



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:08 PM UTC

PDB ID : 8S6Y / pdb_00008s6y
Title : Co-crystal structure of TEAD1 with OPN-9652
Authors : Aplin, A.E.
Deposited on : 2024-02-28
Resolution : 2.03 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

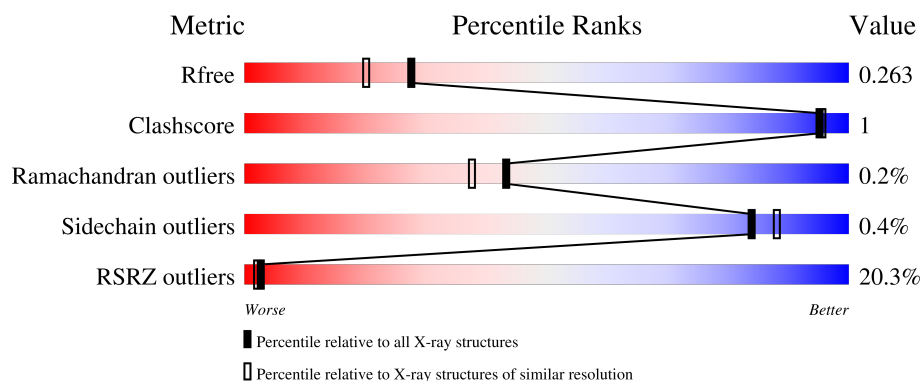
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	AAA	217	 17% 93% 5% •
1	BBB	217	 15% 96% •
1	CCC	217	 16% 97% ••
1	DDD	217	 32% 97% ••

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8177 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 Transcriptional enhancer factor TEF-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	212	Total	C	N	O	S	40	11	0
			1811	1149	313	334	15			
1	BBB	216	Total	C	N	O	S	24	9	0
			1824	1158	315	334	17			
1	CCC	215	Total	C	N	O	S	34	16	0
			1862	1176	326	345	15			
1	DDD	213	Total	C	N	O	S	61	6	0
			1781	1135	305	326	15			

There are 24 discrepancies between the modelled and reference sequences:

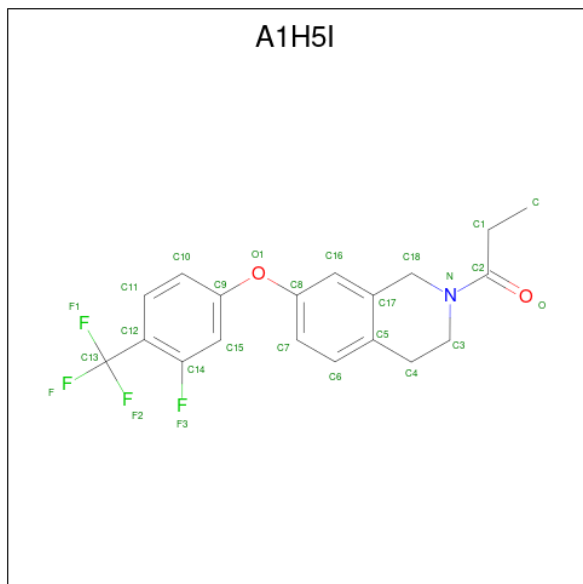
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	ALA	deletion	UNP P28347
AAA	?	-	ASN	deletion	UNP P28347
AAA	248	CYS	SER	conflict	UNP P28347
AAA	249	PRO	TYR	conflict	UNP P28347
AAA	251	ALA	ASP	conflict	UNP P28347
AAA	253	PRO	LEU	conflict	UNP P28347
BBB	?	-	ALA	deletion	UNP P28347
BBB	?	-	ASN	deletion	UNP P28347
BBB	246	CYS	SER	conflict	UNP P28347
BBB	247	PRO	TYR	conflict	UNP P28347
BBB	251	ALA	ASP	conflict	UNP P28347
BBB	253	PRO	LEU	conflict	UNP P28347
CCC	?	-	ALA	deletion	UNP P28347
CCC	?	-	ASN	deletion	UNP P28347
CCC	246	CYS	SER	conflict	UNP P28347
CCC	249	PRO	TYR	conflict	UNP P28347
CCC	251	ALA	ASP	conflict	UNP P28347
CCC	253	PRO	LEU	conflict	UNP P28347
DDD	?	-	ALA	deletion	UNP P28347
DDD	?	-	ASN	deletion	UNP P28347
DDD	246	CYS	SER	conflict	UNP P28347

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	247	PRO	TYR	conflict	UNP P28347
DDD	251	ALA	ASP	conflict	UNP P28347
DDD	253	PRO	LEU	conflict	UNP P28347

- Molecule 2 is 1-[7-[3-fluoranyl-4-(trifluoromethyl)phenoxy]-3,4-dihydro-1 {H}-isoquinolin-2-yl]propan-1-one (CCD ID: A1H5I) (formula: C₁₉H₁₇F₄NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	0	1
			34	23	8	1	2		
2	BBB	1	Total	C	F	N	O	0	1
			34	23	8	1	2		
2	CCC	1	Total	C	F	N	O	0	1
			34	23	8	1	2		
2	DDD	1	Total	C	F	N	O	0	1
			34	23	8	1	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



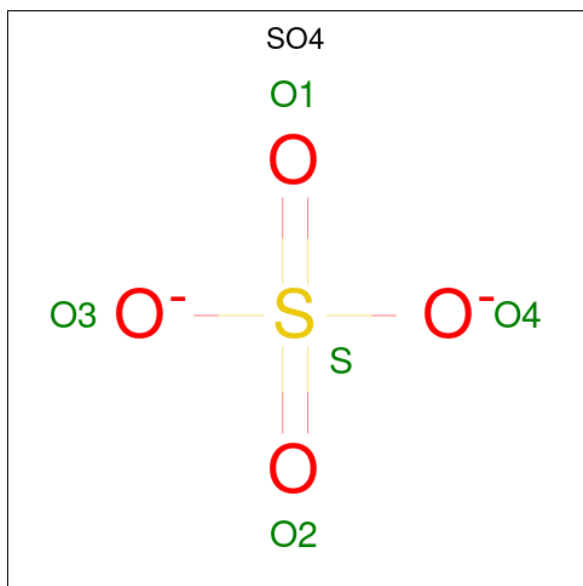
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



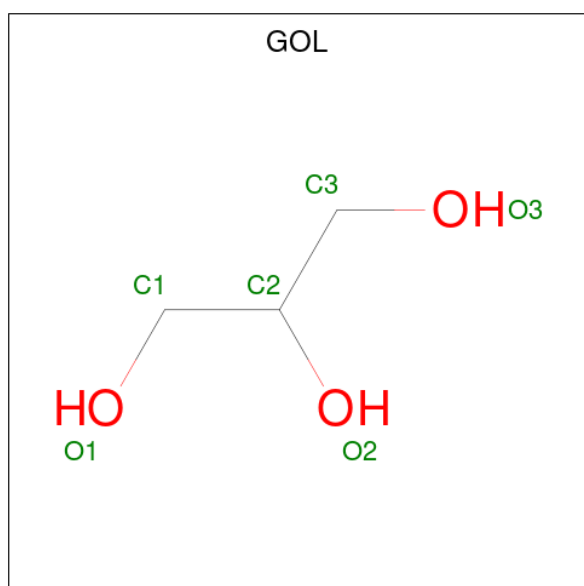
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O S 5 4 1	0	0
4	AAA	1	Total O S 5 4 1	0	0

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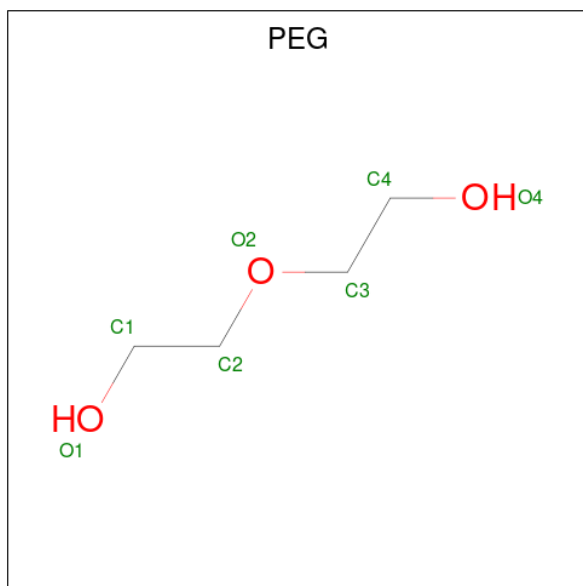
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	O	S	0	0
			5	4	1		
4	AAA	1	Total	O	S	0	0
			5	4	1		
4	BBB	1	Total	O	S	0	0
			5	4	1		
4	BBB	1	Total	O	S	0	0
			5	4	1		
4	BBB	1	Total	O	S	0	0
			5	4	1		
4	CCC	1	Total	O	S	0	0
			5	4	1		
4	CCC	1	Total	O	S	0	0
			5	4	1		
4	CCC	1	Total	O	S	0	0
			5	4	1		
4	DDD	1	Total	O	S	0	0
			5	4	1		
4	DDD	1	Total	O	S	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		

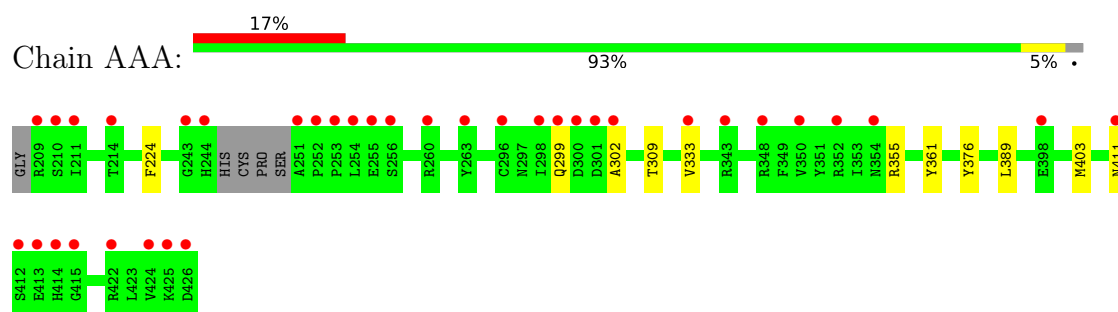
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	134	Total	O	0	0
			134	134		
7	BBB	166	Total	O	0	0
			166	166		
7	CCC	161	Total	O	0	0
			161	161		
7	DDD	130	Total	O	0	0
			130	130		

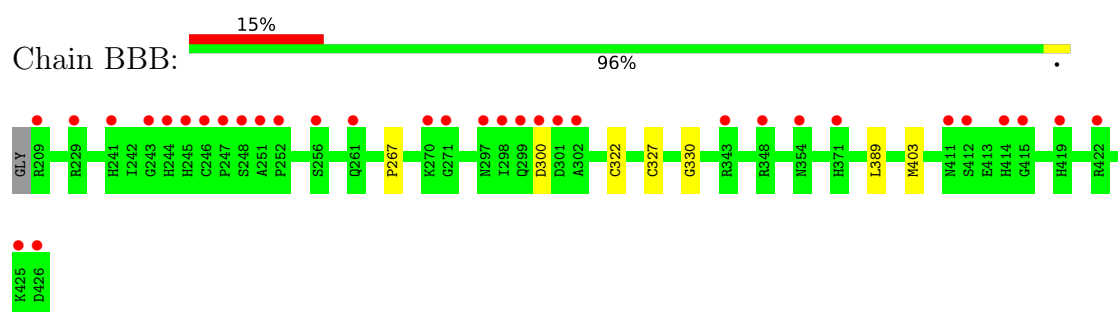
3 Residue-property plots [i](#)

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.

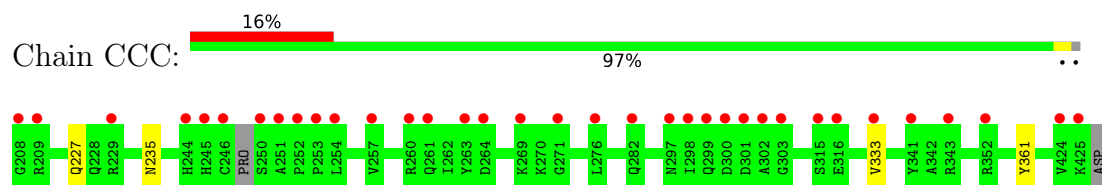
- Molecule 1: Transcriptional enhancer factor TEF-1



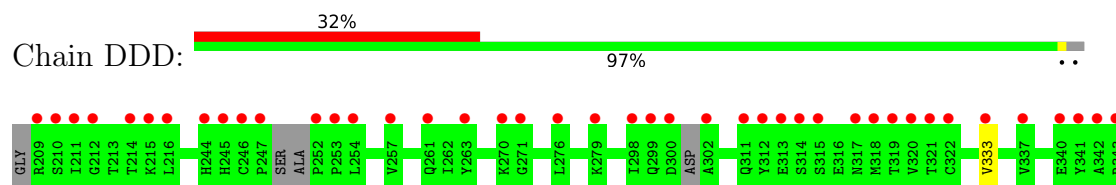
- Molecule 1: Transcriptional enhancer factor TEF-1

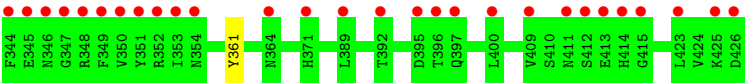


- Molecule 1: Transcriptional enhancer factor TEF-1



- Molecule 1: Transcriptional enhancer factor TEF-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.96Å 120.96Å 155.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	104.75 – 2.03 104.75 – 2.03	Depositor EDS
% Data completeness (in resolution range)	95.2 (104.75-2.03) 95.2 (104.75-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.258 0.226 , 0.263	Depositor DCC
R_{free} test set	647 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8177	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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: SO4, EDO, A1H5I, PEG, 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	AAA	1.01	0/1851	1.31	0/2493
1	BBB	0.99	0/1867	1.29	1/2516 (0.0%)
1	CCC	1.02	0/1902	1.27	0/2560
1	DDD	1.01	0/1822	1.27	0/2454
All	All	1.01	0/7442	1.29	1/10023 (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	BBB	300	ASP	CA-CB-CG	8.44	121.04	112.60

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	AAA	1811	0	1760	4	0
1	BBB	1824	0	1766	6	0
1	CCC	1862	0	1802	6	0
1	DDD	1781	0	1733	1	0
2	AAA	34	0	0	0	0
2	BBB	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	34	0	0	0	0
2	DDD	34	0	0	0	0
3	AAA	24	0	36	0	0
3	BBB	24	0	36	0	0
3	CCC	36	0	54	0	0
3	DDD	8	0	12	0	0
4	AAA	20	0	0	0	0
4	BBB	15	0	0	0	0
4	CCC	15	0	0	0	0
4	DDD	10	0	0	0	0
5	AAA	6	0	8	0	0
6	BBB	7	0	10	0	0
6	DDD	7	0	10	0	0
7	AAA	134	0	0	0	0
7	BBB	166	0	0	0	0
7	CCC	161	0	0	1	1
7	DDD	130	0	0	0	0
All	All	8177	0	7227	17	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 1.

The worst 5 of 17 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:BBB:389[B]:LEU:HD23	1:BBB:403[B]:MET:HE3	1.41	1.02
1:BBB:389[B]:LEU:HD23	1:BBB:403[B]:MET:CE	2.05	0.87
1:BBB:322[B]:CYS:SG	1:BBB:389[B]:LEU:HD11	2.15	0.86
1:CCC:235[B]:ASN:HD22	1:CCC:235[B]:ASN:C	1.86	0.82
1:BBB:322[B]:CYS:SG	1:BBB:389[B]:LEU:CD1	2.85	0.65

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)
7:CCC:627:HOH:O	7:CCC:627:HOH:O[6_555]	2.10	0.10

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	AAA	219/217 (101%)	215 (98%)	2 (1%)	2 (1%)	14	7
1	BBB	221/217 (102%)	216 (98%)	5 (2%)	0	100	100
1	CCC	227/217 (105%)	223 (98%)	4 (2%)	0	100	100
1	DDD	213/217 (98%)	210 (99%)	3 (1%)	0	100	100
All	All	880/868 (101%)	864 (98%)	14 (2%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	302	ALA
1	AAA	355	ARG

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	AAA	203/196 (104%)	200 (98%)	3 (2%)	57	58
1	BBB	205/196 (105%)	205 (100%)	0	100	100
1	CCC	209/196 (107%)	209 (100%)	0	100	100
1	DDD	200/196 (102%)	200 (100%)	0	100	100
All	All	817/784 (104%)	814 (100%)	3 (0%)	84	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	299	GLN
1	AAA	376	TYR
1	AAA	411	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1H5I	CCC	501[A]	-	28,28,28	0.52	0	41,41,41	1.39	6 (14%)
4	SO4	BBB	506	-	4,4,4	0.33	0	6,6,6	0.08	0
3	EDO	CCC	508	-	3,3,3	0.09	0	2,2,2	0.23	0
4	SO4	CCC	506	-	4,4,4	0.34	0	6,6,6	0.08	0
3	EDO	BBB	509	-	3,3,3	0.12	0	2,2,2	0.29	0
3	EDO	CCC	502	-	3,3,3	0.08	0	2,2,2	0.18	0
6	PEG	BBB	508	-	6,6,6	0.16	0	5,5,5	0.17	0
3	EDO	AAA	505	-	3,3,3	0.07	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	BBB	511	-	3,3,3	0.10	0	2,2,2	0.26	0
3	EDO	BBB	510	-	3,3,3	0.09	0	2,2,2	0.18	0
2	A1H5I	DDD	501[B]	-	28,28,28	0.55	0	41,41,41	1.37	6 (14%)
4	SO4	DDD	505	-	4,4,4	0.36	0	6,6,6	0.07	0
3	EDO	BBB	502	-	3,3,3	0.07	0	2,2,2	0.29	0
3	EDO	AAA	507	-	3,3,3	0.09	0	2,2,2	0.22	0
3	EDO	DDD	503	-	3,3,3	0.11	0	2,2,2	0.28	0
4	SO4	BBB	507	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	AAA	504	-	4,4,4	0.34	0	6,6,6	0.07	0
2	A1H5I	AAA	501[B]	-	28,28,28	0.56	0	41,41,41	1.38	8 (19%)
3	EDO	BBB	504	-	3,3,3	0.11	0	2,2,2	0.27	0
2	A1H5I	BBB	501[B]	-	28,28,28	0.54	0	41,41,41	1.46	9 (21%)
3	EDO	CCC	513	-	3,3,3	0.08	0	2,2,2	0.17	0
2	A1H5I	CCC	501[B]	-	28,28,28	0.52	0	41,41,41	1.36	7 (17%)
4	SO4	AAA	503	-	4,4,4	0.34	0	6,6,6	0.07	0
3	EDO	CCC	503	-	3,3,3	0.09	0	2,2,2	0.20	0
6	PEG	DDD	504	-	6,6,6	0.20	0	5,5,5	0.18	0
4	SO4	CCC	505	-	4,4,4	0.34	0	6,6,6	0.11	0
4	SO4	AAA	510	-	4,4,4	0.36	0	6,6,6	0.07	0
4	SO4	CCC	507	-	4,4,4	0.34	0	6,6,6	0.08	0
3	EDO	AAA	509	-	3,3,3	0.09	0	2,2,2	0.13	0
3	EDO	BBB	503	-	3,3,3	0.10	0	2,2,2	0.27	0
3	EDO	AAA	502	-	3,3,3	0.09	0	2,2,2	0.34	0
3	EDO	AAA	508	-	3,3,3	0.06	0	2,2,2	0.15	0
4	SO4	AAA	506	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	DDD	506	-	4,4,4	0.34	0	6,6,6	0.07	0
5	GOL	AAA	511	-	5,5,5	0.13	0	5,5,5	0.45	0
4	SO4	BBB	505	-	4,4,4	0.36	0	6,6,6	0.09	0
3	EDO	CCC	504	-	3,3,3	0.07	0	2,2,2	0.15	0
2	A1H5I	DDD	501[A]	-	28,28,28	0.55	0	41,41,41	1.39	7 (17%)
3	EDO	CCC	510	-	3,3,3	0.13	0	2,2,2	0.20	0
3	EDO	CCC	512	-	3,3,3	0.10	0	2,2,2	0.20	0
3	EDO	CCC	511	-	3,3,3	0.11	0	2,2,2	0.34	0
3	EDO	DDD	502	-	3,3,3	0.12	0	2,2,2	0.19	0
3	EDO	AAA	512	-	3,3,3	0.07	0	2,2,2	0.26	0
2	A1H5I	BBB	501[A]	-	28,28,28	0.54	0	41,41,41	1.47	8 (19%)
3	EDO	CCC	509	-	3,3,3	0.09	0	2,2,2	0.22	0
2	A1H5I	AAA	501[A]	-	28,28,28	0.54	0	41,41,41	1.34	6 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H5I	CCC	501[A]	-	-	3/16/25/25	0/3/3/3
3	EDO	CCC	508	-	-	0/1/1/1	-
3	EDO	BBB	509	-	-	1/1/1/1	-
3	EDO	CCC	502	-	-	0/1/1/1	-
6	PEG	BBB	508	-	-	1/4/4/4	-
3	EDO	AAA	505	-	-	0/1/1/1	-
3	EDO	BBB	511	-	-	0/1/1/1	-
3	EDO	BBB	510	-	-	0/1/1/1	-
2	A1H5I	DDD	501[B]	-	-	3/16/25/25	0/3/3/3
3	EDO	BBB	502	-	-	1/1/1/1	-
3	EDO	AAA	507	-	-	0/1/1/1	-
3	EDO	DDD	503	-	-	0/1/1/1	-
2	A1H5I	AAA	501[B]	-	-	6/16/25/25	0/3/3/3
3	EDO	BBB	504	-	-	1/1/1/1	-
2	A1H5I	BBB	501[B]	-	-	6/16/25/25	0/3/3/3
3	EDO	CCC	513	-	-	0/1/1/1	-
2	A1H5I	CCC	501[B]	-	-	3/16/25/25	0/3/3/3
3	EDO	CCC	503	-	-	1/1/1/1	-
6	PEG	DDD	504	-	-	1/4/4/4	-
3	EDO	AAA	509	-	-	1/1/1/1	-
3	EDO	BBB	503	-	-	0/1/1/1	-
3	EDO	AAA	502	-	-	1/1/1/1	-
3	EDO	AAA	508	-	-	1/1/1/1	-
5	GOL	AAA	511	-	-	2/4/4/4	-
3	EDO	CCC	504	-	-	1/1/1/1	-
2	A1H5I	DDD	501[A]	-	-	6/16/25/25	0/3/3/3
3	EDO	CCC	510	-	-	1/1/1/1	-
3	EDO	CCC	512	-	-	0/1/1/1	-
3	EDO	CCC	511	-	-	1/1/1/1	-
3	EDO	DDD	502	-	-	0/1/1/1	-
3	EDO	AAA	512	-	-	0/1/1/1	-
2	A1H5I	BBB	501[A]	-	-	6/16/25/25	0/3/3/3
3	EDO	CCC	509	-	-	0/1/1/1	-
2	A1H5I	AAA	501[A]	-	-	6/16/25/25	0/3/3/3

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	501[B]	A1H5I	C15-C14-C12	-3.52	120.05	123.88
2	AAA	501[B]	A1H5I	F2-C13-C12	-3.31	106.78	112.65
2	AAA	501[B]	A1H5I	C15-C14-C12	-3.30	120.29	123.88
2	BBB	501[A]	A1H5I	F2-C13-C12	-3.21	106.95	112.65
2	CCC	501[B]	A1H5I	C15-C14-C12	-3.12	120.48	123.88

There are no chirality outliers.

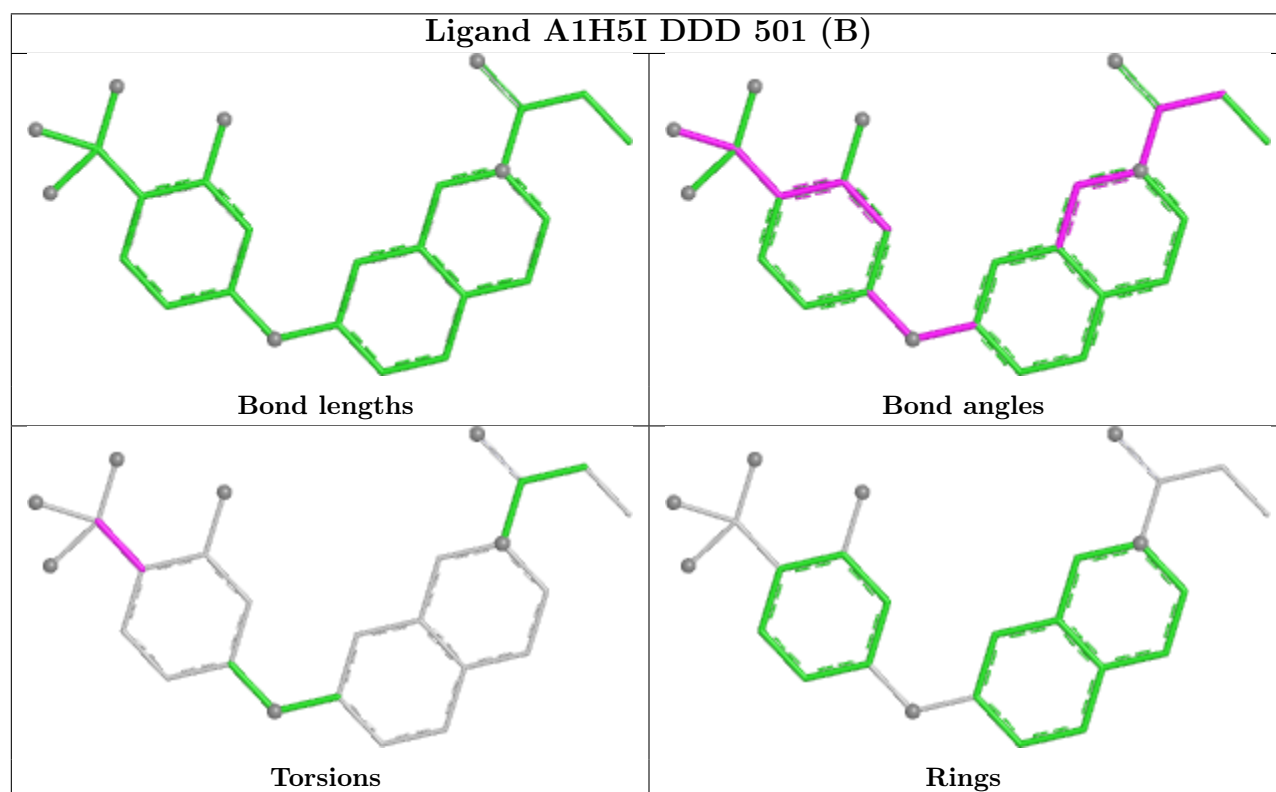
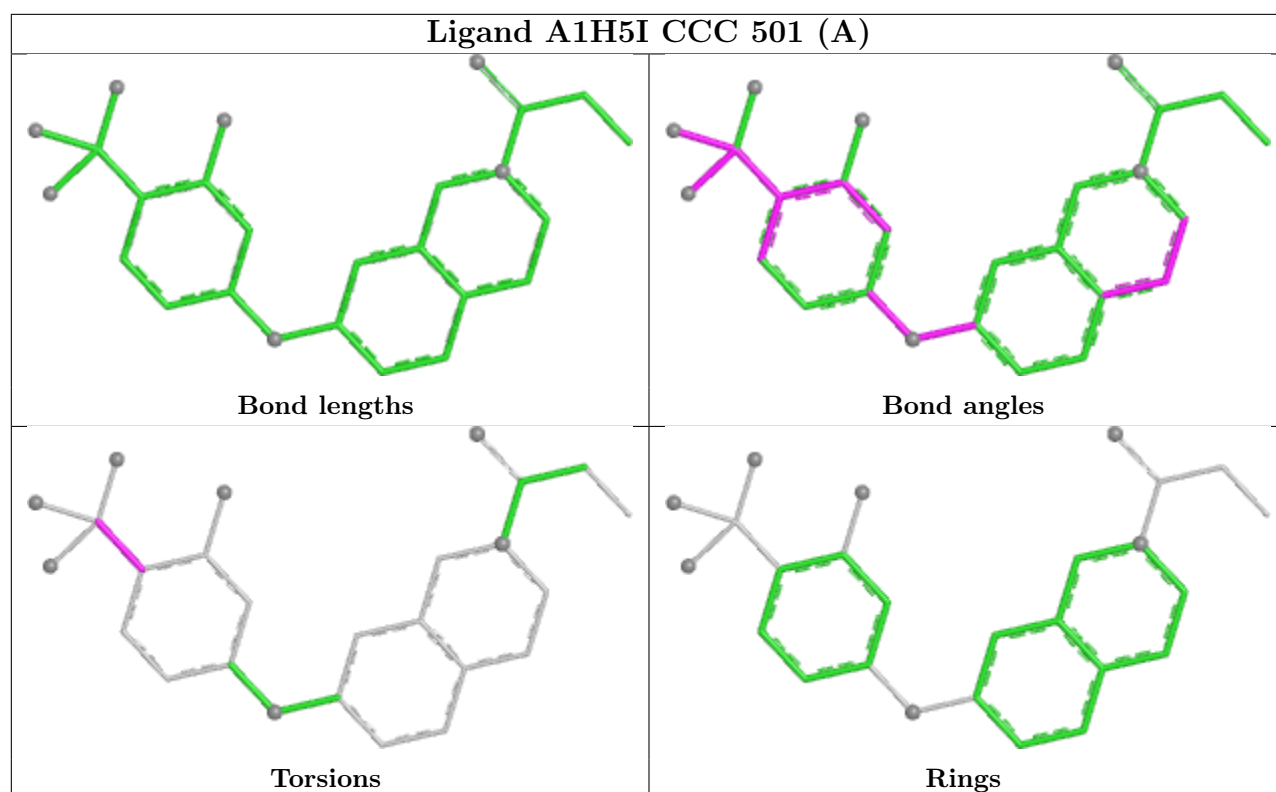
5 of 53 torsion outliers are listed below:

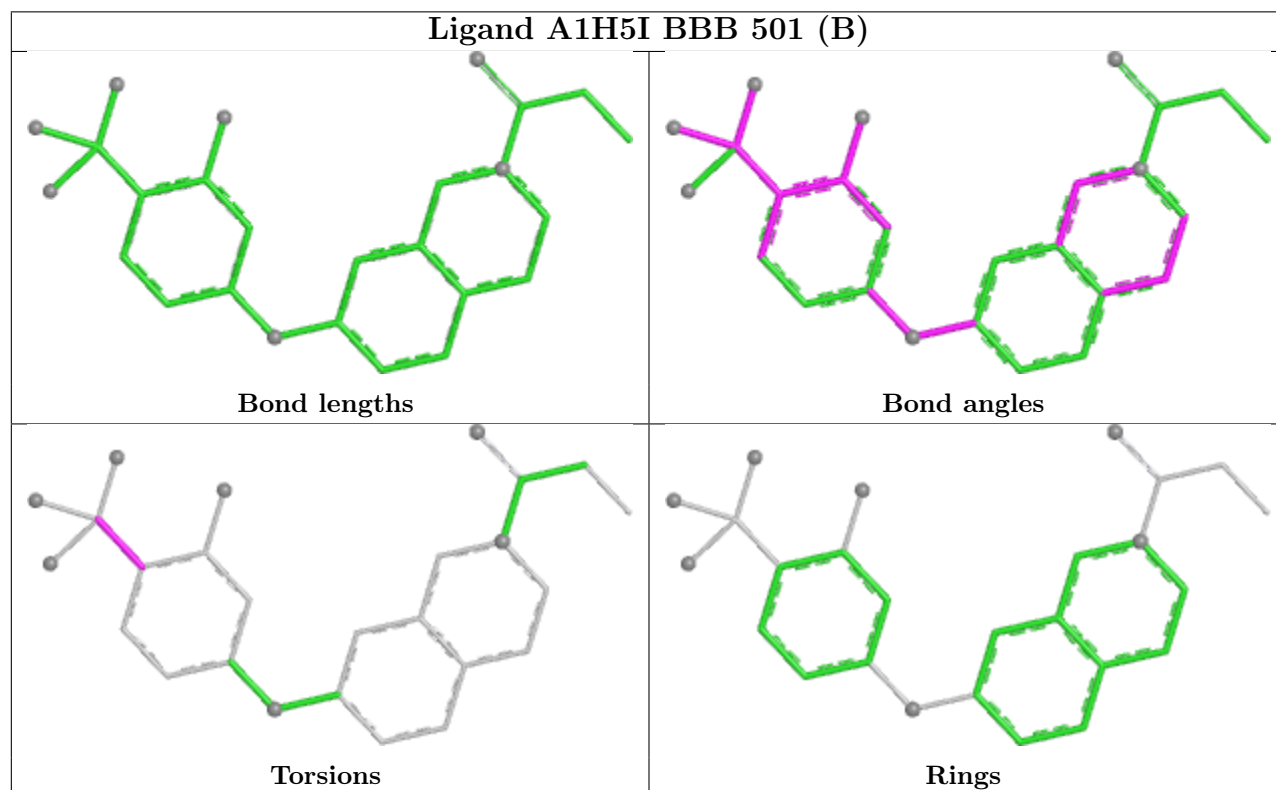
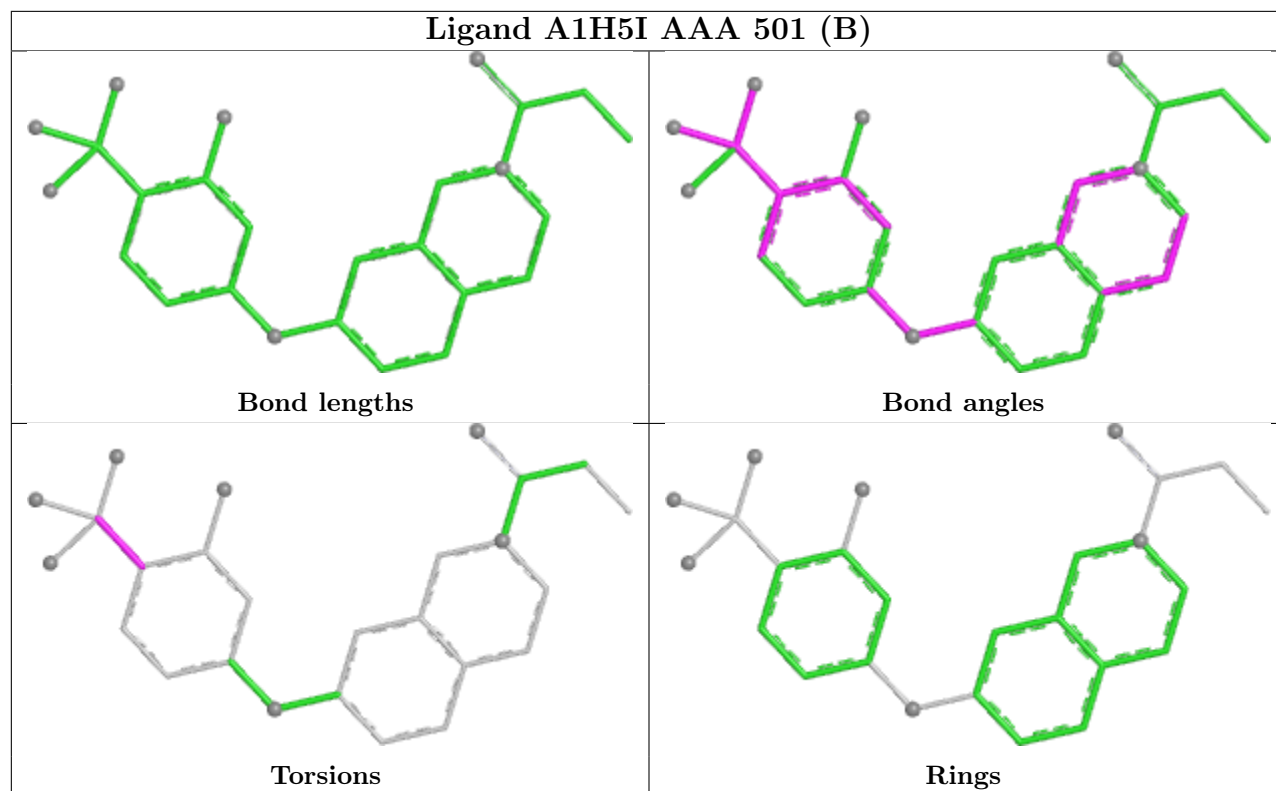
Mol	Chain	Res	Type	Atoms
2	AAA	501[A]	A1H5I	C14-C12-C13-F2
2	AAA	501[A]	A1H5I	C14-C12-C13-F1
2	AAA	501[A]	A1H5I	C14-C12-C13-F
2	AAA	501[B]	A1H5I	C14-C12-C13-F2
2	AAA	501[B]	A1H5I	C14-C12-C13-F1

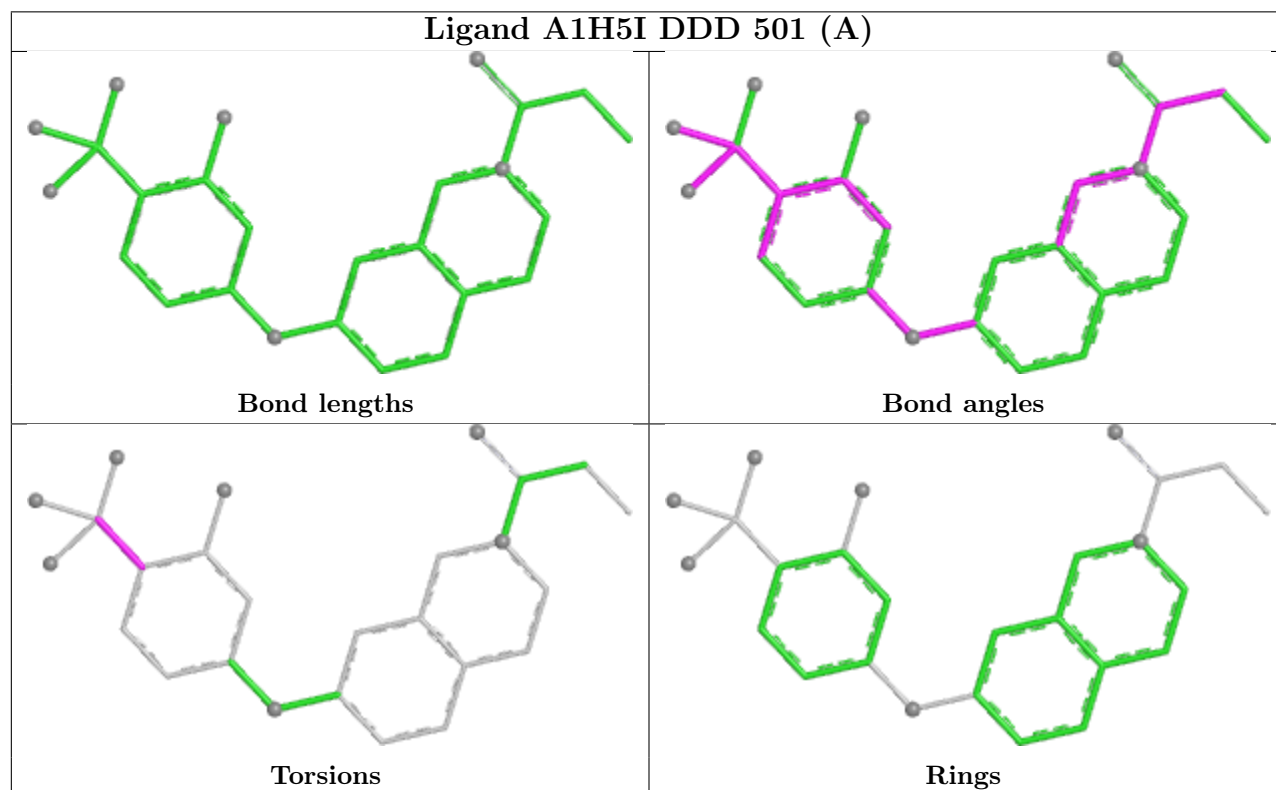
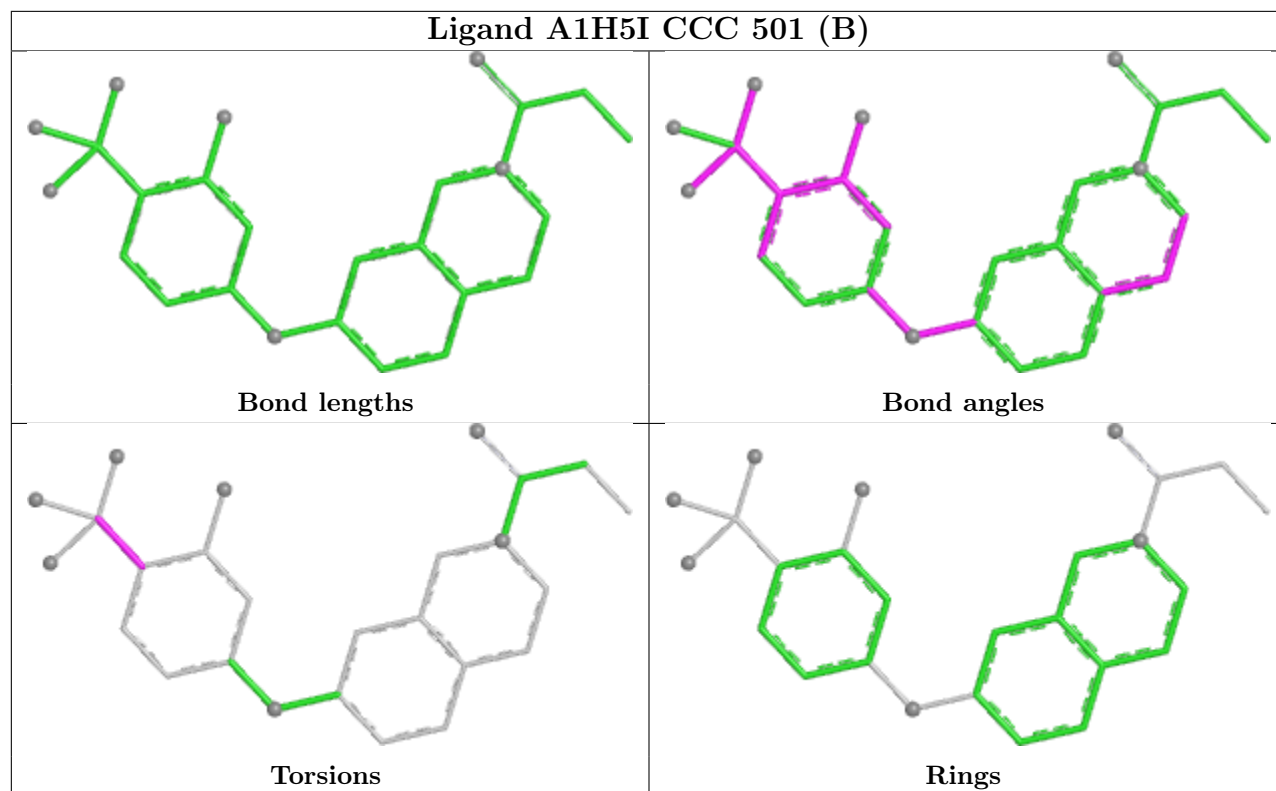
There are no ring outliers.

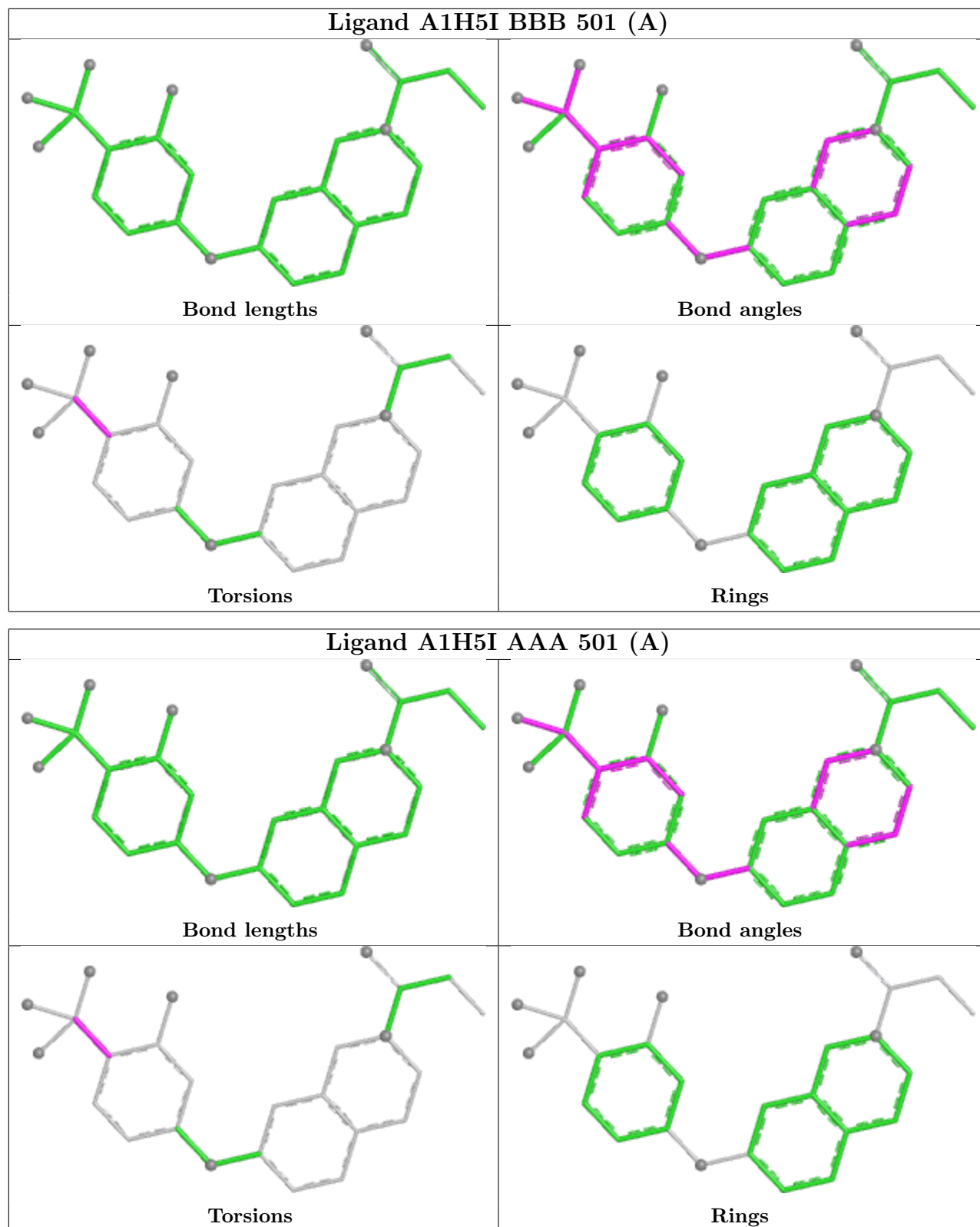
No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	BBB	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BBB	248:SER	C	251:ALA	N	3.99

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	AAA	212/217 (97%)	1.11	36 (16%)	4 4	15, 40, 68, 96	25 (11%)
1	BBB	216/217 (99%)	0.91	33 (15%)	5 5	14, 35, 66, 92	26 (12%)
1	CCC	215/217 (99%)	0.96	35 (16%)	4 4	13, 36, 70, 103	30 (13%)
1	DDD	213/217 (98%)	1.55	70 (32%)	1 0	18, 43, 70, 113	28 (13%)
All	All	856/868 (98%)	1.13	174 (20%)	3 2	13, 38, 69, 113	109 (12%)

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	349	PHE	8.9
1	DDD	344	PHE	8.1
1	CCC	251	ALA	6.8
1	AAA	414	HIS	6.7
1	BBB	300	ASP	6.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	AAA	507	4/4	0.70	0.25	69,71,71,72	0
3	EDO	BBB	509	4/4	0.71	0.34	75,77,78,83	0
3	EDO	CCC	504	4/4	0.72	0.27	73,75,76,77	0
4	SO4	AAA	503	5/5	0.72	0.14	95,98,98,98	0
4	SO4	CCC	506	5/5	0.73	0.14	87,90,90,93	0
4	SO4	DDD	506	5/5	0.75	0.13	99,99,100,103	0
3	EDO	AAA	509	4/4	0.76	0.28	82,84,84,86	0
3	EDO	AAA	512	4/4	0.78	0.26	72,73,74,76	0
4	SO4	CCC	507	5/5	0.79	0.12	96,96,98,99	0
4	SO4	AAA	506	5/5	0.80	0.13	87,88,88,91	0
4	SO4	AAA	504	5/5	0.80	0.14	89,90,92,92	0
6	PEG	DDD	504	7/7	0.80	0.21	71,73,74,75	0
3	EDO	AAA	508	4/4	0.81	0.23	66,66,66,66	0
3	EDO	DDD	503	4/4	0.82	0.23	59,60,61,62	0
3	EDO	CCC	508	4/4	0.82	0.25	69,69,69,71	0
3	EDO	BBB	503	4/4	0.84	0.17	69,70,71,71	0
3	EDO	CCC	503	4/4	0.85	0.23	60,61,62,65	0
3	EDO	CCC	510	4/4	0.86	0.24	53,54,54,54	0
3	EDO	CCC	512	4/4	0.86	0.21	58,61,63,63	0
4	SO4	AAA	510	5/5	0.86	0.14	64,65,67,67	0
5	GOL	AAA	511	6/6	0.86	0.20	59,60,63,66	0
4	SO4	BBB	507	5/5	0.86	0.10	90,90,92,93	0
3	EDO	BBB	511	4/4	0.87	0.18	63,63,64,64	0
3	EDO	CCC	511	4/4	0.87	0.19	57,58,58,58	0
3	EDO	BBB	504	4/4	0.87	0.24	64,66,69,72	0
3	EDO	CCC	513	4/4	0.87	0.20	72,74,75,76	0
3	EDO	CCC	509	4/4	0.87	0.23	73,73,74,74	0
3	EDO	AAA	502	4/4	0.88	0.20	59,60,61,64	0
3	EDO	DDD	502	4/4	0.89	0.14	41,42,43,45	0
4	SO4	BBB	505	5/5	0.89	0.14	51,51,55,56	0
4	SO4	BBB	506	5/5	0.89	0.09	85,85,86,87	0
6	PEG	BBB	508	7/7	0.90	0.18	56,66,72,73	0
3	EDO	BBB	502	4/4	0.90	0.13	33,36,38,40	0
3	EDO	CCC	502	4/4	0.91	0.13	41,45,46,47	0
4	SO4	CCC	505	5/5	0.91	0.10	58,58,59,62	0
3	EDO	AAA	505	4/4	0.92	0.12	35,37,37,38	0
4	SO4	DDD	505	5/5	0.93	0.08	62,62,63,64	0
2	A1H5I	DDD	501[B]	26/26	0.94	0.09	31,33,35,37	8
2	A1H5I	DDD	501[A]	26/26	0.94	0.09	31,33,35,37	8
2	A1H5I	AAA	501[A]	26/26	0.95	0.08	26,29,31,31	8
2	A1H5I	AAA	501[B]	26/26	0.95	0.08	26,29,31,31	8
3	EDO	BBB	510	4/4	0.95	0.12	44,47,49,51	0
2	A1H5I	BBB	501[A]	26/26	0.96	0.06	30,32,33,34	8

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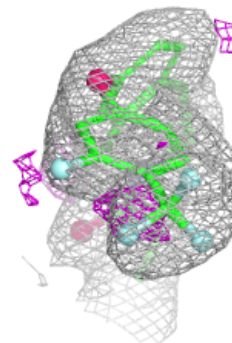
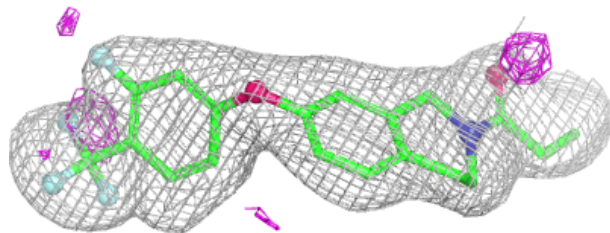
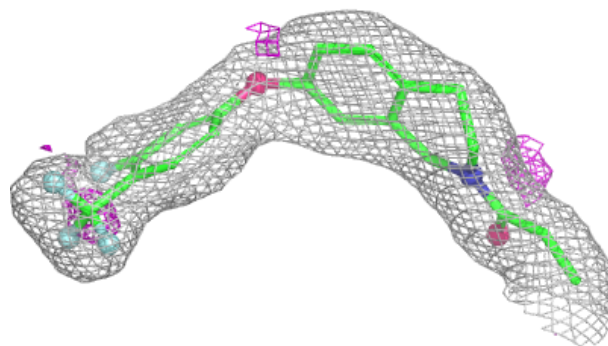
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1H5I	BBB	501[B]	26/26	0.96	0.06	30,32,33,34	8
2	A1H5I	CCC	501[A]	26/26	0.96	0.07	29,31,32,33	8
2	A1H5I	CCC	501[B]	26/26	0.96	0.07	29,31,32,33	8

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.

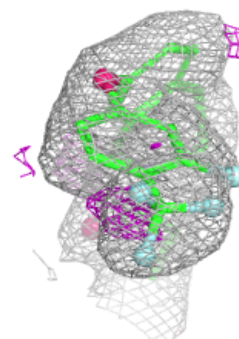
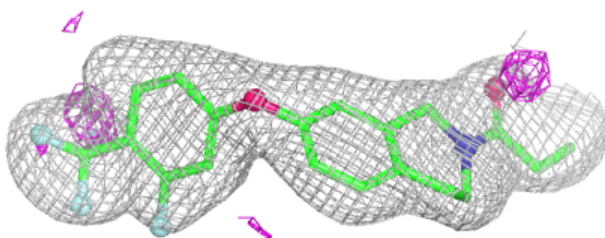
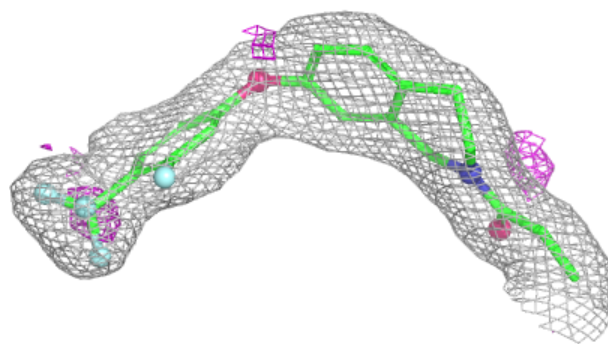
Electron density around A1H5I DDD 501 (B):

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

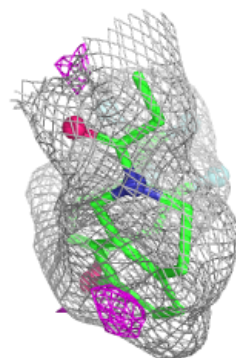
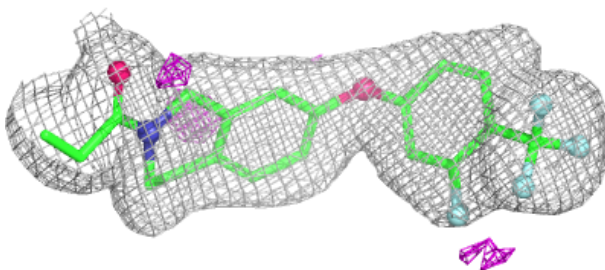
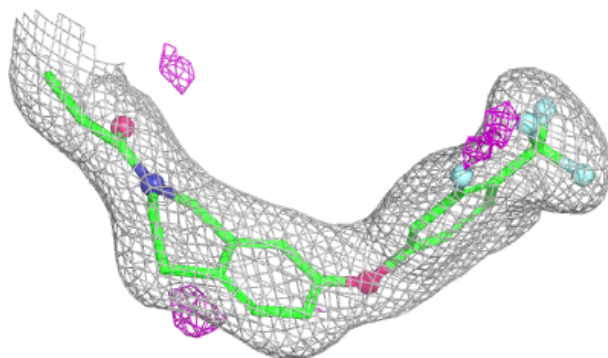


Electron density around A1H5I DDD 501 (A):

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

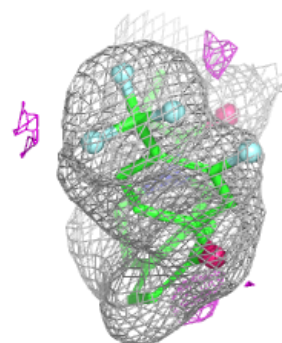
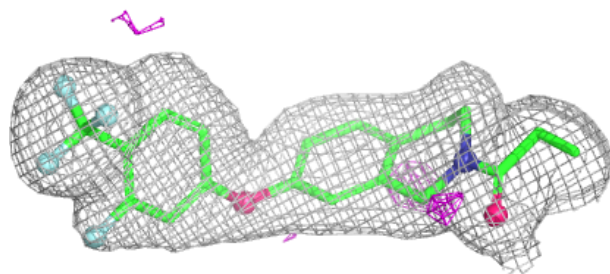
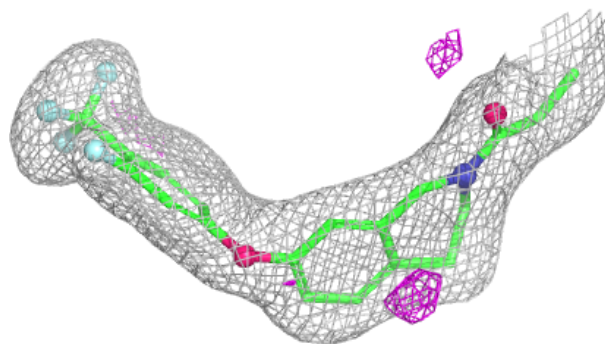
**Electron density around A1H5I AAA 501 (A):**

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and green (positive)

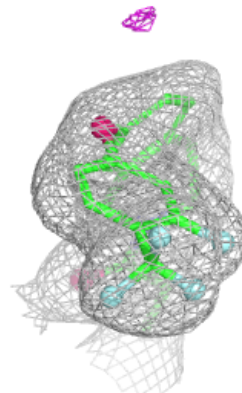
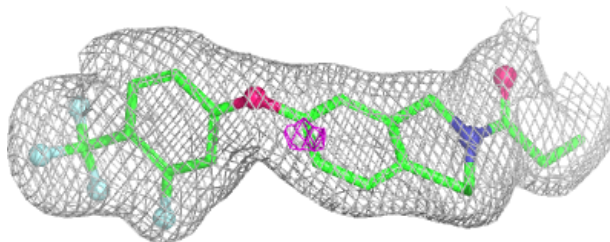
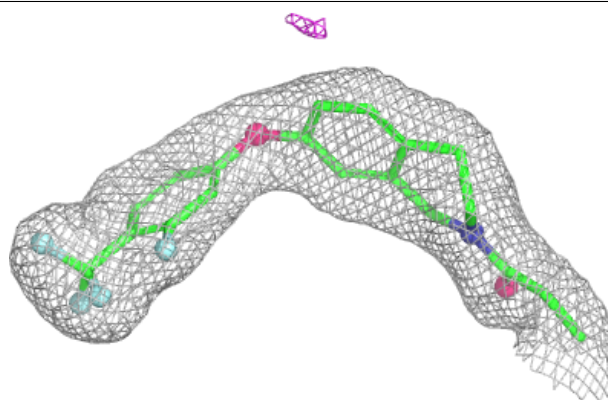


Electron density around A1H5I AAA 501 (B):

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

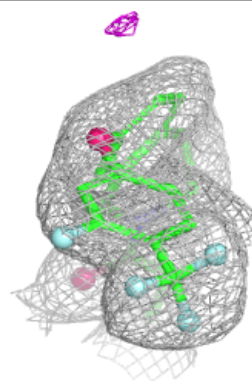
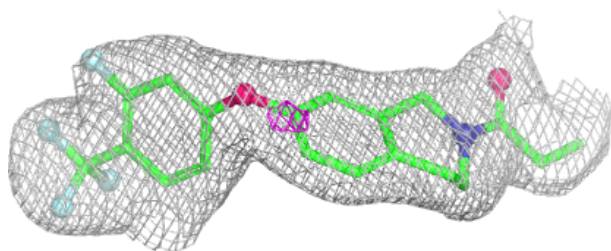
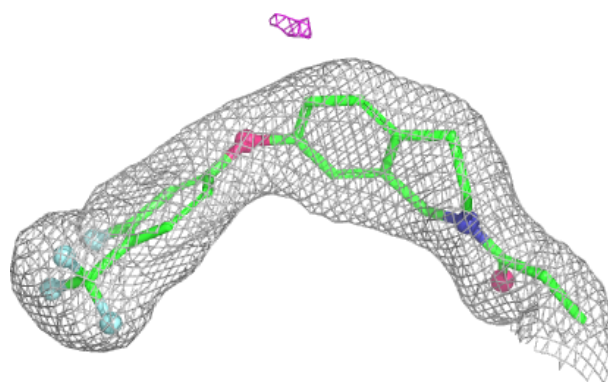
**Electron density around A1H5I BBB 501 (A):**

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and green (positive)

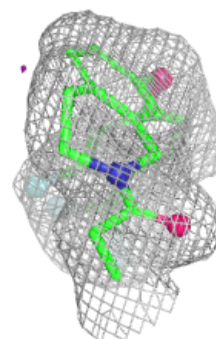
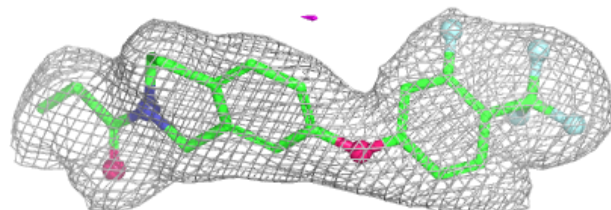
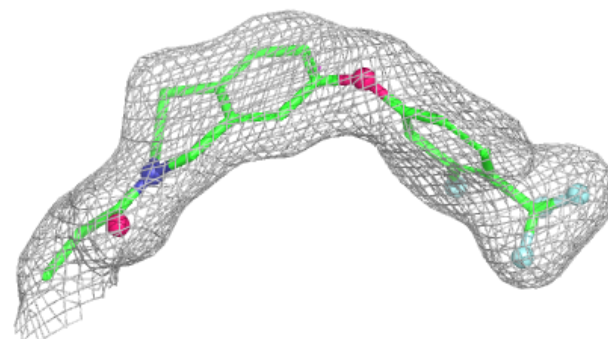


Electron density around A1H5I BBB 501 (B):

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

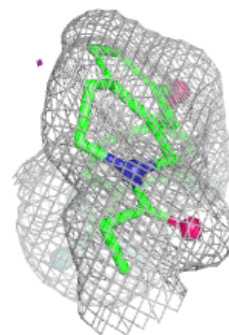
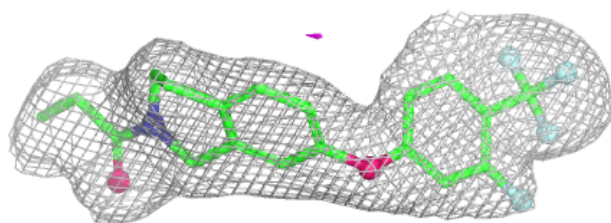
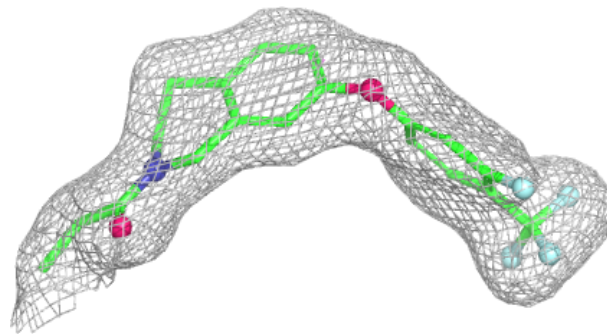
**Electron density around A1H5I CCC 501 (A):**

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



Electron density around A1H5I CCC 501 (B):

$2mF_o - DF_c$ (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.