAL
1	E	80	ILE
1	E	83	LEU
1	E	92	ASN
1	E	99	VAL
1	E	131	ASP
1	E	134	SER
1	E	140	LEU

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Mol	Chain	Res	Type
1	E	149	SER
1	E	150	ARG
1	E	154	LEU
1	E	158	GLU
1	E	161	ILE
1	E	165	ILE
1	E	168	SER
1	E	179	ARG
1	E	188	LYS
1	E	198	VAL
1	E	201	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	45	ASN
1	A	61	HIS
1	A	114	GLN
1	A	157	GLN
2	B	46	GLN
2	B	61	HIS
2	B	177	GLN
1	C	3	GLN
1	C	46	GLN
1	C	61	HIS
1	C	147	HIS
1	D	46	GLN
1	D	55	GLN
1	E	3	GLN
1	E	108	ASN
1	E	155	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	E	301	-	14,14,15	1.28	3 (21%)	17,19,21	1.62	3 (17%)
4	L0B	D	1205	-	27,27,27	0.78	0	33,36,36	1.59	8 (24%)
5	GOL	E	1206	-	5,5,5	1.12	1 (20%)	5,5,5	2.88	2 (40%)
4	L0B	A	1205	-	27,27,27	0.92	0	33,36,36	1.12	3 (9%)
6	9Z0	B	1208	-	14,14,14	2.23	4 (28%)	18,18,18	2.02	7 (38%)
3	NAG	E	302	-	14,14,15	1.62	4 (28%)	17,19,21	1.99	5 (29%)
6	9Z0	E	1207	-	14,14,14	2.09	3 (21%)	18,18,18	1.76	5 (27%)
3	NAG	B	301	-	14,14,15	1.29	2 (14%)	17,19,21	1.60	6 (35%)
3	NAG	B	302	-	14,14,15	1.74	6 (42%)	17,19,21	2.10	4 (23%)
5	GOL	D	1206	-	5,5,5	1.04	0	5,5,5	2.31	1 (20%)
6	9Z0	C	1207	-	14,14,14	2.20	3 (21%)	18,18,18	1.69	6 (33%)
4	L0B	E	1205	-	27,27,27	0.64	0	33,36,36	1.06	4 (12%)
3	NAG	A	302	-	14,14,15	1.58	4 (28%)	17,19,21	1.95	4 (23%)
5	GOL	A	1206	-	5,5,5	0.94	0	5,5,5	1.43	1 (20%)
3	NAG	C	302	-	14,14,15	1.63	4 (28%)	17,19,21	2.02	4 (23%)
3	NAG	D	302	-	14,14,15	1.57	3 (21%)	17,19,21	1.96	4 (23%)
4	L0B	C	1205	-	27,27,27	0.81	1 (3%)	33,36,36	1.49	3 (9%)
3	NAG	A	301	-	14,14,15	1.35	3 (21%)	17,19,21	1.74	6 (35%)
6	9Z0	D	1207	-	14,14,14	2.33	3 (21%)	18,18,18	1.77	5 (27%)
4	L0B	B	1207	-	27,27,27	0.77	0	33,36,36	1.27	6 (18%)
5	GOL	C	1206	-	5,5,5	1.54	1 (20%)	5,5,5	2.79	3 (60%)
3	NAG	C	301	-	14,14,15	1.40	3 (21%)	17,19,21	1.72	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	9Z0	A	1207	-	14,14,14	2.26	3 (21%)	18,18,18	1.81	6 (33%)
3	NAG	D	301	-	14,14,15	1.30	2 (14%)	17,19,21	2.24	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	301	-	-	0/6/23/26	0/1/1/1
4	L0B	D	1205	-	-	0/16/30/30	0/3/3/3
5	GOL	E	1206	-	-	2/4/4/4	-
4	L0B	A	1205	-	-	1/16/30/30	0/3/3/3
6	9Z0	B	1208	-	-	1/9/9/9	0/1/1/1
3	NAG	E	302	-	-	3/6/23/26	0/1/1/1
6	9Z0	E	1207	-	-	1/9/9/9	0/1/1/1
3	NAG	B	301	-	-	0/6/23/26	0/1/1/1
3	NAG	B	302	-	-	2/6/23/26	0/1/1/1
5	GOL	D	1206	-	-	2/4/4/4	-
6	9Z0	C	1207	-	-	1/9/9/9	0/1/1/1
4	L0B	E	1205	-	-	0/16/30/30	0/3/3/3
3	NAG	A	302	-	-	2/6/23/26	0/1/1/1
5	GOL	A	1206	-	-	4/4/4/4	-
3	NAG	C	302	-	-	2/6/23/26	0/1/1/1
3	NAG	D	302	-	-	2/6/23/26	0/1/1/1
4	L0B	C	1205	-	-	2/16/30/30	0/3/3/3
3	NAG	A	301	-	-	0/6/23/26	0/1/1/1
6	9Z0	D	1207	-	-	1/9/9/9	0/1/1/1
4	L0B	B	1207	-	-	2/16/30/30	0/3/3/3
5	GOL	C	1206	-	-	3/4/4/4	-
3	NAG	C	301	-	-	0/6/23/26	0/1/1/1
6	9Z0	A	1207	-	-	1/9/9/9	0/1/1/1
3	NAG	D	301	-	-	0/6/23/26	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1208	9Z0	C02-N03	6.48	1.44	1.33
6	A	1207	9Z0	C02-N03	6.34	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1207	9Z0	C02-N03	6.07	1.43	1.33
6	C	1207	9Z0	C02-N03	6.05	1.43	1.33
6	D	1207	9Z0	C02-N03	5.99	1.43	1.33
6	D	1207	9Z0	BR2-C12	4.87	1.96	1.86
6	C	1207	9Z0	BR2-C12	4.64	1.96	1.86
6	A	1207	9Z0	BR2-C12	4.46	1.95	1.86
6	E	1207	9Z0	BR2-C12	3.86	1.94	1.86
6	B	1208	9Z0	BR2-C12	3.66	1.94	1.86
6	D	1207	9Z0	BR1-C10	3.01	1.95	1.88
3	C	302	NAG	C1-C2	2.98	1.56	1.52
3	E	302	NAG	C1-C2	2.90	1.56	1.52
3	B	302	NAG	C1-C2	2.82	1.56	1.52
3	D	302	NAG	C1-C2	2.77	1.56	1.52
3	A	302	NAG	C1-C2	2.73	1.56	1.52
3	B	302	NAG	C4-C3	2.65	1.59	1.52
3	E	301	NAG	C1-C2	2.63	1.55	1.52
3	C	301	NAG	C4-C3	2.61	1.59	1.52
3	C	301	NAG	C3-C2	2.61	1.58	1.52
3	C	302	NAG	C3-C2	2.61	1.58	1.52
3	A	302	NAG	C3-C2	2.60	1.58	1.52
5	C	1206	GOL	O2-C2	-2.58	1.35	1.43
6	A	1207	9Z0	BR1-C10	2.57	1.94	1.88
3	D	302	NAG	C3-C2	2.57	1.57	1.52
3	B	301	NAG	C4-C3	2.56	1.59	1.52
3	E	302	NAG	C4-C5	2.56	1.58	1.53
3	B	301	NAG	C3-C2	2.55	1.57	1.52
3	A	301	NAG	C3-C2	2.49	1.57	1.52
3	B	302	NAG	O5-C5	2.42	1.48	1.43
3	A	301	NAG	C4-C5	2.40	1.58	1.53
3	D	301	NAG	C4-C3	2.40	1.58	1.52
3	E	301	NAG	C3-C2	2.38	1.57	1.52
6	B	1208	9Z0	BR1-C10	2.29	1.93	1.88
3	B	302	NAG	C3-C2	2.28	1.57	1.52
6	B	1208	9Z0	C08-N14	-2.27	1.33	1.37
3	E	301	NAG	C4-C3	2.26	1.58	1.52
6	C	1207	9Z0	BR1-C10	2.24	1.93	1.88
3	D	301	NAG	C4-C5	2.22	1.57	1.53
3	E	302	NAG	C4-C3	2.20	1.58	1.52
3	C	301	NAG	O5-C1	-2.19	1.40	1.43
3	A	302	NAG	C4-C3	2.19	1.58	1.52
3	B	302	NAG	O3-C3	2.15	1.48	1.43
3	C	302	NAG	C4-C5	2.14	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	NAG	C4-C5	2.10	1.57	1.53
3	C	302	NAG	C4-C3	2.09	1.57	1.52
3	E	302	NAG	C3-C2	2.09	1.56	1.52
3	A	302	NAG	C4-C5	2.07	1.57	1.53
3	A	301	NAG	C4-C3	2.05	1.57	1.52
5	E	1206	GOL	C1-C2	-2.04	1.44	1.51
3	D	302	NAG	C4-C3	2.02	1.57	1.52
6	E	1207	9Z0	BR1-C10	2.02	1.93	1.88
4	C	1205	L0B	C17-C16	-2.01	1.48	1.51

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	NAG	C1-O5-C5	6.32	120.65	112.19
3	D	302	NAG	C1-O5-C5	5.91	120.10	112.19
3	E	302	NAG	C1-O5-C5	5.78	119.94	112.19
5	E	1206	GOL	C3-C2-C1	-5.68	90.95	111.80
3	A	302	NAG	C1-O5-C5	5.67	119.78	112.19
3	C	302	NAG	C1-O5-C5	5.55	119.62	112.19
4	C	1205	L0B	C22-N1-C9	-5.38	108.80	113.16
4	D	1205	L0B	C12-C9-C8	-5.33	106.19	112.77
3	D	301	NAG	C1-O5-C5	-4.60	106.03	112.19
5	D	1206	GOL	C3-C2-C1	-4.59	94.97	111.80
3	C	301	NAG	C1-C2-N2	-4.53	103.29	110.43
5	C	1206	GOL	O1-C1-C2	-4.32	90.91	110.38
3	E	301	NAG	C1-C2-N2	-4.30	103.66	110.43
3	D	301	NAG	C8-C7-N2	-4.14	109.26	116.12
6	A	1207	9Z0	C05-C04-N03	3.85	123.00	112.20
3	D	301	NAG	C1-C2-N2	-3.82	104.41	110.43
4	A	1205	L0B	C22-N1-C11	-3.80	110.08	113.16
4	C	1205	L0B	C12-C9-C8	-3.71	108.19	112.77
3	C	302	NAG	C1-C2-N2	3.67	116.22	110.43
6	E	1207	9Z0	C04-C05-C06	3.64	118.47	112.95
4	B	1207	L0B	C22-N1-C11	-3.61	110.24	113.16
6	B	1208	9Z0	C04-C05-C06	3.59	118.40	112.95
3	A	301	NAG	C1-O5-C5	-3.58	107.39	112.19
6	A	1207	9Z0	C04-C05-C06	3.55	118.33	112.95
6	D	1207	9Z0	C04-C05-C06	3.54	118.32	112.95
6	D	1207	9Z0	C05-C04-N03	3.48	121.97	112.20
5	C	1206	GOL	O2-C2-C1	-3.39	95.13	109.18
3	B	302	NAG	C1-C2-N2	3.38	115.76	110.43
3	D	302	NAG	C1-C2-N2	3.37	115.74	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1208	9Z0	C08-C02-N03	3.33	121.38	116.80
3	A	302	NAG	C1-C2-N2	3.31	115.66	110.43
3	E	302	NAG	C1-C2-N2	3.22	115.50	110.43
4	D	1205	L0B	C22-N1-C11	-3.15	110.61	113.16
6	C	1207	9Z0	C05-C04-N03	3.09	120.85	112.20
3	B	301	NAG	C1-O5-C5	-3.07	108.08	112.19
6	E	1207	9Z0	BR2-C12-N14	3.05	127.74	122.21
6	B	1208	9Z0	O01-C02-C08	-3.01	117.21	121.09
6	A	1207	9Z0	BR2-C12-N14	2.96	127.59	122.21
6	C	1207	9Z0	BR2-C12-N14	2.94	127.55	122.21
5	C	1206	GOL	C3-C2-C1	-2.90	101.15	111.80
6	B	1208	9Z0	BR2-C12-C10	-2.84	123.56	128.91
6	C	1207	9Z0	C08-C02-N03	2.83	120.70	116.80
3	B	302	NAG	O4-C4-C5	2.81	116.23	109.32
3	C	302	NAG	C4-C3-C2	2.77	115.08	111.02
4	A	1205	L0B	C12-C9-C8	-2.70	109.44	112.77
5	E	1206	GOL	O1-C1-C2	-2.66	98.40	110.38
4	E	1205	L0B	C14-C11-C13	-2.66	108.34	112.94
4	B	1207	L0B	C22-N1-C9	-2.65	111.01	113.16
6	B	1208	9Z0	BR2-C12-N14	2.62	126.96	122.21
3	E	301	NAG	C1-O5-C5	-2.62	108.68	112.19
3	C	301	NAG	O3-C3-C4	2.61	116.53	110.38
4	B	1207	L0B	C14-C11-C13	-2.61	108.42	112.94
6	B	1208	9Z0	C05-C04-N03	2.61	119.52	112.20
3	C	302	NAG	C8-C7-N2	-2.60	111.81	116.12
3	B	302	NAG	C4-C3-C2	2.60	114.83	111.02
4	E	1205	L0B	C22-N1-C9	-2.59	111.06	113.16
3	A	301	NAG	C4-C3-C2	-2.55	107.28	111.02
6	E	1207	9Z0	C08-C02-N03	2.55	120.31	116.80
4	D	1205	L0B	O2-C16-C14	2.53	114.08	108.69
6	A	1207	9Z0	C09-C08-C02	-2.52	123.49	132.80
3	D	302	NAG	C4-C3-C2	2.50	114.69	111.02
3	A	302	NAG	C4-C3-C2	2.46	114.62	111.02
5	A	1206	GOL	C3-C2-C1	-2.44	102.84	111.80
4	B	1207	L0B	C9-C8-C3	2.43	116.98	112.92
3	D	301	NAG	C4-C3-C2	-2.43	107.45	111.02
3	A	301	NAG	O4-C4-C3	2.43	116.10	110.38
3	C	301	NAG	C4-C3-C2	-2.40	107.50	111.02
6	B	1208	9Z0	C09-C08-C02	-2.40	123.96	132.80
3	A	302	NAG	C8-C7-N2	-2.38	112.17	116.12
3	E	302	NAG	O4-C4-C5	2.37	115.17	109.32
6	A	1207	9Z0	BR2-C12-C10	-2.35	124.49	128.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1205	L0B	C14-C16-C17	-2.35	106.64	111.63
3	A	301	NAG	C1-C2-N2	-2.34	106.75	110.43
4	D	1205	L0B	C8-C3-C1	-2.31	116.24	118.73
6	E	1207	9Z0	BR2-C12-C10	-2.27	124.63	128.91
6	E	1207	9Z0	C05-C04-N03	2.26	118.54	112.20
4	B	1207	L0B	C12-C9-C8	-2.25	109.99	112.77
4	D	1205	L0B	O1-C3-C8	2.25	123.38	120.70
3	E	302	NAG	O7-C7-N2	2.25	125.95	121.98
3	B	301	NAG	O3-C3-C4	2.24	115.66	110.38
3	C	301	NAG	C1-O5-C5	-2.22	109.21	112.19
4	A	1205	L0B	C14-C11-C13	-2.20	109.14	112.94
4	D	1205	L0B	C15-C12-C9	2.19	114.98	110.81
3	A	301	NAG	C2-N2-C7	2.17	125.81	122.90
6	C	1207	9Z0	O01-C02-N03	-2.17	119.44	123.35
3	B	301	NAG	C4-C3-C2	-2.17	107.84	111.02
4	E	1205	L0B	C12-C9-C8	-2.15	110.12	112.77
3	D	302	NAG	C2-N2-C7	2.14	125.77	122.90
4	B	1207	L0B	C8-C3-C1	-2.14	116.42	118.73
6	D	1207	9Z0	C09-C08-C02	-2.11	125.00	132.80
3	E	301	NAG	O3-C3-C4	2.09	115.31	110.38
4	D	1205	L0B	C14-C16-C17	-2.08	107.20	111.63
4	D	1205	L0B	C14-C11-C13	-2.08	109.34	112.94
6	D	1207	9Z0	C02-C08-N14	2.07	128.20	120.53
3	B	301	NAG	C8-C7-N2	-2.07	112.69	116.12
4	E	1205	L0B	O1-C3-C8	2.07	123.16	120.70
6	C	1207	9Z0	C04-C05-C06	2.06	116.08	112.95
3	B	301	NAG	O4-C4-C3	2.05	115.20	110.38
3	E	302	NAG	C8-C7-N2	-2.04	112.74	116.12
3	B	301	NAG	C2-N2-C7	2.01	125.60	122.90
6	C	1207	9Z0	BR2-C12-C10	-2.01	125.13	128.91
6	D	1207	9Z0	BR1-C10-C12	2.01	129.92	126.29
3	A	301	NAG	O5-C1-C2	-2.01	108.18	111.29
6	A	1207	9Z0	C02-C08-N14	2.01	127.95	120.53

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1207	L0B	C3-C8-C9-N1
4	C	1205	L0B	C11-C14-C16-O2
5	A	1206	GOL	C1-C2-C3-O3
5	A	1206	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	1206	GOL	O1-C1-C2-C3
5	D	1206	GOL	C1-C2-C3-O3
5	E	1206	GOL	C1-C2-C3-O3
5	E	1206	GOL	O2-C2-C3-O3
6	C	1207	9Z0	N03-C04-C05-C06
6	D	1207	9Z0	C04-C05-C06-O07
6	E	1207	9Z0	N03-C04-C05-C06
6	B	1208	9Z0	C04-C05-C06-O07
3	D	302	NAG	C4-C5-C6-O6
3	A	302	NAG	C4-C5-C6-O6
3	B	302	NAG	C4-C5-C6-O6
5	D	1206	GOL	O2-C2-C3-O3
3	C	302	NAG	C4-C5-C6-O6
3	C	302	NAG	O5-C5-C6-O6
3	D	302	NAG	O5-C5-C6-O6
3	E	302	NAG	C4-C5-C6-O6
3	B	302	NAG	O5-C5-C6-O6
3	A	302	NAG	O5-C5-C6-O6
3	E	302	NAG	O5-C5-C6-O6
5	A	1206	GOL	O1-C1-C2-C3
5	C	1206	GOL	O1-C1-C2-O2
6	A	1207	9Z0	C04-C05-C06-O07
5	C	1206	GOL	C1-C2-C3-O3
4	A	1205	L0B	N1-C11-C14-C16
4	C	1205	L0B	C3-C8-C9-C12
5	A	1206	GOL	O1-C1-C2-O2
3	E	302	NAG	C1-C2-N2-C7
4	B	1207	L0B	C3-C8-C9-C12

There are no ring outliers.

20 monomers are involved in 45 short contacts:

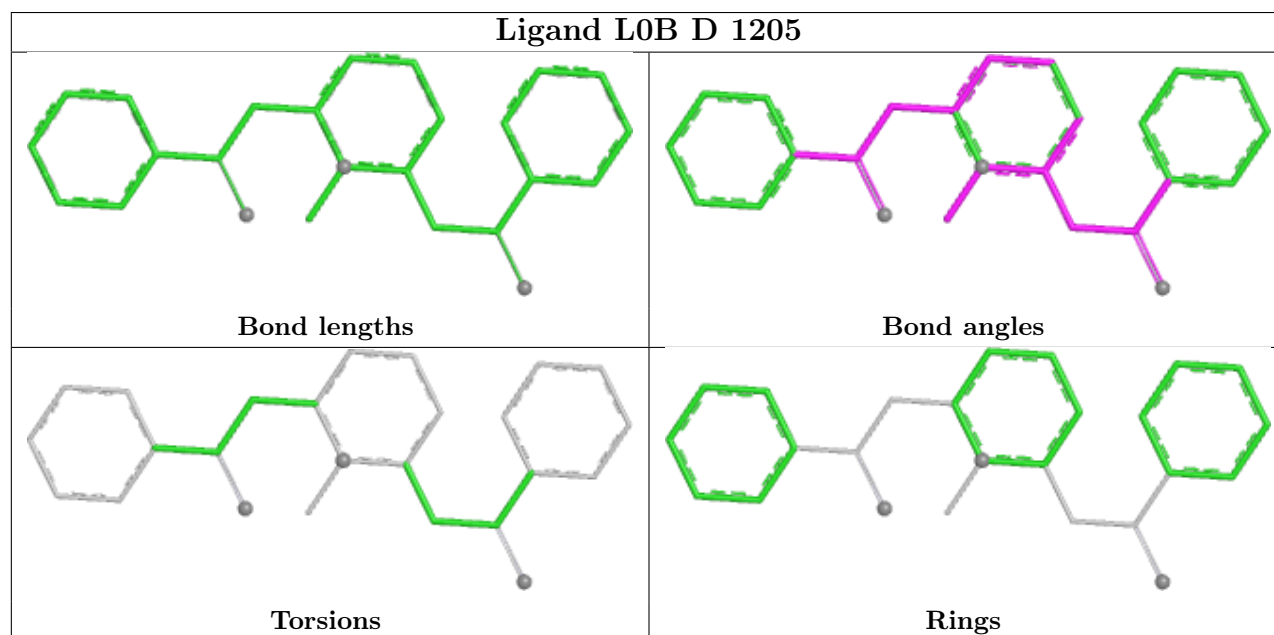
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	301	NAG	6	0
4	D	1205	L0B	4	0
5	E	1206	GOL	1	0
6	B	1208	9Z0	3	0
3	E	302	NAG	3	0
3	B	301	NAG	3	0
3	B	302	NAG	2	0
5	D	1206	GOL	3	0
3	A	302	NAG	2	0

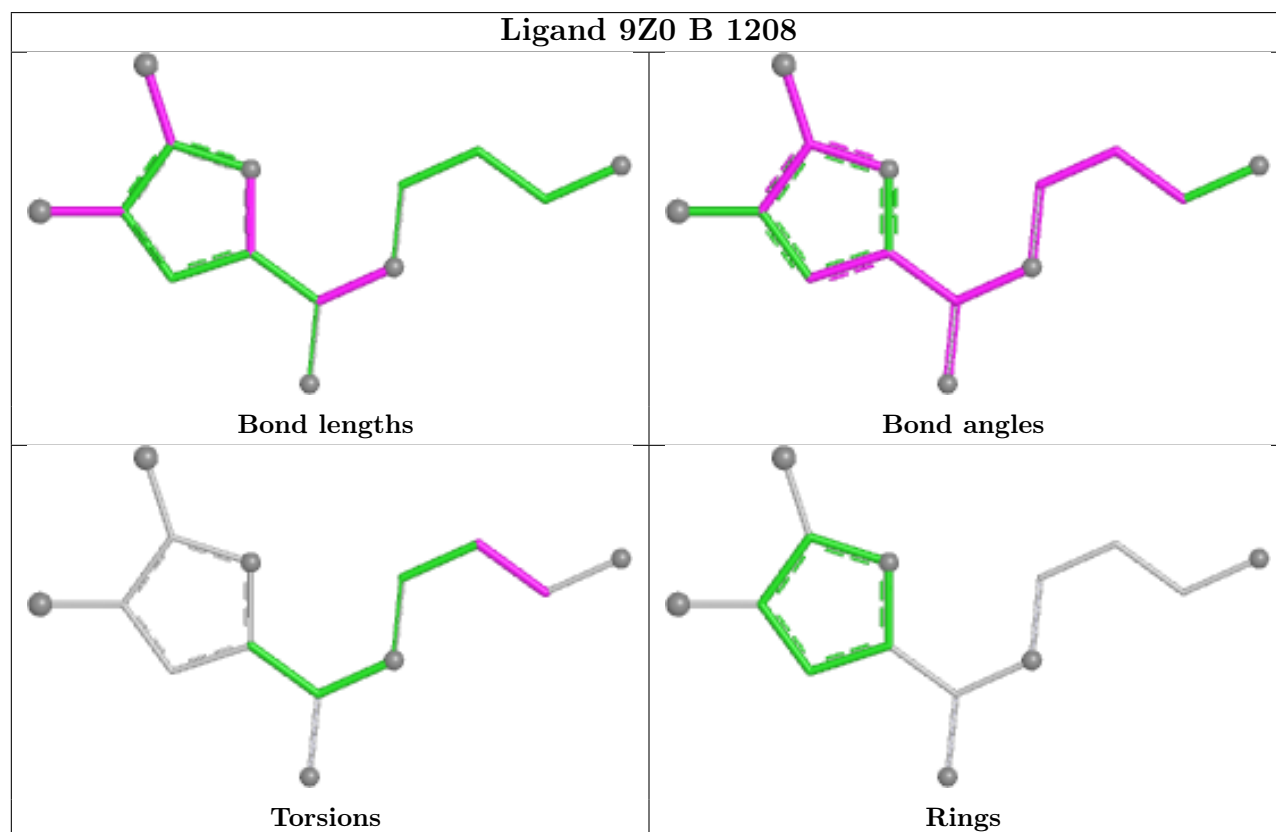
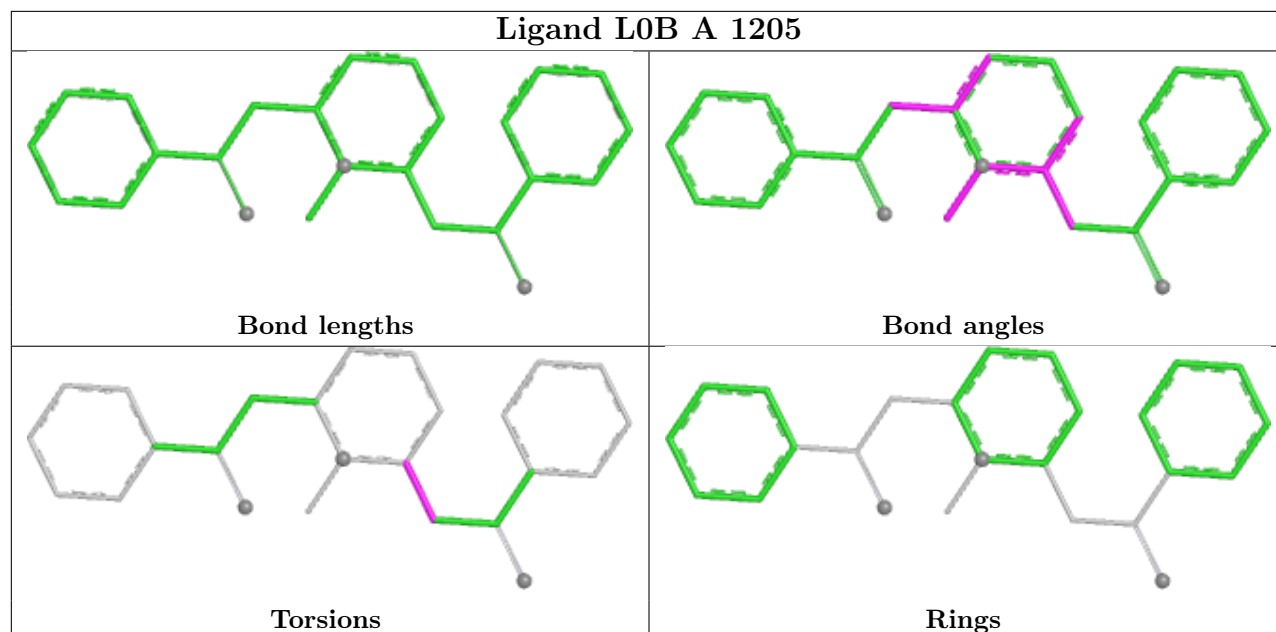
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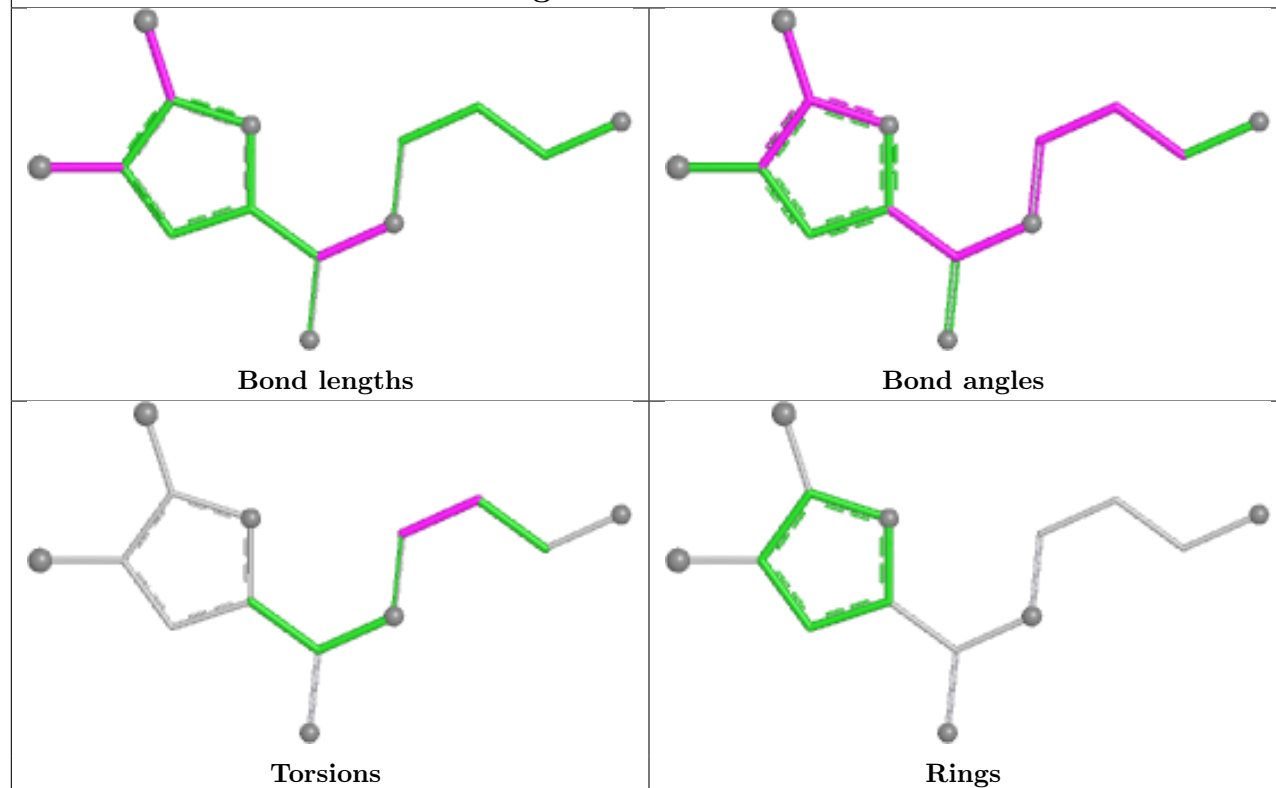
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1206	GOL	2	0
3	C	302	NAG	2	0
3	D	302	NAG	3	0
4	C	1205	L0B	4	0
3	A	301	NAG	4	0
6	D	1207	9Z0	1	0
4	B	1207	L0B	1	0
5	C	1206	GOL	4	0
3	C	301	NAG	2	0
6	A	1207	9Z0	1	0
3	D	301	NAG	6	0

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.

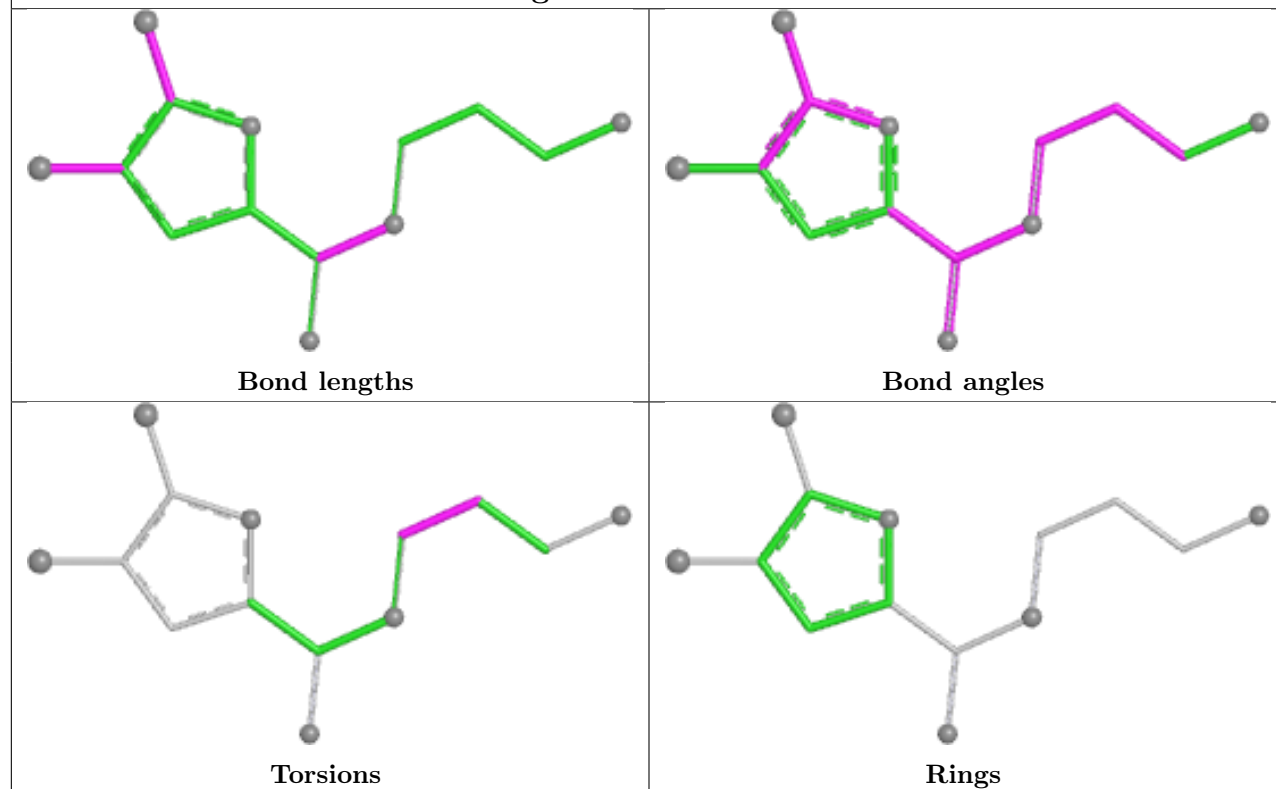


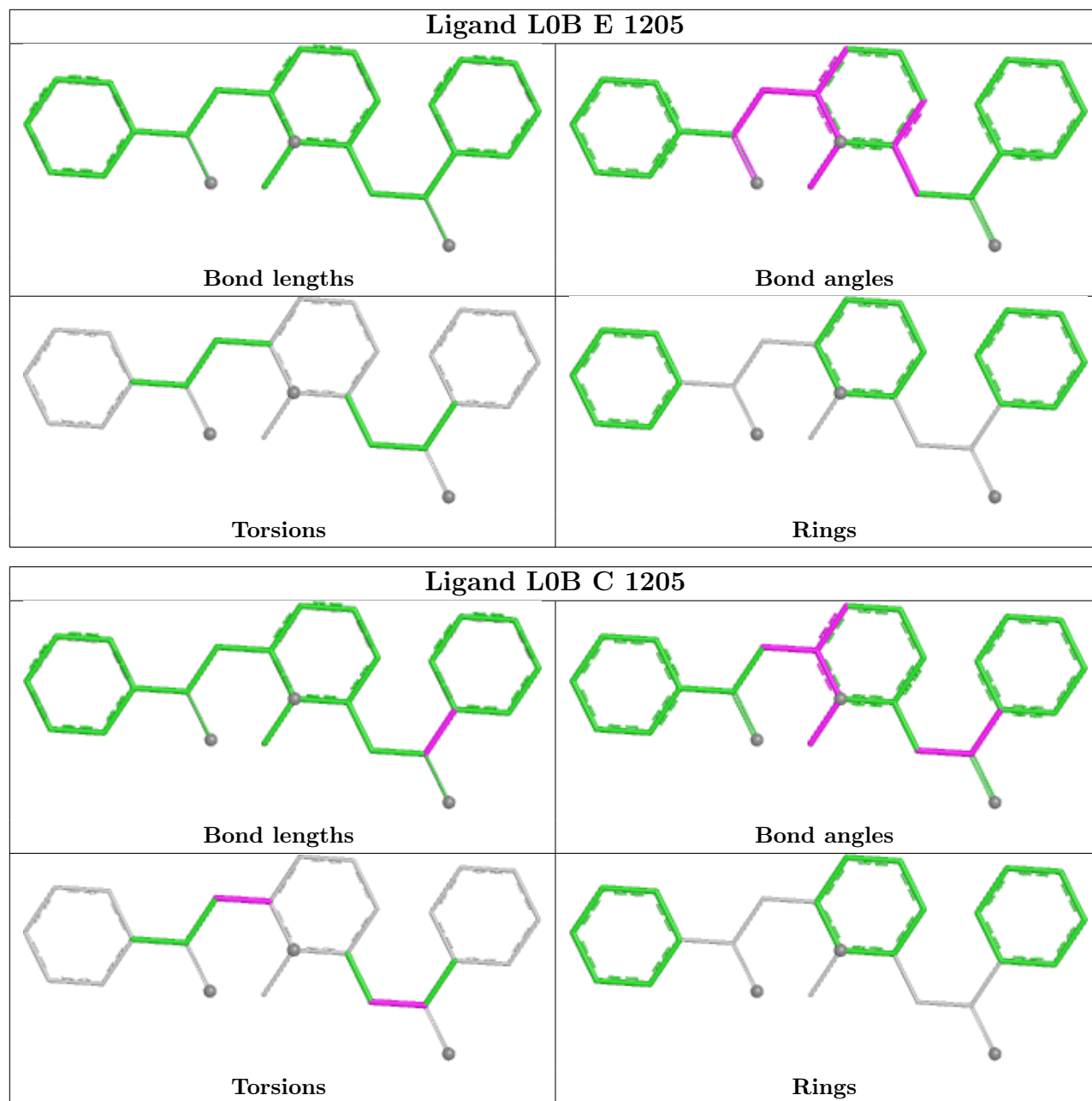


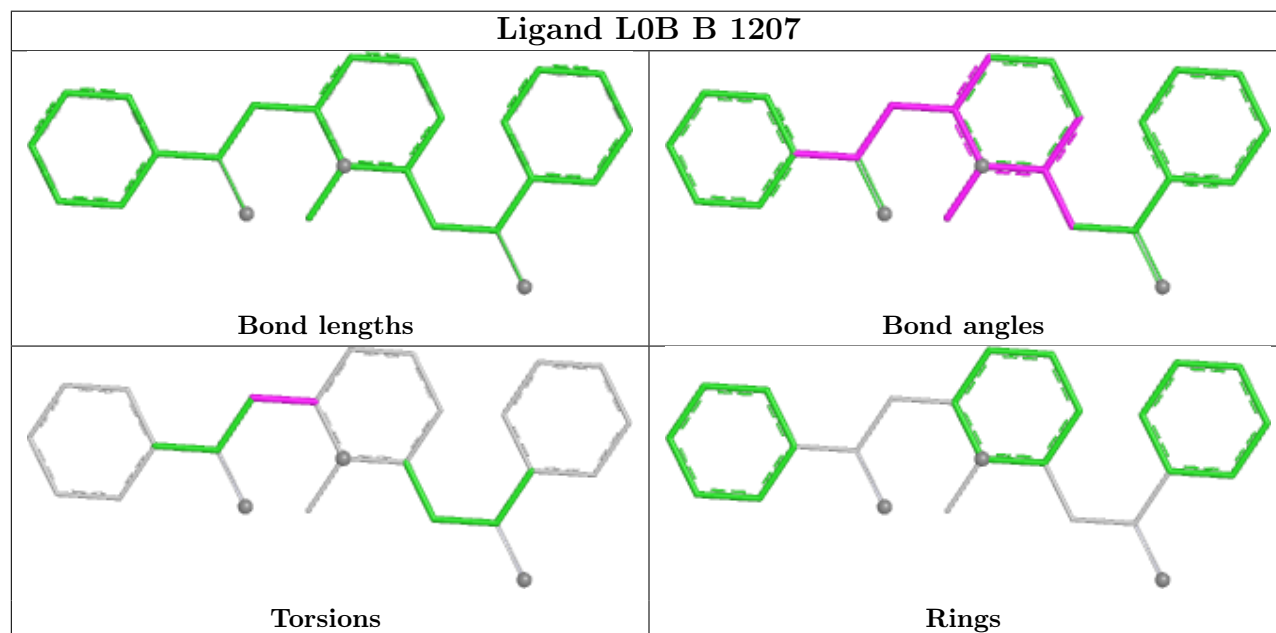
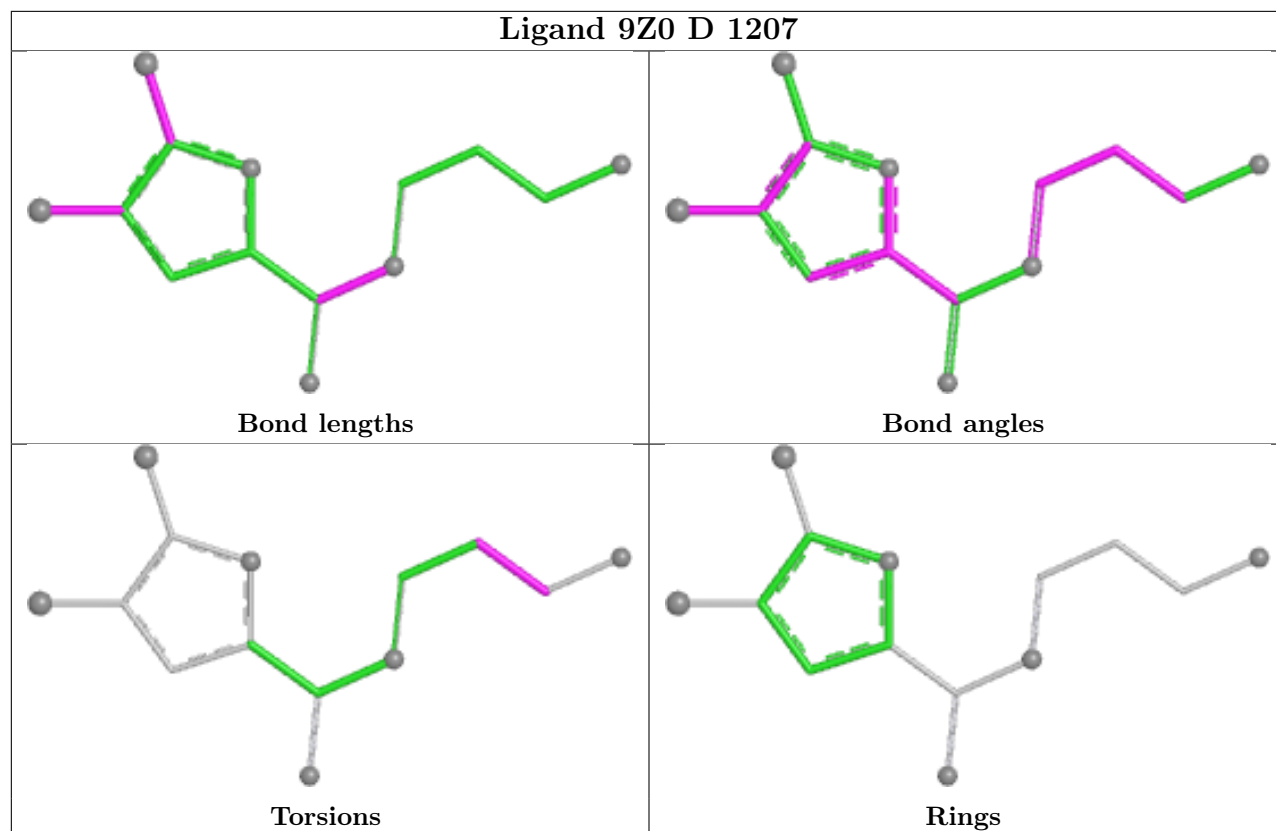
Ligand 9Z0 E 1207

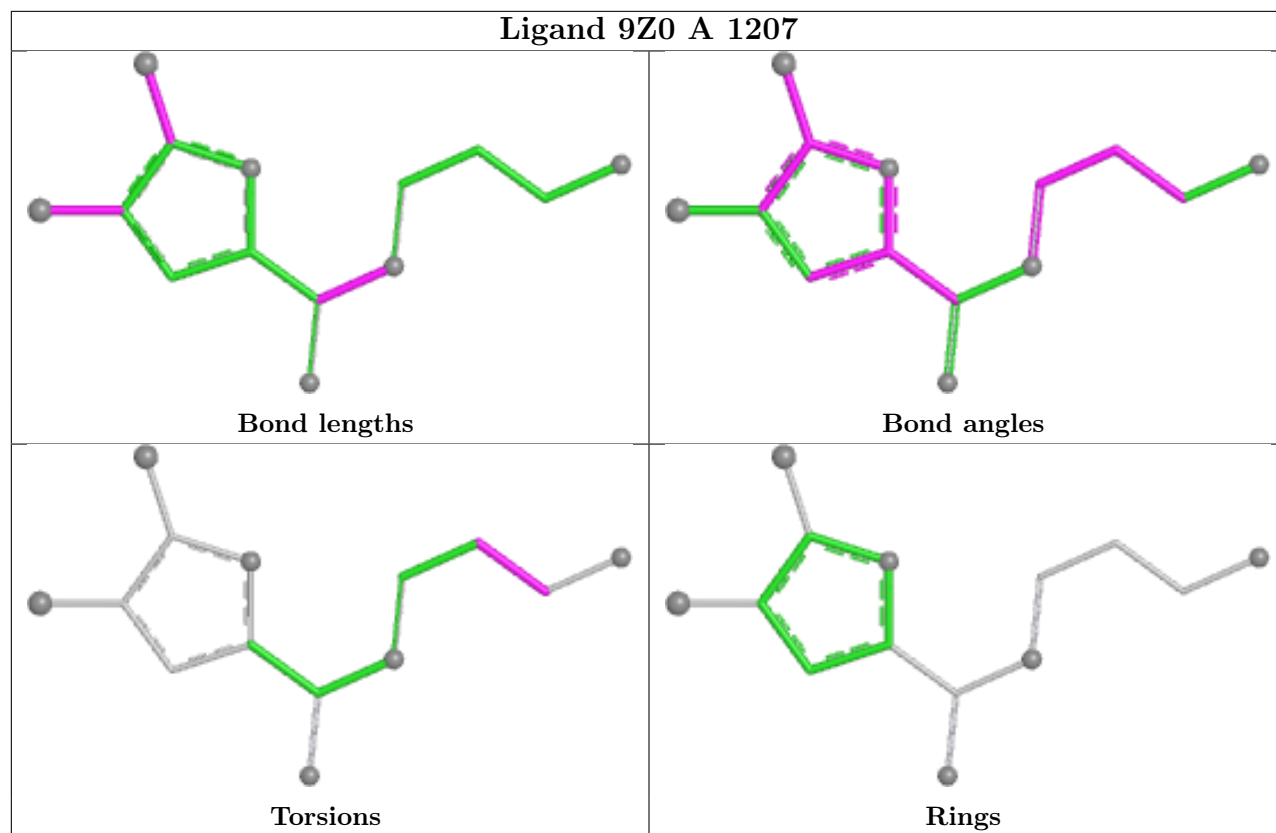


Ligand 9Z0 C 1207









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	205/205 (100%)	-0.39	1 (0%) 87 85	47, 78, 136, 155	0
1	C	205/205 (100%)	-0.42	2 (0%) 79 74	51, 79, 138, 160	0
1	D	205/205 (100%)	-0.46	3 (1%) 72 65	45, 70, 110, 158	0
1	E	205/205 (100%)	-0.45	1 (0%) 87 85	45, 72, 120, 137	0
2	B	207/207 (100%)	-0.25	0 100 100	56, 96, 142, 187	0
All	All	1027/1027 (100%)	-0.39	7 (0%) 84 80	45, 79, 136, 187	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	GLY	2.7
1	C	161	ILE	2.5
1	E	10	LEU	2.4
1	D	0	GLY	2.3
1	D	52	PHE	2.2
1	D	10	LEU	2.2
1	A	10	LEU	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 ⓘ

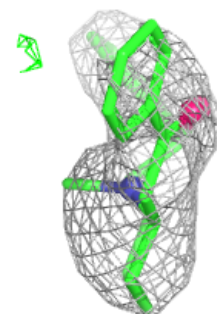
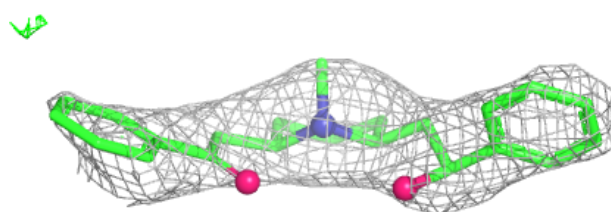
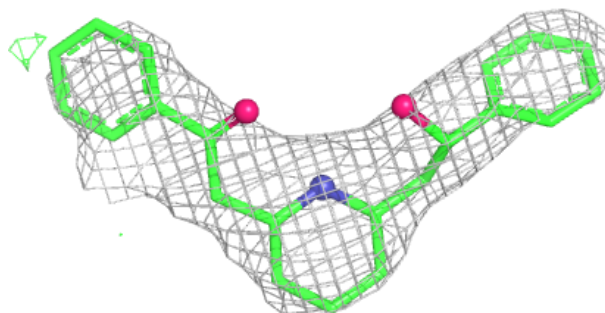
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	302	14/15	0.56	0.12	123,132,143,144	0
3	NAG	C	302	14/15	0.68	0.14	157,168,177,181	0
3	NAG	D	302	14/15	0.77	0.11	154,158,167,168	0
3	NAG	A	302	14/15	0.78	0.10	141,149,156,159	0
3	NAG	B	301	14/15	0.83	0.10	117,126,132,134	0
3	NAG	E	302	14/15	0.85	0.10	116,124,135,136	0
3	NAG	C	301	14/15	0.87	0.08	100,106,117,117	0
3	NAG	E	301	14/15	0.89	0.08	84,91,97,98	0
3	NAG	D	301	14/15	0.90	0.08	86,92,96,98	0
3	NAG	A	301	14/15	0.91	0.06	91,97,106,107	0
4	L0B	A	1205	25/25	0.91	0.13	57,74,295,300	0
5	GOL	C	1206	6/6	0.91	0.14	66,67,68,70	0
5	GOL	D	1206	6/6	0.92	0.14	72,73,74,77	0
6	9Z0	B	1208	14/14	0.92	0.16	25,86,240,251	2
5	GOL	E	1206	6/6	0.93	0.13	65,67,69,73	0
4	L0B	B	1207	25/25	0.93	0.13	45,86,171,300	0
4	L0B	E	1205	25/25	0.94	0.12	36,75,167,260	0
5	GOL	A	1206	6/6	0.94	0.13	99,100,101,101	0
6	9Z0	C	1207	14/14	0.94	0.11	47,61,104,126	2
6	9Z0	D	1207	14/14	0.94	0.13	27,67,202,297	2
4	L0B	D	1205	25/25	0.95	0.09	27,60,97,136	0
4	L0B	C	1205	25/25	0.95	0.10	40,78,115,189	0
6	9Z0	A	1207	14/14	0.95	0.11	34,65,190,236	2
6	9Z0	E	1207	14/14	0.96	0.11	23,46,148,205	2

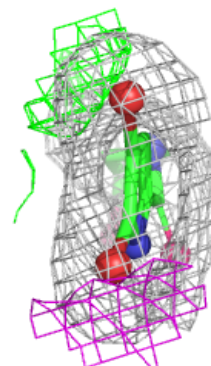
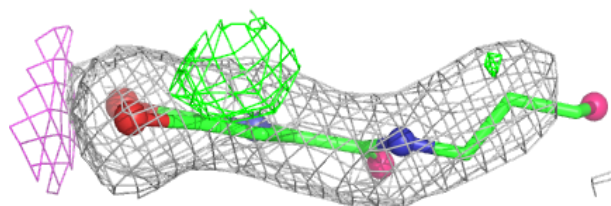
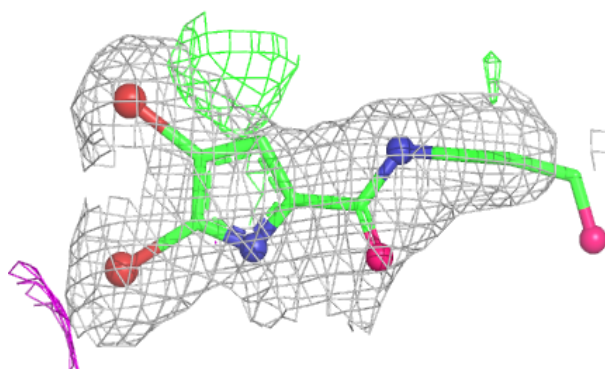
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L0B 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)

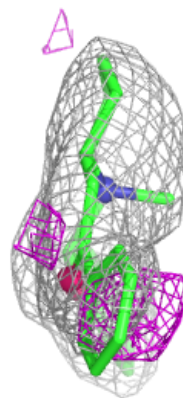
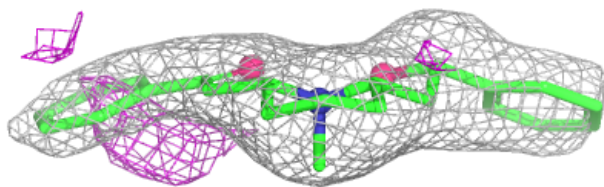
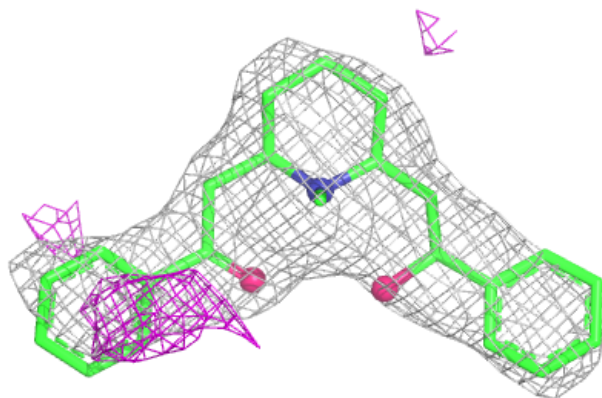
**Electron density around 9Z0 B 1208:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

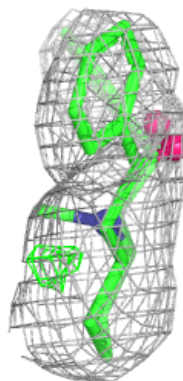
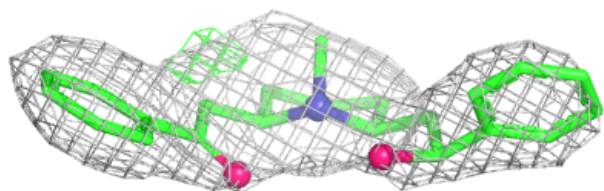
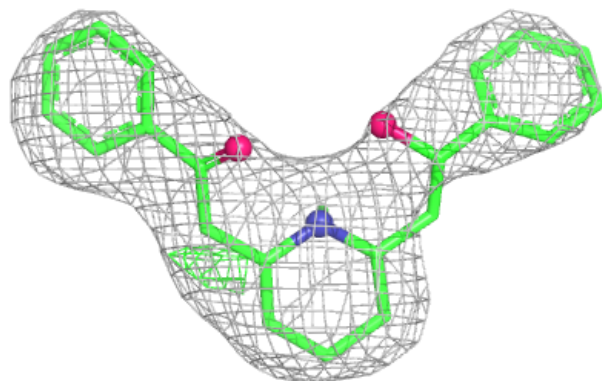


Electron density around L0B B 1207:

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

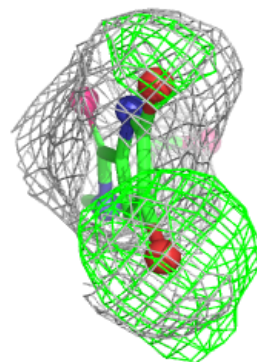
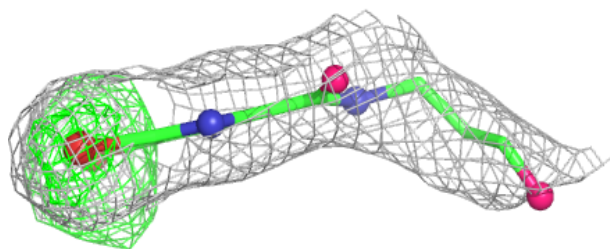
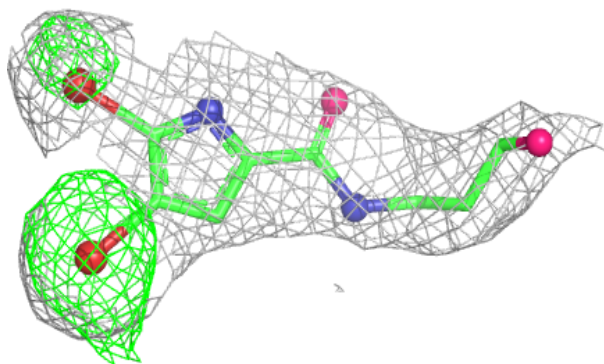
**Electron density around L0B E 1205:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

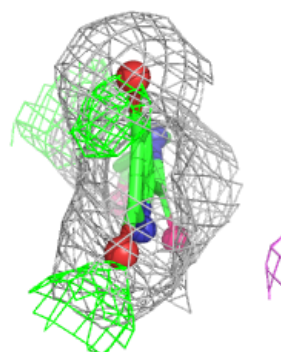
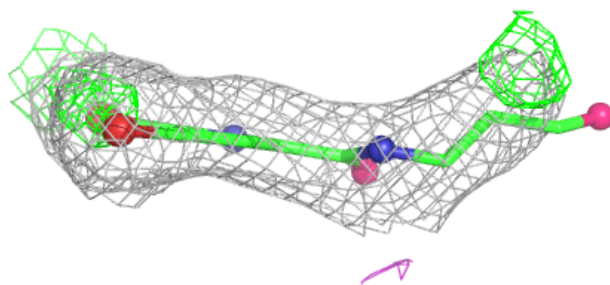
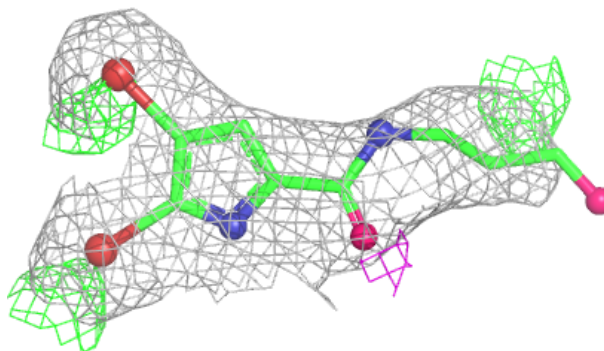


Electron density around 9Z0 C 1207:

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

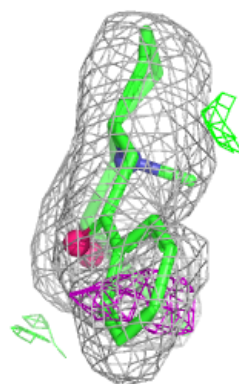
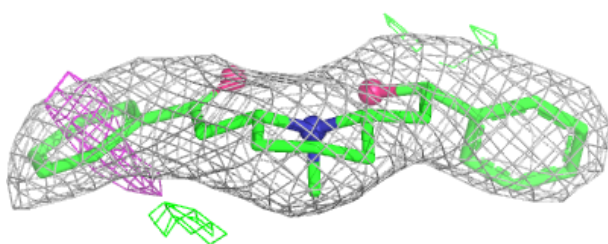
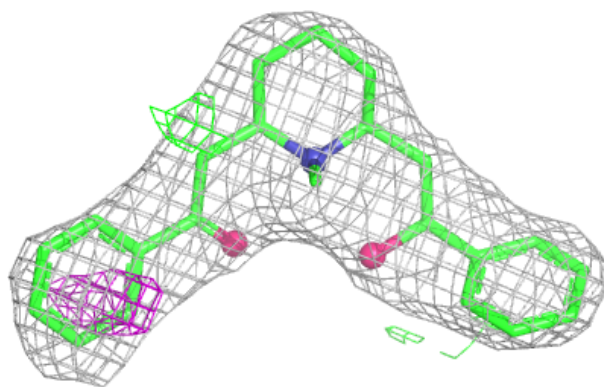
**Electron density around 9Z0 D 1207:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

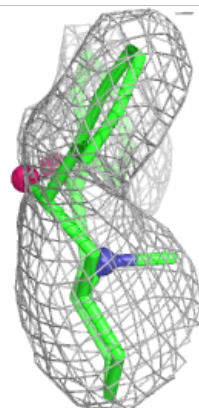
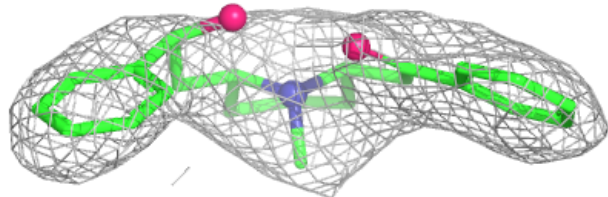
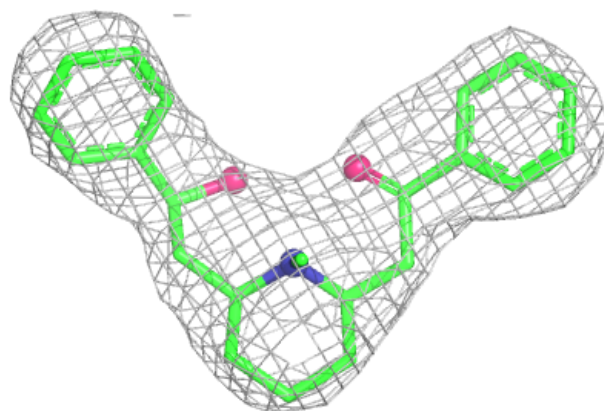


Electron density around L0B D 1205:

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

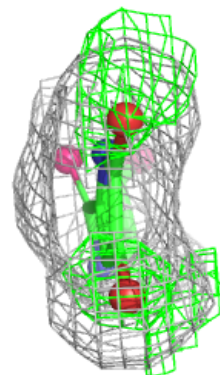
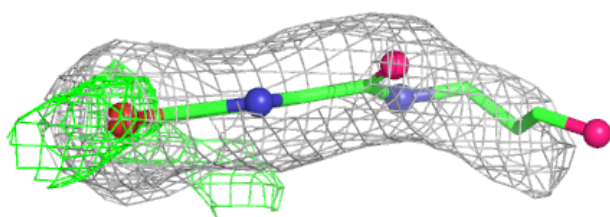
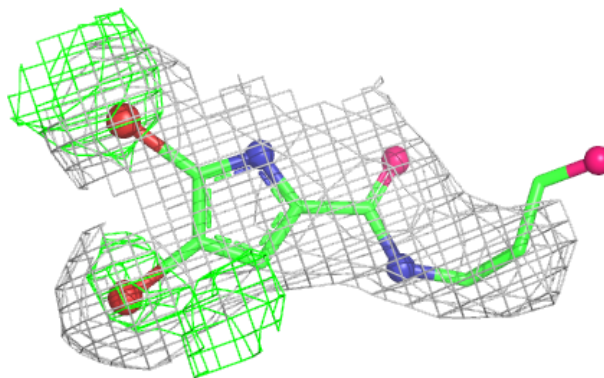
**Electron density around L0B C 1205:**

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

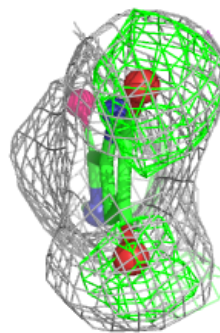
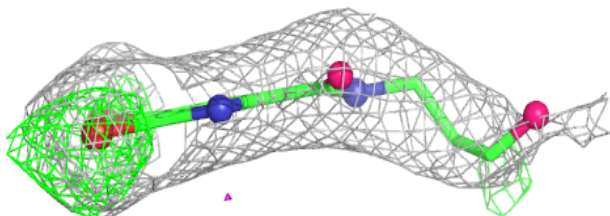
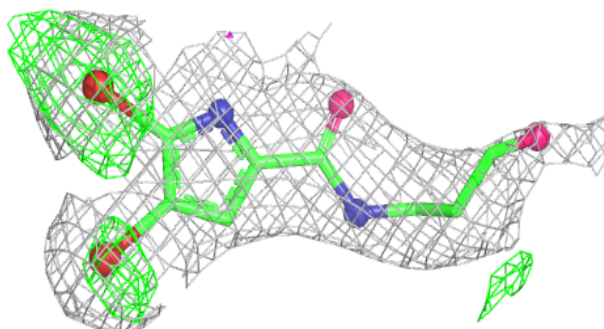


Electron density around 9Z0 A 1207:

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

**Electron density around 9Z0 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](#)

There are no such residues in this entry.