



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:24 PM UTC

PDB ID : 3K5C / pdb_00003k5c
Title : Human BACE-1 complex with NB-216
Authors : Rondeau, J.-M.
Deposited on : 2009-10-07
Resolution : 2.12 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

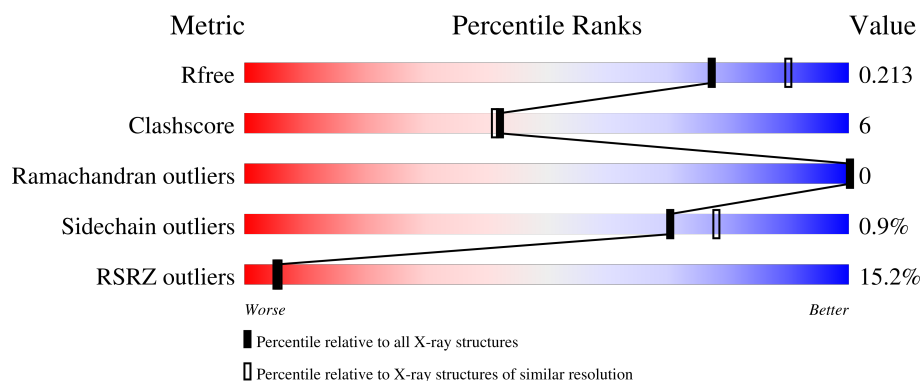
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	402	13% 80% 13% 6%
1	B	402	16% 82% 11% 6%
1	C	402	14% 79% 15% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9519 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.

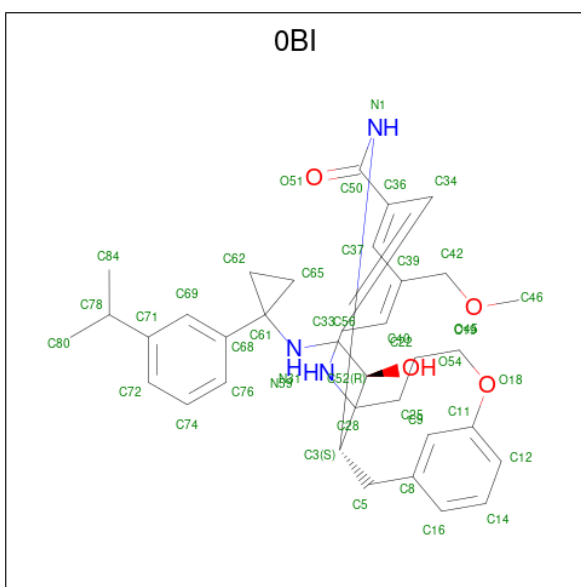
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	381	Total	C	N	O	S	0	0	0
			2993	1917	497	565	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33P	GLY	-	expression tag	UNP P56817
A	34P	PRO	-	expression tag	UNP P56817
B	33P	GLY	-	expression tag	UNP P56817
B	34P	PRO	-	expression tag	UNP P56817
C	33P	GLY	-	expression tag	UNP P56817
C	34P	PRO	-	expression tag	UNP P56817

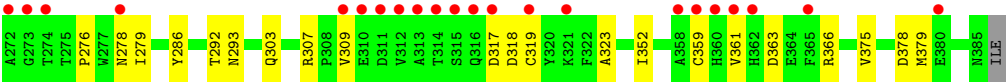
- Molecule 2 is (4S)-4-[(1R)-1-hydroxy-2-({1-[3-(1-methylethyl)phenyl]cyclopropyl}amino)ethyl]-19-(methoxymethyl)-11-oxa-3,16-diazatric yclo[15.3.1.1 6,10]docosa-1(21),6(22),7,9,17,19-hexaen-2-one (CCD ID: 0BI) (formula: C₃₅H₄₅N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 42	C 35	N 3	O 4	0	0
2	B	1	Total 42	C 35	N 3	O 4	0	0
2	C	1	Total 42	C 35	N 3	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	162	Total O 162 162	0	0
3	B	135	Total O 135 135	0	0
3	C	171	Total O 171 171	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.75Å 103.19Å 100.14Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	70.55 – 2.12 70.55 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.55-2.12) 99.8 (70.55-2.12)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.12Å)	Xtriage
Refinement program	CNS, CNX 2005	Depositor
R, R_{free}	0.200 , 0.220 0.194 , 0.213	Depositor DCC
R_{free} test set	9103 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9519	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: 0BI

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	0.34	0/3041	0.67	0/4133
1	B	0.34	0/3041	0.69	0/4133
1	C	0.35	0/3070	0.69	0/4173
All	All	0.35	0/9152	0.68	0/12439

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2966	0	2875	37	0
1	B	2966	0	2875	35	0
1	C	2993	0	2899	46	0
2	A	42	0	45	1	0
2	B	42	0	45	1	0
2	C	42	0	45	2	0
3	A	162	0	0	2	0
3	B	135	0	0	0	0
3	C	171	0	0	3	0
All	All	9519	0	8784	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (113) 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:367:THR:H	1:C:211:GLN:HE22	1.19	0.85
1:A:267:LEU:H	1:A:267:LEU:HD23	1.48	0.74
1:B:267:LEU:H	1:B:267:LEU:HD23	1.55	0.72
1:C:255:GLU:OE1	1:C:270:TRP:NE1	2.26	0.69
1:C:267:LEU:HD23	1:C:267:LEU:H	1.58	0.69
1:B:9:LYS:N	1:B:9:LYS:HD2	2.10	0.66
1:A:46(P):SER:HB3	3:A:539:HOH:O	1.96	0.65
1:C:268:VAL:O	1:C:319:CYS:HA	1.97	0.63
1:C:9:LYS:HD3	1:C:168:ALA:HB3	1.79	0.63
1:A:367:THR:H	1:C:211:GLN:NE2	1.95	0.63
1:B:205:ARG:NH2	1:B:212:ASP:HB2	2.14	0.62
1:A:72:THR:HB	2:A:387:0BI:H37	1.81	0.62
1:A:267:LEU:HD12	1:A:319:CYS:HB3	1.85	0.59
1:A:233:ASN:HD22	1:A:325:SER:HG	1.51	0.57
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.88	0.56
1:C:267:LEU:HD13	1:C:309:VAL:CG2	2.36	0.56
1:A:68:TYR:CD1	1:B:3:VAL:HG11	2.41	0.55
1:B:9:LYS:HZ2	1:B:114:ASN:HB2	1.71	0.55
1:C:65:LYS:HD3	3:C:540:HOH:O	2.07	0.55
1:A:254:THR:HG23	1:C:278:ASN:OD1	2.07	0.55
1:C:269:CYS:HA	1:C:318:ASP:O	2.07	0.55
1:A:258:PRO:O	1:A:261:PHE:HB3	2.07	0.55
1:C:258:PRO:O	1:C:261:PHE:HB3	2.07	0.55
1:C:72:THR:HB	2:C:387:0BI:H37	1.88	0.54
1:A:335:ALA:O	1:A:339:GLU:HG3	2.07	0.54
1:B:9:LYS:NZ	1:B:114:ASN:HB2	2.23	0.53
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.90	0.53
1:C:303:GLN:HB2	1:C:361:VAL:HG11	1.91	0.53
1:B:276:PRO:O	1:B:279:ILE:HG12	2.09	0.53
1:A:278:ASN:HD22	1:A:278:ASN:H	1.57	0.52
1:C:110:ILE:HB	1:C:113:SER:HB3	1.91	0.52
1:B:110:ILE:HB	1:B:113:SER:HB3	1.91	0.52
1:B:357:SER:O	1:B:360:HIS:HB3	2.10	0.52
1:A:110:ILE:HB	1:A:113:SER:HB3	1.92	0.52
1:C:159:PHE:HB3	1:C:160:PRO:HD2	1.92	0.52
1:B:258:PRO:O	1:B:261:PHE:HB3	2.09	0.51
1:B:267:LEU:HD13	1:B:309:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:TRP:O	1:B:317:ASP:HB3	2.10	0.51
1:C:75:LYS:NZ	3:C:521:HOH:O	2.42	0.51
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.93	0.51
1:C:12:GLN:OE1	1:C:113:SER:HA	2.11	0.50
1:C:276:PRO:O	1:C:279:ILE:HG12	2.12	0.49
1:C:363:ASP:HB3	1:C:366:ARG:O	2.13	0.49
1:C:293:ASN:HA	1:C:375:VAL:HA	1.93	0.49
1:B:63:LEU:HG	1:B:81:GLY:HA2	1.95	0.48
1:A:125:GLU:OE2	1:A:195:ARG:NH2	2.44	0.48
1:B:267:LEU:HD13	1:B:309:VAL:HG21	1.95	0.48
1:C:125:GLU:HG2	1:C:197:TRP:HB3	1.95	0.48
1:B:199:TYR:HB3	1:B:352:ILE:HD11	1.94	0.48
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.95	0.48
1:C:267:LEU:HD13	1:C:309:VAL:HG21	1.96	0.48
1:B:197:TRP:CG	1:B:198:TYR:H	2.33	0.47
1:C:249:LYS:HE2	1:C:262:TRP:CD1	2.49	0.47
1:A:197:TRP:CG	1:A:198:TYR:H	2.32	0.47
1:B:72:THR:HB	2:B:387:OBI:H37	1.97	0.47
1:A:249:LYS:HE2	1:A:262:TRP:CD1	2.50	0.46
1:C:267:LEU:HD23	1:C:267:LEU:N	2.26	0.46
1:C:197:TRP:CG	1:C:198:TYR:H	2.33	0.46
1:C:199:TYR:HB3	1:C:352:ILE:HD11	1.96	0.46
1:A:222:TYR:HA	1:A:223:ASP:HA	1.65	0.45
1:C:270:TRP:O	1:C:317:ASP:HB3	2.16	0.45
1:B:212:ASP:O	1:B:214:LYS:HG3	2.16	0.45
1:A:8:GLY:C	1:A:170:VAL:HG22	2.42	0.45
1:A:211:GLN:HB2	3:A:455:HOH:O	2.16	0.45
1:C:202:ILE:CD1	1:C:379:MET:HG3	2.46	0.45
1:C:63:LEU:HG	1:C:81:GLY:HA2	1.99	0.45
1:A:232:THR:O	1:A:336:VAL:HG13	2.17	0.44
1:A:267:LEU:HD13	1:A:309:VAL:CG2	2.47	0.44
1:A:211:GLN:HB2	1:A:211:GLN:HE21	1.65	0.44
1:B:174:MET:HE3	1:B:176:ILE:HD11	1.99	0.44
1:C:359:CYS:SG	1:C:359:CYS:O	2.76	0.44
1:C:267:LEU:HD13	1:C:309:VAL:HG23	1.98	0.44
1:A:95:VAL:HG11	1:A:140:LEU:HA	2.00	0.44
1:B:8:GLY:C	1:B:9:LYS:HD2	2.42	0.44
1:B:9:LYS:N	1:B:9:LYS:CD	2.81	0.44
1:C:202:ILE:HD11	1:C:379:MET:HG3	2.00	0.44
1:B:249:LYS:HE2	1:B:262:TRP:CD1	2.52	0.43
1:C:205:ARG:HB3	1:C:286:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ARG:HG3	1:C:323:ALA:HB2	1.99	0.43
1:B:125:GLU:O	1:B:125:GLU:HG3	2.17	0.43
1:B:222:TYR:HA	1:B:223:ASP:HA	1.63	0.43
1:C:95:VAL:HG11	1:C:140:LEU:HA	2.00	0.43
1:C:78:GLY:HA3	1:C:101:ALA:O	2.18	0.43
1:C:363:ASP:CG	3:C:416:HOH:O	2.62	0.42
1:A:9:LYS:HD2	1:A:12:GLN:OE1	2.19	0.42
1:A:301:LEU:HD13	1:A:363:ASP:HB2	2.02	0.42
1:B:267:LEU:HD23	1:B:267:LEU:N	2.28	0.42
1:C:65:LYS:HE2	1:C:65:LYS:HB2	1.95	0.42
1:A:8:GLY:O	1:A:170:VAL:HG22	2.19	0.42
1:C:292:THR:HG21	1:C:378:ASP:HB3	2.00	0.42
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.55	0.42
1:C:232:THR:OG1	2:C:387:OBI:H28	2.20	0.42
1:A:269:CYS:HA	1:A:318:ASP:O	2.20	0.41
1:B:309:VAL:HG11	1:B:321:LYS:HG3	2.02	0.41
1:A:205:ARG:HB3	1:A:286:TYR:HB2	2.02	0.41
1:B:95:VAL:HG11	1:B:140:LEU:HA	2.02	0.41
1:A:365:PHE:CG	1:C:250:ALA:HB1	2.56	0.41
1:C:91:PRO:HD3	1:C:176:ILE:HB	2.03	0.41
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.51	0.41
1:B:126:ILE:HG23	1:B:197:TRP:HB2	2.03	0.41
1:B:278:ASN:H	1:B:278:ASN:HD22	1.69	0.41
1:C:47(P):PHE:CZ	1:C:178:GLY:HA3	2.56	0.41
1:A:63:LEU:HG	1:A:81:GLY:HA2	2.02	0.41
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.86	0.41
1:B:267:LEU:HD12	1:B:319:CYS:HB3	2.02	0.41
1:C:222:TYR:HA	1:C:223:ASP:HA	1.63	0.41
1:C:379:MET:HE2	1:C:379:MET:HB2	1.71	0.41
1:A:78:GLY:HA3	1:A:101:ALA:O	2.21	0.41
1:A:197:TRP:CD1	1:A:197:TRP:N	2.89	0.41
1:B:64:ARG:HA	1:B:79:GLU:OE2	2.20	0.41
1:A:76:TRP:HB2	1:A:102:ILE:HG23	2.03	0.40
1:B:197:TRP:N	1:B:197:TRP:CD1	2.89	0.40
1:A:198:TYR:CE2	1:A:224:LYS:HE3	2.56	0.40

There are no symmetry-related clashes.

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	373/402 (93%)	365 (98%)	8 (2%)	0	100	100
1	B	373/402 (93%)	361 (97%)	12 (3%)	0	100	100
1	C	377/402 (94%)	363 (96%)	14 (4%)	0	100	100
All	All	1123/1206 (93%)	1089 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	322/342 (94%)	319 (99%)	3 (1%)	70	78
1	B	322/342 (94%)	318 (99%)	4 (1%)	63	71
1	C	324/342 (95%)	322 (99%)	2 (1%)	78	85
All	All	968/1026 (94%)	959 (99%)	9 (1%)	70	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	TRP
1	A	211	GLN
1	A	267	LEU
1	B	125	GLU
1	B	169	SER

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Mol	Chain	Res	Type
1	B	197	TRP
1	B	267	LEU
1	C	197	TRP
1	C	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	114	ASN
1	A	233	ASN
1	A	326	GLN
1	A	362	HIS
1	A	385	ASN
1	B	89	HIS
1	B	114	ASN
1	B	181	HIS
1	B	278	ASN
1	B	326	GLN
1	C	89	HIS
1	C	98	ASN
1	C	114	ASN
1	C	211	GLN
1	C	326	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0BI	A	387	-	45,46,46	1.57	6 (13%)	60,64,64	1.12	5 (8%)
2	0BI	B	387	-	45,46,46	1.56	5 (11%)	60,64,64	1.12	6 (10%)
2	0BI	C	387	-	45,46,46	1.59	6 (13%)	60,64,64	1.13	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0BI	A	387	-	-	4/41/48/48	0/4/5/5
2	0BI	B	387	-	-	4/41/48/48	0/4/5/5
2	0BI	C	387	-	-	4/41/48/48	0/4/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	387	0BI	C65-C61	3.87	1.55	1.51
2	A	387	0BI	C65-C61	3.81	1.55	1.51
2	B	387	0BI	C65-C61	3.65	1.55	1.51
2	A	387	0BI	C62-C61	3.30	1.54	1.51
2	C	387	0BI	C62-C61	3.17	1.54	1.51
2	B	387	0BI	C62-C61	2.96	1.54	1.51
2	B	387	0BI	C69-C71	2.41	1.42	1.39
2	C	387	0BI	C72-C71	2.39	1.42	1.39
2	C	387	0BI	C69-C71	2.29	1.42	1.39
2	C	387	0BI	C56-C52	2.29	1.55	1.52
2	B	387	0BI	C9-C11	2.28	1.42	1.39
2	A	387	0BI	C69-C71	2.28	1.42	1.39
2	B	387	0BI	C72-C71	2.11	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	387	0BI	C9-C11	2.06	1.42	1.39
2	A	387	0BI	C56-C52	2.06	1.55	1.52
2	A	387	0BI	C34-C33	2.05	1.42	1.39
2	C	387	0BI	C9-C11	2.04	1.42	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	387	0BI	C62-C61-N59	-4.10	113.42	117.30
2	A	387	0BI	C62-C61-N59	-3.77	113.72	117.30
2	B	387	0BI	C62-C61-C68	-3.72	114.06	118.78
2	B	387	0BI	C62-C61-N59	-3.72	113.78	117.30
2	A	387	0BI	C62-C61-C68	-3.66	114.13	118.78
2	C	387	0BI	C62-C61-C68	-3.42	114.44	118.78
2	A	387	0BI	C19-O18-C11	2.80	125.20	117.93
2	C	387	0BI	C19-O18-C11	2.77	125.13	117.93
2	B	387	0BI	C19-O18-C11	2.41	124.21	117.93
2	A	387	0BI	C3-N1-C50	2.39	127.29	122.94
2	A	387	0BI	C36-C50-N1	2.32	121.34	117.04
2	B	387	0BI	C36-C50-N1	2.27	121.24	117.04
2	B	387	0BI	O54-C52-C56	-2.25	105.24	109.67
2	C	387	0BI	C36-C50-N1	2.21	121.15	117.04
2	C	387	0BI	C3-N1-C50	2.18	126.91	122.94
2	B	387	0BI	C3-N1-C50	2.16	126.88	122.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	387	0BI	C39-C42-O45-C46
2	B	387	0BI	C39-C42-O45-C46
2	C	387	0BI	C39-C42-O45-C46
2	B	387	0BI	C22-C19-O18-C11
2	C	387	0BI	C22-C19-O18-C11
2	A	387	0BI	C22-C19-O18-C11
2	A	387	0BI	C62-C61-C68-C69
2	A	387	0BI	C62-C61-C68-C76
2	B	387	0BI	C62-C61-C68-C69
2	B	387	0BI	C62-C61-C68-C76
2	C	387	0BI	C62-C61-C68-C69
2	C	387	0BI	C62-C61-C68-C76

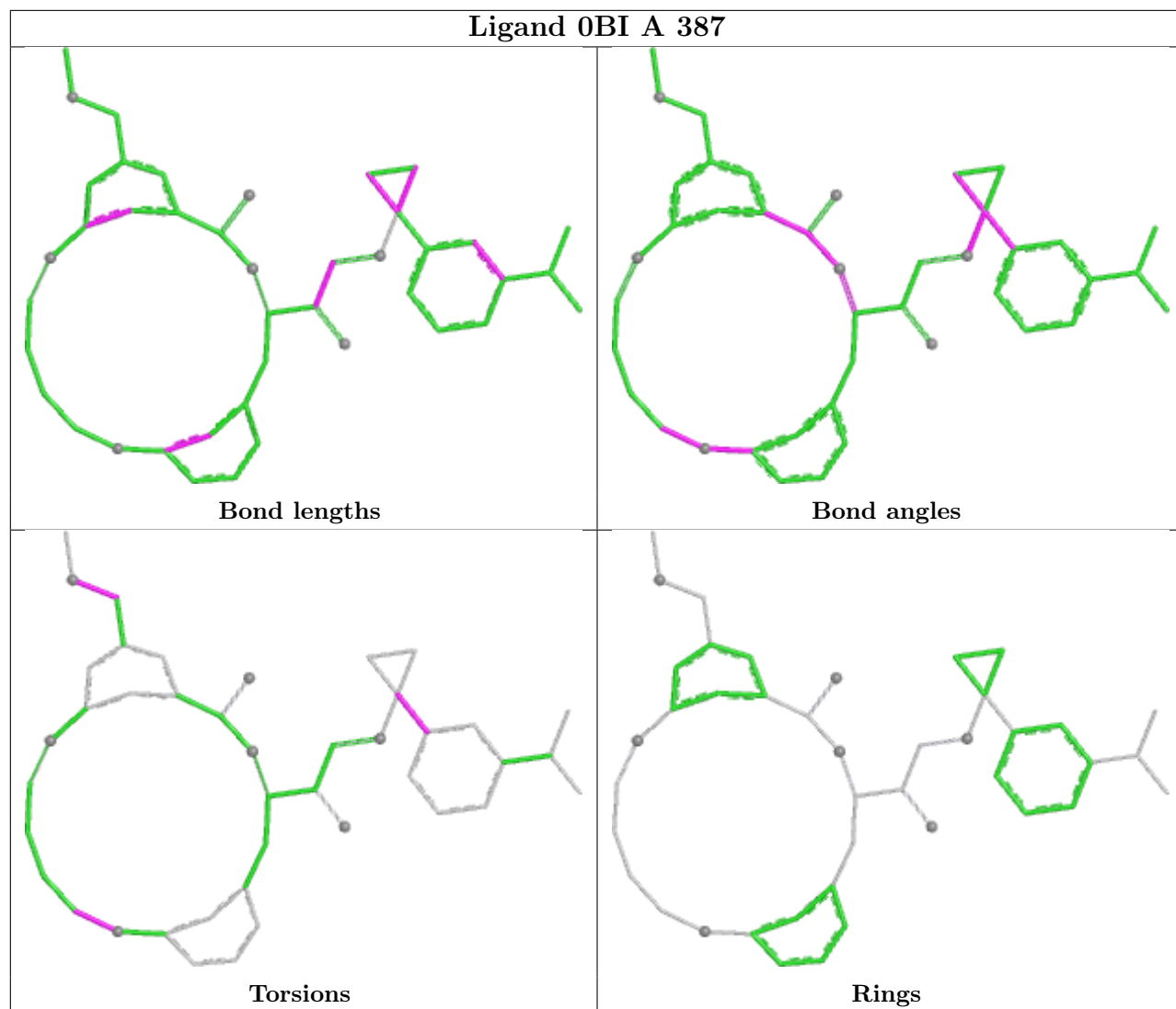
There are no ring outliers.

3 monomers are involved in 4 short contacts:

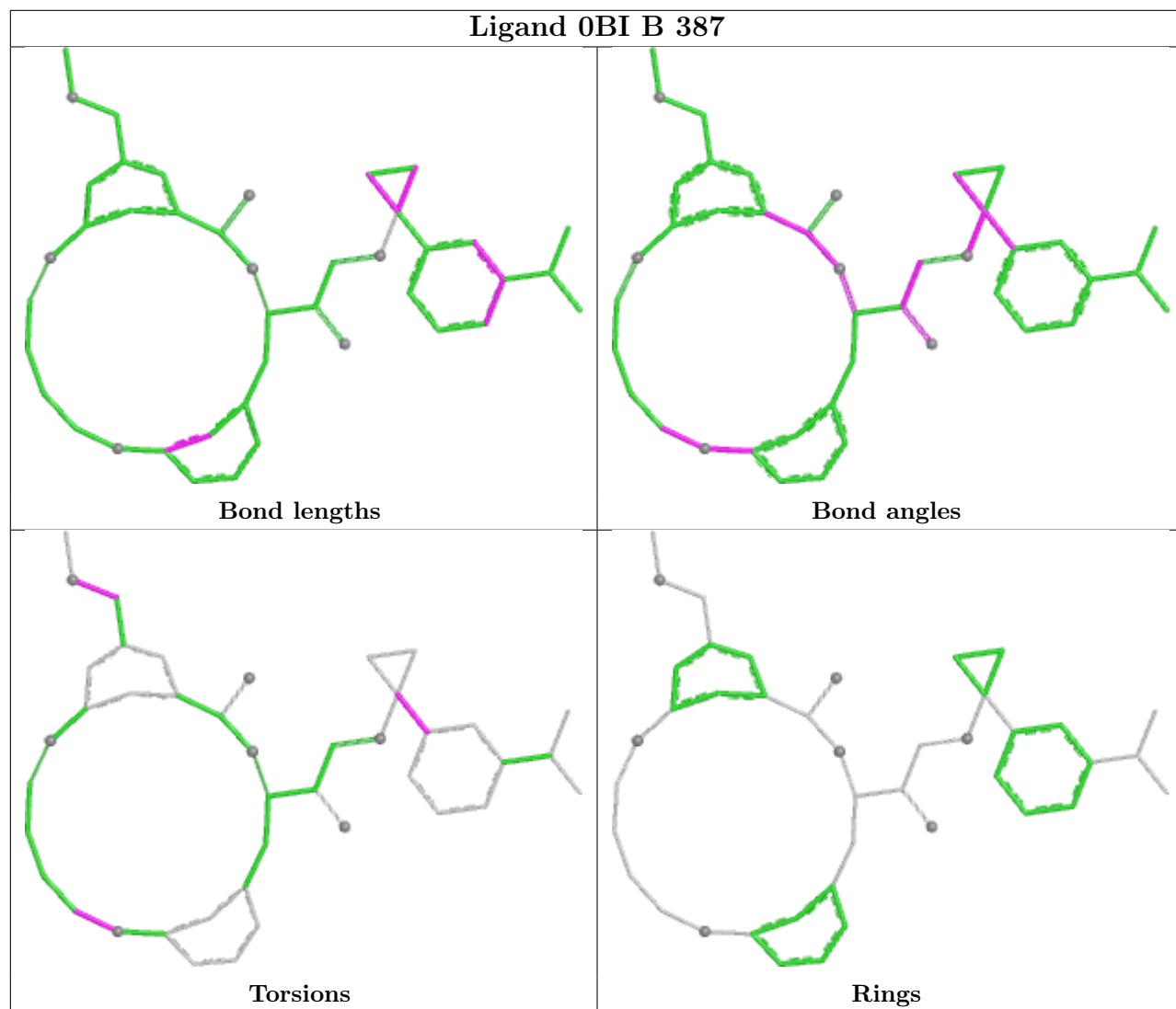
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	387	0BI	1	0
2	B	387	0BI	1	0
2	C	387	0BI	2	0

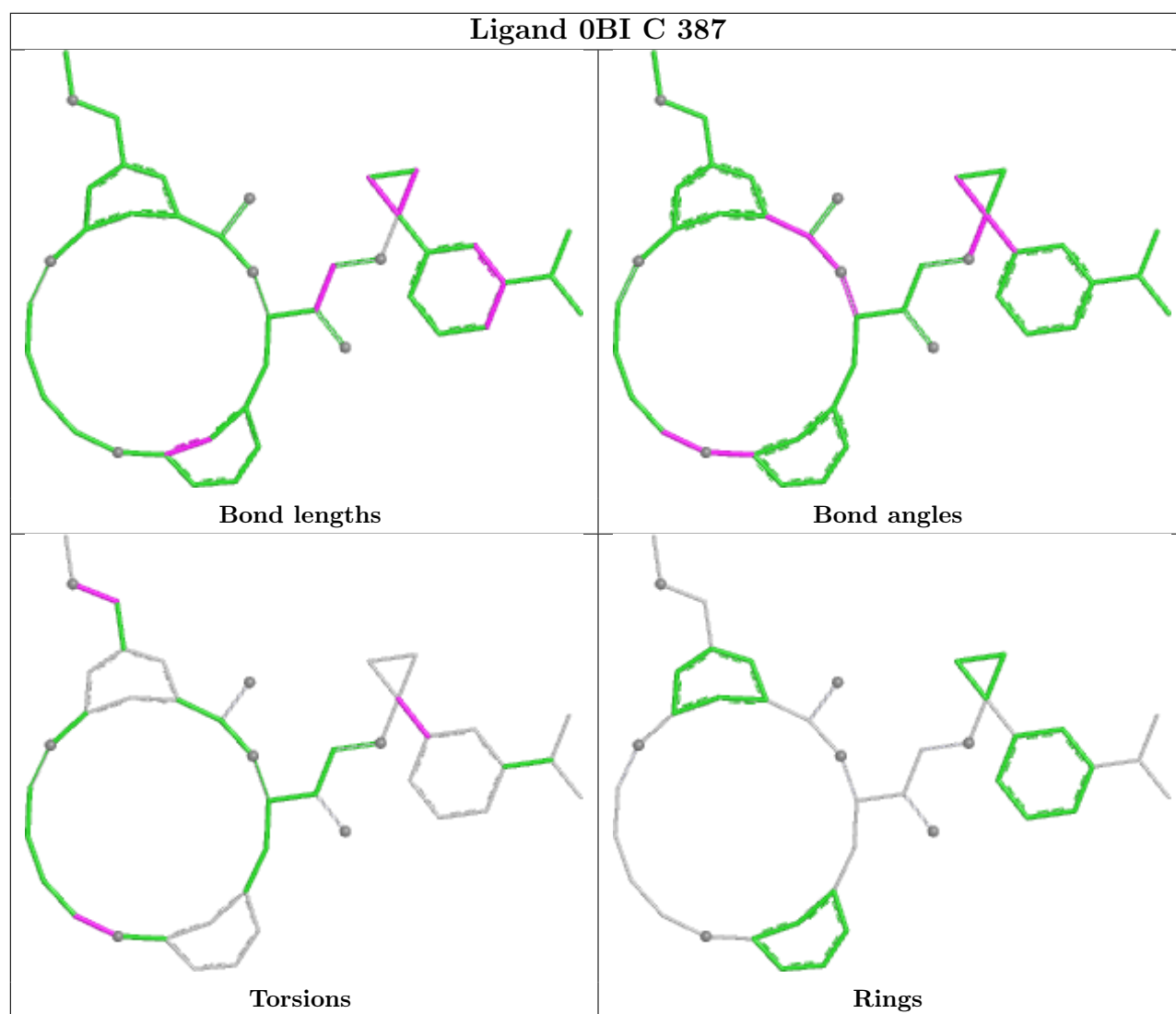
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 0BI A 387



Ligand 0BI B 387





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	377/402 (93%)	0.72	53 (14%) 6 7	28, 44, 81, 116	0
1	B	377/402 (93%)	0.85	63 (16%) 4 5	27, 45, 85, 118	0
1	C	381/402 (94%)	0.78	57 (14%) 5 6	29, 44, 83, 116	0
All	All	1135/1206 (94%)	0.78	173 (15%) 5 5	27, 45, 84, 118	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	VAL	9.4
1	B	361	VAL	8.3
1	C	312	VAL	8.0
1	B	314	THR	7.3
1	B	312	VAL	7.3
1	B	313	ALA	7.2
1	A	313	ALA	6.8
1	A	314	THR	6.4
1	B	267	LEU	6.3
1	B	315	SER	6.3
1	A	272	ALA	5.8
1	C	168	ALA	5.8
1	C	258	PRO	5.8
1	C	313	ALA	5.6
1	A	258	PRO	5.5
1	C	272	ALA	5.5
1	A	273	GLY	5.4
1	C	159	PHE	5.4
1	B	258	PRO	5.3
1	C	269	CYS	5.3
1	C	160	PRO	5.2
1	C	158	GLY	5.1
1	C	267	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	256	LYS	4.8
1	C	361	VAL	4.8
1	B	257	PHE	4.7
1	C	46(P)	SER	4.6
1	C	362	HIS	4.6
1	A	157	ALA	4.5
1	B	250	ALA	4.4
1	A	365	PHE	4.4
1	B	309	VAL	4.3
1	A	317	ASP	4.3
1	C	254	THR	4.3
1	B	46(P)	SER	4.3
1	A	316	GLN	4.2
1	C	314	THR	4.2
1	C	257	PHE	4.2
1	A	266	GLN	4.1
1	A	267	LEU	4.1
1	B	273	GLY	4.1
1	A	256	LYS	4.1
1	C	315	SER	4.0
1	C	264	GLY	4.0
1	C	271	GLN	3.9
1	C	359	CYS	3.9
1	C	157	ALA	3.9
1	A	254	THR	3.9
1	C	365	PHE	3.9
1	B	359	CYS	3.8
1	C	263	LEU	3.8
1	C	268	VAL	3.8
1	A	269	CYS	3.7
1	C	259	ASP	3.7
1	B	277	TRP	3.7
1	C	317	ASP	3.7
1	B	278	ASN	3.6
1	A	311	ASP	3.6
1	B	254	THR	3.6
1	B	308	PRO	3.6
1	A	309	VAL	3.5
1	A	253	SER	3.5
1	A	315	SER	3.5
1	B	365	PHE	3.5
1	B	272	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	362	HIS	3.5
1	B	157	ALA	3.5
1	C	311	ASP	3.5
1	B	362	HIS	3.5
1	B	263	LEU	3.4
1	B	271	GLN	3.4
1	C	260	GLY	3.4
1	B	360	HIS	3.4
1	C	49	HIS	3.4
1	B	319	CYS	3.4
1	B	320	TYR	3.4
1	C	321	LYS	3.3
1	C	309	VAL	3.3
1	C	261	PHE	3.3
1	B	262	TRP	3.3
1	A	259	ASP	3.3
1	A	257	PHE	3.1
1	B	274	THR	3.1
1	B	268	VAL	3.1
1	C	310	GLU	3.0
1	A	319	CYS	3.0
1	B	340	GLY	3.0
1	C	270	TRP	3.0
1	C	145	HIS	3.0
1	A	55	GLN	3.0
1	C	319	CYS	3.0
1	B	266	GLN	3.0
1	A	268	VAL	3.0
1	B	265	GLU	3.0
1	B	317	ASP	3.0
1	A	60	TYR	3.0
1	A	318	ASP	2.9
1	B	252	SER	2.9
1	C	214	LYS	2.9
1	A	264	GLY	2.9
1	A	360	HIS	2.9
1	B	276	PRO	2.8
1	C	316	GLN	2.8
1	C	273	GLY	2.8
1	A	361	VAL	2.8
1	C	169	SER	2.8
1	A	156	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	170	VAL	2.8
1	B	269	CYS	2.8
1	B	316	GLN	2.7
1	C	253	SER	2.7
1	B	47	PHE	2.7
1	A	271	GLN	2.7
1	A	308	PRO	2.7
1	B	270	TRP	2.7
1	B	318	ASP	2.7
1	A	262	TRP	2.6
1	C	278	ASN	2.6
1	B	9	LYS	2.6
1	A	251	ALA	2.6
1	A	56	LEU	2.6
1	C	68	TYR	2.6
1	C	266	GLN	2.6
1	A	265	GLU	2.6
1	B	275	THR	2.6
1	A	169	SER	2.6
1	A	263	LEU	2.6
1	B	260	GLY	2.5
1	C	66	GLY	2.5
1	A	73	GLN	2.5
1	B	22	SER	2.5
1	C	56	LEU	2.5
1	B	60	TYR	2.5
1	C	156	GLY	2.5
1	B	311	ASP	2.4
1	B	49	HIS	2.4
1	B	209	ASN	2.4
1	A	46(P)	SER	2.4
1	B	253	SER	2.4
1	C	256	LYS	2.4
1	C	360	HIS	2.4
1	B	306	LEU	2.3
1	A	359	CYS	2.3
1	C	380	GLU	2.3
1	A	270	TRP	2.3
1	C	73	GLN	2.3
1	A	142	LYS	2.3
1	A	261	PHE	2.3
1	A	58	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	2.3
1	B	264	GLY	2.3
1	A	10	SER	2.3
1	B	279	ILE	2.3
1	C	274	THR	2.3
1	A	260	GLY	2.3
1	B	249	LYS	2.3
1	B	259	ASP	2.2
1	A	320	TYR	2.2
1	B	61	ARG	2.2
1	C	358	ALA	2.2
1	B	211	GLN	2.2
1	C	60	TYR	2.2
1	B	300	ILE	2.2
1	C	1	GLU	2.2
1	A	9	LYS	2.2
1	B	280	PHE	2.1
1	B	251	ALA	2.1
1	B	44	PRO	2.1
1	C	262	TRP	2.1
1	B	51	TYR	2.1
1	A	255	GLU	2.0
1	C	265	GLU	2.0
1	B	310	GLU	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](#)

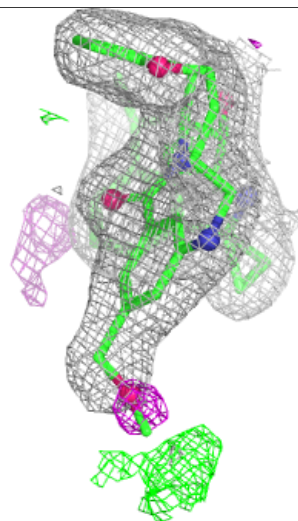
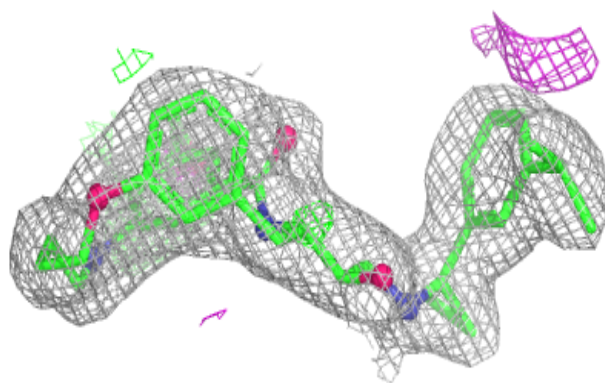
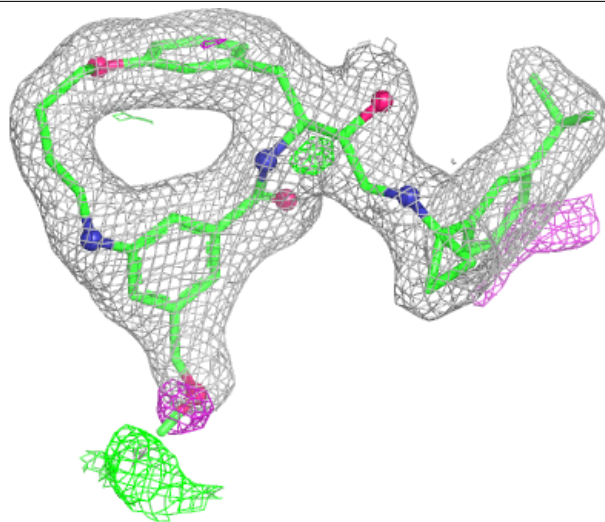
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	OBI	A	387	42/42	0.94	0.10	30,36,44,59	0
2	OBI	B	387	42/42	0.95	0.09	31,37,43,58	0
2	OBI	C	387	42/42	0.96	0.08	31,36,44,59	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.

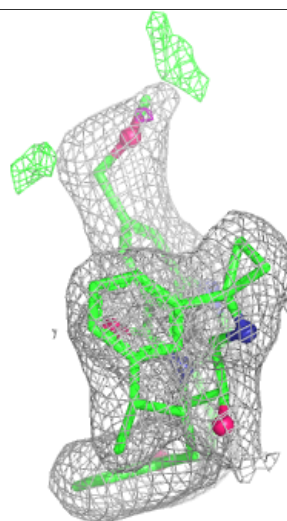
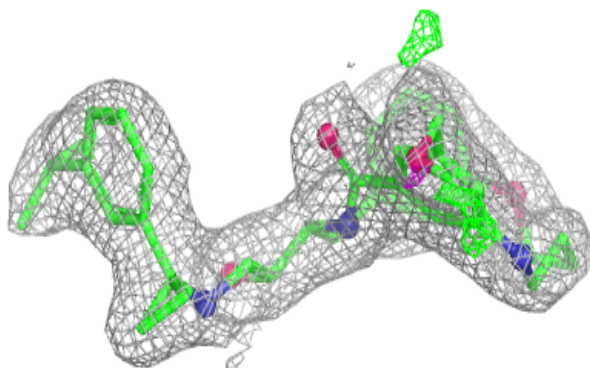
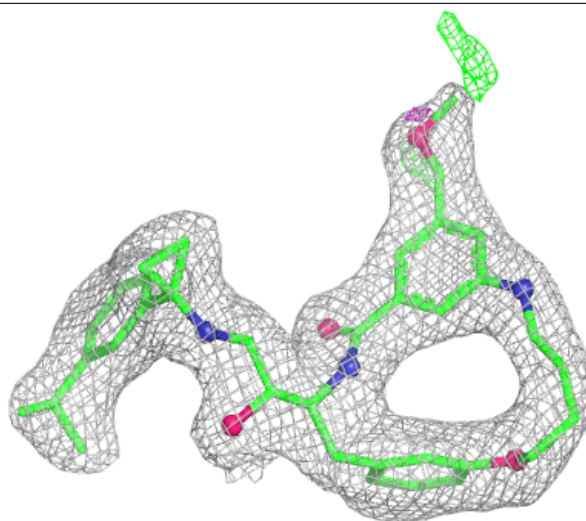
Electron density around OBI A 387:

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



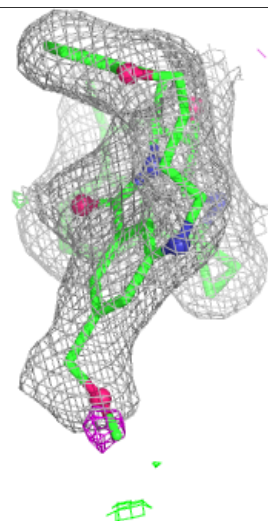
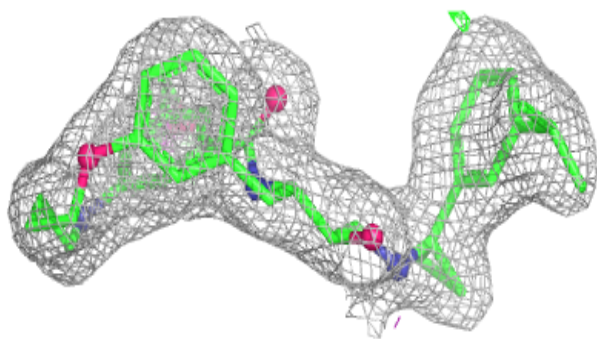
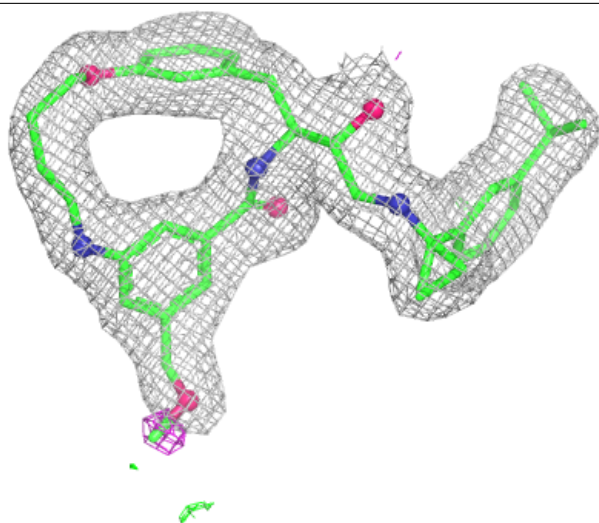
Electron density around 0BI B 387:

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



Electron density around 0BI C 387:

$2mF_o-DF_c$ (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.