Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 08:30 AM EST

PDB ID	:	3OZ1
Title	:	cIAP1-BIR3 domain in complex with the Smac-mimetic compound Smac066
Authors	:	Cossu, F.; Malvezzi, F.; Mastrangelo, E.; Canevari, G.; Bolognesi, M.; Milani, M.
Deposited on	:	2010-09-24
Resolution	:	3.00 Å(reported)

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

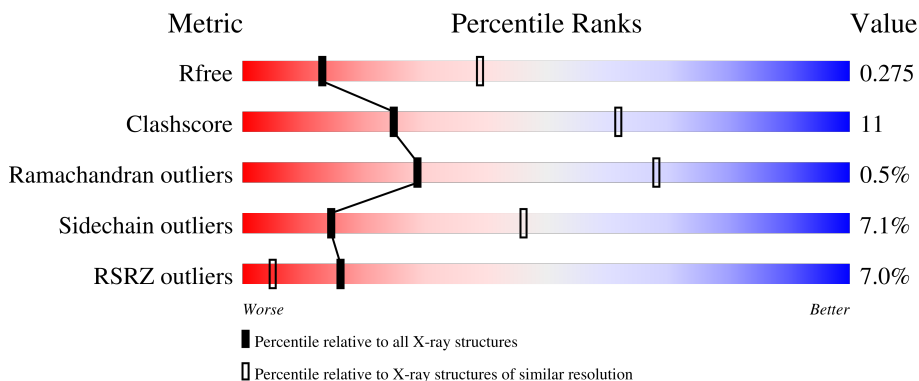|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		11
Ramachandran outliers		0.5%
Sidechain outliers		7.1%
RSRZ outliers		7.0%

Worse　　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	122	72%　　　　11%　·　16%
1	B	122	78%　　　　5%　·　15%
1	C	122	69%　　　10%　6%　16%
1	D	122	24%　　58%　　22%　·　16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3579 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 Baculoviral IAP repeat-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			845	540	145	151	9			
1	B	104	Total	C	N	O	S	0	0	0
			852	544	146	153	9			
1	C	103	Total	C	N	O	S	0	0	0
			850	543	148	150	9			
1	D	102	Total	C	N	O	S	0	0	0
			839	537	144	149	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	MET	-	expression tag	UNP Q13490
A	358	LEU	-	expression tag	UNP Q13490
A	359	GLU	-	expression tag	UNP Q13490
A	360	HIS	-	expression tag	UNP Q13490
A	361	HIS	-	expression tag	UNP Q13490
A	362	HIS	-	expression tag	UNP Q13490
A	363	HIS	-	expression tag	UNP Q13490
A	364	HIS	-	expression tag	UNP Q13490
A	365	HIS	-	expression tag	UNP Q13490
B	244	MET	-	expression tag	UNP Q13490
B	358	LEU	-	expression tag	UNP Q13490
B	359	GLU	-	expression tag	UNP Q13490
B	360	HIS	-	expression tag	UNP Q13490
B	361	HIS	-	expression tag	UNP Q13490
B	362	HIS	-	expression tag	UNP Q13490
B	363	HIS	-	expression tag	UNP Q13490
B	364	HIS	-	expression tag	UNP Q13490
B	365	HIS	-	expression tag	UNP Q13490
C	244	MET	-	expression tag	UNP Q13490
C	358	LEU	-	expression tag	UNP Q13490
C	359	GLU	-	expression tag	UNP Q13490

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	360	HIS	-	expression tag	UNP Q13490
C	361	HIS	-	expression tag	UNP Q13490
C	362	HIS	-	expression tag	UNP Q13490
C	363	HIS	-	expression tag	UNP Q13490
C	364	HIS	-	expression tag	UNP Q13490
C	365	HIS	-	expression tag	UNP Q13490
D	244	MET	-	expression tag	UNP Q13490
D	358	LEU	-	expression tag	UNP Q13490
D	359	GLU	-	expression tag	UNP Q13490
D	360	HIS	-	expression tag	UNP Q13490
D	361	HIS	-	expression tag	UNP Q13490
D	362	HIS	-	expression tag	UNP Q13490
D	363	HIS	-	expression tag	UNP Q13490
D	364	HIS	-	expression tag	UNP Q13490
D	365	HIS	-	expression tag	UNP Q13490

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is (3S,6S,7R,9aS)-7-[2-(benzylamino)ethyl]-N-(diphenylmethyl)-6-{[(2S)-2-(methylamino)butanoyl]amino}-5-oxooctahydro-1H-pyrrolo[1,2-a]azepine-3-carboxamide (three-letter code: BMB) (formula: $C_{37}H_{47}N_5O_3$).

BMB
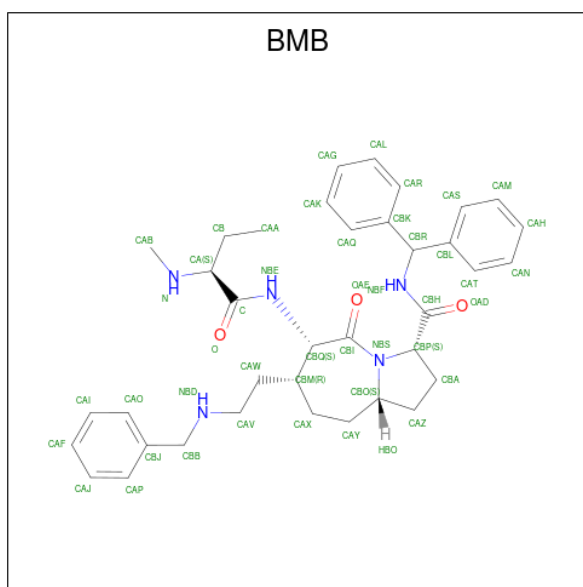
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 45	C 37	N 5	O 3	0	0
3	B	1	Total 45	C 37	N 5	O 3	0	0
3	C	1	Total 45	C 37	N 5	O 3	0	0
3	D	1	Total 45	C 37	N 5	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	3	Total 3	O 3	0	0
4	C	4	Total 4	O 4	0	0
4	D	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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: Baculoviral IAP repeat-containing protein 2

Chain A:

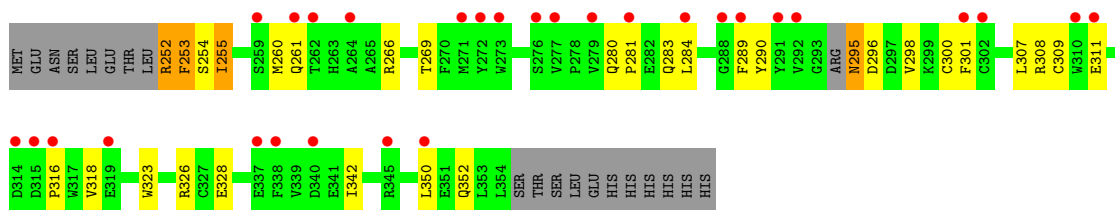- Molecule 1: Baculoviral IAP repeat-containing protein 2

Chain B:

- Molecule 1: Baculoviral IAP repeat-containing protein 2

Chain C:

- Molecule 1: Baculoviral IAP repeat-containing protein 2

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	113.59Å　114.63Å　92.96Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	60.93　–　3.00 60.93　–　3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (60.93-3.00) 95.3 (60.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.01 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.192　,　0.257 0.210　,　0.275	Depositor DCC
R_{free} test set	575 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 102.3	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.048 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3579	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 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMB

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	0.51	0/872	0.69	0/1180
1	B	0.53	0/879	0.69	0/1190
1	C	0.58	0/877	0.72	0/1186
1	D	0.50	0/865	0.70	0/1169
All	All	0.53	0/3493	0.70	0/4725

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	845	0	790	8	0
1	B	852	0	797	8	0
1	C	850	0	798	34	0
1	D	839	0	784	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	45	0	47	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	47	0	0
3	C	45	0	47	1	0
3	D	45	0	47	4	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
All	All	3579	0	3357	74	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 11.

All (74) 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:C:350:LEU:C	1:C:350:LEU:HD12	1.57	1.18
1:C:252:ARG:CG	1:C:252:ARG:HH11	1.57	1.15
1:D:254:SER:C	1:D:255:ILE:HD13	1.69	1.11
1:D:255:ILE:HD13	1:D:255:ILE:N	1.66	1.10
1:C:252:ARG:HH11	1:C:252:ARG:HG2	1.17	1.07
1:C:252:ARG:HH11	1:C:252:ARG:CB	1.69	1.04
1:C:252:ARG:NH1	1:C:252:ARG:HB3	1.72	1.03
1:C:350:LEU:HD12	1:C:350:LEU:O	1.60	1.01
1:C:350:LEU:C	1:C:350:LEU:CD1	2.30	1.00
1:D:254:SER:C	1:D:255:ILE:CD1	2.30	1.00
1:C:252:ARG:CB	1:C:252:ARG:NH1	2.30	0.93
1:D:255:ILE:N	1:D:255:ILE:CD1	2.30	0.88
1:C:252:ARG:HG2	1:C:252:ARG:NH1	1.88	0.87
1:B:345:ARG:HH11	1:B:345:ARG:HG3	1.42	0.85
1:C:252:ARG:O	1:C:253:PHE:CD2	2.30	0.84
1:D:253:PHE:HB3	1:D:255:ILE:HD11	1.62	0.80
1:C:350:LEU:O	1:C:350:LEU:CD1	2.30	0.77
1:C:350:LEU:HD11	1:C:354:LEU:HD13	1.70	0.73
1:C:252:ARG:O	1:C:253:PHE:HD2	1.72	0.72
1:A:332:ARG:HH11	1:B:331:ILE:HG21	1.55	0.72
1:C:350:LEU:CD1	1:C:354:LEU:HD13	2.21	0.71
1:D:254:SER:O	1:D:255:ILE:HD12	1.92	0.70
1:C:296:ASP:OD1	1:C:296:ASP:C	2.30	0.68
1:D:254:SER:C	1:D:255:ILE:HD12	2.14	0.67
1:D:283:GLN:HB3	1:D:316:PRO:HG2	1.79	0.64
1:D:253:PHE:CZ	1:D:328:GLU:HB3	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:HG2	1:A:349:LEU:HD21	1.82	0.62
1:B:345:ARG:HG3	1:B:345:ARG:NH1	2.12	0.62
1:C:295:ASN:O	1:C:296:ASP:CB	2.48	0.62
1:B:322:LYS:HG2	1:B:349:LEU:HD21	1.85	0.58
1:C:349:LEU:O	1:C:352:GLN:HG2	2.04	0.57
1:C:352:GLN:HG3	1:C:353:LEU:N	2.19	0.57
1:D:284:LEU:HD22	1:D:298:VAL:HG11	1.87	0.57
1:D:254:SER:CA	1:D:255:ILE:HD13	2.35	0.57
1:C:252:ARG:HB3	1:C:252:ARG:CZ	2.34	0.57
1:D:308:ARG:HB3	3:D:600:BMB:HAK	1.86	0.56
1:C:252:ARG:C	1:C:253:PHE:CD2	2.80	0.55
1:C:258:LEU:O	1:C:261:GLN:HB2	2.09	0.52
1:C:350:LEU:HD12	1:C:351:GLU:N	2.21	0.52
1:C:350:LEU:HB2	1:D:350:LEU:HD13	1.91	0.52
1:A:348:HIS:HB3	1:A:351:GLU:HG2	1.92	0.52
1:C:295:ASN:O	1:C:296:ASP:OD1	2.29	0.50
1:D:323:TRP:CE2	3:D:600:BMB:HBO	2.46	0.49
1:D:307:LEU:HD22	3:D:600:BMB:HAAB	1.93	0.48
1:D:308:ARG:HH12	3:D:600:BMB:CAT	2.27	0.48
1:B:354:LEU:HA	1:B:354:LEU:HD12	1.38	0.48
1:C:349:LEU:HD12	1:C:349:LEU:HA	1.70	0.48
1:D:295:ASN:HB3	1:D:296:ASP:H	1.56	0.48
1:C:253:PHE:O	1:C:254:SER:OG	2.30	0.47
1:D:318:VAL:HG13	1:D:342:ILE:HD12	1.97	0.47
3:A:600:BMB:CAT	3:A:600:BMB:HAR	2.44	0.46
1:A:258:LEU:O	1:A:261:GLN:HB2	2.15	0.46
1:B:318:VAL:HG13	1:B:342:ILE:HD12	1.97	0.45
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.76	0.45
1:C:295:ASN:O	1:C:296:ASP:HB3	2.16	0.45
1:D:252:ARG:HB2	1:D:253:PHE:H	1.51	0.45
1:C:349:LEU:HD12	1:C:352:GLN:NE2	2.30	0.45
1:C:351:GLU:OE2	1:D:326:ARG:NH1	2.50	0.45
1:C:294:ARG:HG3	1:C:295:ASN:HB2	1.98	0.45
1:C:295:ASN:O	1:C:296:ASP:CG	2.55	0.45
1:D:260:MET:HB3	1:D:266:ARG:HG2	1.98	0.44
1:A:282:GLU:H	1:A:282:GLU:HG3	1.46	0.44
1:D:280:GLN:HG2	1:D:283:GLN:HE22	1.82	0.44
1:A:284:LEU:O	1:A:289:PHE:HB2	2.17	0.44
1:A:318:VAL:HG13	1:A:342:ILE:HD12	1.99	0.44
1:D:290:TYR:HE2	1:D:301:PHE:HA	1.84	0.43
3:C:600:BMB:CAT	3:C:600:BMB:HAR	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:PHE:HB3	1:D:298:VAL:HB	2.01	0.42
1:C:296:ASP:CG	1:C:296:ASP:O	2.58	0.42
1:C:318:VAL:HG13	1:C:342:ILE:HD12	2.01	0.42
1:D:289:PHE:HA	1:D:300:CYS:HA	2.03	0.41
1:B:322:LYS:NZ	1:B:349:LEU:HD11	2.34	0.41
1:A:349:LEU:HA	1:A:352:GLN:HB2	2.02	0.40
1:C:332:ARG:HH11	1:C:332:ARG:HB3	1.86	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	101/122 (83%)	96 (95%)	5 (5%)	0	100	100
1	B	102/122 (84%)	99 (97%)	3 (3%)	0	100	100
1	C	101/122 (83%)	95 (94%)	5 (5%)	1 (1%)	15	53
1	D	98/122 (80%)	89 (91%)	8 (8%)	1 (1%)	15	53
All	All	402/488 (82%)	379 (94%)	21 (5%)	2 (0%)	29	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	PRO
1	C	255	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/110 (83%)	87 (96%)	4 (4%)	28	65
1	B	92/110 (84%)	87 (95%)	5 (5%)	22	57
1	C	91/110 (83%)	83 (91%)	8 (9%)	10	36
1	D	90/110 (82%)	81 (90%)	9 (10%)	7	29
All	All	364/440 (83%)	338 (93%)	26 (7%)	14	46

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

Mol	Chain	Res	Type
1	A	253	PHE
1	A	282	GLU
1	A	332	ARG
1	A	353	LEU
1	B	254	SER
1	B	345	ARG
1	B	349	LEU
1	B	354	LEU
1	B	355	SER
1	C	252	ARG
1	C	271	MET
1	C	294	ARG
1	C	296	ASP
1	C	349	LEU
1	C	350	LEU
1	C	352	GLN
1	C	354	LEU
1	D	252	ARG
1	D	253	PHE
1	D	255	ILE
1	D	261	GLN
1	D	269	THR
1	D	295	ASN
1	D	309	CYS
1	D	311	GLU
1	D	352	GLN

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

Mol	Chain	Res	Type
1	B	352	GLN
1	C	352	GLN
1	D	257	ASN
1	D	280	GLN
1	D	283	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	BMB	A	600	-	47,49,49	0.66	0	53,66,66	1.05	3 (5%)
3	BMB	D	600	-	47,49,49	0.78	1 (2%)	53,66,66	1.31	5 (9%)
3	BMB	C	600	-	47,49,49	0.75	0	53,66,66	1.06	2 (3%)
3	BMB	B	600	-	47,49,49	0.71	0	53,66,66	1.15	3 (5%)

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	BMB	A	600	-	-	8/35/65/65	0/5/5/5
3	BMB	D	600	-	-	12/35/65/65	0/5/5/5
3	BMB	C	600	-	-	8/35/65/65	0/5/5/5
3	BMB	B	600	-	-	9/35/65/65	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	BMB	CBL-CBR	2.05	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	600	BMB	OAE-CBI-NBS	-3.98	117.28	121.69
3	D	600	BMB	CBL-CBR-NBF	3.97	118.39	111.30
3	B	600	BMB	OAE-CBI-NBS	-3.76	117.53	121.69
3	D	600	BMB	CBP-NBS-CBI	3.68	123.57	118.60
3	D	600	BMB	CBA-CBP-NBS	3.42	106.37	103.09
3	D	600	BMB	OAE-CBI-NBS	-3.19	118.15	121.69
3	A	600	BMB	OAE-CBI-NBS	-3.13	118.22	121.69
3	D	600	BMB	CAZ-CBO-NBS	3.00	105.07	101.70
3	C	600	BMB	CBP-NBS-CBI	2.49	121.97	118.60
3	B	600	BMB	CBP-NBS-CBI	2.27	121.67	118.60
3	A	600	BMB	CBP-NBS-CBI	2.21	121.58	118.60
3	B	600	BMB	CBB-NBD-CAV	-2.16	106.00	113.41
3	A	600	BMB	CBL-CBR-CBK	2.09	116.88	112.33

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	BMB	CAV-CAW-CBM-CBQ
3	D	600	BMB	N-CA-CB-CAA
3	D	600	BMB	NBD-CAV-CAW-CBM
3	D	600	BMB	CAV-CAW-CBM-CBQ
3	D	600	BMB	CBM-CBQ-NBE-C
3	D	600	BMB	CBL-CBR-NBF-CBH
3	D	600	BMB	OAD-CBH-CBP-CBA
3	D	600	BMB	NBF-CBH-CBP-CBA
3	A	600	BMB	CBJ-CBB-NBD-CAV
3	B	600	BMB	CBJ-CBB-NBD-CAV

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	600	BMB	CBJ-CBB-NBD-CAV
3	D	600	BMB	CBJ-CBB-NBD-CAV
3	B	600	BMB	CAW-CAV-NBD-CBB
3	A	600	BMB	CB-CA-N-CAB
3	B	600	BMB	CB-CA-N-CAB
3	C	600	BMB	CB-CA-N-CAB
3	A	600	BMB	CAV-CAW-CBM-CAX
3	B	600	BMB	CAV-CAW-CBM-CAX
3	C	600	BMB	CAV-CAW-CBM-CAX
3	D	600	BMB	CAV-CAW-CBM-CAX
3	B	600	BMB	CAV-CAW-CBM-CBQ
3	C	600	BMB	CAV-CAW-CBM-CBQ
3	B	600	BMB	CAR-CBK-CBR-CBL
3	C	600	BMB	CAR-CBK-CBR-CBL
3	A	600	BMB	CAR-CBK-CBR-CBL
3	B	600	BMB	CAQ-CBK-CBR-CBL
3	C	600	BMB	CAQ-CBK-CBR-CBL
3	A	600	BMB	NBD-CAV-CAW-CBM
3	B	600	BMB	NBD-CAV-CAW-CBM
3	C	600	BMB	NBD-CAV-CAW-CBM
3	D	600	BMB	CB-CA-N-CAB
3	A	600	BMB	C-CA-CB-CAA
3	B	600	BMB	C-CA-CB-CAA
3	C	600	BMB	C-CA-CB-CAA
3	D	600	BMB	OAD-CBH-CBP-NBS
3	D	600	BMB	CAT-CBL-CBR-NBF
3	A	600	BMB	CAQ-CBK-CBR-CBL

There are no ring outliers.

3 monomers are involved in 6 short contacts:

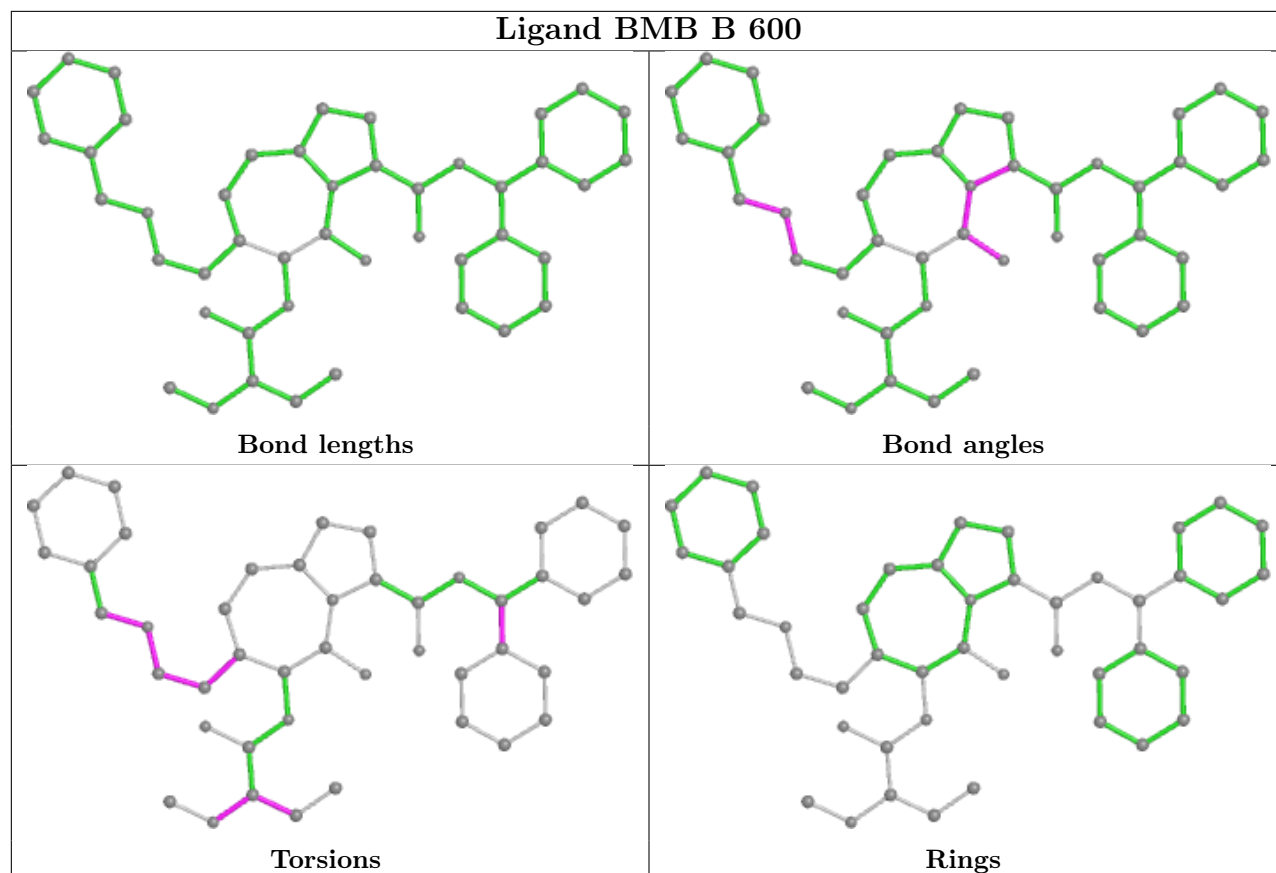| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	BMB	1	0
3	D	600	BMB	4	0
3	C	600	BMB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BMB A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand BMB D 600

Bond lengths

Bond angles

Torsions

Rings

Ligand BMB C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand BMB B 600
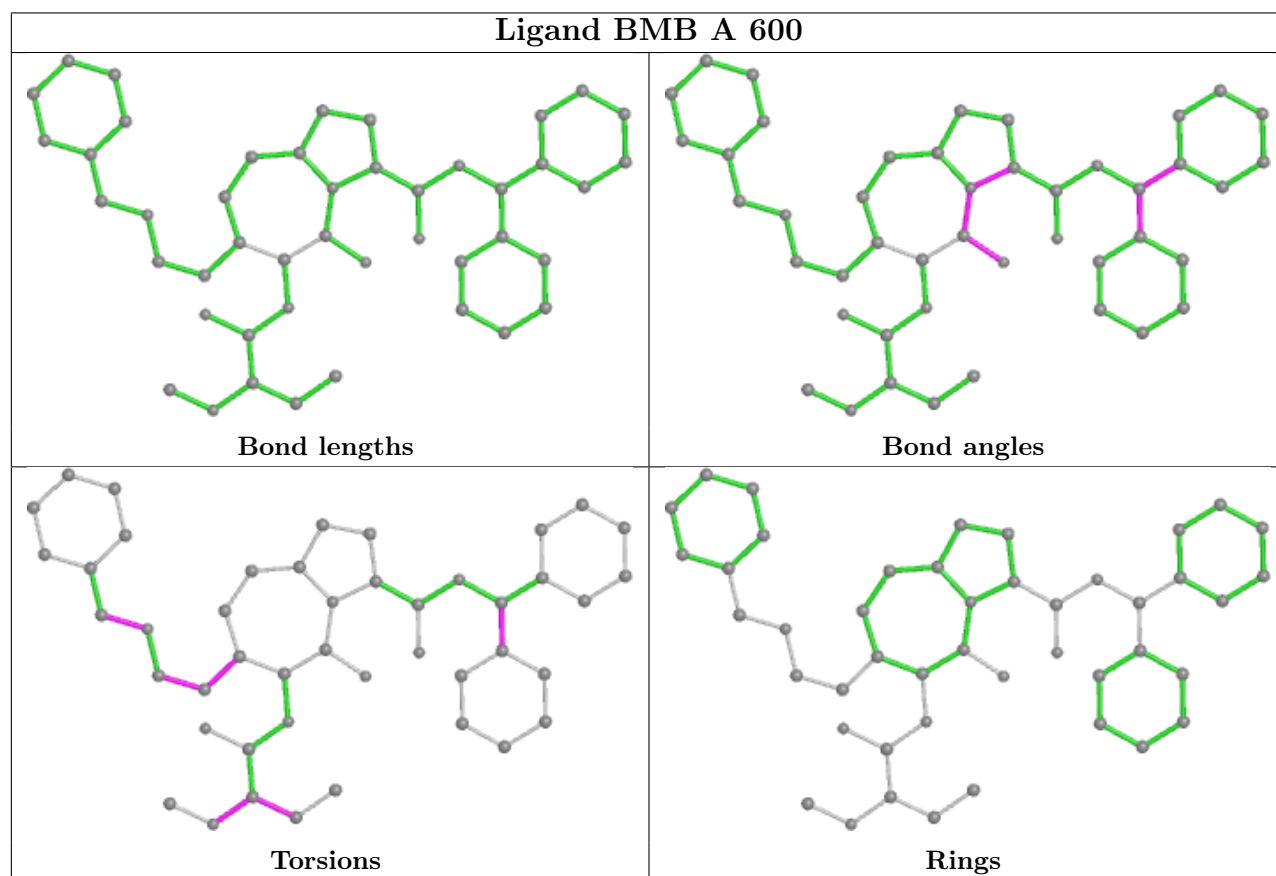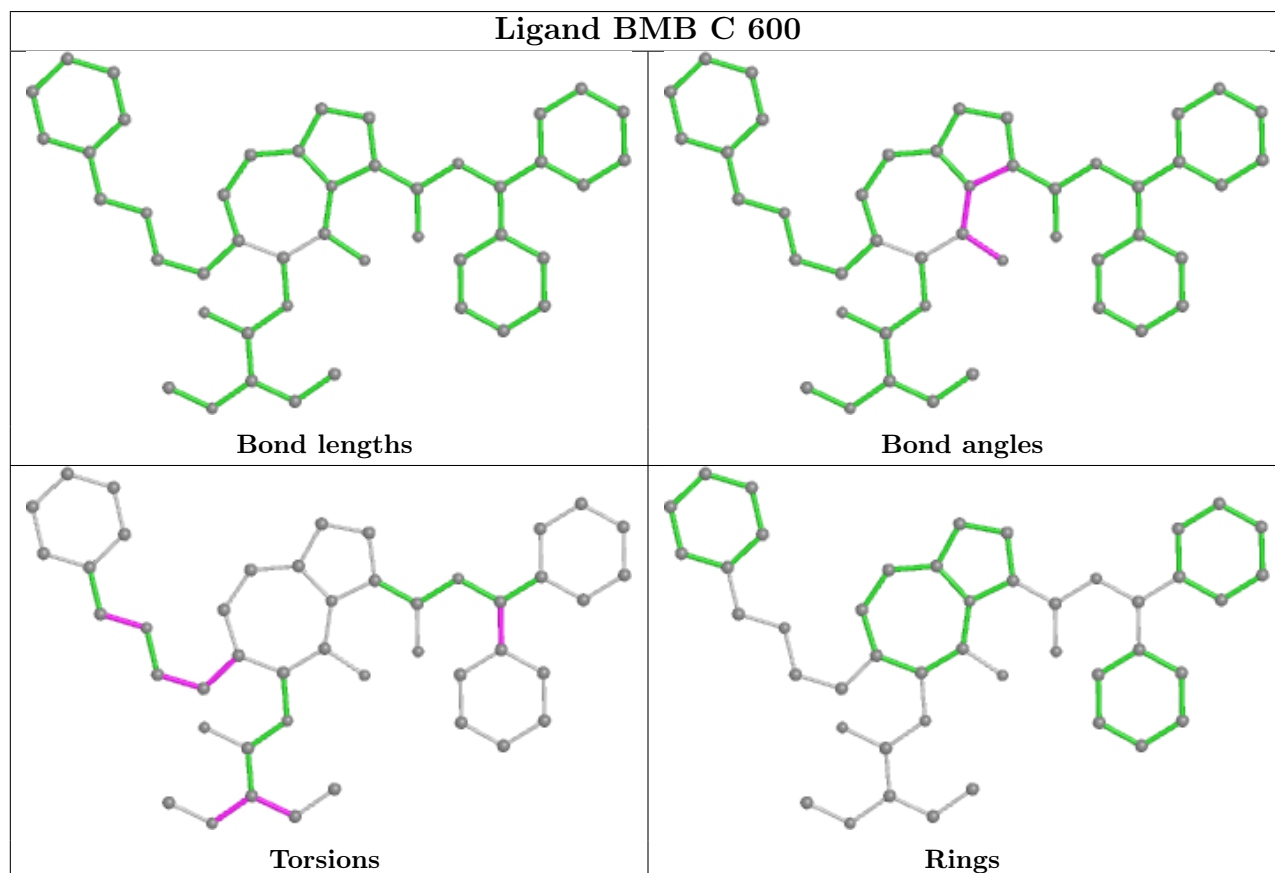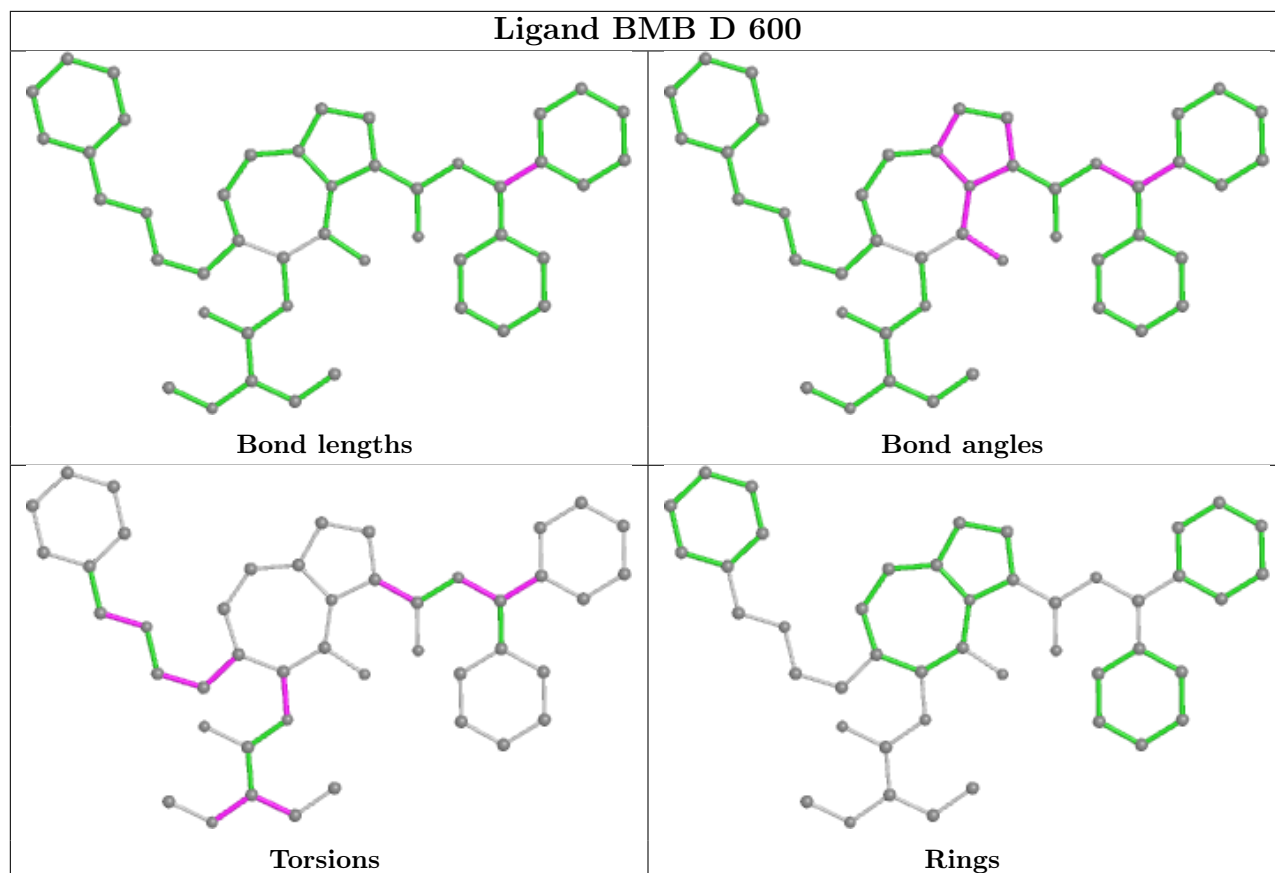
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	103/122 (84%)	0.15	0	100	100	45, 71, 114, 131	4 (3%)
1	B	104/122 (85%)	-0.08	0	100	100	41, 64, 97, 122	3 (2%)
1	C	103/122 (84%)	-0.05	0	100	100	41, 61, 96, 120	3 (2%)
1	D	102/122 (83%)	1.44	29 (28%)	0	0	77, 122, 167, 179	9 (8%)
All	All	412/488 (84%)	0.36	29 (7%)	16	5	41, 74, 149, 179	19 (4%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	271	MET	6.5
1	D	314	ASP	5.0
1	D	279	VAL	4.7
1	D	284	LEU	4.6
1	D	273	TRP	3.9
1	D	281	PRO	3.9
1	D	264	ALA	3.7
1	D	310	TRP	3.4
1	D	311	GLU	3.4
1	D	291	TYR	3.3
1	D	277	VAL	3.2
1	D	276	SER	3.0
1	D	340	ASP	3.0
1	D	292	VAL	2.9
1	D	262	THR	2.7
1	D	315	ASP	2.5
1	D	288	GLY	2.5
1	D	289	PHE	2.5
1	D	259	SER	2.4
1	D	302	CYS	2.3
1	D	316	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	301	PHE	2.3
1	D	345	ARG	2.2
1	D	319	GLU	2.2
1	D	272	TYR	2.2
1	D	338	PHE	2.2
1	D	261	GLN	2.1
1	D	337	GLU	2.1
1	D	350	LEU	2.0

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

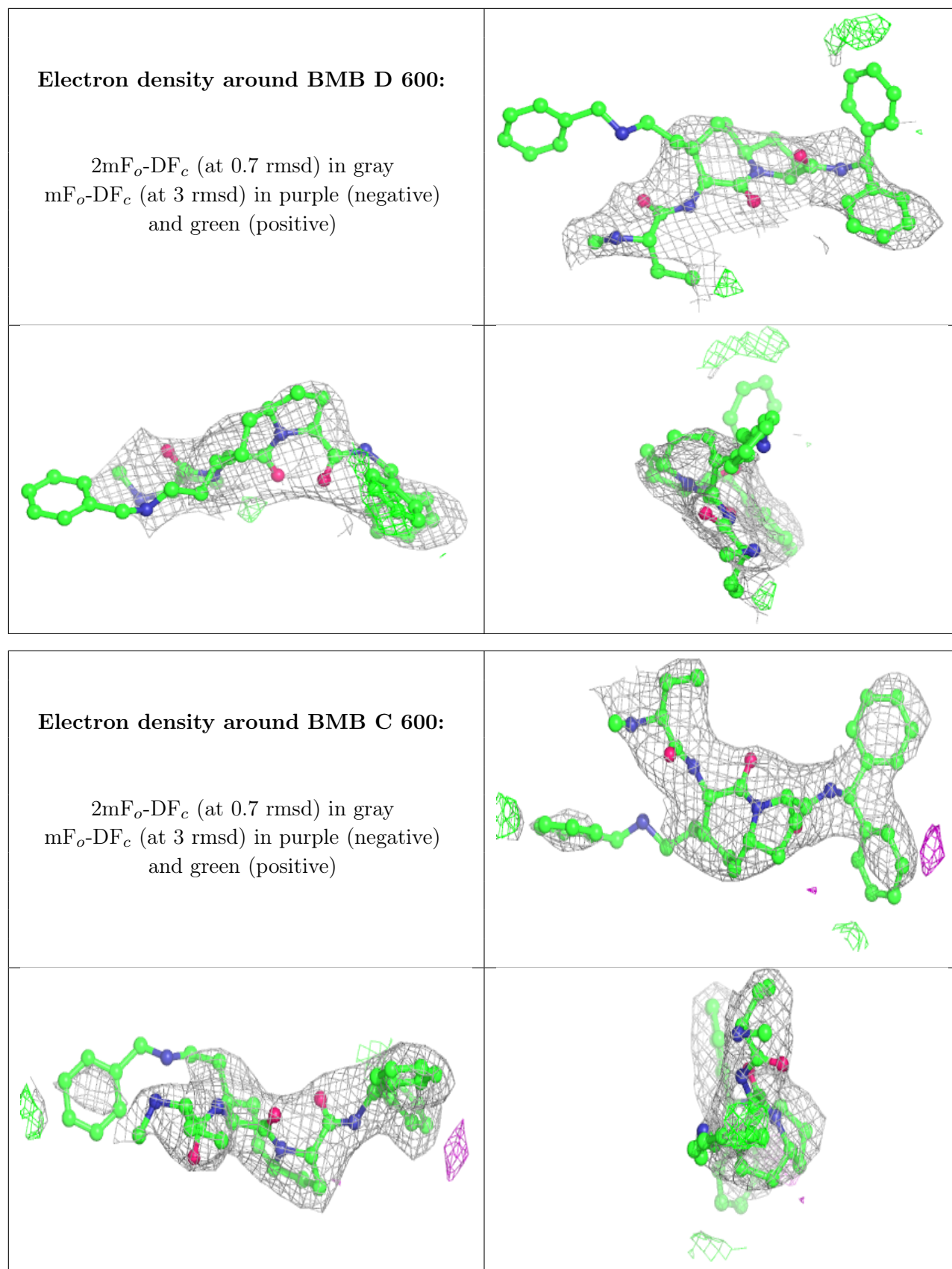There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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	BMB	D	600	45/45	0.89	0.45	62,118,264,284	0
3	BMB	C	600	45/45	0.92	0.27	19,75,216,277	0
3	BMB	A	600	45/45	0.95	0.34	16,74,197,262	0
3	BMB	B	600	45/45	0.96	0.26	16,76,239,281	0
2	ZN	B	501	1/1	0.99	0.17	55,55,55,55	0
2	ZN	D	501	1/1	0.99	0.13	100,100,100,100	0
2	ZN	A	501	1/1	0.99	0.17	59,59,59,59	0
2	ZN	C	501	1/1	1.00	0.19	53,53,53,53	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.
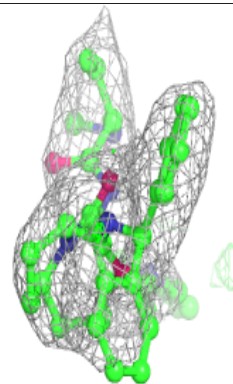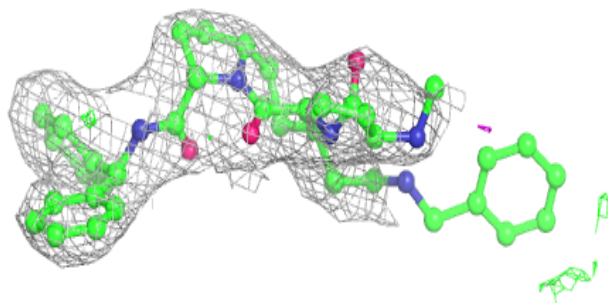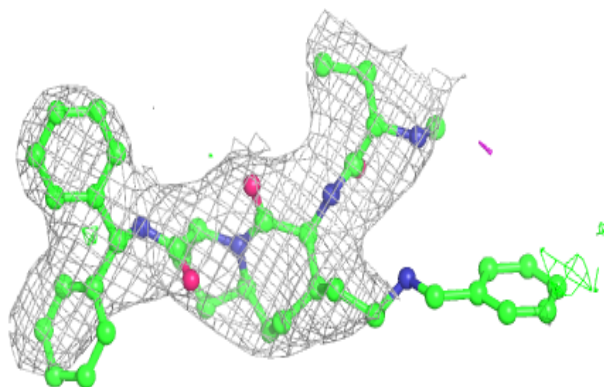
Electron density around BMB D 600:

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

Electron density around BMB C 600:

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

Electron density around BMB A 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
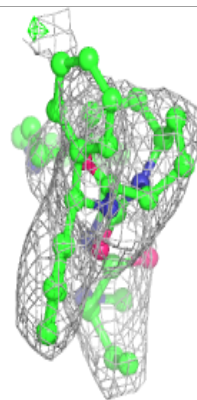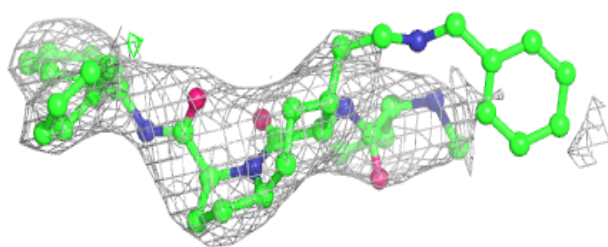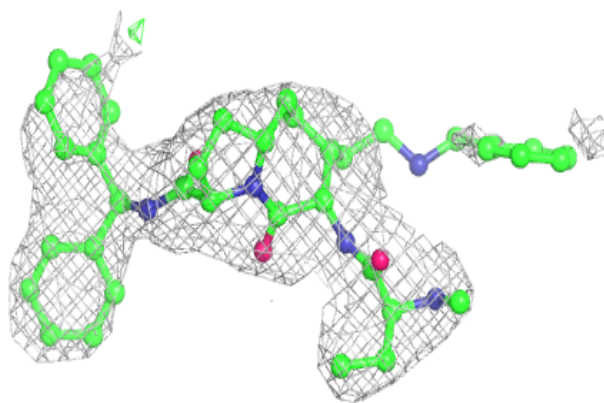
Electron density around BMB B 600:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.