



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:17 AM UTC

PDB ID : 1U1G / pdb_00001u1g
Title : Structure of E. coli uridine phosphorylase complexed to 5-(m-(benzyloxy)benzyl)barbituric acid (BBBA)
Authors : Bu, W.; Settembre, E.C.; Ealick, S.E.
Deposited on : 2004-07-15
Resolution : 1.95 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:

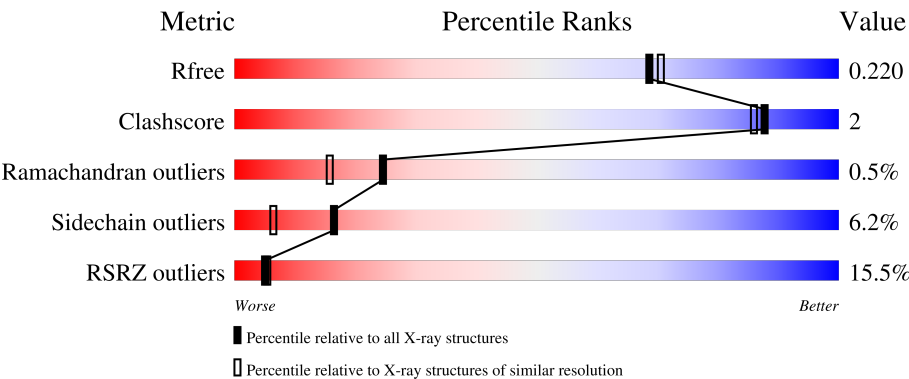
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	256	12% 89% 6% .
1	B	256	24% 89% 9% ..
1	C	256	4% 89% 8% ..
1	D	256	9% 90% 7% .
1	E	256	13% 88% 8% ..

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Mol	Chain	Length	Quality of chain
1	F	256	

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
2	K	A	1002	-	-	-	X
3	BBB	B	4300	-	X	-	-
3	BBB	E	7300	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12025 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1825	1144	316	354	11			
1	B	251	Total	C	N	O	S	0	0	0
			1879	1178	326	364	11			
1	C	250	Total	C	N	O	S	0	0	0
			1870	1172	324	363	11			
1	D	250	Total	C	N	O	S	0	0	0
			1870	1172	324	363	11			
1	E	247	Total	C	N	O	S	0	0	0
			1842	1154	320	357	11			
1	F	250	Total	C	N	O	S	0	0	0
			1870	1172	324	363	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P12758
A	-1	SER	-	cloning artifact	UNP P12758
A	0	HIS	-	cloning artifact	UNP P12758
A	1	MET	-	cloning artifact	UNP P12758
B	-2	GLY	-	cloning artifact	UNP P12758
B	-1	SER	-	cloning artifact	UNP P12758
B	0	HIS	-	cloning artifact	UNP P12758
B	1	MET	-	cloning artifact	UNP P12758
C	-2	GLY	-	cloning artifact	UNP P12758
C	-1	SER	-	cloning artifact	UNP P12758
C	0	HIS	-	cloning artifact	UNP P12758
C	1	MET	-	cloning artifact	UNP P12758
D	-2	GLY	-	cloning artifact	UNP P12758
D	-1	SER	-	cloning artifact	UNP P12758
D	0	HIS	-	cloning artifact	UNP P12758
D	1	MET	-	cloning artifact	UNP P12758
E	-2	GLY	-	cloning artifact	UNP P12758

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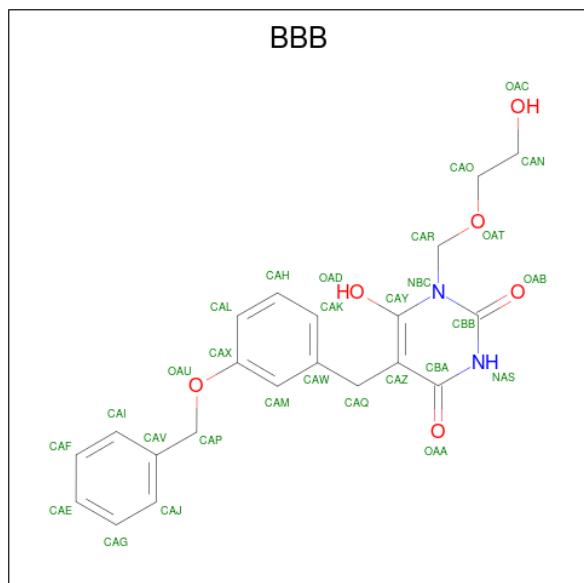
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	cloning artifact	UNP P12758
E	0	HIS	-	cloning artifact	UNP P12758
E	1	MET	-	cloning artifact	UNP P12758
F	-2	GLY	-	cloning artifact	UNP P12758
F	-1	SER	-	cloning artifact	UNP P12758
F	0	HIS	-	cloning artifact	UNP P12758
F	1	MET	-	cloning artifact	UNP P12758

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0

- Molecule 3 is 1-((2-HYDROXYETHOXY)METHYL)-5-(3-(BENZYLOXY)BENZYL)-6-HYDROXYPYRIMIDINE-2,4(1H,3H)-DIONE (CCD ID: BBB) (formula: C₂₁H₂₂N₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 29 21 2 6	0	0
3	B	1	Total C N O 29 21 2 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			29	21	2	6		
3	D	1	Total	C	N	O	0	0
			29	21	2	6		
3	E	1	Total	C	N	O	0	0
			29	21	2	6		
3	F	1	Total	C	N	O	0	0
			29	21	2	6		

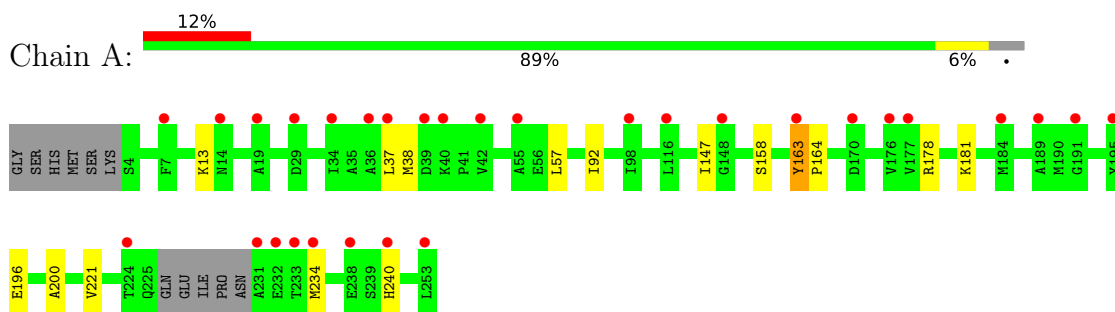
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	106	Total	O	0	0
			106	106		
4	C	147	Total	O	0	0
			147	147		
4	D	130	Total	O	0	0
			130	130		
4	E	90	Total	O	0	0
			90	90		
4	F	76	Total	O	0	0
			76	76		

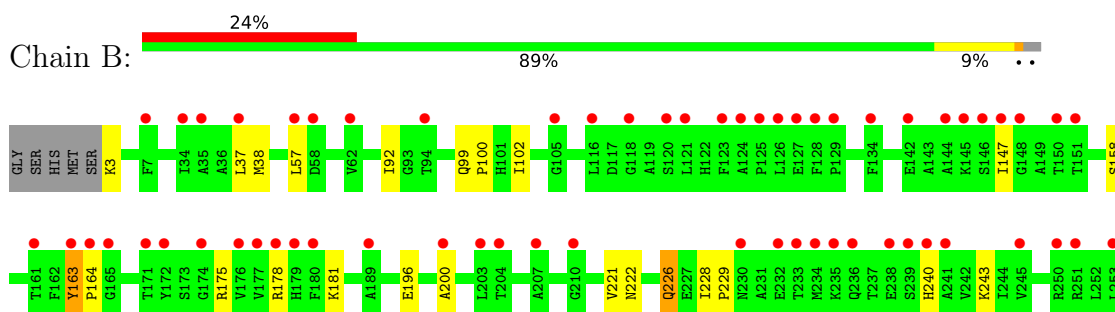
3 Residue-property plots [i](#)

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.

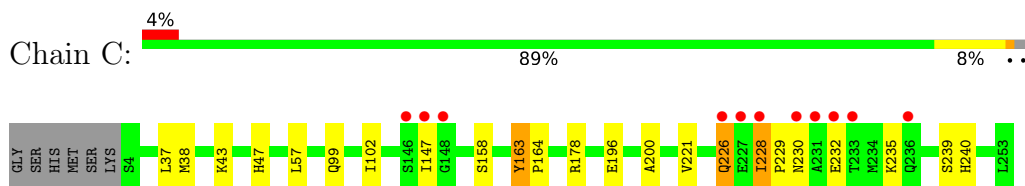
- Molecule 1: Uridine phosphorylase



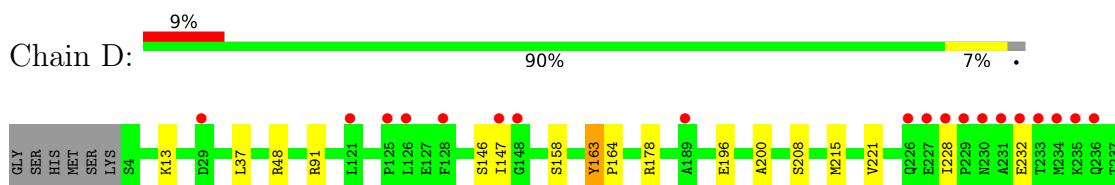
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

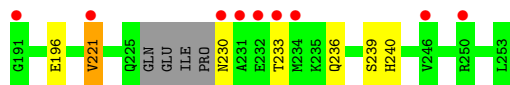
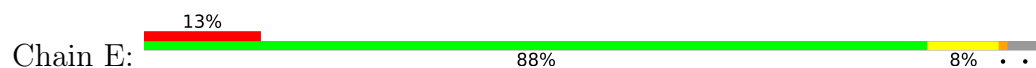


- Molecule 1: Uridine phosphorylase

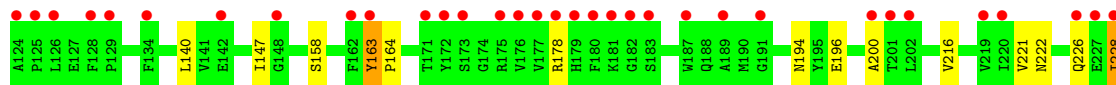
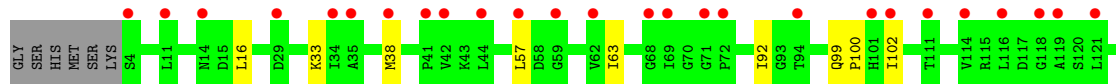
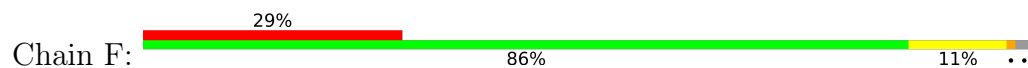




• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.68Å 127.12Å 143.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 1.95 49.39 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.39-1.95) 93.6 (49.39-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.200 , 0.221 0.199 , 0.220	Depositor DCC
R_{free} test set	8280 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	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	0.91	EDS
Total number of atoms	12025	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: K, BBB

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	0.46	0/1855	0.85	0/2519
1	B	0.45	0/1911	0.85	0/2595
1	C	0.48	0/1902	0.85	0/2584
1	D	0.48	0/1902	0.86	0/2584
1	E	0.44	0/1872	0.84	0/2541
1	F	0.43	0/1902	0.83	1/2584 (0.0%)
All	All	0.46	0/11344	0.85	1/15407 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	194	ASN	N-CA-C	5.03	115.95	108.60

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	1825	0	1813	4	0
1	B	1879	0	1876	9	0
1	C	1870	0	1863	8	0
1	D	1870	0	1862	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1842	0	1832	8	0
1	F	1870	0	1863	11	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	29	0	21	0	0
3	B	29	0	21	0	0
3	C	29	0	21	0	0
3	D	29	0	21	0	0
3	E	29	0	21	1	0
3	F	29	0	21	0	0
4	A	143	0	0	0	0
4	B	106	0	0	1	0
4	C	147	0	0	1	0
4	D	130	0	0	0	0
4	E	90	0	0	1	0
4	F	76	0	0	0	0
All	All	12025	0	11235	44	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 2.

All (44) 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:B:222:ASN:H	1:B:226:GLN:HE21	1.45	0.64
1:B:38:MET:HG2	1:B:57:LEU:HD13	1.87	0.56
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.88	0.55
1:B:175:ARG:NH2	4:B:4318:HOH:O	2.39	0.54
1:E:38:MET:HG2	1:E:57:LEU:HD13	1.90	0.54
1:F:163:TYR:HB2	1:F:164:PRO:HD3	1.92	0.51
1:A:163:TYR:HB2	1:A:164:PRO:HD3	1.93	0.51
1:A:38:MET:HG2	1:A:57:LEU:HD13	1.94	0.50
1:F:38:MET:HG2	1:F:57:LEU:HD13	1.94	0.50
1:E:230:ASN:HD22	1:E:233:THR:H	1.61	0.49
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.94	0.48
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.96	0.48
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.94	0.48
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.96	0.48
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.44	0.48
1:F:241:ALA:HA	1:F:244:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:HIS:HE1	4:C:5386:HOH:O	1.97	0.47
1:C:38:MET:HG2	1:C:57:LEU:HD13	1.96	0.47
1:B:99:GLN:HB2	1:B:102:ILE:HD12	1.99	0.45
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.99	0.45
1:C:99:GLN:HB2	1:C:102:ILE:HD12	1.98	0.45
1:D:163:TYR:HB2	1:D:164:PRO:HD3	1.99	0.45
1:D:163:TYR:HB2	1:D:164:PRO:CD	2.46	0.45
1:F:163:TYR:HB2	1:F:164:PRO:CD	2.47	0.45
1:F:228:ILE:HA	1:F:229:PRO:HD3	1.84	0.44
1:C:163:TYR:HB2	1:C:164:PRO:CD	2.48	0.43
1:D:91:ARG:HG2	1:D:215:MET:SD	2.59	0.43
1:C:163:TYR:HB2	1:C:164:PRO:HD3	2.00	0.43
1:A:163:TYR:HB2	1:A:164:PRO:CD	2.48	0.43
1:E:9:LEU:HB3	1:E:11:LEU:HD12	2.01	0.43
1:A:158:SER:HB3	1:A:200:ALA:HB2	2.01	0.42
1:B:99:GLN:HA	1:B:100:PRO:HD3	1.91	0.42
1:C:228:ILE:HA	1:C:229:PRO:HD3	1.82	0.42
1:B:163:TYR:HB2	1:B:164:PRO:CD	2.50	0.42
1:F:99:GLN:HB2	1:F:102:ILE:HD12	2.02	0.42
1:C:226:GLN:HE21	1:C:226:GLN:HB2	1.64	0.42
1:D:208:SER:HB2	1:E:190:MET:HG2	2.02	0.41
1:F:140:LEU:HD22	1:F:216:VAL:HB	2.02	0.41
1:B:228:ILE:HA	1:B:229:PRO:HD3	1.86	0.41
1:F:102:ILE:O	1:F:222:ASN:ND2	2.54	0.41
1:E:175:ARG:NH1	4:E:7341:HOH:O	2.53	0.40
1:F:16:LEU:HD22	1:F:63:ILE:HG13	2.02	0.40
1:E:221:VAL:HG11	3:E:7300:BBB:HAK	2.04	0.40
1:F:99:GLN:HA	1:F:100:PRO:HD3	1.91	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	241/256 (94%)	237 (98%)	3 (1%)	1 (0%)	30	21
1	B	249/256 (97%)	246 (99%)	2 (1%)	1 (0%)	30	21
1	C	248/256 (97%)	245 (99%)	2 (1%)	1 (0%)	30	21
1	D	248/256 (97%)	245 (99%)	2 (1%)	1 (0%)	30	21
1	E	243/256 (95%)	238 (98%)	4 (2%)	1 (0%)	30	21
1	F	248/256 (97%)	238 (96%)	8 (3%)	2 (1%)	16	8
All	All	1477/1536 (96%)	1449 (98%)	21 (1%)	7 (0%)	24	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	TYR
1	B	163	TYR
1	C	163	TYR
1	D	163	TYR
1	E	163	TYR
1	F	163	TYR
1	F	229	PRO

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	193/206 (94%)	183 (95%)	10 (5%)	21	9
1	B	200/206 (97%)	189 (94%)	11 (6%)	19	8
1	C	199/206 (97%)	186 (94%)	13 (6%)	15	6
1	D	199/206 (97%)	186 (94%)	13 (6%)	15	6
1	E	195/206 (95%)	182 (93%)	13 (7%)	15	5
1	F	199/206 (97%)	186 (94%)	13 (6%)	15	6
All	All	1185/1236 (96%)	1112 (94%)	73 (6%)	16	6

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	37	LEU
1	A	92	ILE
1	A	147	ILE
1	A	178	ARG
1	A	181	LYS
1	A	196	GLU
1	A	221	VAL
1	A	234	MET
1	A	240	HIS
1	B	3	LYS
1	B	37	LEU
1	B	92	ILE
1	B	147	ILE
1	B	178	ARG
1	B	181	LYS
1	B	196	GLU
1	B	221	VAL
1	B	226	GLN
1	B	240	HIS
1	B	243	LYS
1	C	37	LEU
1	C	43	LYS
1	C	147	ILE
1	C	178	ARG
1	C	196	GLU
1	C	221	VAL
1	C	226	GLN
1	C	228	ILE
1	C	230	ASN
1	C	232	GLU
1	C	235	LYS
1	C	239	SER
1	C	240	HIS
1	D	13	LYS
1	D	37	LEU
1	D	48	ARG
1	D	146	SER
1	D	147	ILE
1	D	178	ARG
1	D	196	GLU
1	D	221	VAL
1	D	228	ILE

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Mol	Chain	Res	Type
1	D	232	GLU
1	D	239	SER
1	D	240	HIS
1	D	243	LYS
1	E	3	LYS
1	E	13	LYS
1	E	14	ASN
1	E	37	LEU
1	E	92	ILE
1	E	146	SER
1	E	147	ILE
1	E	181	LYS
1	E	196	GLU
1	E	221	VAL
1	E	236	GLN
1	E	239	SER
1	E	240	HIS
1	F	33	LYS
1	F	92	ILE
1	F	147	ILE
1	F	178	ARG
1	F	196	GLU
1	F	221	VAL
1	F	226	GLN
1	F	228	ILE
1	F	233	THR
1	F	239	SER
1	F	240	HIS
1	F	245	VAL
1	F	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	B	47	HIS
1	B	101	HIS
1	B	226	GLN
1	C	17	GLN
1	C	47	HIS
1	C	101	HIS
1	C	226	GLN

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Mol	Chain	Res	Type
1	C	230	ASN
1	D	47	HIS
1	E	17	GLN
1	E	47	HIS
1	E	101	HIS
1	E	152	HIS
1	E	230	ASN
1	F	17	GLN
1	F	101	HIS
1	F	152	HIS
1	F	225	GLN
1	F	236	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	BBB	B	4300	-	31,31,31	2.71	22 (70%)	36,41,41	3.01	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BBB	D	6300	-	31,31,31	2.71	22 (70%)	36,41,41	3.06	8 (22%)
3	BBB	F	8300	-	31,31,31	2.70	22 (70%)	36,41,41	3.05	9 (25%)
3	BBB	E	7300	-	31,31,31	2.70	22 (70%)	36,41,41	3.13	11 (30%)
3	BBB	C	5300	-	31,31,31	2.69	22 (70%)	36,41,41	3.07	9 (25%)
3	BBB	A	3300	-	31,31,31	2.71	22 (70%)	36,41,41	3.08	9 (25%)

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	BBB	B	4300	-	-	4/14/14/14	0/3/3/3
3	BBB	D	6300	-	-	3/14/14/14	0/3/3/3
3	BBB	F	8300	-	-	3/14/14/14	0/3/3/3
3	BBB	E	7300	-	-	3/14/14/14	0/3/3/3
3	BBB	C	5300	-	-	3/14/14/14	0/3/3/3
3	BBB	A	3300	-	-	4/14/14/14	0/3/3/3

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4300	BBB	CAQ-CAZ	4.41	1.57	1.51
3	F	8300	BBB	CAQ-CAZ	4.35	1.57	1.51
3	C	5300	BBB	CAQ-CAZ	4.34	1.57	1.51
3	A	3300	BBB	CAQ-CAZ	4.33	1.57	1.51
3	D	6300	BBB	CAQ-CAZ	4.31	1.57	1.51
3	E	7300	BBB	CAQ-CAZ	4.30	1.57	1.51
3	C	5300	BBB	CAM-CAX	4.27	1.46	1.39
3	D	6300	BBB	CAM-CAX	4.23	1.46	1.39
3	E	7300	BBB	CAM-CAX	4.20	1.45	1.39
3	A	3300	BBB	CAM-CAX	4.17	1.45	1.39
3	F	8300	BBB	CAM-CAX	4.12	1.45	1.39
3	B	4300	BBB	CAM-CAX	4.07	1.45	1.39
3	B	4300	BBB	CAP-CAV	-3.84	1.41	1.50
3	C	5300	BBB	CAP-CAV	-3.83	1.41	1.50
3	D	6300	BBB	CAP-CAV	-3.82	1.41	1.50
3	A	3300	BBB	CAP-CAV	-3.81	1.41	1.50
3	F	8300	BBB	CAP-CAV	-3.81	1.41	1.50
3	E	7300	BBB	CAP-CAV	-3.78	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4300	BBB	CBB-NBC	3.62	1.44	1.39
3	F	8300	BBB	CBB-NBC	3.57	1.43	1.39
3	A	3300	BBB	CBB-NBC	3.55	1.43	1.39
3	E	7300	BBB	CBB-NBC	3.52	1.43	1.39
3	A	3300	BBB	CAF-CAI	3.47	1.44	1.38
3	B	4300	BBB	CAF-CAI	3.47	1.44	1.38
3	C	5300	BBB	CAF-CAI	3.45	1.44	1.38
3	D	6300	BBB	CAF-CAI	3.44	1.44	1.38
3	E	7300	BBB	CAF-CAI	3.44	1.44	1.38
3	C	5300	BBB	CBB-NBC	3.44	1.43	1.39
3	D	6300	BBB	CBB-NBC	3.43	1.43	1.39
3	F	8300	BBB	CAF-CAI	3.43	1.44	1.38
3	D	6300	BBB	CAG-CAJ	3.42	1.44	1.38
3	A	3300	BBB	CAH-CAK	3.41	1.44	1.38
3	C	5300	BBB	CAG-CAJ	3.39	1.44	1.38
3	B	4300	BBB	CAH-CAK	3.38	1.44	1.38
3	D	6300	BBB	CAE-CAG	3.38	1.45	1.38
3	B	4300	BBB	CAG-CAJ	3.38	1.44	1.38
3	E	7300	BBB	CAG-CAJ	3.38	1.44	1.38
3	F	8300	BBB	CAL-CAX	3.37	1.45	1.38
3	B	4300	BBB	CAE-CAG	3.37	1.45	1.38
3	F	8300	BBB	CAE-CAG	3.36	1.45	1.38
3	A	3300	BBB	CAL-CAX	3.35	1.45	1.38
3	D	6300	BBB	CAH-CAK	3.35	1.44	1.38
3	E	7300	BBB	CAH-CAK	3.35	1.44	1.38
3	B	4300	BBB	CAL-CAX	3.35	1.45	1.38
3	A	3300	BBB	CAG-CAJ	3.35	1.44	1.38
3	A	3300	BBB	CAI-CAV	3.35	1.45	1.38
3	D	6300	BBB	CAL-CAX	3.34	1.45	1.38
3	E	7300	BBB	CAE-CAG	3.34	1.45	1.38
3	F	8300	BBB	CAH-CAK	3.34	1.44	1.38
3	A	3300	BBB	CAE-CAG	3.34	1.45	1.38
3	D	6300	BBB	CAJ-CAV	3.33	1.45	1.38
3	C	5300	BBB	CAI-CAV	3.33	1.45	1.38
3	F	8300	BBB	CAG-CAJ	3.32	1.44	1.38
3	A	3300	BBB	CAJ-CAV	3.32	1.45	1.38
3	E	7300	BBB	CAI-CAV	3.32	1.45	1.38
3	F	8300	BBB	CAI-CAV	3.31	1.45	1.38
3	D	6300	BBB	CAI-CAV	3.30	1.45	1.38
3	C	5300	BBB	CAE-CAG	3.30	1.45	1.38
3	E	7300	BBB	CAL-CAX	3.30	1.44	1.38
3	C	5300	BBB	CAJ-CAV	3.30	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4300	BBB	CAI-CAV	3.29	1.45	1.38
3	C	5300	BBB	CAH-CAK	3.29	1.44	1.38
3	B	4300	BBB	CAJ-CAV	3.28	1.45	1.38
3	F	8300	BBB	CAJ-CAV	3.28	1.45	1.38
3	C	5300	BBB	CAL-CAX	3.25	1.44	1.38
3	E	7300	BBB	CAJ-CAV	3.25	1.45	1.38
3	D	6300	BBB	CAF-CAE	3.07	1.45	1.38
3	B	4300	BBB	CAF-CAE	3.06	1.45	1.38
3	E	7300	BBB	CAK-CAW	3.04	1.44	1.38
3	C	5300	BBB	CAF-CAE	3.02	1.44	1.38
3	F	8300	BBB	CAF-CAE	3.00	1.44	1.38
3	E	7300	BBB	CAF-CAE	2.99	1.44	1.38
3	A	3300	BBB	CAF-CAE	2.99	1.44	1.38
3	A	3300	BBB	CAM-CAW	2.98	1.44	1.39
3	B	4300	BBB	CAK-CAW	2.98	1.44	1.38
3	E	7300	BBB	CAM-CAW	2.98	1.44	1.39
3	A	3300	BBB	CAK-CAW	2.97	1.44	1.38
3	D	6300	BBB	CAK-CAW	2.96	1.44	1.38
3	F	8300	BBB	CAH-CAL	2.96	1.44	1.38
3	D	6300	BBB	CAM-CAW	2.95	1.44	1.39
3	F	8300	BBB	CAK-CAW	2.95	1.44	1.38
3	C	5300	BBB	CAM-CAW	2.94	1.44	1.39
3	C	5300	BBB	CAK-CAW	2.92	1.44	1.38
3	E	7300	BBB	CAH-CAL	2.90	1.43	1.38
3	A	3300	BBB	CAH-CAL	2.89	1.43	1.38
3	B	4300	BBB	CAH-CAL	2.89	1.43	1.38
3	B	4300	BBB	CAZ-CAY	2.88	1.43	1.36
3	B	4300	BBB	CAM-CAW	2.88	1.44	1.39
3	F	8300	BBB	CAM-CAW	2.86	1.44	1.39
3	D	6300	BBB	CAH-CAL	2.86	1.43	1.38
3	C	5300	BBB	CAH-CAL	2.86	1.43	1.38
3	A	3300	BBB	OAU-CAP	2.84	1.52	1.43
3	E	7300	BBB	CAZ-CAY	2.84	1.43	1.36
3	D	6300	BBB	CAZ-CAY	2.83	1.43	1.36
3	E	7300	BBB	OAU-CAP	2.83	1.52	1.43
3	F	8300	BBB	CAZ-CAY	2.82	1.43	1.36
3	F	8300	BBB	OAU-CAP	2.82	1.52	1.43
3	B	4300	BBB	OAU-CAP	2.81	1.52	1.43
3	C	5300	BBB	OAU-CAP	2.80	1.52	1.43
3	D	6300	BBB	OAU-CAP	2.78	1.52	1.43
3	A	3300	BBB	CAZ-CAY	2.75	1.43	1.36
3	C	5300	BBB	CAZ-CAY	2.75	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3300	BBB	CBB-NAS	2.56	1.42	1.38
3	B	4300	BBB	CBB-NAS	2.51	1.42	1.38
3	D	6300	BBB	CAR-NBC	-2.50	1.41	1.46
3	D	6300	BBB	CBB-NAS	2.45	1.42	1.38
3	E	7300	BBB	CBB-NAS	2.43	1.42	1.38
3	F	8300	BBB	CBB-NAS	2.43	1.42	1.38
3	C	5300	BBB	CBB-NAS	2.42	1.42	1.38
3	F	8300	BBB	CAR-NBC	-2.42	1.41	1.46
3	B	4300	BBB	CAR-NBC	-2.40	1.41	1.46
3	C	5300	BBB	CAR-NBC	-2.39	1.41	1.46
3	E	7300	BBB	CAR-NBC	-2.36	1.41	1.46
3	A	3300	BBB	CAR-NBC	-2.35	1.41	1.46
3	E	7300	BBB	CAQ-CAW	2.33	1.55	1.51
3	A	3300	BBB	CAQ-CAW	2.32	1.55	1.51
3	D	6300	BBB	CAQ-CAW	2.29	1.55	1.51
3	B	4300	BBB	CAQ-CAW	2.27	1.55	1.51
3	C	5300	BBB	CAQ-CAW	2.24	1.55	1.51
3	F	8300	BBB	CAQ-CAW	2.23	1.55	1.51
3	A	3300	BBB	CBA-NAS	2.17	1.42	1.38
3	D	6300	BBB	CBA-NAS	2.10	1.42	1.38
3	B	4300	BBB	CBA-NAS	2.07	1.42	1.38
3	E	7300	BBB	CBA-NAS	2.07	1.42	1.38
3	F	8300	BBB	CBA-NAS	2.06	1.42	1.38
3	A	3300	BBB	CAY-NBC	2.06	1.45	1.39
3	C	5300	BBB	CAY-NBC	2.05	1.45	1.39
3	C	5300	BBB	CBA-NAS	2.05	1.42	1.38
3	F	8300	BBB	CAY-NBC	2.05	1.45	1.39
3	B	4300	BBB	CAY-NBC	2.04	1.45	1.39
3	E	7300	BBB	CAY-NBC	2.02	1.45	1.39
3	D	6300	BBB	CAY-NBC	2.01	1.45	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7300	BBB	CAP-OAU-CAX	13.25	149.18	117.62
3	D	6300	BBB	CAP-OAU-CAX	13.04	148.68	117.62
3	C	5300	BBB	CAP-OAU-CAX	12.94	148.43	117.62
3	A	3300	BBB	CAP-OAU-CAX	12.82	148.16	117.62
3	F	8300	BBB	CAP-OAU-CAX	12.74	147.97	117.62
3	B	4300	BBB	CAP-OAU-CAX	12.56	147.53	117.62
3	D	6300	BBB	CAZ-CBA-NAS	8.14	121.88	115.70
3	A	3300	BBB	CAZ-CBA-NAS	7.98	121.76	115.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7300	BBB	CAZ-CBA-NAS	7.90	121.70	115.70
3	B	4300	BBB	CAZ-CBA-NAS	7.89	121.69	115.70
3	F	8300	BBB	CAZ-CBA-NAS	7.78	121.61	115.70
3	C	5300	BBB	CAZ-CBA-NAS	7.72	121.57	115.70
3	E	7300	BBB	OAD-CAY-CAZ	-5.16	118.49	124.64
3	A	3300	BBB	OAD-CAY-CAZ	-5.13	118.53	124.64
3	C	5300	BBB	OAD-CAY-CAZ	-5.05	118.62	124.64
3	F	8300	BBB	OAD-CAY-CAZ	-4.90	118.81	124.64
3	B	4300	BBB	OAD-CAY-CAZ	-4.79	118.94	124.64
3	D	6300	BBB	CBA-NAS-CBB	-4.69	121.19	127.34
3	D	6300	BBB	OAD-CAY-CAZ	-4.64	119.11	124.64
3	A	3300	BBB	CBA-NAS-CBB	-4.62	121.29	127.34
3	E	7300	BBB	CBA-NAS-CBB	-4.57	121.35	127.34
3	F	8300	BBB	CBA-NAS-CBB	-4.56	121.36	127.34
3	C	5300	BBB	CBA-NAS-CBB	-4.48	121.47	127.34
3	B	4300	BBB	CBA-NAS-CBB	-4.47	121.47	127.34
3	C	5300	BBB	CBB-NBC-CAY	-3.64	119.18	122.49
3	F	8300	BBB	CBB-NBC-CAY	-3.62	119.20	122.49
3	A	3300	BBB	OAT-CAR-NBC	3.58	119.81	111.46
3	B	4300	BBB	CBB-NBC-CAY	-3.53	119.28	122.49
3	C	5300	BBB	OAT-CAR-NBC	3.49	119.61	111.46
3	E	7300	BBB	CBB-NBC-CAY	-3.49	119.32	122.49
3	F	8300	BBB	OAT-CAR-NBC	3.49	119.59	111.46
3	E	7300	BBB	OAT-CAR-NBC	3.48	119.59	111.46
3	A	3300	BBB	CBB-NBC-CAY	-3.43	119.38	122.49
3	B	4300	BBB	OAT-CAR-NBC	3.30	119.17	111.46
3	D	6300	BBB	CBB-NBC-CAY	-3.15	119.63	122.49
3	D	6300	BBB	OAT-CAR-NBC	3.09	118.66	111.46
3	A	3300	BBB	OAA-CBA-CAZ	-2.33	121.69	124.56
3	C	5300	BBB	CAZ-CAY-NBC	2.27	122.62	120.48
3	F	8300	BBB	OAB-CBB-NAS	-2.25	117.34	121.49
3	B	4300	BBB	CAZ-CAY-NBC	2.24	122.59	120.48
3	A	3300	BBB	CAZ-CAY-NBC	2.20	122.56	120.48
3	E	7300	BBB	CAZ-CAY-NBC	2.20	122.55	120.48
3	B	4300	BBB	OAB-CBB-NAS	-2.18	117.46	121.49
3	F	8300	BBB	CAZ-CAY-NBC	2.15	122.50	120.48
3	D	6300	BBB	OAA-CBA-NAS	-2.15	116.08	120.11
3	E	7300	BBB	OAU-CAP-CAV	2.11	115.36	109.16
3	F	8300	BBB	OAA-CBA-NAS	-2.10	116.17	120.11
3	C	5300	BBB	OAA-CBA-CAZ	-2.09	121.98	124.56
3	E	7300	BBB	OAA-CBA-CAZ	-2.09	121.98	124.56
3	A	3300	BBB	OAB-CBB-NAS	-2.09	117.64	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4300	BBB	OAA-CBA-NAS	-2.08	116.21	120.11
3	E	7300	BBB	OAB-CBB-NAS	-2.07	117.67	121.49
3	D	6300	BBB	OAA-CBA-CAZ	-2.07	122.02	124.56
3	C	5300	BBB	OAB-CBB-NAS	-2.06	117.69	121.49
3	E	7300	BBB	OAA-CBA-NAS	-2.02	116.31	120.11
3	B	4300	BBB	OAA-CBA-CAZ	-2.01	122.09	124.56

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	6300	BBB	CAV-CAP-OAU-CAX
3	D	6300	BBB	CAL-CAX-OAU-CAP
3	B	4300	BBB	CAV-CAP-OAU-CAX
3	F	8300	BBB	CAV-CAP-OAU-CAX
3	B	4300	BBB	CAL-CAX-OAU-CAP
3	F	8300	BBB	CAL-CAX-OAU-CAP
3	D	6300	BBB	CAM-CAX-OAU-CAP
3	A	3300	BBB	CAL-CAX-OAU-CAP
3	F	8300	BBB	CAM-CAX-OAU-CAP
3	A	3300	BBB	CAM-CAX-OAU-CAP
3	B	4300	BBB	CAM-CAX-OAU-CAP
3	A	3300	BBB	CAV-CAP-OAU-CAX
3	C	5300	BBB	CAL-CAX-OAU-CAP
3	E	7300	BBB	CAV-CAP-OAU-CAX
3	E	7300	BBB	CAL-CAX-OAU-CAP
3	E	7300	BBB	CAM-CAX-OAU-CAP
3	C	5300	BBB	CAM-CAX-OAU-CAP
3	C	5300	BBB	CAV-CAP-OAU-CAX
3	A	3300	BBB	OAC-CAN-CAO-OAT
3	B	4300	BBB	OAC-CAN-CAO-OAT

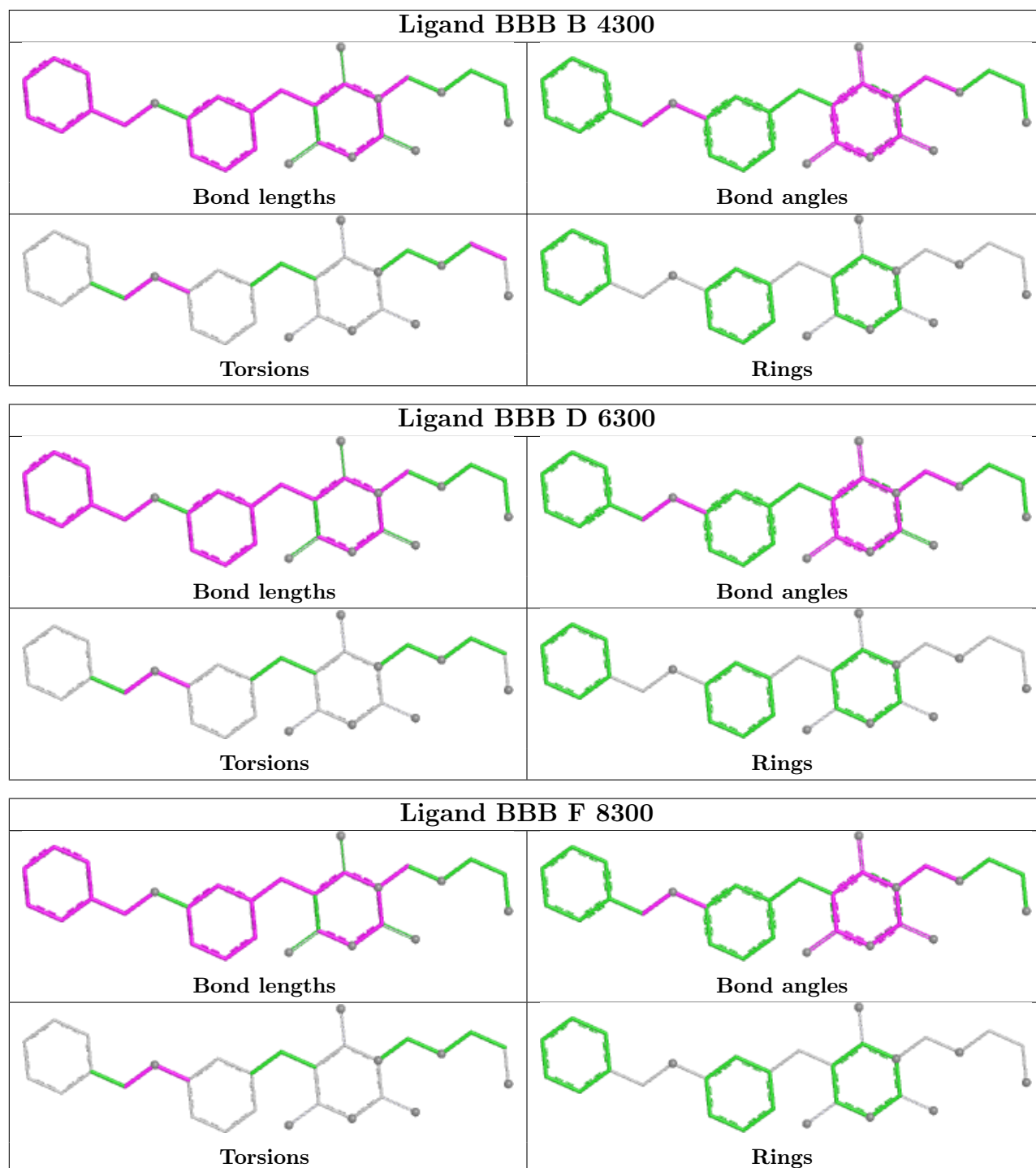
There are no ring outliers.

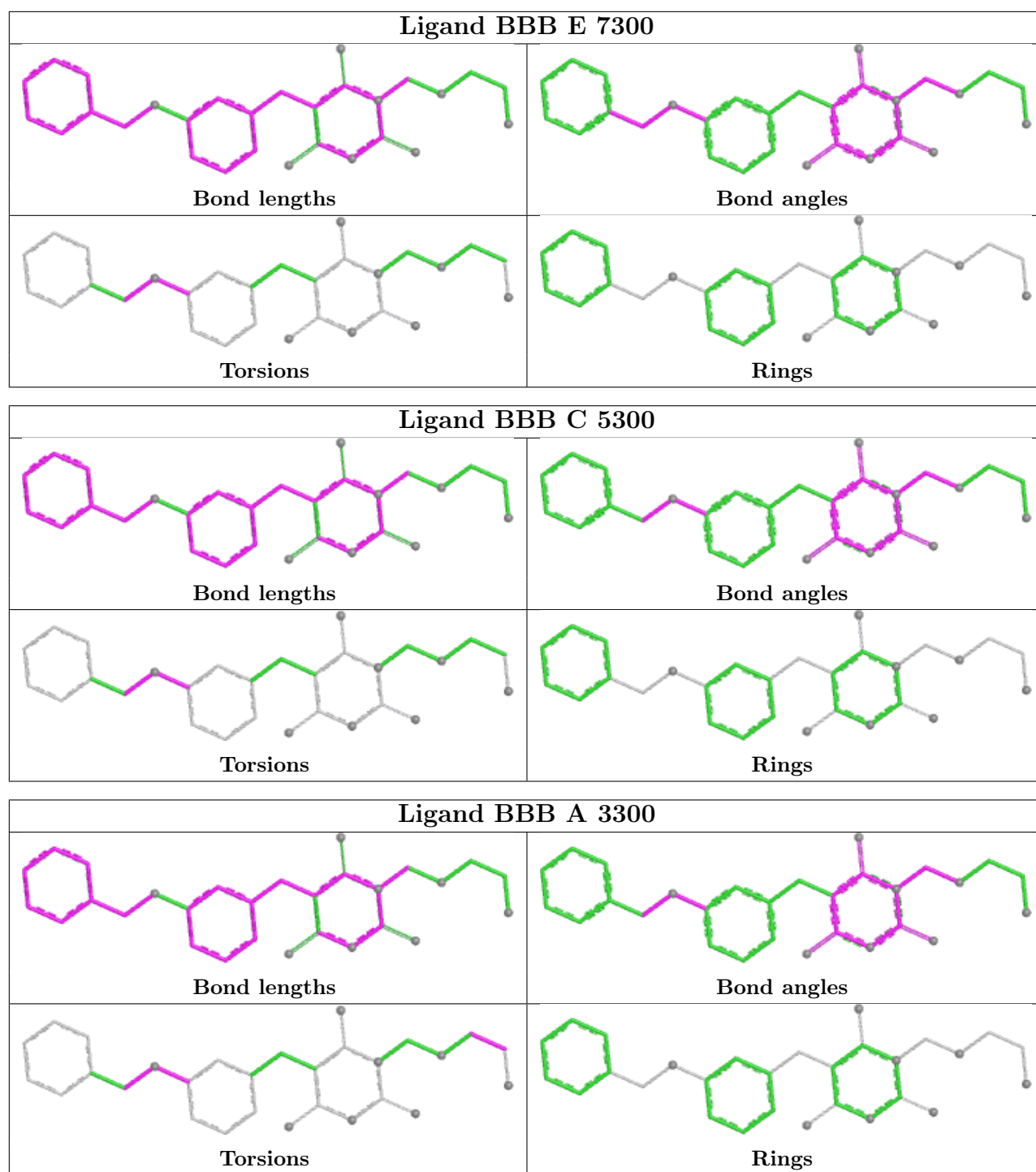
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7300	BBB	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	245/256 (95%)	0.90	30 (12%)	8 10	13, 14, 18, 24	0
1	B	251/256 (98%)	1.45	61 (24%)	2 2	12, 14, 17, 21	0
1	C	250/256 (97%)	0.33	11 (4%)	39 45	12, 14, 21, 24	0
1	D	250/256 (97%)	0.66	22 (8%)	15 18	12, 14, 21, 24	0
1	E	247/256 (96%)	1.07	33 (13%)	7 8	13, 15, 17, 21	0
1	F	250/256 (97%)	1.60	74 (29%)	1 1	13, 15, 18, 20	0
All	All	1493/1536 (97%)	1.00	231 (15%)	5 5	12, 14, 18, 24	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	229	PRO	5.7
1	B	121	LEU	5.1
1	D	228	ILE	4.9
1	F	126	LEU	4.8
1	B	125	PRO	4.6
1	F	121	LEU	4.5
1	F	228	ILE	4.5
1	B	177	VAL	4.5
1	F	230	ASN	4.4
1	B	148	GLY	4.3
1	B	126	LEU	4.2
1	A	189	ALA	4.2
1	F	180	PHE	4.2
1	B	232	GLU	4.2
1	B	172	TYR	4.1
1	F	71	GLY	3.9
1	B	147	ILE	3.9
1	F	236	GLN	3.9
1	B	118	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	227	GLU	3.9
1	D	232	GLU	3.8
1	A	14	ASN	3.8
1	B	234	MET	3.7
1	D	230	ASN	3.7
1	D	227	GLU	3.7
1	F	59	GLY	3.6
1	A	238	GLU	3.6
1	D	236	GLN	3.6
1	F	229	PRO	3.6
1	E	4	SER	3.6
1	B	124	ALA	3.6
1	B	171	THR	3.5
1	A	176	VAL	3.5
1	A	36	ALA	3.5
1	D	235	LYS	3.5
1	F	125	PRO	3.4
1	F	181	LYS	3.4
1	F	177	VAL	3.4
1	F	148	GLY	3.4
1	B	233	THR	3.4
1	F	182	GLY	3.4
1	B	241	ALA	3.3
1	B	128	PHE	3.3
1	A	148	GLY	3.3
1	D	234	MET	3.3
1	B	180	PHE	3.3
1	B	144	ALA	3.2
1	B	151	THR	3.2
1	E	182	GLY	3.2
1	A	170	ASP	3.2
1	E	147	ILE	3.1
1	F	233	THR	3.1
1	A	234	MET	3.1
1	E	148	GLY	3.1
1	F	252	LEU	3.1
1	B	250	ARG	3.1
1	B	239	SER	3.1
1	F	118	GLY	3.1
1	E	230	ASN	3.1
1	E	62	VAL	3.1
1	F	227	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	134	PHE	3.0
1	D	240	HIS	3.0
1	F	189	ALA	3.0
1	D	121	LEU	3.0
1	B	7	PHE	3.0
1	F	128	PHE	3.0
1	B	58	ASP	3.0
1	F	42	VAL	3.0
1	B	134	PHE	3.0
1	E	234	MET	3.0
1	F	102	ILE	3.0
1	F	191	GLY	2.9
1	C	228	ILE	2.9
1	D	126	LEU	2.9
1	F	235	LYS	2.9
1	F	172	TYR	2.9
1	B	230	ASN	2.9
1	A	253	LEU	2.9
1	F	247	GLU	2.9
1	D	29	ASP	2.9
1	B	37	LEU	2.9
1	B	176	VAL	2.8
1	B	240	HIS	2.8
1	C	226	GLN	2.8
1	D	128	PHE	2.8
1	F	232	GLU	2.8
1	A	233	THR	2.8
1	F	14	ASN	2.8
1	B	142	GLU	2.8
1	F	57	LEU	2.8
1	B	200	ALA	2.7
1	A	7	PHE	2.7
1	F	241	ALA	2.7
1	E	18	GLY	2.7
1	D	233	THR	2.7
1	F	183	SER	2.7
1	B	105	GLY	2.7
1	B	116	LEU	2.7
1	B	207	ALA	2.6
1	F	171	THR	2.6
1	B	238	GLU	2.6
1	E	232	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	146	SER	2.6
1	F	69	ILE	2.6
1	F	240	HIS	2.6
1	A	177	VAL	2.6
1	E	246	VAL	2.6
1	A	232	GLU	2.6
1	B	253	LEU	2.6
1	F	226	GLN	2.6
1	F	62	VAL	2.6
1	F	246	VAL	2.6
1	B	178	ARG	2.6
1	B	129	PRO	2.5
1	E	178	ARG	2.5
1	F	72	PRO	2.5
1	B	123	PHE	2.5
1	F	116	LEU	2.5
1	F	201	THR	2.5
1	E	29	ASP	2.5
1	B	174	GLY	2.5
1	D	148	GLY	2.5
1	E	10	GLY	2.5
1	E	189	ALA	2.5
1	E	169	TYR	2.5
1	F	179	HIS	2.5
1	F	38	MET	2.5
1	B	235	LYS	2.5
1	A	231	ALA	2.4
1	F	200	ALA	2.4
1	F	237	THR	2.4
1	E	187	TRP	2.4
1	B	127	GLU	2.4
1	A	37	LEU	2.4
1	F	34	ILE	2.4
1	B	150	THR	2.4
1	F	231	ALA	2.4
1	F	178	ARG	2.4
1	F	142	GLU	2.4
1	B	120	SER	2.4
1	B	94	THR	2.4
1	B	34	ILE	2.4
1	E	191	GLY	2.4
1	F	187	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	147	ILE	2.3
1	F	119	ALA	2.3
1	C	148	GLY	2.3
1	F	202	LEU	2.3
1	A	195	TYR	2.3
1	D	189	ALA	2.3
1	F	124	ALA	2.3
1	A	34	ILE	2.3
1	B	236	GLN	2.3
1	E	116	LEU	2.3
1	F	11	LEU	2.3
1	A	240	HIS	2.3
1	E	221	VAL	2.3
1	C	230	ASN	2.3
1	F	101	HIS	2.3
1	B	204	THR	2.3
1	E	250	ARG	2.2
1	B	163	TYR	2.2
1	B	189	ALA	2.2
1	D	226	GLN	2.2
1	B	245	VAL	2.2
1	E	42	VAL	2.2
1	B	179	HIS	2.2
1	B	203	LEU	2.2
1	F	44	LEU	2.2
1	A	191	GLY	2.2
1	A	19	ALA	2.2
1	A	29	ASP	2.2
1	A	55	ALA	2.2
1	D	231	ALA	2.2
1	E	231	ALA	2.2
1	F	162	PHE	2.2
1	B	62	VAL	2.2
1	F	176	VAL	2.2
1	A	224	THR	2.2
1	B	161	THR	2.2
1	F	111	THR	2.2
1	C	236	GLN	2.2
1	E	183	SER	2.2
1	F	173	SER	2.2
1	D	125	PRO	2.2
1	C	147	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	232	GLU	2.2
1	F	94	THR	2.2
1	F	29	ASP	2.2
1	C	146	SER	2.2
1	D	239	SER	2.2
1	F	4	SER	2.2
1	B	164	PRO	2.2
1	C	231	ALA	2.2
1	F	35	ALA	2.2
1	F	175	ARG	2.2
1	D	238	GLU	2.1
1	F	163	TYR	2.1
1	F	220	ILE	2.1
1	E	20	THR	2.1
1	F	239	SER	2.1
1	B	57	LEU	2.1
1	A	40	LYS	2.1
1	E	3	LYS	2.1
1	A	184	MET	2.1
1	B	35	ALA	2.1
1	E	27	ASP	2.1
1	E	176	VAL	2.1
1	E	38	MET	2.1
1	F	129	PRO	2.1
1	A	98	ILE	2.1
1	E	12	THR	2.1
1	E	142	GLU	2.1
1	F	68	GLY	2.1
1	F	114	VAL	2.1
1	A	116	LEU	2.1
1	E	57	LEU	2.1
1	A	39	ASP	2.1
1	B	251	ARG	2.1
1	B	145	LYS	2.0
1	C	233	THR	2.0
1	B	165	GLY	2.0
1	E	175	ARG	2.0
1	F	243	LYS	2.0
1	B	210	GLY	2.0
1	E	233	THR	2.0
1	A	163	TYR	2.0
1	F	41	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	42	VAL	2.0
1	F	219	VAL	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](#)

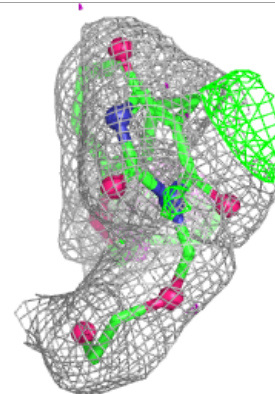
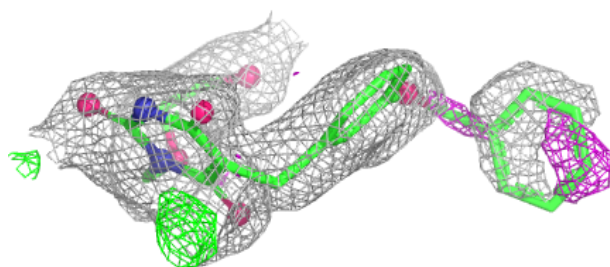
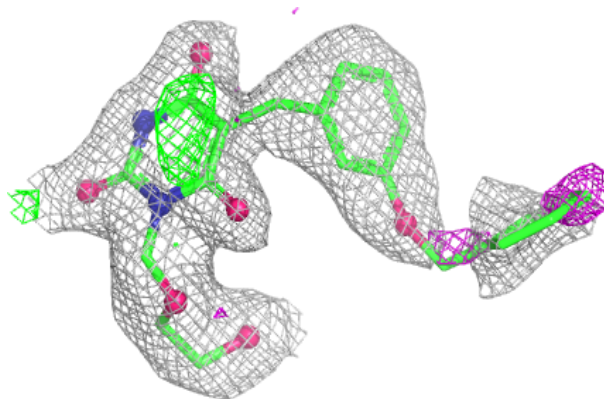
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	K	A	1002	1/1	0.74	0.46	62,62,62,62	0
3	BBB	F	8300	29/29	0.77	0.17	42,43,46,46	0
2	K	E	1003	1/1	0.80	0.39	63,63,63,63	0
3	BBB	B	4300	29/29	0.82	0.15	36,37,41,41	0
3	BBB	A	3300	29/29	0.85	0.14	33,36,44,44	0
3	BBB	E	7300	29/29	0.87	0.12	36,37,45,45	0
3	BBB	C	5300	29/29	0.90	0.11	27,30,40,40	0
3	BBB	D	6300	29/29	0.91	0.11	29,32,40,41	0
2	K	C	1001	1/1	0.95	0.29	49,49,49,49	0

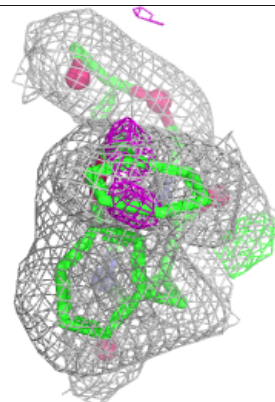
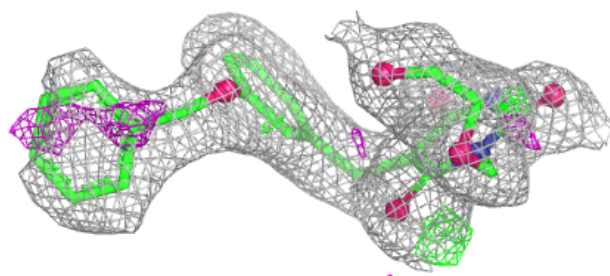
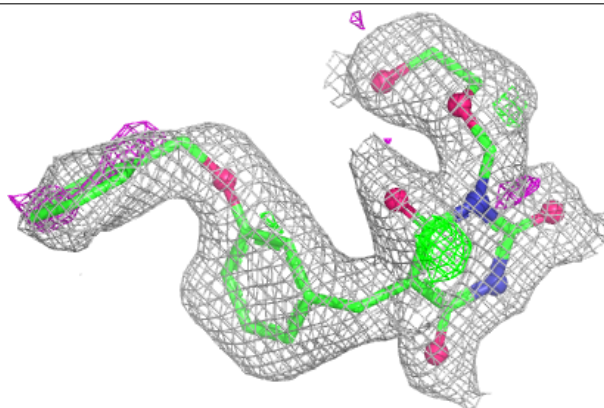
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BBB F 8300:

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

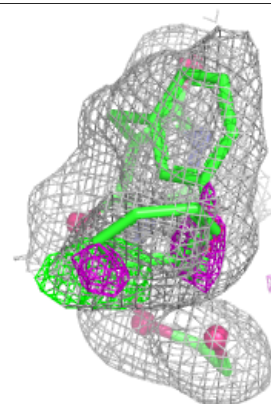
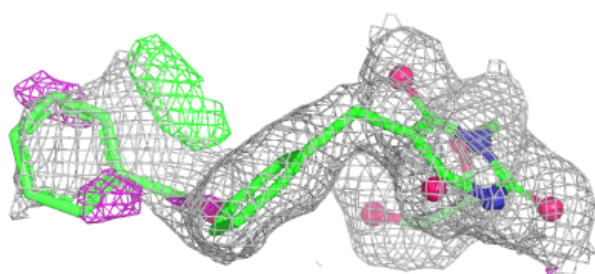
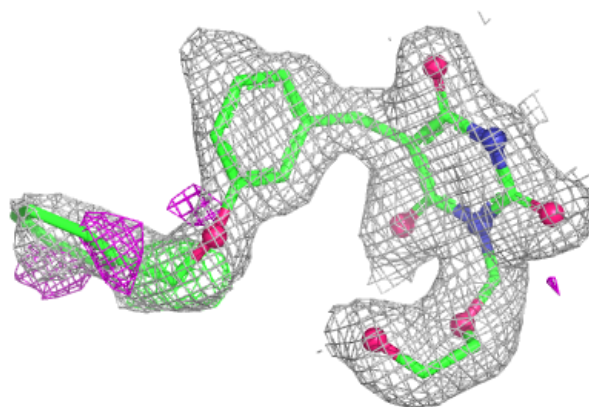
**Electron density around BBB B 4300:**

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

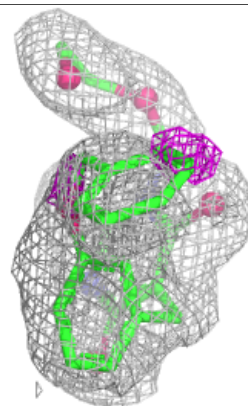
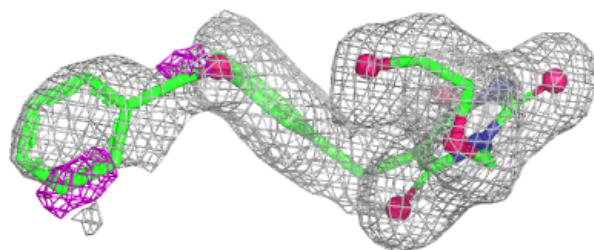
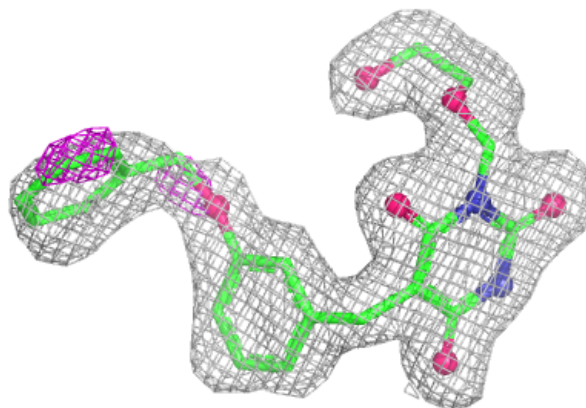


Electron density around BBB A 3300:

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

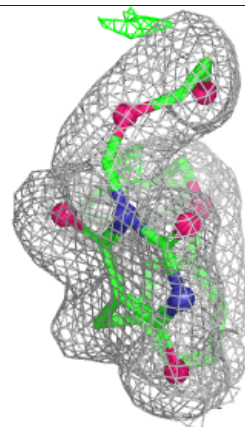
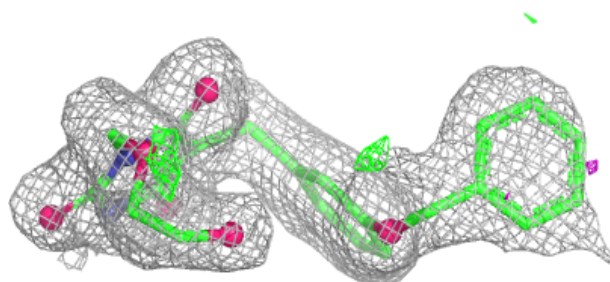
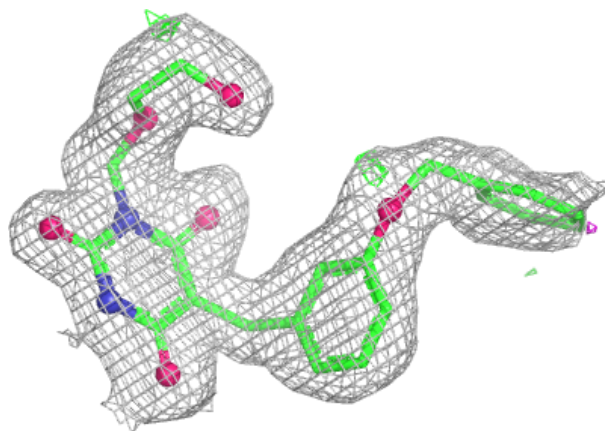
**Electron density around BBB E 7300:**

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



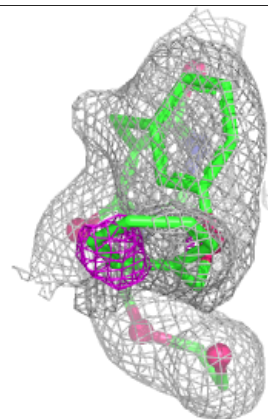
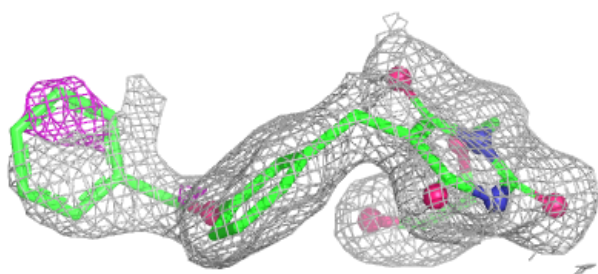
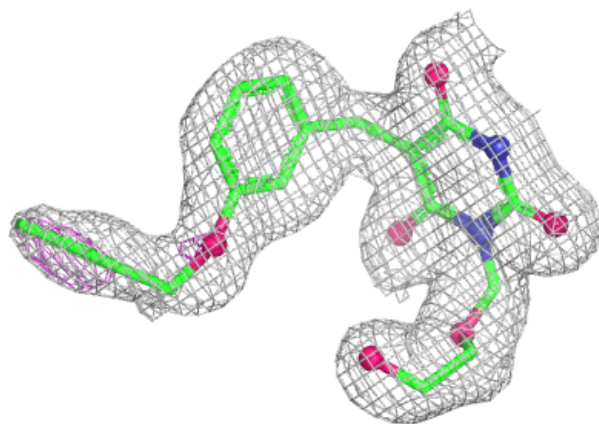
Electron density around BBB C 5300:

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



Electron density around BBB D 6300:

$2mF_o-DF_c$ (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.