



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 09:24 PM UTC

PDB ID : 9DU1 / pdb_00009du1
Title : Co-crystal structure of the ternary complex of human FKBP12, BRD9 bromo domain and Compound 1
Authors : Romanowski, M.J.; Viscomi, J.S.
Deposited on : 2024-10-02
Resolution : 2.01 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

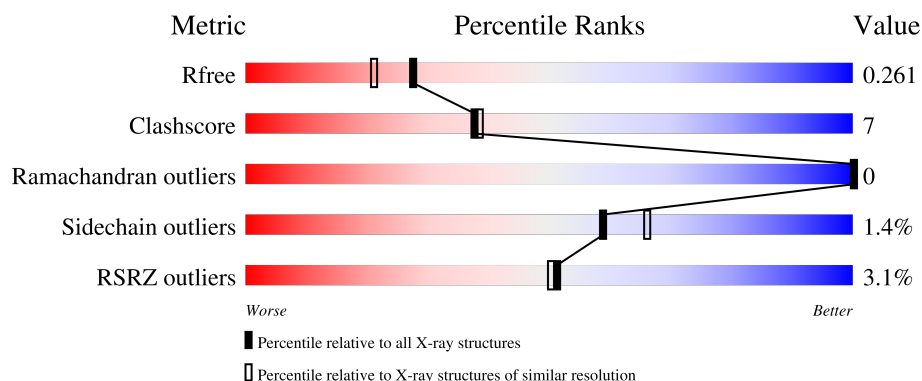
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	109	
1	B	109	
1	C	109	
1	D	109	
2	E	116	

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Mol	Chain	Length	Quality of chain
2	F	116	
2	G	116	
2	H	116	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7707 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 Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			840	532	147	156	5			
1	B	109	Total	C	N	O	S	0	0	0
			846	535	148	158	5			
1	C	108	Total	C	N	O	S	0	1	0
			848	537	150	156	5			
1	D	109	Total	C	N	O	S	0	0	0
			846	535	148	158	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P62942
B	-1	SER	-	expression tag	UNP P62942
C	-1	SER	-	expression tag	UNP P62942
D	-1	SER	-	expression tag	UNP P62942

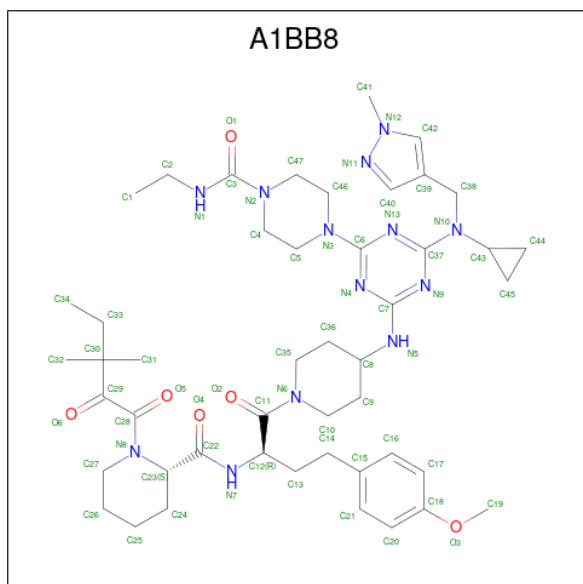
- Molecule 2 is a protein called Bromodomain-containing protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	103	Total	C	N	O	S	0	0	0
			826	537	135	146	8			
2	F	101	Total	C	N	O	S	0	0	0
			808	526	131	143	8			
2	G	102	Total	C	N	O	S	0	0	0
			817	531	132	146	8			
2	H	101	Total	C	N	O	S	0	1	0
			815	531	133	143	8			

There are 20 discrepancies between the modelled and reference sequences:

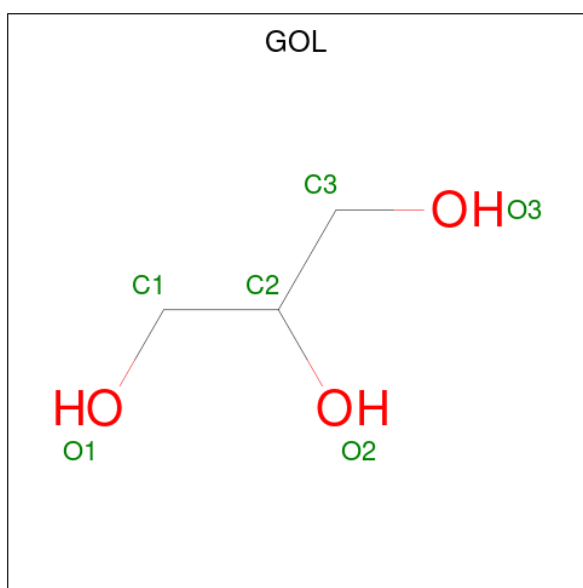
Chain	Residue	Modelled	Actual	Comment	Reference
E	125	GLY	-	expression tag	UNP Q9H8M2
E	126	PRO	-	expression tag	UNP Q9H8M2
E	127	LEU	-	expression tag	UNP Q9H8M2
E	128	GLY	-	expression tag	UNP Q9H8M2
E	129	SER	-	expression tag	UNP Q9H8M2
F	125	GLY	-	expression tag	UNP Q9H8M2
F	126	PRO	-	expression tag	UNP Q9H8M2
F	127	LEU	-	expression tag	UNP Q9H8M2
F	128	GLY	-	expression tag	UNP Q9H8M2
F	129	SER	-	expression tag	UNP Q9H8M2
G	125	GLY	-	expression tag	UNP Q9H8M2
G	126	PRO	-	expression tag	UNP Q9H8M2
G	127	LEU	-	expression tag	UNP Q9H8M2
G	128	GLY	-	expression tag	UNP Q9H8M2
G	129	SER	-	expression tag	UNP Q9H8M2
H	125	GLY	-	expression tag	UNP Q9H8M2
H	126	PRO	-	expression tag	UNP Q9H8M2
H	127	LEU	-	expression tag	UNP Q9H8M2
H	128	GLY	-	expression tag	UNP Q9H8M2
H	129	SER	-	expression tag	UNP Q9H8M2

- Molecule 3 is 4-[4-{cyclopropyl}[(1-methyl-1H-pyrazol-4-yl)methyl]amino}-6-({1-[(2R)-2-{[(2S)-1-(3,3-dimethyl-2-oxopentanoyl)piperidine-2-carbonyl]amino}-4-(4-methoxyphenyl)butanoyl]piperidin-4-yl}amino)-1,3,5-triazin-2-yl]-N-ethylpiperazine-1-carboxamide (CCD ID: A1BB8) (formula: C₄₇H₆₉N₁₃O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			66	47	13	6		
3	D	1	Total	C	N	O	0	0
			66	47	13	6		
3	G	1	Total	C	N	O	0	0
			66	47	13	6		
3	H	1	Total	C	N	O	0	0
			66	47	13	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	87	Total	O	0	0
			87	87		
5	C	117	Total	O	0	0
			117	117		
5	D	80	Total	O	0	0
			80	80		
5	E	86	Total	O	0	0
			86	86		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	93	Total 93	O 93	0	0
5	G	123	Total 123	O 123	0	0
5	H	101	Total 101	O 101	0	0

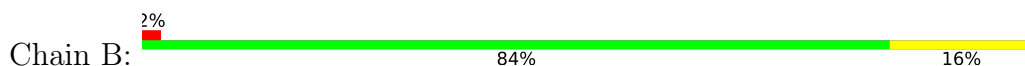
3 Residue-property plots [i](#)

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

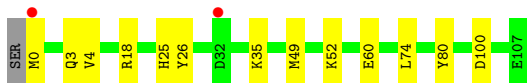
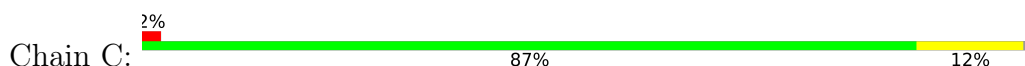
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



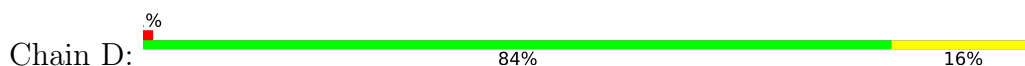
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



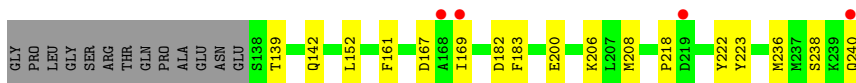
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



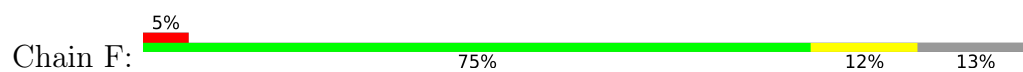
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Bromodomain-containing protein 9



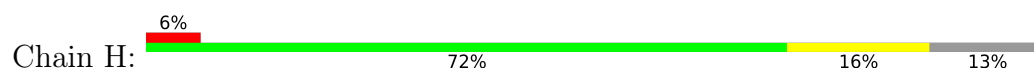
- Molecule 2: Bromodomain-containing protein 9



- Molecule 2: Bromodomain-containing protein 9



- Molecule 2: Bromodomain-containing protein 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.16Å 97.51Å 100.00Å 90.00° 93.69° 90.00°	Depositor
Resolution (Å)	59.04 – 2.01 59.04 – 2.01	Depositor EDS
% Data completeness (in resolution range)	94.0 (59.04-2.01) 81.4 (59.04-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.224 , 0.259 0.225 , 0.261	Depositor DCC
R_{free} test set	3621 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7707	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% 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: A1BB8, GOL

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	0.31	0/859	0.67	0/1156
1	B	0.35	0/865	0.74	0/1164
1	C	0.31	0/870	0.66	0/1170
1	D	0.33	0/865	0.73	0/1164
2	E	0.31	0/848	0.68	0/1142
2	F	0.29	0/830	0.65	0/1119
2	G	0.32	0/839	0.73	0/1131
2	H	0.31	0/841	0.71	0/1134
All	All	0.32	0/6817	0.70	0/9180

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	840	0	840	6	0
1	B	846	0	845	15	0
1	C	848	0	853	9	0
1	D	846	0	845	12	0
2	E	826	0	815	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	808	0	794	10	0
2	G	817	0	800	19	0
2	H	815	0	801	15	0
3	B	66	0	0	0	0
3	D	66	0	0	0	0
3	G	66	0	0	0	0
3	H	66	0	0	0	0
4	F	6	0	8	2	0
5	A	104	0	0	3	0
5	B	87	0	0	5	0
5	C	117	0	0	5	0
5	D	80	0	0	5	0
5	E	86	0	0	6	1
5	F	93	0	0	3	0
5	G	123	0	0	12	1
5	H	101	0	0	6	0
All	All	7707	0	6601	95	1

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 7.

All (95) 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)
2:G:142:GLN:O	5:G:401:HOH:O	1.84	0.95
1:D:79:ASP:OD2	5:D:301:HOH:O	1.91	0.89
2:E:222:TYR:OH	5:E:301:HOH:O	1.91	0.89
1:D:18:ARG:NH2	5:D:303:HOH:O	2.09	0.86
2:F:171:PRO:O	5:F:401:HOH:O	1.96	0.82
2:G:200:GLU:OE2	5:G:402:HOH:O	1.97	0.81
2:F:138:SER:N	5:F:402:HOH:O	2.14	0.81
2:G:174:SER:OG	5:G:403:HOH:O	2.02	0.77
2:H:146:GLU:OE2	2:H:150:ARG:NH2	2.19	0.75
1:D:18:ARG:O	5:D:302:HOH:O	2.08	0.72
2:H:217:ARG:NH1	5:H:405:HOH:O	2.24	0.69
2:G:145:LEU:N	5:G:401:HOH:O	2.24	0.69
1:B:71:ARG:NH1	5:B:306:HOH:O	2.26	0.69
1:C:0:MET:N	5:C:203:HOH:O	2.24	0.68
2:E:200:GLU:OE1	5:E:302:HOH:O	2.10	0.68
2:H:227:LYS:NZ	5:H:406:HOH:O	2.25	0.68
2:G:194:GLU:OE2	5:G:404:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:O	5:A:201:HOH:O	2.11	0.67
2:H:199:THR:O	5:H:402:HOH:O	2.11	0.67
2:H:194:GLU:OE1	5:H:403:HOH:O	2.14	0.66
1:B:0:MET:HA	1:B:0:MET:HE2	1.78	0.66
2:F:172:GLY:HA2	2:F:175:MET:HE3	1.76	0.65
1:C:80:TYR:OH	5:C:201:HOH:O	2.14	0.64
1:D:52:LYS:HG2	1:D:54:GLU:HG3	1.81	0.63
2:G:175:MET:HG3	5:G:403:HOH:O	2.00	0.61
1:C:60:GLU:OE2	5:C:202:HOH:O	2.16	0.61
2:E:152:LEU:HG	2:E:236:MET:HE1	1.82	0.60
1:B:104:LEU:O	1:B:105:LYS:HD3	2.01	0.60
1:B:52:LYS:O	5:B:301:HOH:O	2.17	0.59
1:A:107:GLU:OE1	5:A:202:HOH:O	2.17	0.58
2:G:179:HIS:HD2	5:G:498:HOH:O	1.89	0.56
2:G:194:GLU:O	5:G:405:HOH:O	2.18	0.55
2:E:238:SER:HA	5:E:329:HOH:O	2.07	0.54
2:G:163:PHE:O	5:G:406:HOH:O	2.19	0.54
1:C:49:MET:SD	1:C:52:LYS:HD2	2.48	0.54
1:D:17:LYS:HD2	1:D:20:GLN:OE1	2.08	0.54
1:D:54:GLU:OE2	5:D:304:HOH:O	2.18	0.54
2:H:213:MET:CE	2:H:227:LYS:HD2	2.39	0.53
1:C:35:LYS:NZ	5:C:204:HOH:O	2.39	0.52
1:D:13:ARG:HD3	5:D:342:HOH:O	2.08	0.52
2:F:146:GLU:HG3	2:F:190:ILE:HG21	1.92	0.52
1:B:0:MET:HE1	2:H:228:LYS:C	2.35	0.51
2:F:155:LYS:NZ	5:F:404:HOH:O	2.41	0.51
1:B:0:MET:HE3	2:H:232:ALA:HB2	1.92	0.51
1:D:42:ARG:HD3	2:E:167:ASP:HB3	1.93	0.51
2:G:231:HIS:CE1	2:G:235:LYS:HD3	2.46	0.51
2:E:139:THR:H	2:E:142:GLN:HE21	1.58	0.50
1:A:5:GLU:OE2	5:A:203:HOH:O	2.20	0.47
2:E:182:ASP:OD1	5:E:303:HOH:O	2.21	0.46
1:B:57:ARG:NH1	5:B:311:HOH:O	2.36	0.46
1:D:26:TYR:HA	1:D:100:ASP:O	2.16	0.46
2:G:155:LYS:HE3	2:G:232:ALA:HB1	1.98	0.46
1:B:87:HIS:HE1	4:F:301:GOL:H2	1.81	0.46
2:G:137:GLU:OE1	5:G:407:HOH:O	2.21	0.46
2:E:240:GLN:HG3	5:E:304:HOH:O	2.15	0.46
2:H:163:PHE:O	5:H:404:HOH:O	2.21	0.46
2:E:183:PHE:CE1	2:E:208:MET:HE1	2.51	0.46
2:E:218:PRO:HA	2:E:223:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:GLN:HG2	2:H:183:PHE:CD2	2.51	0.45
2:G:153:GLN:HG2	2:G:183:PHE:CD2	2.52	0.45
2:H:183:PHE:CZ	2:H:208:MET:HE1	2.51	0.45
2:E:139:THR:H	2:E:142:GLN:NE2	2.15	0.45
2:H:149:LEU:HG	5:H:422:HOH:O	2.16	0.44
1:D:2:VAL:O	2:G:228:LYS:NZ	2.51	0.44
1:D:16:PRO:HB2	1:D:50:LEU:HD12	2.00	0.44
2:H:146:GLU:CD	2:H:146:GLU:C	2.86	0.44
1:B:52:LYS:HA	1:B:52:LYS:HD3	1.86	0.43
1:C:26:TYR:HA	1:C:100:ASP:O	2.18	0.43
1:B:54:GLU:OE2	5:B:302:HOH:O	2.21	0.43
1:C:3:GLN:HB3	5:C:208:HOH:O	2.17	0.43
2:G:170:ALA:HB1	2:G:215:TYR:OH	2.18	0.43
2:F:152:LEU:HD21	2:F:233:GLY:HA2	2.01	0.43
2:F:152:LEU:HG	2:F:236:MET:HE1	2.01	0.43
2:G:170:ALA:HB1	2:G:215:TYR:CZ	2.53	0.42
2:E:139:THR:HG23	2:E:142:GLN:HE21	1.85	0.42
2:H:213:MET:HE3	2:H:227:LYS:HD2	2.01	0.41
1:B:42:ARG:HD3	2:F:167:ASP:HB3	2.02	0.41
2:G:175:MET:HG3	5:G:487:HOH:O	2.19	0.41
1:A:26:TYR:HA	1:A:100:ASP:O	2.21	0.41
1:C:4:VAL:HG22	1:C:74:LEU:HD22	2.01	0.41
1:A:57:ARG:HD3	1:A:80:TYR:CD2	2.56	0.41
1:B:42:ARG:HG3	5:B:360:HOH:O	2.20	0.41
2:G:139:THR:OG1	2:G:141:ILE:HG22	2.20	0.41
2:F:145:LEU:HD22	2:F:201:PHE:CG	2.55	0.41
2:G:146:GLU:N	5:G:401:HOH:O	1.99	0.41
1:C:18[B]:ARG:CG	1:C:18[B]:ARG:HH11	2.34	0.41
2:E:139:THR:HG23	2:E:142:GLN:NE2	2.35	0.41
2:F:215:TYR:O	4:F:301:GOL:O3	2.38	0.41
1:B:91:ILE:HA	1:B:92:PRO:HD3	1.96	0.41
2:H:170:ALA:HB1	2:H:215:TYR:CZ	2.56	0.40
1:B:4:VAL:HG22	1:B:74:LEU:HD22	2.03	0.40
2:E:161:PHE:HA	5:E:321:HOH:O	2.21	0.40
1:A:4:VAL:HG22	1:A:74:LEU:HD22	2.03	0.40
1:B:16:PRO:C	1:B:17:LYS:HD2	2.47	0.40
1:D:4:VAL:HG22	1:D:74:LEU:HD22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:360:HOH:O	5:G:464:HOH:O[2_545]	2.02	0.18

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	106/109 (97%)	104 (98%)	2 (2%)	0	100	100
1	B	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
1	C	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
1	D	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
2	E	101/116 (87%)	101 (100%)	0	0	100	100
2	F	99/116 (85%)	99 (100%)	0	0	100	100
2	G	100/116 (86%)	100 (100%)	0	0	100	100
2	H	100/116 (86%)	100 (100%)	0	0	100	100
All	All	827/900 (92%)	816 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	90/91 (99%)	89 (99%)	1 (1%)	65	73
1	B	91/91 (100%)	89 (98%)	2 (2%)	45	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	91/91 (100%)	90 (99%)	1 (1%)	65	73
1	D	91/91 (100%)	89 (98%)	2 (2%)	45	50
2	E	88/101 (87%)	86 (98%)	2 (2%)	44	49
2	F	86/101 (85%)	86 (100%)	0	100	100
2	G	87/101 (86%)	87 (100%)	0	100	100
2	H	87/101 (86%)	85 (98%)	2 (2%)	44	49
All	All	711/768 (93%)	701 (99%)	10 (1%)	59	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	B	25	HIS
1	B	79	ASP
1	C	25	HIS
1	D	-1	SER
1	D	25	HIS
2	E	169	ILE
2	E	206	LYS
2	H	138	SER
2	H	169	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	B	94	HIS
1	C	94	HIS
1	D	53	GLN
1	D	65	GLN
2	E	142	GLN
2	G	147	HIS
2	G	151	GLN
2	G	158	HIS
2	G	231	HIS

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 ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A1BB8	B	201	-	72,72,72	6.99	60 (83%)	95,102,102	2.79	32 (33%)
3	A1BB8	D	201	-	72,72,72	7.12	61 (84%)	95,102,102	2.84	30 (31%)
3	A1BB8	G	301	-	72,72,72	6.88	60 (83%)	95,102,102	3.43	41 (43%)
3	A1BB8	H	301	-	72,72,72	6.92	59 (81%)	95,102,102	3.30	42 (44%)
4	GOL	F	301	-	5,5,5	1.15	1 (20%)	5,5,5	1.10	0

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	A1BB8	B	201	-	-	12/67/100/100	0/7/7/7
3	A1BB8	D	201	-	-	9/67/100/100	0/7/7/7
3	A1BB8	G	301	-	-	6/67/100/100	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1BB8	H	301	-	-	10/67/100/100	0/7/7/7
4	GOL	F	301	-	-	4/4/4/4	-

All (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	A1BB8	C7-N5	17.51	1.55	1.34
3	B	201	A1BB8	C7-N5	16.87	1.54	1.34
3	H	301	A1BB8	C7-N5	15.56	1.53	1.34
3	B	201	A1BB8	C11-N6	15.42	1.57	1.35
3	D	201	A1BB8	C11-N6	15.38	1.57	1.35
3	G	301	A1BB8	C7-N5	15.37	1.52	1.34
3	G	301	A1BB8	C11-N6	15.34	1.57	1.35
3	H	301	A1BB8	C11-N6	15.15	1.57	1.35
3	D	201	A1BB8	C17-C16	14.11	1.61	1.38
3	D	201	A1BB8	C21-C20	14.06	1.61	1.38
3	B	201	A1BB8	C21-C20	13.77	1.61	1.38
3	H	301	A1BB8	C17-C16	13.63	1.60	1.38
3	G	301	A1BB8	C17-C16	13.57	1.60	1.38
3	G	301	A1BB8	C21-C20	13.51	1.60	1.38
3	B	201	A1BB8	C17-C16	13.40	1.60	1.38
3	D	201	A1BB8	C28-N8	13.39	1.54	1.34
3	H	301	A1BB8	C21-C20	13.22	1.60	1.38
3	B	201	A1BB8	C28-N8	12.90	1.53	1.34
3	H	301	A1BB8	C28-N8	12.56	1.52	1.34
3	B	201	A1BB8	C20-C18	12.23	1.61	1.38
3	G	301	A1BB8	C28-N8	12.19	1.52	1.34
3	G	301	A1BB8	C20-C18	12.13	1.61	1.38
3	H	301	A1BB8	C20-C18	12.06	1.61	1.38
3	D	201	A1BB8	C17-C18	12.06	1.61	1.38
3	H	301	A1BB8	C17-C18	12.03	1.61	1.38
3	G	301	A1BB8	C17-C18	11.90	1.61	1.38
3	B	201	A1BB8	C17-C18	11.89	1.61	1.38
3	D	201	A1BB8	C20-C18	11.79	1.60	1.38
3	G	301	A1BB8	C16-C15	11.54	1.61	1.38
3	H	301	A1BB8	C16-C15	11.47	1.61	1.38
3	B	201	A1BB8	C21-C15	11.41	1.61	1.38
3	D	201	A1BB8	C16-C15	11.35	1.61	1.38
3	G	301	A1BB8	C21-C15	11.28	1.61	1.38
3	H	301	A1BB8	C21-C15	11.16	1.60	1.38
3	D	201	A1BB8	C21-C15	11.14	1.60	1.38
3	H	301	A1BB8	N12-N11	11.10	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	A1BB8	C16-C15	11.01	1.60	1.38
3	D	201	A1BB8	C22-N7	10.87	1.57	1.34
3	G	301	A1BB8	N12-N11	10.63	1.47	1.35
3	D	201	A1BB8	N12-N11	10.57	1.47	1.35
3	B	201	A1BB8	N12-N11	10.50	1.47	1.35
3	H	301	A1BB8	C37-N10	10.46	1.55	1.36
3	D	201	A1BB8	C38-N10	10.35	1.56	1.45
3	B	201	A1BB8	C22-N7	10.35	1.56	1.34
3	D	201	A1BB8	C37-N10	10.19	1.54	1.36
3	H	301	A1BB8	C38-N10	10.13	1.56	1.45
3	G	301	A1BB8	C22-N7	10.09	1.55	1.34
3	B	201	A1BB8	C6-N4	10.04	1.53	1.34
3	H	301	A1BB8	C22-N7	10.04	1.55	1.34
3	D	201	A1BB8	C6-N4	10.01	1.53	1.34
3	H	301	A1BB8	C37-N9	9.95	1.53	1.34
3	G	301	A1BB8	C38-N10	9.92	1.55	1.45
3	D	201	A1BB8	C37-N9	9.88	1.52	1.34
3	B	201	A1BB8	C6-N13	9.85	1.52	1.34
3	B	201	A1BB8	C37-N9	9.84	1.52	1.34
3	D	201	A1BB8	C6-N13	9.84	1.52	1.34
3	B	201	A1BB8	C38-N10	9.79	1.55	1.45
3	H	301	A1BB8	C6-N13	9.75	1.52	1.34
3	G	301	A1BB8	C37-N10	9.65	1.53	1.36
3	G	301	A1BB8	C6-N13	9.59	1.52	1.34
3	G	301	A1BB8	C6-N4	9.56	1.52	1.34
3	D	201	A1BB8	C37-N13	9.52	1.52	1.34
3	B	201	A1BB8	C37-N10	9.29	1.53	1.36
3	G	301	A1BB8	C37-N9	9.29	1.51	1.34
3	H	301	A1BB8	C37-N13	9.28	1.51	1.34
3	B	201	A1BB8	C37-N13	8.98	1.51	1.34
3	G	301	A1BB8	C37-N13	8.91	1.51	1.34
3	D	201	A1BB8	C3-N2	8.85	1.51	1.36
3	H	301	A1BB8	C6-N4	8.82	1.51	1.34
3	G	301	A1BB8	C23-N8	8.57	1.58	1.47
3	G	301	A1BB8	C3-N2	8.46	1.51	1.36
3	D	201	A1BB8	C23-N8	8.29	1.57	1.47
3	B	201	A1BB8	C3-N2	8.23	1.50	1.36
3	B	201	A1BB8	C23-N8	8.13	1.57	1.47
3	H	301	A1BB8	C3-N2	8.12	1.50	1.36
3	H	301	A1BB8	C23-N8	7.95	1.57	1.47
3	H	301	A1BB8	C41-N12	7.82	1.55	1.46
3	B	201	A1BB8	C6-N3	7.76	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	A1BB8	C6-N3	7.67	1.51	1.35
3	D	201	A1BB8	C27-N8	7.57	1.59	1.47
3	G	301	A1BB8	C30-C29	7.56	1.62	1.53
3	B	201	A1BB8	C41-N12	7.51	1.55	1.46
3	B	201	A1BB8	C27-N8	7.44	1.59	1.47
3	D	201	A1BB8	C41-N12	7.39	1.55	1.46
3	G	301	A1BB8	C27-N8	7.39	1.59	1.47
3	H	301	A1BB8	C6-N3	7.18	1.50	1.35
3	H	301	A1BB8	C35-N6	7.17	1.59	1.47
3	G	301	A1BB8	C35-N6	7.15	1.59	1.47
3	B	201	A1BB8	C28-C29	7.11	1.62	1.53
3	D	201	A1BB8	C10-N6	7.04	1.59	1.47
3	G	301	A1BB8	C6-N3	7.03	1.50	1.35
3	H	301	A1BB8	C27-N8	6.96	1.58	1.47
3	B	201	A1BB8	C10-N6	6.96	1.59	1.47
3	H	301	A1BB8	C30-C29	6.95	1.61	1.53
3	G	301	A1BB8	C41-N12	6.92	1.54	1.46
3	H	301	A1BB8	C7-N9	6.90	1.53	1.34
3	D	201	A1BB8	C28-C29	6.90	1.62	1.53
3	B	201	A1BB8	C30-C29	6.86	1.61	1.53
3	G	301	A1BB8	C5-N3	6.76	1.58	1.46
3	H	301	A1BB8	C28-C29	6.75	1.62	1.53
3	H	301	A1BB8	C46-N3	6.67	1.58	1.46
3	D	201	A1BB8	C35-N6	6.67	1.59	1.47
3	G	301	A1BB8	C28-C29	6.60	1.61	1.53
3	D	201	A1BB8	C42-N12	6.60	1.41	1.34
3	B	201	A1BB8	C35-N6	6.59	1.58	1.47
3	D	201	A1BB8	C30-C29	6.57	1.61	1.53
3	B	201	A1BB8	C7-N4	6.54	1.52	1.34
3	D	201	A1BB8	C7-N9	6.52	1.52	1.34
3	B	201	A1BB8	C5-N3	6.49	1.57	1.46
3	B	201	A1BB8	C7-N9	6.45	1.52	1.34
3	G	301	A1BB8	C7-N9	6.44	1.52	1.34
3	H	301	A1BB8	C10-N6	6.42	1.58	1.47
3	D	201	A1BB8	C8-N5	6.35	1.60	1.46
3	B	201	A1BB8	C42-N12	6.34	1.41	1.34
3	D	201	A1BB8	C7-N4	6.32	1.52	1.34
3	G	301	A1BB8	C46-N3	6.30	1.57	1.46
3	H	301	A1BB8	C5-N3	6.24	1.57	1.46
3	D	201	A1BB8	C46-N3	6.22	1.57	1.46
3	D	201	A1BB8	C5-N3	6.21	1.57	1.46
3	B	201	A1BB8	C46-N3	6.19	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	A1BB8	C42-N12	6.12	1.41	1.34
3	G	301	A1BB8	C8-N5	6.10	1.59	1.46
3	H	301	A1BB8	C42-N12	6.08	1.40	1.34
3	H	301	A1BB8	C7-N4	5.92	1.51	1.34
3	H	301	A1BB8	C8-N5	5.87	1.59	1.46
3	H	301	A1BB8	C40-N11	5.82	1.41	1.32
3	D	201	A1BB8	C45-C43	5.81	1.61	1.48
3	D	201	A1BB8	C44-C43	5.79	1.61	1.48
3	G	301	A1BB8	C40-N11	5.75	1.41	1.32
3	B	201	A1BB8	C8-N5	5.71	1.58	1.46
3	D	201	A1BB8	C40-N11	5.71	1.41	1.32
3	B	201	A1BB8	C40-N11	5.66	1.41	1.32
3	G	301	A1BB8	C7-N4	5.63	1.50	1.34
3	B	201	A1BB8	C32-C30	5.63	1.64	1.53
3	B	201	A1BB8	C45-C43	5.63	1.61	1.48
3	G	301	A1BB8	C44-C43	5.62	1.61	1.48
3	H	301	A1BB8	C32-C30	5.59	1.64	1.53
3	H	301	A1BB8	C45-C43	5.59	1.60	1.48
3	G	301	A1BB8	C45-C43	5.59	1.60	1.48
3	B	201	A1BB8	C44-C43	5.58	1.60	1.48
3	G	301	A1BB8	C32-C30	5.54	1.64	1.53
3	H	301	A1BB8	C44-C43	5.53	1.60	1.48
3	D	201	A1BB8	O3-C18	5.27	1.48	1.37
3	B	201	A1BB8	C31-C30	5.21	1.63	1.53
3	D	201	A1BB8	C32-C30	5.19	1.63	1.53
3	D	201	A1BB8	C31-C30	5.14	1.63	1.53
3	G	301	A1BB8	O3-C18	4.97	1.47	1.37
3	G	301	A1BB8	C10-N6	4.93	1.55	1.47
3	H	301	A1BB8	C31-C30	4.88	1.63	1.53
3	G	301	A1BB8	C31-C30	4.85	1.62	1.53
3	B	201	A1BB8	O3-C18	4.79	1.47	1.37
3	D	201	A1BB8	C3-N1	4.77	1.53	1.34
3	H	301	A1BB8	C3-N1	4.75	1.53	1.34
3	H	301	A1BB8	O3-C18	4.73	1.46	1.37
3	G	301	A1BB8	C3-N1	4.72	1.53	1.34
3	D	201	A1BB8	C43-N10	4.66	1.55	1.47
3	B	201	A1BB8	C3-N1	4.62	1.53	1.34
3	H	301	A1BB8	C43-N10	4.54	1.55	1.47
3	B	201	A1BB8	C43-N10	4.37	1.55	1.47
3	G	301	A1BB8	C36-C35	4.33	1.64	1.52
3	H	301	A1BB8	C38-C39	4.27	1.63	1.50
3	B	201	A1BB8	C38-C39	4.23	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	A1BB8	C38-C39	4.05	1.62	1.50
3	H	301	A1BB8	C14-C15	3.98	1.63	1.51
3	G	301	A1BB8	C38-C39	3.98	1.62	1.50
3	B	201	A1BB8	C14-C15	3.96	1.62	1.51
3	D	201	A1BB8	C14-C15	3.96	1.62	1.51
3	G	301	A1BB8	C43-N10	3.95	1.54	1.47
3	G	301	A1BB8	C14-C15	3.84	1.62	1.51
3	D	201	A1BB8	C36-C35	3.68	1.62	1.52
3	H	301	A1BB8	C36-C35	3.62	1.62	1.52
3	H	301	A1BB8	C45-C44	3.60	1.61	1.48
3	B	201	A1BB8	C45-C44	3.54	1.61	1.48
3	G	301	A1BB8	C45-C44	3.54	1.61	1.48
3	D	201	A1BB8	C45-C44	3.54	1.61	1.48
3	G	301	A1BB8	C12-N7	3.51	1.53	1.45
3	H	301	A1BB8	C12-N7	3.45	1.53	1.45
3	D	201	A1BB8	C13-C12	3.44	1.61	1.53
3	B	201	A1BB8	C36-C35	3.42	1.61	1.52
3	B	201	A1BB8	C13-C12	3.39	1.61	1.53
3	B	201	A1BB8	C12-N7	3.39	1.52	1.45
3	D	201	A1BB8	C9-C10	3.37	1.61	1.52
3	B	201	A1BB8	C9-C10	3.24	1.61	1.52
3	D	201	A1BB8	C12-N7	3.24	1.52	1.45
3	G	301	A1BB8	C36-C8	3.19	1.59	1.52
3	H	301	A1BB8	C13-C12	3.15	1.60	1.53
3	B	201	A1BB8	C23-C22	3.14	1.60	1.52
3	G	301	A1BB8	C13-C12	3.13	1.60	1.53
3	G	301	A1BB8	C23-C22	3.13	1.60	1.52
3	D	201	A1BB8	C23-C22	3.12	1.60	1.52
3	H	301	A1BB8	C24-C23	3.11	1.60	1.53
3	G	301	A1BB8	C24-C23	3.03	1.60	1.53
3	H	301	A1BB8	C9-C10	3.02	1.60	1.52
3	D	201	A1BB8	C24-C23	3.01	1.60	1.53
3	H	301	A1BB8	C23-C22	2.99	1.60	1.52
3	D	201	A1BB8	C26-C27	2.94	1.61	1.51
3	B	201	A1BB8	C36-C8	2.89	1.58	1.52
3	H	301	A1BB8	C36-C8	2.85	1.58	1.52
3	G	301	A1BB8	C34-C33	2.72	1.63	1.51
3	H	301	A1BB8	C40-C39	2.69	1.45	1.40
3	D	201	A1BB8	C36-C8	2.68	1.58	1.52
3	B	201	A1BB8	C24-C23	2.67	1.59	1.53
3	B	201	A1BB8	C26-C27	2.66	1.60	1.51
3	B	201	A1BB8	C13-C14	2.63	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	A1BB8	C12-C11	2.63	1.58	1.53
3	D	201	A1BB8	C47-C46	2.62	1.61	1.51
3	H	301	A1BB8	C34-C33	2.61	1.62	1.51
3	D	201	A1BB8	C12-C11	2.59	1.58	1.53
3	G	301	A1BB8	C2-N1	2.58	1.54	1.46
3	D	201	A1BB8	C34-C33	2.57	1.62	1.51
3	H	301	A1BB8	C26-C27	2.53	1.59	1.51
3	D	201	A1BB8	C13-C14	2.53	1.63	1.52
3	D	201	A1BB8	C5-C4	2.51	1.60	1.51
3	G	301	A1BB8	C9-C10	2.49	1.59	1.52
3	G	301	A1BB8	C47-C46	2.48	1.60	1.51
3	G	301	A1BB8	C26-C27	2.47	1.59	1.51
3	B	201	A1BB8	C34-C33	2.46	1.62	1.51
3	H	301	A1BB8	C2-N1	2.46	1.54	1.46
3	H	301	A1BB8	C47-C46	2.44	1.60	1.51
3	B	201	A1BB8	C47-C46	2.41	1.60	1.51
3	B	201	A1BB8	C5-C4	2.39	1.60	1.51
3	D	201	A1BB8	C40-C39	2.39	1.44	1.40
3	B	201	A1BB8	C40-C39	2.36	1.44	1.40
3	B	201	A1BB8	C12-C11	2.35	1.57	1.53
3	H	301	A1BB8	C13-C14	2.33	1.62	1.52
3	G	301	A1BB8	C5-C4	2.31	1.59	1.51
3	H	301	A1BB8	C1-C2	2.31	1.62	1.48
3	D	201	A1BB8	C2-N1	2.30	1.53	1.46
3	B	201	A1BB8	C1-C2	2.30	1.62	1.48
3	G	301	A1BB8	C1-C2	2.30	1.62	1.48
3	G	301	A1BB8	C40-C39	2.29	1.44	1.40
3	B	201	A1BB8	C2-N1	2.24	1.53	1.46
3	D	201	A1BB8	C1-C2	2.24	1.62	1.48
4	F	301	GOL	C3-C2	2.21	1.60	1.51
3	H	301	A1BB8	C12-C11	2.21	1.57	1.53
3	H	301	A1BB8	C5-C4	2.20	1.59	1.51
3	G	301	A1BB8	C13-C14	2.19	1.62	1.52
3	D	201	A1BB8	C42-C39	2.07	1.45	1.38
3	B	201	A1BB8	C42-C39	2.06	1.45	1.38
3	G	301	A1BB8	C42-C39	2.05	1.45	1.38
3	D	201	A1BB8	O3-C19	2.03	1.48	1.42

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	A1BB8	C39-C40-N11	-12.09	107.16	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	A1BB8	C39-C40-N11	-11.79	107.31	113.14
3	D	201	A1BB8	C37-N9-C7	11.11	123.22	113.84
3	B	201	A1BB8	C39-C40-N11	-10.78	107.81	113.14
3	D	201	A1BB8	C39-C40-N11	-10.64	107.88	113.14
3	G	301	A1BB8	C12-C11-N6	10.28	134.34	118.85
3	G	301	A1BB8	C37-N9-C7	10.26	122.50	113.84
3	H	301	A1BB8	C41-N12-N11	9.45	127.61	120.03
3	H	301	A1BB8	C12-C11-N6	9.24	132.77	118.85
3	B	201	A1BB8	C37-N9-C7	9.14	121.56	113.84
3	H	301	A1BB8	C37-N9-C7	8.79	121.26	113.84
3	G	301	A1BB8	O2-C11-N6	-8.35	111.64	121.61
3	H	301	A1BB8	N9-C37-N10	8.31	126.25	116.96
3	H	301	A1BB8	C42-N12-N11	-7.85	107.62	112.08
3	G	301	A1BB8	C41-N12-N11	7.69	126.20	120.03
3	D	201	A1BB8	C42-N12-N11	-7.61	107.76	112.08
3	B	201	A1BB8	C42-N12-N11	-7.55	107.79	112.08
3	H	301	A1BB8	C40-N11-N12	7.48	108.52	104.41
3	B	201	A1BB8	C41-N12-N11	7.33	125.91	120.03
3	D	201	A1BB8	C41-N12-N11	7.33	125.91	120.03
3	B	201	A1BB8	C40-N11-N12	7.02	108.27	104.41
3	D	201	A1BB8	C40-N11-N12	6.98	108.24	104.41
3	G	301	A1BB8	C40-N11-N12	6.96	108.23	104.41
3	G	301	A1BB8	C42-N12-N11	-6.84	108.20	112.08
3	B	201	A1BB8	C12-C11-N6	6.70	128.94	118.85
3	G	301	A1BB8	C36-C8-N5	6.70	121.56	110.77
3	D	201	A1BB8	C12-C11-N6	6.33	128.38	118.85
3	G	301	A1BB8	C9-C8-N5	-6.30	100.62	110.77
3	H	301	A1BB8	O2-C11-N6	-6.22	114.19	121.61
3	D	201	A1BB8	C13-C12-N7	-5.74	99.54	110.91
3	G	301	A1BB8	C7-N5-C8	5.42	132.75	124.32
3	G	301	A1BB8	C35-N6-C11	5.29	143.09	123.30
3	H	301	A1BB8	N9-C37-N13	-5.21	117.01	126.27
3	H	301	A1BB8	C35-C36-C8	-5.17	102.50	110.67
3	D	201	A1BB8	C6-N4-C7	5.15	118.19	113.84
3	G	301	A1BB8	N9-C37-N10	5.11	122.67	116.96
3	G	301	A1BB8	O5-C28-C29	4.90	124.34	116.28
3	D	201	A1BB8	N9-C7-N4	-4.66	118.61	126.26
3	B	201	A1BB8	C6-N4-C7	4.63	117.74	113.84
3	B	201	A1BB8	N5-C7-N4	4.62	124.35	117.09
3	H	301	A1BB8	C36-C8-N5	4.62	118.21	110.77
3	H	301	A1BB8	C13-C12-N7	-4.59	101.83	110.91
3	G	301	A1BB8	N9-C37-N13	-4.55	118.19	126.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	A1BB8	N9-C37-N13	-4.54	118.20	126.27
3	H	301	A1BB8	C10-C9-C8	-4.52	103.54	110.67
3	B	201	A1BB8	C13-C12-N7	-4.49	102.02	110.91
3	G	301	A1BB8	C46-C47-N2	-4.32	101.83	110.42
3	D	201	A1BB8	C26-C27-N8	4.29	117.29	110.65
3	D	201	A1BB8	N5-C7-N4	4.23	123.73	117.09
3	G	301	A1BB8	N5-C7-N4	4.21	123.70	117.09
3	B	201	A1BB8	N9-C7-N4	-4.12	119.51	126.26
3	G	301	A1BB8	C29-C28-N8	-4.07	114.59	119.25
3	H	301	A1BB8	C6-N13-C37	4.05	120.20	113.63
3	G	301	A1BB8	C44-C43-N10	-4.02	111.15	118.82
3	H	301	A1BB8	O5-C28-C29	3.95	122.78	116.28
3	B	201	A1BB8	C10-C9-C8	-3.93	104.47	110.67
3	G	301	A1BB8	C13-C12-N7	-3.89	103.21	110.91
3	D	201	A1BB8	N13-C37-N10	3.72	121.11	116.96
3	H	301	A1BB8	C35-N6-C11	3.69	137.13	123.30
3	B	201	A1BB8	O5-C28-C29	3.69	122.34	116.28
3	G	301	A1BB8	C35-N6-C10	-3.62	105.30	112.68
3	H	301	A1BB8	C46-C47-N2	-3.60	103.26	110.42
3	H	301	A1BB8	O2-C11-C12	-3.59	113.04	119.61
3	B	201	A1BB8	N9-C37-N13	-3.57	119.92	126.27
3	G	301	A1BB8	C5-C4-N2	-3.55	103.36	110.42
3	B	201	A1BB8	O2-C11-N6	-3.50	117.43	121.61
3	G	301	A1BB8	N9-C7-N4	-3.45	120.60	126.26
3	G	301	A1BB8	C14-C13-C12	-3.42	106.29	113.21
3	G	301	A1BB8	C35-C36-C8	-3.41	105.28	110.67
3	H	301	A1BB8	C14-C13-C12	-3.38	106.37	113.21
3	B	201	A1BB8	C35-C36-C8	-3.36	105.36	110.67
3	B	201	A1BB8	N4-C6-N3	3.36	121.90	117.12
3	D	201	A1BB8	O2-C11-N6	-3.35	117.62	121.61
3	D	201	A1BB8	N9-C37-N10	3.34	120.69	116.96
3	G	301	A1BB8	C9-C10-N6	-3.29	104.21	110.66
3	H	301	A1BB8	C11-C12-N7	-3.29	100.46	108.97
3	H	301	A1BB8	C5-N3-C46	3.27	118.92	111.57
3	B	201	A1BB8	O2-C11-C12	-3.27	113.63	119.61
3	B	201	A1BB8	C38-N10-C43	3.25	121.77	118.14
3	B	201	A1BB8	C26-C27-N8	3.24	115.66	110.65
3	H	301	A1BB8	C26-C27-N8	3.21	115.61	110.65
3	B	201	A1BB8	N13-C37-N10	3.20	120.54	116.96
3	H	301	A1BB8	C41-N12-C42	-3.16	124.77	127.94
3	G	301	A1BB8	C13-C14-C15	-3.13	102.91	113.22
3	G	301	A1BB8	C10-N6-C11	-3.12	111.60	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	A1BB8	C10-C9-C8	-3.12	105.75	110.67
3	D	201	A1BB8	C6-N13-C37	3.09	118.65	113.63
3	H	301	A1BB8	C9-C10-N6	3.09	116.72	110.66
3	D	201	A1BB8	O2-C11-C12	-3.07	113.99	119.61
3	H	301	A1BB8	C24-C23-C22	-3.07	106.40	112.17
3	G	301	A1BB8	O2-C11-C12	-3.06	114.01	119.61
3	H	301	A1BB8	C5-N3-C6	-3.05	115.63	121.67
3	D	201	A1BB8	O5-C28-C29	2.99	121.20	116.28
3	G	301	A1BB8	C5-N3-C46	2.95	118.21	111.57
3	G	301	A1BB8	C11-C12-N7	-2.95	101.33	108.97
3	H	301	A1BB8	C13-C14-C15	-2.88	103.74	113.22
3	B	201	A1BB8	C13-C14-C15	-2.82	103.95	113.22
3	G	301	A1BB8	C24-C23-C22	-2.81	106.90	112.17
3	B	201	A1BB8	C11-C12-N7	-2.80	101.72	108.97
3	G	301	A1BB8	C42-C39-C40	2.79	108.86	103.18
3	H	301	A1BB8	C5-C4-N2	-2.75	104.96	110.42
3	B	201	A1BB8	C6-N13-C37	2.73	118.06	113.63
3	H	301	A1BB8	N9-C7-N4	-2.67	121.88	126.26
3	G	301	A1BB8	O1-C3-N2	-2.67	117.94	121.67
3	G	301	A1BB8	C6-N13-C37	2.66	117.94	113.63
3	H	301	A1BB8	C42-C39-C40	2.64	108.55	103.18
3	G	301	A1BB8	C5-N3-C6	-2.63	116.47	121.67
3	H	301	A1BB8	C10-N6-C11	-2.58	113.64	123.30
3	G	301	A1BB8	C21-C15-C16	2.57	122.05	118.23
3	H	301	A1BB8	O1-C3-N2	-2.57	118.08	121.67
3	H	301	A1BB8	N4-C6-N3	2.53	120.72	117.12
3	D	201	A1BB8	C35-N6-C10	-2.51	107.58	112.68
3	H	301	A1BB8	C29-C28-N8	-2.50	116.39	119.25
3	B	201	A1BB8	C44-C43-N10	-2.47	114.11	118.82
3	H	301	A1BB8	C21-C15-C16	2.47	121.90	118.23
3	D	201	A1BB8	C10-C9-C8	-2.44	106.81	110.67
3	B	201	A1BB8	C1-C2-N1	-2.43	103.44	111.53
3	B	201	A1BB8	C42-C39-C40	2.42	108.11	103.18
3	D	201	A1BB8	C42-C39-C40	2.42	108.11	103.18
3	H	301	A1BB8	C44-C43-N10	-2.39	114.26	118.82
3	H	301	A1BB8	C26-C25-C24	2.38	116.31	111.42
3	H	301	A1BB8	C24-C23-N8	2.37	113.73	110.55
3	D	201	A1BB8	C46-C47-N2	-2.37	105.70	110.42
3	H	301	A1BB8	C19-O3-C18	-2.37	112.42	117.50
3	D	201	A1BB8	C35-C36-C8	-2.35	106.96	110.67
3	D	201	A1BB8	N4-C6-N3	2.34	120.44	117.12
3	G	301	A1BB8	C41-N12-C42	-2.33	125.60	127.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	A1BB8	C6-N4-C7	2.32	115.80	113.84
3	B	201	A1BB8	C46-C47-N2	-2.30	105.83	110.42
3	B	201	A1BB8	N9-C37-N10	2.30	119.53	116.96
3	H	301	A1BB8	C9-C8-N5	-2.29	107.08	110.77
3	D	201	A1BB8	C38-N10-C43	2.28	120.69	118.14
3	D	201	A1BB8	C13-C14-C15	-2.26	105.77	113.22
3	B	201	A1BB8	C35-N6-C11	2.25	131.72	123.30
3	D	201	A1BB8	C11-C12-N7	-2.25	103.15	108.97
3	G	301	A1BB8	C6-N4-C7	2.24	115.73	113.84
3	G	301	A1BB8	N4-C6-N3	2.23	120.29	117.12
3	B	201	A1BB8	C21-C15-C16	2.19	121.49	118.23
3	D	201	A1BB8	C36-C8-N5	2.17	114.27	110.77
3	B	201	A1BB8	C19-O3-C18	-2.14	112.91	117.50
3	D	201	A1BB8	C35-N6-C11	2.12	131.22	123.30
3	B	201	A1BB8	C35-N6-C10	-2.11	108.38	112.68
3	D	201	A1BB8	C5-C4-N2	-2.06	106.32	110.42
3	H	301	A1BB8	O4-C22-N7	-2.01	119.36	122.96
3	G	301	A1BB8	C26-C27-N8	2.00	113.75	110.65

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	A1BB8	C28-C29-C30-C33
3	B	201	A1BB8	O6-C29-C30-C33
3	B	201	A1BB8	N13-C37-N10-C43
3	B	201	A1BB8	C9-C8-N5-C7
3	D	201	A1BB8	O6-C29-C30-C33
3	D	201	A1BB8	C29-C30-C33-C34
3	D	201	A1BB8	C31-C30-C33-C34
3	D	201	A1BB8	C32-C30-C33-C34
3	D	201	A1BB8	C9-C8-N5-C7
3	G	301	A1BB8	C29-C30-C33-C34
3	G	301	A1BB8	C36-C8-N5-C7
3	H	301	A1BB8	C44-C43-N10-C37
3	H	301	A1BB8	C45-C43-N10-C37
3	H	301	A1BB8	C45-C43-N10-C38
3	H	301	A1BB8	C29-C30-C33-C34
3	H	301	A1BB8	N10-C38-C39-C40
3	H	301	A1BB8	C36-C8-N5-C7
4	F	301	GOL	O1-C1-C2-C3
4	F	301	GOL	O1-C1-C2-O2

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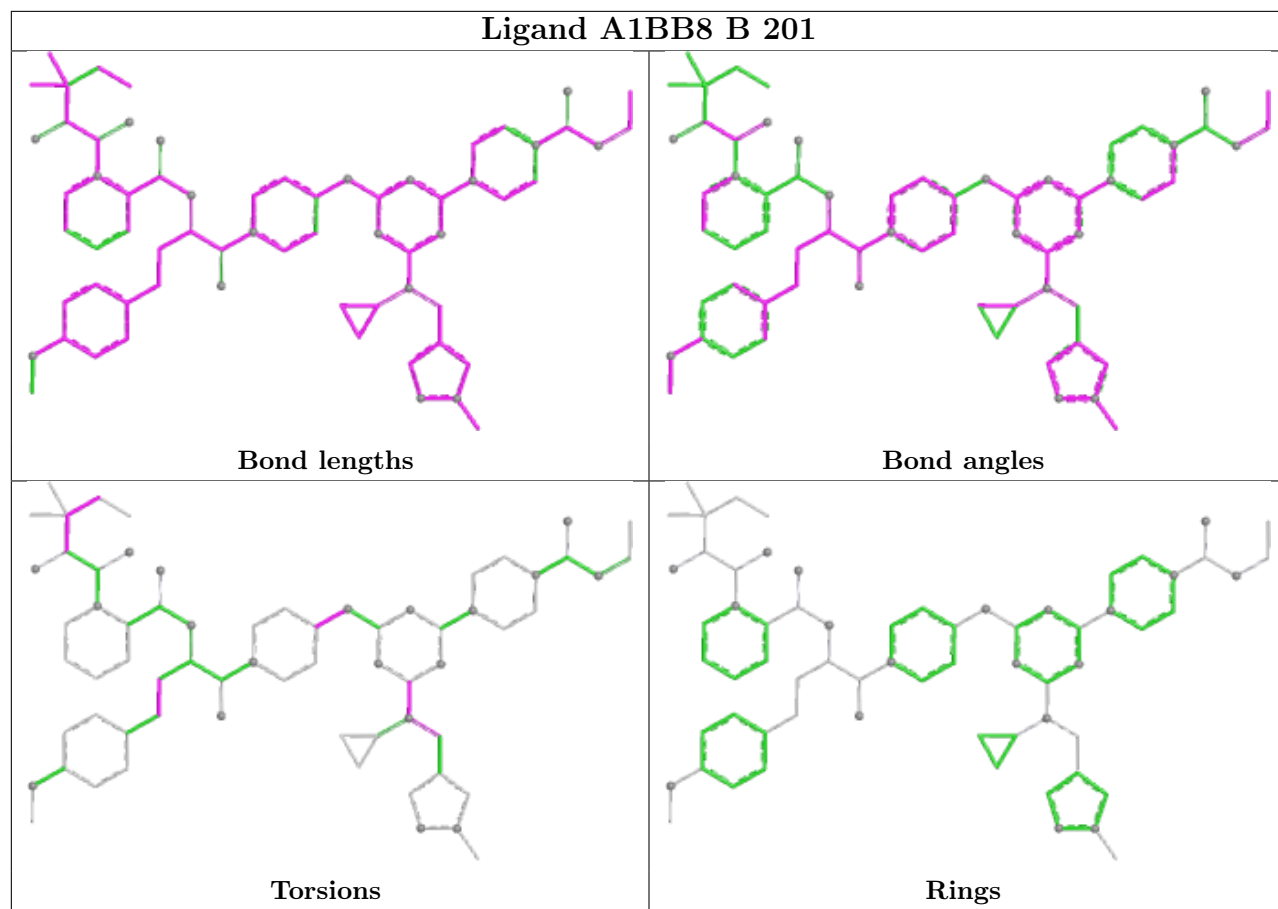
Mol	Chain	Res	Type	Atoms
4	F	301	GOL	C1-C2-C3-O3
3	B	201	A1BB8	N13-C37-N10-C38
4	F	301	GOL	O2-C2-C3-O3
3	B	201	A1BB8	N9-C37-N10-C38
3	D	201	A1BB8	N9-C37-N10-C38
3	D	201	A1BB8	N13-C37-N10-C38
3	B	201	A1BB8	N9-C37-N10-C43
3	D	201	A1BB8	N13-C37-N10-C43
3	D	201	A1BB8	N9-C37-N10-C43
3	B	201	A1BB8	C31-C30-C33-C34
3	B	201	A1BB8	C32-C30-C33-C34
3	G	301	A1BB8	C31-C30-C33-C34
3	G	301	A1BB8	C32-C30-C33-C34
3	H	301	A1BB8	C31-C30-C33-C34
3	H	301	A1BB8	C32-C30-C33-C34
3	H	301	A1BB8	N10-C38-C39-C42
3	B	201	A1BB8	C29-C30-C33-C34
3	G	301	A1BB8	C44-C43-N10-C37
3	G	301	A1BB8	C45-C43-N10-C37
3	H	301	A1BB8	C9-C8-N5-C7
3	B	201	A1BB8	C12-C13-C14-C15
3	B	201	A1BB8	C39-C38-N10-C43

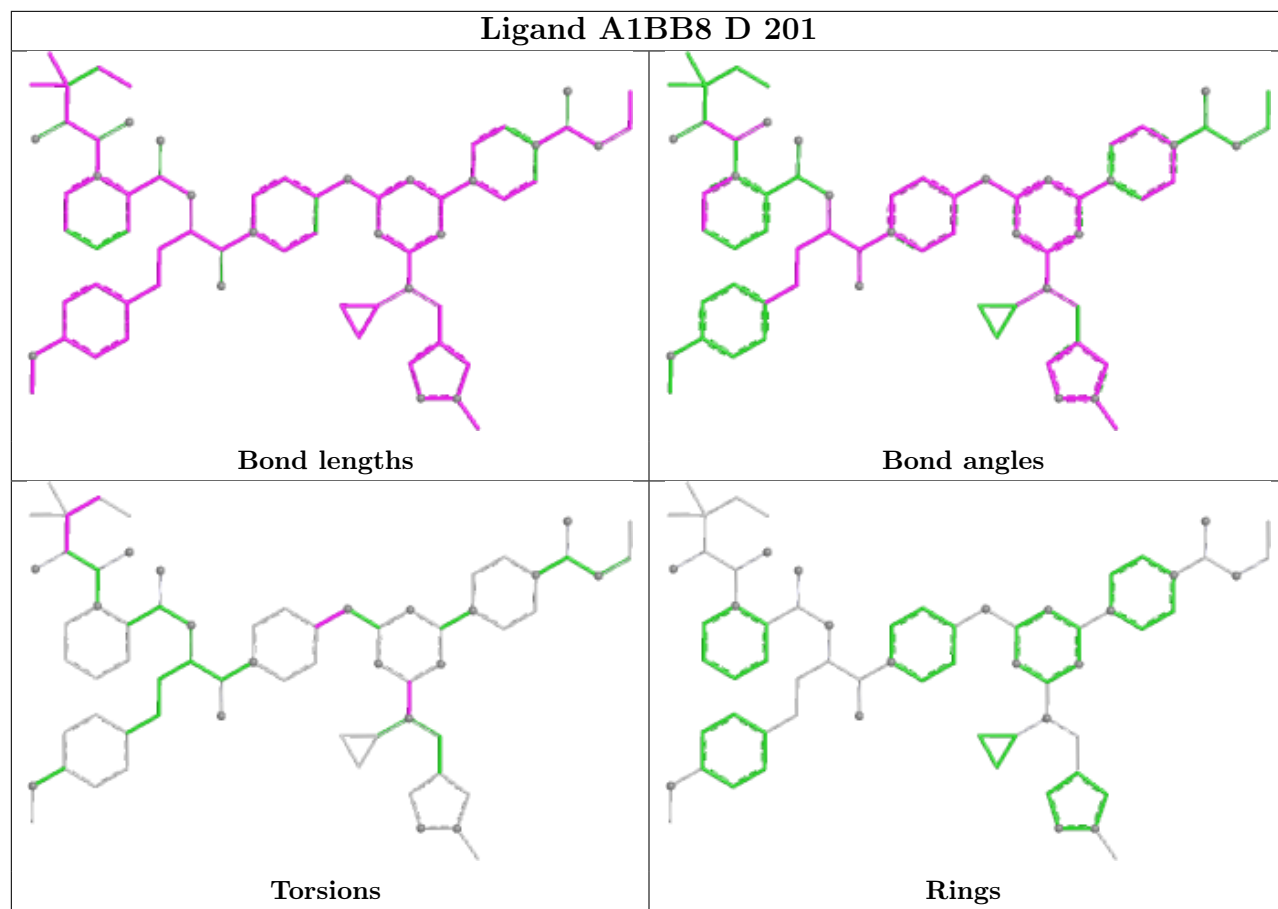
There are no ring outliers.

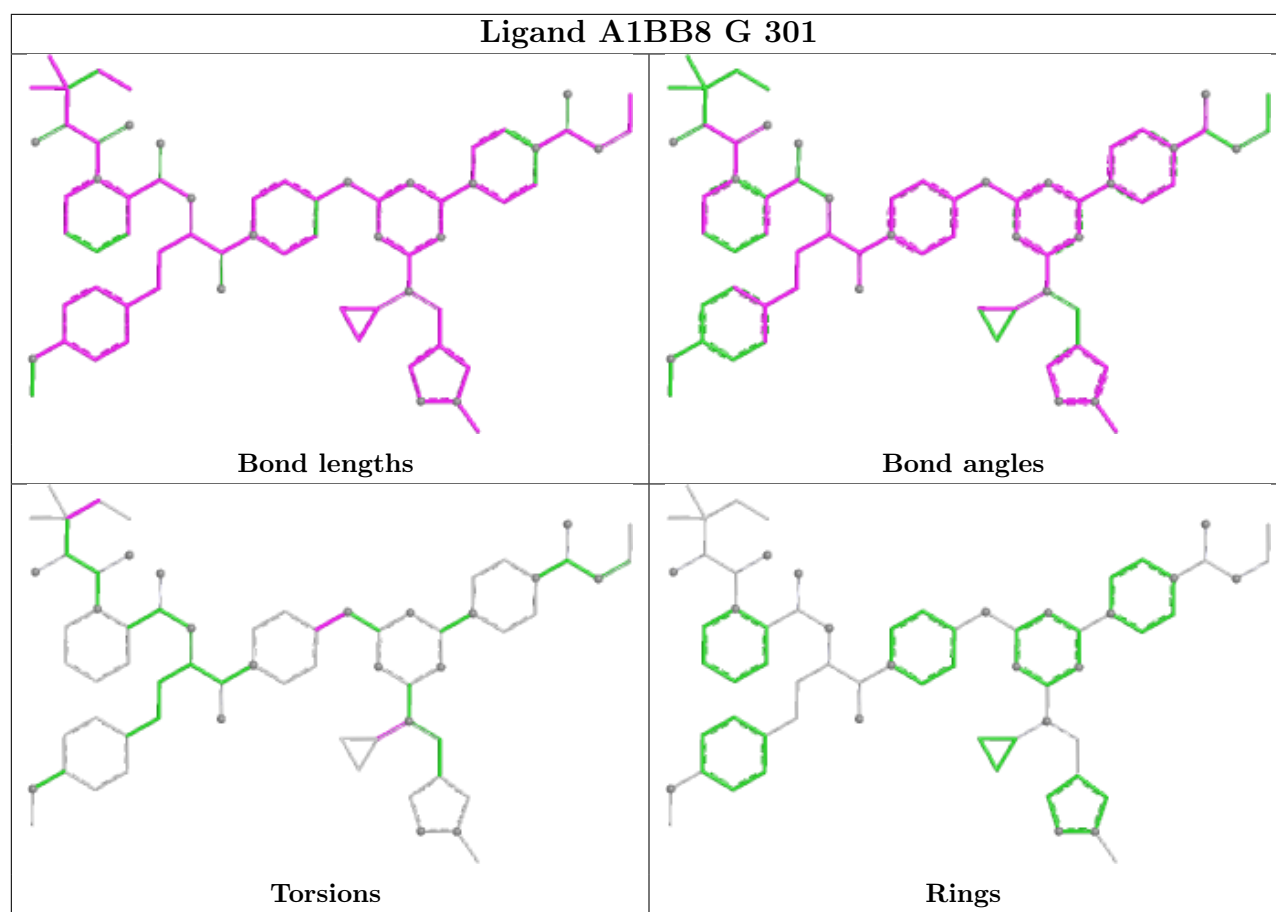
1 monomer is involved in 2 short contacts:

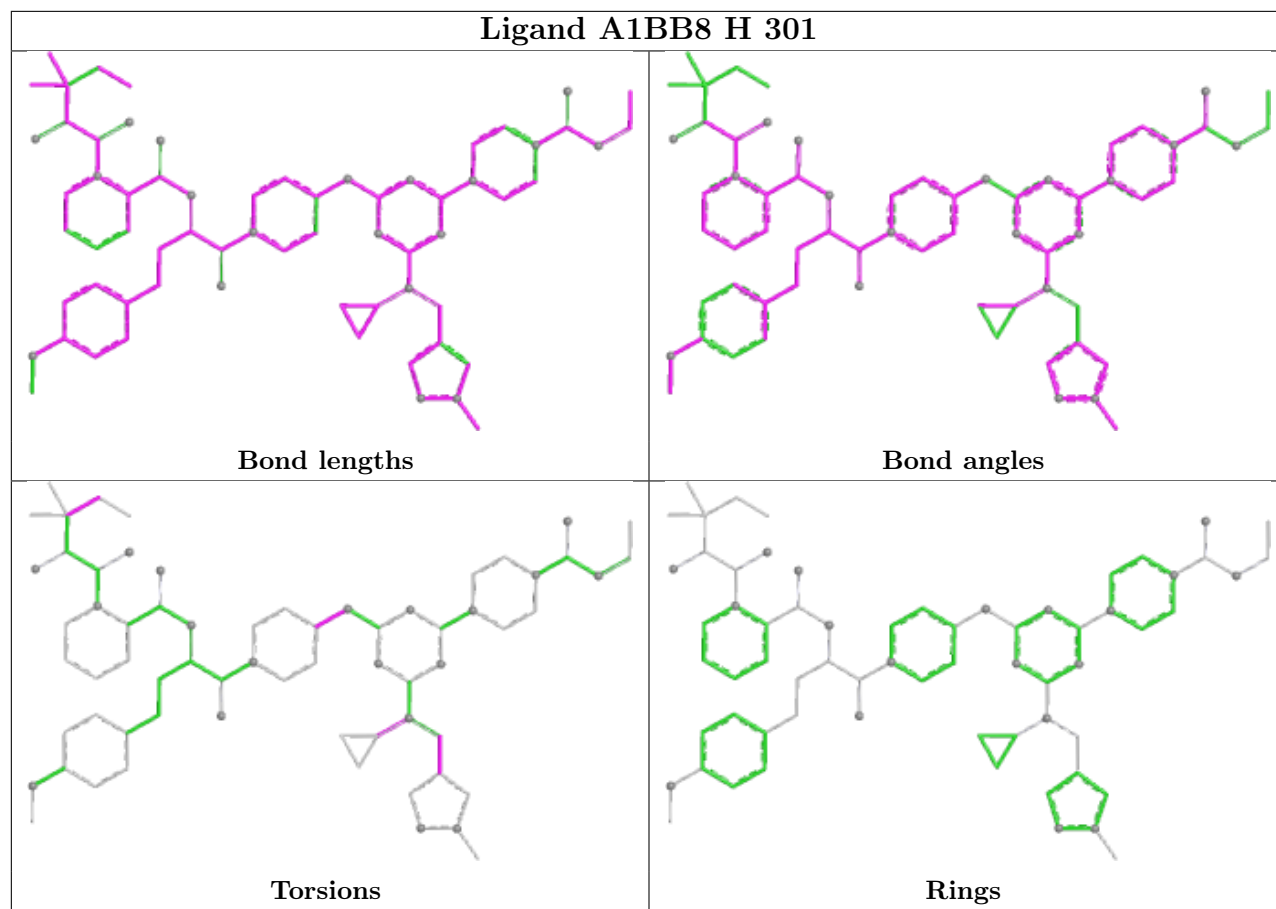
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	301	GOL	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	108/109 (99%)	0.50	3 (2%)	55	54	25, 31, 48, 61	0
1	B	109/109 (100%)	0.56	2 (1%)	67	67	25, 32, 46, 53	0
1	C	108/109 (99%)	0.43	2 (1%)	66	66	20, 32, 46, 51	1 (0%)
1	D	109/109 (100%)	0.67	1 (0%)	81	80	27, 34, 49, 54	0
2	E	103/116 (88%)	0.70	4 (3%)	43	42	27, 38, 54, 62	0
2	F	101/116 (87%)	0.79	6 (5%)	28	27	26, 38, 53, 59	0
2	G	102/116 (87%)	0.54	1 (0%)	79	79	24, 33, 45, 56	0
2	H	101/116 (87%)	0.67	7 (6%)	23	21	22, 34, 42, 51	1 (0%)
All	All	841/900 (93%)	0.61	26 (3%)	51	50	20, 34, 50, 62	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	PRO	3.9
1	A	0	MET	3.6
2	H	175	MET	3.4
1	B	50	LEU	3.2
2	E	240	GLN	3.0
2	H	158	HIS	2.9
1	D	-1	SER	2.9
2	G	175	MET	2.7
1	A	85	THR	2.7
2	E	169	ILE	2.7
2	E	219	ASP	2.6
1	C	32	ASP	2.5
2	F	141	ILE	2.4
1	B	105	LYS	2.4
2	H	219	ASP	2.3
1	C	0	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	193	ASN	2.2
2	H	169	ILE	2.2
2	H	192	ALA	2.1
2	F	154	ARG	2.1
2	F	163	PHE	2.1
2	H	231[A]	HIS	2.1
2	F	219	ASP	2.1
2	H	163	PHE	2.1
2	F	191	VAL	2.0
2	E	168	ALA	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](#)

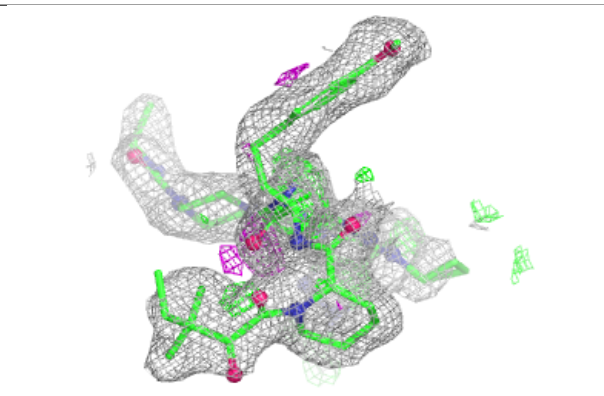
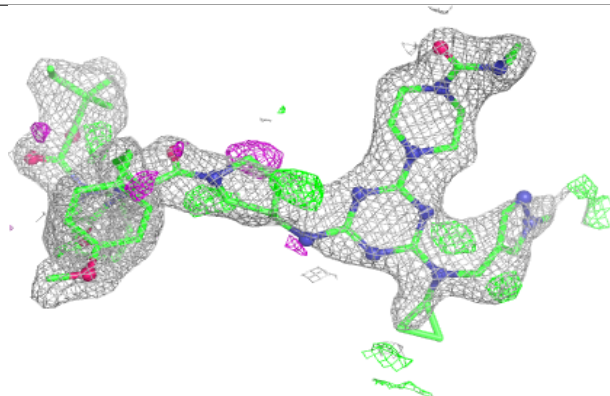
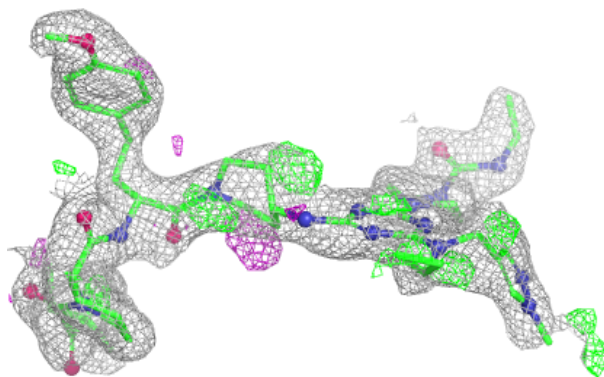
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	F	301	6/6	0.79	0.17	38,45,46,46	0
3	A1BB8	D	201	66/66	0.87	0.16	25,35,56,64	0
3	A1BB8	B	201	66/66	0.88	0.15	21,36,54,63	0
3	A1BB8	H	301	66/66	0.89	0.14	22,32,48,57	0
3	A1BB8	G	301	66/66	0.89	0.13	27,32,45,50	0

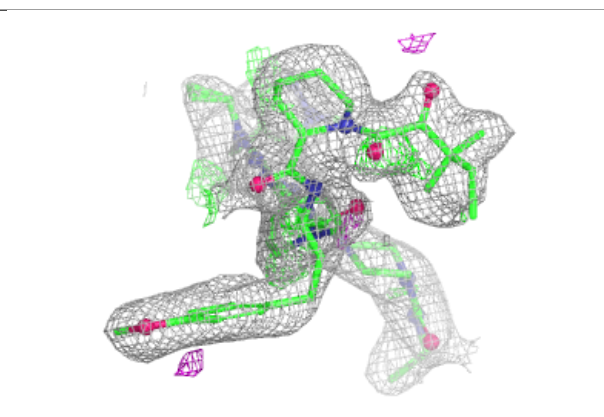
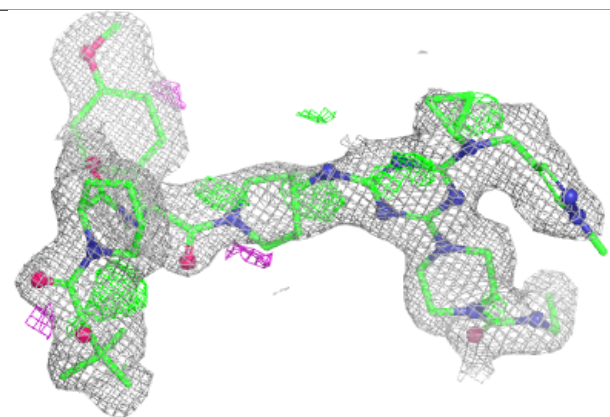
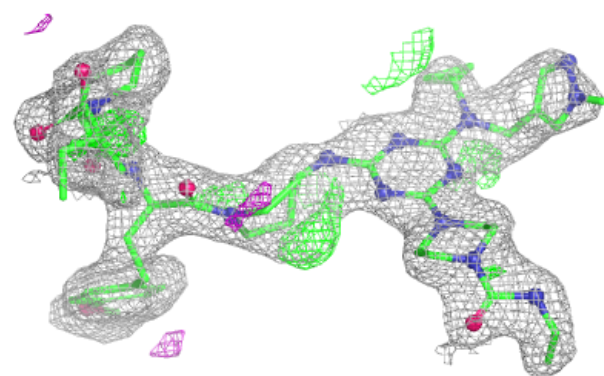
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BB8 D 201:

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

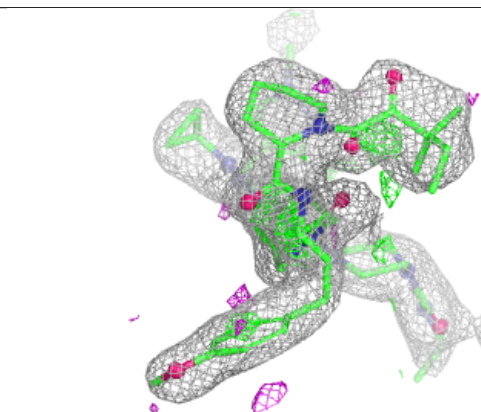
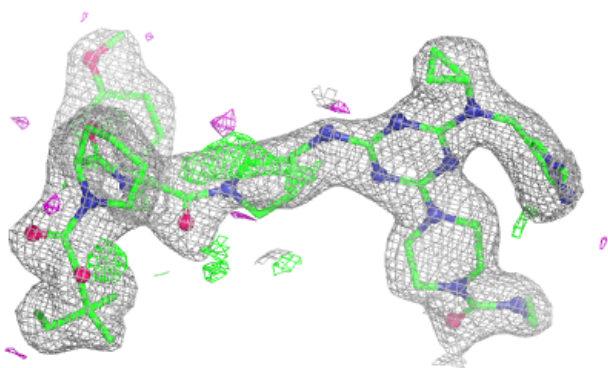
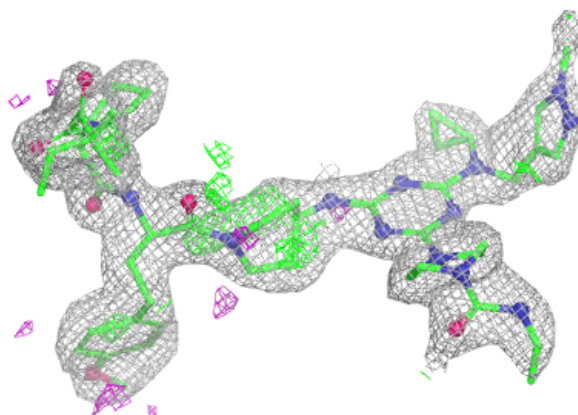
**Electron density around A1BB8 B 201:**

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

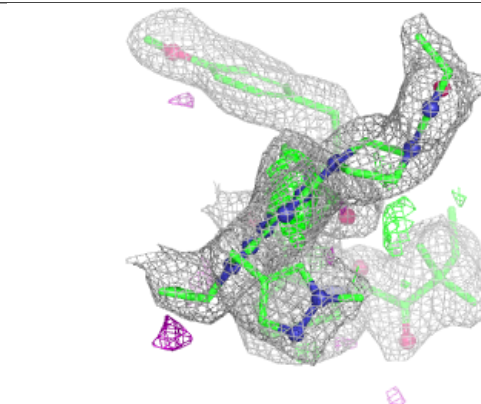
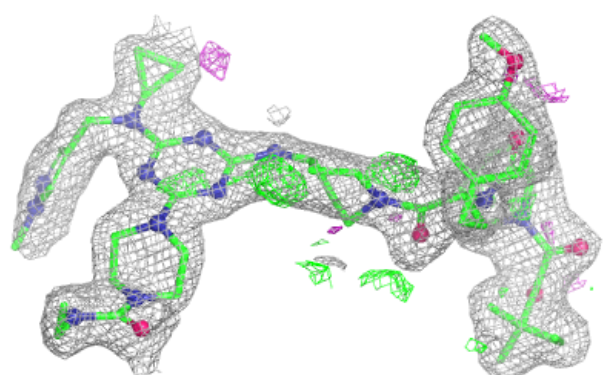
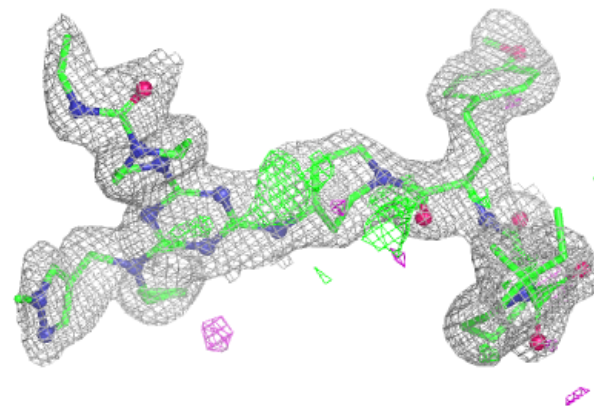


Electron density around A1BB8 H 301:

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

**Electron density around A1BB8 G 301:**

$2mF_o-DF_c$ (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.