



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 05:02 pm GMT

PDB ID : 7PXO
Title : Structure of the Diels Alderase enzyme AbyU, from *Micromonospora maris*,
co-crystallised with a non transformable substrate analogue
Authors : Back, C.R.; Race, P.R.
Deposited on : 2021-10-08
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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

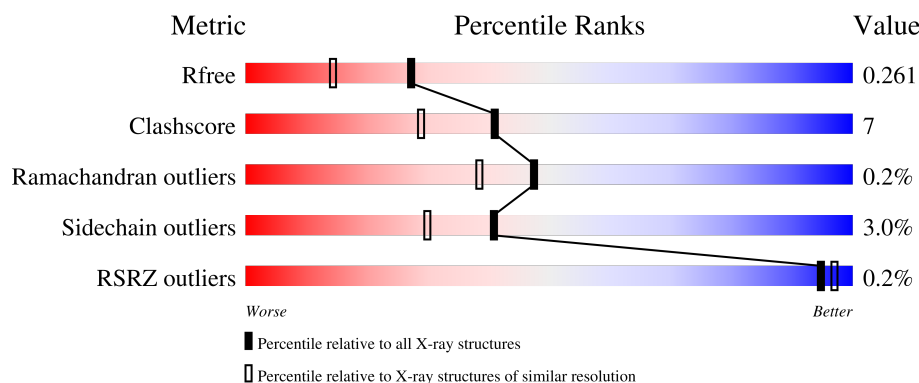
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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	AAA	160	<div> <div style="width: 78%;"></div> <div style="width: 8%;"></div> <div style="width: 15%;"></div> </div> <div>78% 8% 15%</div>
1	BBB	160	<div> <div style="width: 74%;"></div> <div style="width: 11%;"></div> <div style="width: 15%;"></div> </div> <div>74% 11% 15%</div>
1	CCC	160	<div> <div style="width: 76%;"></div> <div style="width: 6%;"></div> <div style="width: 17%;"></div> </div> <div>76% 6% 17%</div>
1	DDD	160	<div> <div style="width: 74%;"></div> <div style="width: 9%;"></div> <div style="width: 18%;"></div> </div> <div>74% 9% 18%</div>

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	8IF	AAA	201	X	-	X	-
2	8IF	BBB	201	X	-	X	-
2	8IF	DDD	201	X	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8560 atoms, of which 4223 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 YD repeat-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	136	Total	C	H	N	O	S	38	0	0
			2093	672	1035	180	205	1			
1	BBB	136	Total	C	H	N	O	S	39	1	0
			2104	675	1042	181	204	2			
1	CCC	133	Total	C	H	N	O	S	37	0	0
			2040	657	1009	174	199	1			
1	DDD	132	Total	C	H	N	O	S	37	0	0
			2026	652	1002	173	198	1			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-18	MET	-	initiating methionine	UNP F4F7G1
AAA	-17	ALA	-	expression tag	UNP F4F7G1
AAA	-16	HIS	-	expression tag	UNP F4F7G1
AAA	-15	HIS	-	expression tag	UNP F4F7G1
AAA	-14	HIS	-	expression tag	UNP F4F7G1
AAA	-13	HIS	-	expression tag	UNP F4F7G1
AAA	-12	HIS	-	expression tag	UNP F4F7G1
AAA	-11	HIS	-	expression tag	UNP F4F7G1
AAA	-10	SER	-	expression tag	UNP F4F7G1
AAA	-9	SER	-	expression tag	UNP F4F7G1
AAA	-8	GLY	-	expression tag	UNP F4F7G1
AAA	-7	LEU	-	expression tag	UNP F4F7G1
AAA	-6	GLU	-	expression tag	UNP F4F7G1
AAA	-5	VAL	-	expression tag	UNP F4F7G1
AAA	-4	LEU	-	expression tag	UNP F4F7G1
AAA	-3	PHE	-	expression tag	UNP F4F7G1
AAA	-2	GLN	-	expression tag	UNP F4F7G1
AAA	-1	GLY	-	expression tag	UNP F4F7G1
AAA	0	PRO	-	expression tag	UNP F4F7G1
BBB	-18	MET	-	initiating methionine	UNP F4F7G1
BBB	-17	ALA	-	expression tag	UNP F4F7G1

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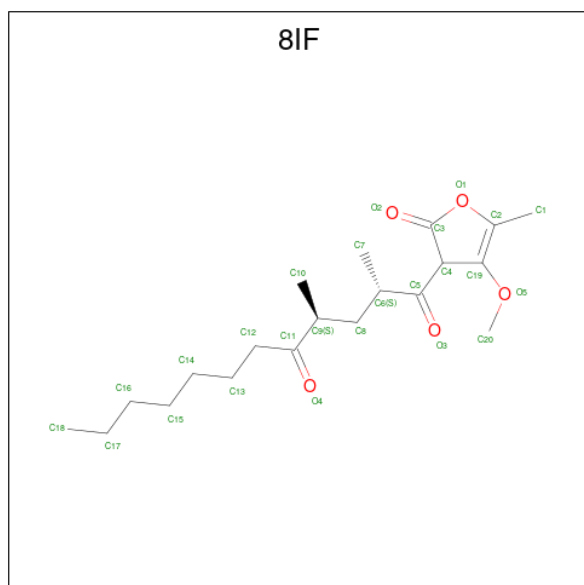
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-16	HIS	-	expression tag	UNP F4F7G1
BBB	-15	HIS	-	expression tag	UNP F4F7G1
BBB	-14	HIS	-	expression tag	UNP F4F7G1
BBB	-13	HIS	-	expression tag	UNP F4F7G1
BBB	-12	HIS	-	expression tag	UNP F4F7G1
BBB	-11	HIS	-	expression tag	UNP F4F7G1
BBB	-10	SER	-	expression tag	UNP F4F7G1
BBB	-9	SER	-	expression tag	UNP F4F7G1
BBB	-8	GLY	-	expression tag	UNP F4F7G1
BBB	-7	LEU	-	expression tag	UNP F4F7G1
BBB	-6	GLU	-	expression tag	UNP F4F7G1
BBB	-5	VAL	-	expression tag	UNP F4F7G1
BBB	-4	LEU	-	expression tag	UNP F4F7G1
BBB	-3	PHE	-	expression tag	UNP F4F7G1
BBB	-2	GLN	-	expression tag	UNP F4F7G1
BBB	-1	GLY	-	expression tag	UNP F4F7G1
BBB	0	PRO	-	expression tag	UNP F4F7G1
CCC	-18	MET	-	initiating methionine	UNP F4F7G1
CCC	-17	ALA	-	expression tag	UNP F4F7G1
CCC	-16	HIS	-	expression tag	UNP F4F7G1
CCC	-15	HIS	-	expression tag	UNP F4F7G1
CCC	-14	HIS	-	expression tag	UNP F4F7G1
CCC	-13	HIS	-	expression tag	UNP F4F7G1
CCC	-12	HIS	-	expression tag	UNP F4F7G1
CCC	-11	HIS	-	expression tag	UNP F4F7G1
CCC	-10	SER	-	expression tag	UNP F4F7G1
CCC	-9	SER	-	expression tag	UNP F4F7G1
CCC	-8	GLY	-	expression tag	UNP F4F7G1
CCC	-7	LEU	-	expression tag	UNP F4F7G1
CCC	-6	GLU	-	expression tag	UNP F4F7G1
CCC	-5	VAL	-	expression tag	UNP F4F7G1
CCC	-4	LEU	-	expression tag	UNP F4F7G1
CCC	-3	PHE	-	expression tag	UNP F4F7G1
CCC	-2	GLN	-	expression tag	UNP F4F7G1
CCC	-1	GLY	-	expression tag	UNP F4F7G1
CCC	0	PRO	-	expression tag	UNP F4F7G1
DDD	-18	MET	-	initiating methionine	UNP F4F7G1
DDD	-17	ALA	-	expression tag	UNP F4F7G1
DDD	-16	HIS	-	expression tag	UNP F4F7G1
DDD	-15	HIS	-	expression tag	UNP F4F7G1
DDD	-14	HIS	-	expression tag	UNP F4F7G1
DDD	-13	HIS	-	expression tag	UNP F4F7G1

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-12	HIS	-	expression tag	UNP F4F7G1
DDD	-11	HIS	-	expression tag	UNP F4F7G1
DDD	-10	SER	-	expression tag	UNP F4F7G1
DDD	-9	SER	-	expression tag	UNP F4F7G1
DDD	-8	GLY	-	expression tag	UNP F4F7G1
DDD	-7	LEU	-	expression tag	UNP F4F7G1
DDD	-6	GLU	-	expression tag	UNP F4F7G1
DDD	-5	VAL	-	expression tag	UNP F4F7G1
DDD	-4	LEU	-	expression tag	UNP F4F7G1
DDD	-3	PHE	-	expression tag	UNP F4F7G1
DDD	-2	GLN	-	expression tag	UNP F4F7G1
DDD	-1	GLY	-	expression tag	UNP F4F7G1
DDD	0	PRO	-	expression tag	UNP F4F7G1

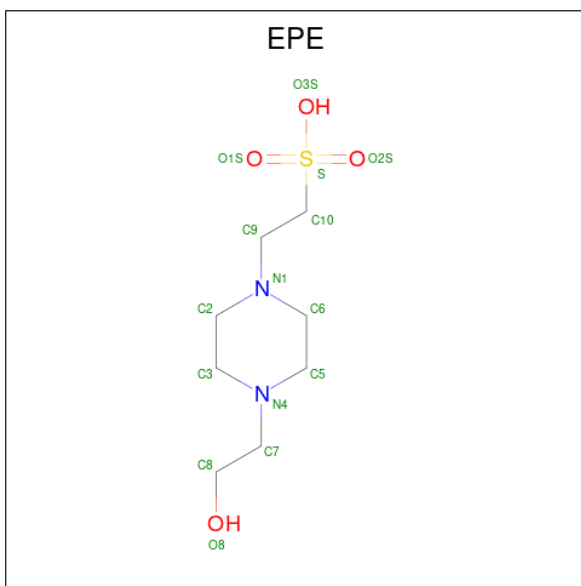
- Molecule 2 is (2 {S},4 {S})-1-(4-methoxy-5-methyl-2-oxidanylidene-3 {H}-furan-3-yl)-2,4-dimethyl-dodecane-1,5-dione (three-letter code: 8IF) (formula: C₂₀H₃₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	0	0
			53	20	28	5		
2	BBB	1	Total	C	H	O	0	0
			53	20	28	5		
2	DDD	1	Total	C	H	O	0	0
			53	20	28	5		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	CCC	1	Total 32	C 8	H 17	N 2	O 4	S 1	1	0
3	CCC	1	Total 32	C 8	H 17	N 2	O 4	S 1	1	0
3	DDD	1	Total 32	C 8	H 17	N 2	O 4	S 1	1	0


- Molecule 4 is water.

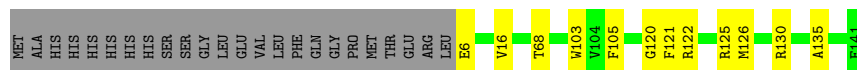
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	13	Total	O	0	0
			13	13		
4	BBB	12	Total	O	0	0
			12	12		
4	CCC	8	Total	O	0	0
			8	8		
4	DDD	9	Total	O	0	0
			9	9		

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: YD repeat-containing protein

Chain AAA: 




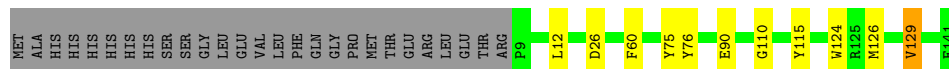
- Molecule 1: YD repeat-containing protein

Chain BBB: 




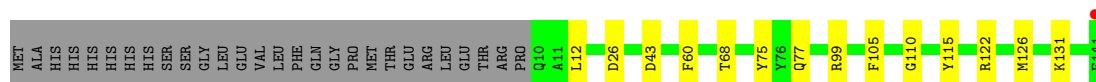
- Molecule 1: YD repeat-containing protein

Chain CCC: 



- Molecule 1: YD repeat-containing protein

Chain DDD: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.57Å 61.56Å 87.78Å 90.00° 112.96° 90.00°	Depositor
Resolution (Å)	49.02 – 1.95 48.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.02-1.95) 99.7 (48.97-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.219 , 0.258 0.225 , 0.261	Depositor DCC
R_{free} test set	2588 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8560	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: 8IF, EPE

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	0.67	0/1080	0.93	0/1468
1	BBB	0.67	0/1084	0.93	0/1473
1	CCC	0.68	0/1053	0.87	0/1431
1	DDD	0.65	0/1045	0.88	0/1420
All	All	0.67	0/4262	0.90	0/5792

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	AAA	1058	1035	1033	10	0
1	BBB	1062	1042	1037	28	0
1	CCC	1031	1009	1008	5	0
1	DDD	1024	1002	1000	5	0
2	AAA	25	28	0	10	0
2	BBB	25	28	0	22	0
2	DDD	25	28	0	5	0
3	CCC	30	34	36	3	0
3	DDD	15	17	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	13	0	0	0	0
4	BBB	12	0	0	0	0
4	CCC	8	0	0	0	0
4	DDD	9	0	0	0	0
All	All	4337	4223	4132	60	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 7.

All (60) 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:126[B]:MET:CE	2:BBB:201:8IF:C13	1.83	1.56
1:BBB:126[B]:MET:HE2	2:BBB:201:8IF:C13	1.36	1.28
1:BBB:126[B]:MET:HE1	2:BBB:201:8IF:C13	1.66	1.05
1:BBB:126[A]:MET:HB2	2:BBB:201:8IF:C15	2.14	0.77
1:BBB:126[A]:MET:HA	2:BBB:201:8IF:C16	2.15	0.74
2:BBB:201:8IF:C12	2:BBB:201:8IF:C7	2.68	0.72
1:BBB:126[A]:MET:CE	1:BBB:129:VAL:HG22	2.23	0.69
1:BBB:126[A]:MET:CA	2:BBB:201:8IF:C16	2.79	0.59
1:BBB:126[A]:MET:SD	1:BBB:129:VAL:HG22	2.43	0.59
1:AAA:130:ARG:HA	2:AAA:201:8IF:C20	2.34	0.58
1:DDD:43:ASP:OD2	2:DDD:201:8IF:C17	2.54	0.56
1:BBB:126[A]:MET:HB2	2:BBB:201:8IF:C16	2.36	0.55
1:AAA:126:MET:SD	2:AAA:201:8IF:C9	2.94	0.55
2:AAA:201:8IF:C14	2:AAA:201:8IF:C2	2.84	0.55
1:DDD:110:GLY:HA3	1:DDD:115:TYR:O	2.07	0.55
1:AAA:126:MET:HB2	2:AAA:201:8IF:C12	2.37	0.55
1:BBB:126[A]:MET:CB	2:BBB:201:8IF:C16	2.86	0.54
2:BBB:201:8IF:C13	2:BBB:201:8IF:C7	2.86	0.53
1:AAA:126:MET:CB	2:AAA:201:8IF:C12	2.86	0.53
1:BBB:99:ARG:HA	1:BBB:126[A]:MET:HE1	1.91	0.52
1:DDD:126:MET:HG3	2:DDD:201:8IF:C12	2.39	0.52
1:AAA:126:MET:CG	2:AAA:201:8IF:C12	2.88	0.52
2:BBB:201:8IF:C20	2:BBB:201:8IF:C1	2.88	0.52
2:BBB:201:8IF:C12	2:BBB:201:8IF:C6	2.90	0.50
1:AAA:126:MET:HG3	2:AAA:201:8IF:C12	2.42	0.50
1:BBB:126[A]:MET:SD	1:BBB:129:VAL:CG2	3.00	0.49
1:BBB:126[A]:MET:HG3	2:BBB:201:8IF:C15	2.43	0.49
1:CCC:126:MET:SD	3:CCC:201:EPE:H91	2.53	0.49
1:BBB:126[A]:MET:CB	2:BBB:201:8IF:C15	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:110:GLY:HA3	1:BBB:115:TYR:O	2.13	0.49
1:BBB:129:VAL:HG12	1:BBB:130:ARG:HG3	1.97	0.47
1:CCC:110:GLY:HA3	1:CCC:115:TYR:O	2.15	0.47
1:BBB:120:GLY:C	1:BBB:121:PHE:CD1	2.88	0.46
1:AAA:120:GLY:C	1:AAA:121:PHE:CD1	2.88	0.46
2:AAA:201:8IF:C15	2:AAA:201:8IF:C1	2.94	0.46
1:BBB:130:ARG:H	2:BBB:201:8IF:C12	2.28	0.46
3:CCC:201:EPE:O3S	3:CCC:201:EPE:N1	2.49	0.46
1:BBB:129:VAL:HA	2:BBB:201:8IF:C13	2.46	0.46
1:CCC:60:PHE:HA	1:CCC:75:TYR:O	2.16	0.46
1:BBB:124:TRP:CZ2	2:BBB:201:8IF:O1	2.69	0.46
1:CCC:124:TRP:CH2	3:CCC:201:EPE:H101	2.51	0.46
2:DDD:201:8IF:C1	2:DDD:201:8IF:C16	2.95	0.45
1:BBB:21:VAL:HG13	1:BBB:131:LYS:C	2.36	0.45
1:BBB:12:LEU:HD11	1:BBB:114:ARG:NH2	2.32	0.44
1:BBB:126[A]:MET:CE	2:BBB:201:8IF:C15	2.97	0.43
1:BBB:66:ARG:HG2	1:BBB:68:THR:HB	2.00	0.43
1:AAA:105:PHE:HA	1:AAA:122:ARG:O	2.19	0.42
1:BBB:129:VAL:HG13	2:BBB:201:8IF:C12	2.49	0.42
1:CCC:76:TYR:O	1:CCC:90:GLU:HA	2.19	0.42
2:DDD:201:8IF:C17	2:DDD:201:8IF:C1	2.96	0.42
1:BBB:126[A]:MET:CG	2:BBB:201:8IF:C15	2.97	0.42
1:DDD:60:PHE:HA	1:DDD:75:TYR:O	2.20	0.41
2:DDD:201:8IF:C2	2:DDD:201:8IF:C14	2.98	0.41
1:BBB:126[A]:MET:HE2	2:BBB:201:8IF:C15	2.51	0.41
1:AAA:103:TRP:CD1	1:AAA:125:ARG:HD3	2.56	0.41
1:AAA:16:VAL:HB	1:AAA:135:ALA:HB3	2.02	0.41
2:AAA:201:8IF:C10	2:AAA:201:8IF:C3	2.99	0.40
2:AAA:201:8IF:C10	2:AAA:201:8IF:C4	2.99	0.40
1:BBB:130:ARG:H	2:BBB:201:8IF:C13	2.35	0.40
1:DDD:105:PHE:HA	1:DDD:122:ARG:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	134/160 (84%)	129 (96%)	5 (4%)	0	100	100
1	BBB	135/160 (84%)	131 (97%)	4 (3%)	0	100	100
1	CCC	131/160 (82%)	125 (95%)	5 (4%)	1 (1%)	19	9
1	DDD	130/160 (81%)	122 (94%)	8 (6%)	0	100	100
All	All	530/640 (83%)	507 (96%)	22 (4%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	129	VAL

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	AAA	110/131 (84%)	108 (98%)	2 (2%)	59	53
1	BBB	110/131 (84%)	108 (98%)	2 (2%)	59	53
1	CCC	107/131 (82%)	104 (97%)	3 (3%)	43	33
1	DDD	106/131 (81%)	100 (94%)	6 (6%)	20	9
All	All	433/524 (83%)	420 (97%)	13 (3%)	41	30

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	6	GLU
1	AAA	68	THR
1	BBB	26	ASP
1	BBB	141	GLU
1	CCC	12	LEU
1	CCC	26	ASP
1	CCC	129	VAL

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Mol	Chain	Res	Type
1	DDD	12	LEU
1	DDD	26	ASP
1	DDD	68	THR
1	DDD	77	GLN
1	DDD	99	ARG
1	DDD	131	LYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	8IF	BBB	201	1	23,25,25	2.00	3 (13%)	23,33,33	2.49	6 (26%)
2	8IF	AAA	201	-	23,25,25	1.77	3 (13%)	23,33,33	2.32	5 (21%)
3	EPE	CCC	202	-	15,15,15	1.61	1 (6%)	18,20,20	1.38	3 (16%)
3	EPE	CCC	201	-	15,15,15	2.41	1 (6%)	18,20,20	1.29	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	DDD	202	-	15,15,15	1.83	1 (6%)	18,20,20	1.59	3 (16%)
2	8IF	DDD	201	-	23,25,25	1.46	2 (8%)	23,33,33	1.83	4 (17%)

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	8IF	BBB	201	1	2/2/8/8	13/25/41/41	0/1/1/1
2	8IF	AAA	201	-	3/3/8/8	8/25/41/41	0/1/1/1
3	EPE	CCC	202	-	-	0/9/19/19	0/1/1/1
3	EPE	CCC	201	-	-	7/9/19/19	0/1/1/1
3	EPE	DDD	202	-	-	7/9/19/19	0/1/1/1
2	8IF	DDD	201	-	3/3/8/8	11/25/41/41	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	201	EPE	C10-S	-8.89	1.64	1.77
2	BBB	201	8IF	C12-C11	-6.92	1.41	1.51
3	DDD	202	EPE	C10-S	-6.43	1.68	1.77
2	AAA	201	8IF	C13-C12	-6.15	1.29	1.52
2	BBB	201	8IF	C13-C12	-5.68	1.31	1.52
2	DDD	201	8IF	C13-C12	-5.65	1.31	1.52
3	CCC	202	EPE	C10-S	-5.54	1.69	1.77
2	AAA	201	8IF	C12-C11	-4.19	1.45	1.51
2	DDD	201	8IF	C12-C11	-3.13	1.46	1.51
2	AAA	201	8IF	C4-C19	-2.59	1.38	1.51
2	BBB	201	8IF	C4-C19	-2.26	1.40	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	201	8IF	O1-C2-C1	7.73	126.35	115.88
2	BBB	201	8IF	O1-C2-C1	7.04	125.41	115.88
2	BBB	201	8IF	O1-C2-C19	-5.67	105.62	108.40
2	DDD	201	8IF	C13-C12-C11	5.63	124.36	114.60
3	DDD	202	EPE	O1S-S-C10	4.64	112.51	106.92
2	DDD	201	8IF	O1-C2-C1	4.55	122.05	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	201	8IF	C13-C12-C11	4.45	122.32	114.60
2	AAA	201	8IF	C13-C12-C11	4.40	122.23	114.60
2	BBB	201	8IF	C14-C13-C12	3.83	126.95	113.19
3	CCC	202	EPE	O3S-S-C10	3.67	111.71	105.77
2	AAA	201	8IF	O3-C5-C6	-3.67	114.46	121.26
2	AAA	201	8IF	C1-C2-C19	-3.52	124.15	131.64
3	DDD	202	EPE	O2S-S-C10	2.81	110.30	106.92
2	DDD	201	8IF	C14-C13-C12	2.72	122.97	113.19
2	DDD	201	8IF	O3-C5-C6	-2.69	116.28	121.26
3	CCC	202	EPE	O3S-S-O2S	-2.60	104.92	111.27
3	CCC	202	EPE	O2S-S-C10	2.59	110.03	106.92
3	DDD	202	EPE	C9-N1-C2	2.37	117.30	111.23
2	BBB	201	8IF	C10-C9-C8	2.36	116.52	111.55
2	AAA	201	8IF	O1-C2-C19	2.24	109.50	108.40
3	CCC	201	EPE	O2S-S-C10	2.13	109.48	106.92
2	BBB	201	8IF	O2-C3-C4	2.08	133.61	129.19
3	CCC	201	EPE	C6-N1-C2	2.03	113.41	108.83

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AAA	201	8IF	C4
2	AAA	201	8IF	C9
2	AAA	201	8IF	C6
2	BBB	201	8IF	C4
2	BBB	201	8IF	C9
2	DDD	201	8IF	C4
2	DDD	201	8IF	C9
2	DDD	201	8IF	C6

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	201	8IF	C6-C8-C9-C10
2	AAA	201	8IF	C4-C19-O5-C20
2	BBB	201	8IF	C3-C4-C5-C6
2	BBB	201	8IF	C19-C4-C5-C6
2	BBB	201	8IF	C11-C12-C13-C14
2	DDD	201	8IF	C11-C12-C13-C14
2	DDD	201	8IF	C4-C19-O5-C20
3	CCC	201	EPE	C8-C7-N4-C3
3	CCC	201	EPE	C9-C10-S-O1S

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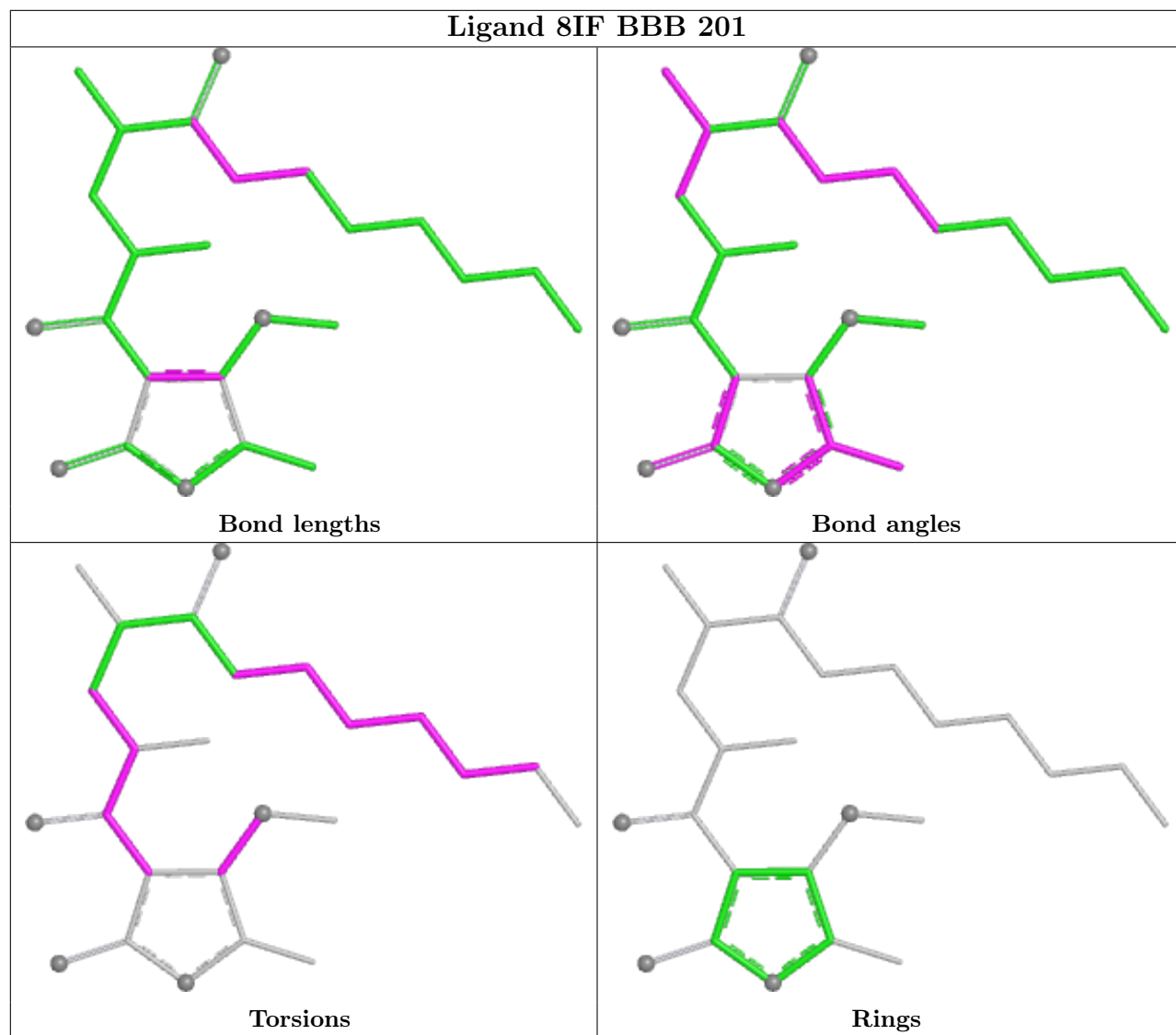
Mol	Chain	Res	Type	Atoms
3	CCC	201	EPE	C9-C10-S-O3S
3	DDD	202	EPE	C10-C9-N1-C2
3	DDD	202	EPE	C9-C10-S-O2S
3	DDD	202	EPE	C9-C10-S-O3S
3	DDD	202	EPE	N4-C7-C8-O8
2	AAA	201	8IF	C11-C12-C13-C14
2	BBB	201	8IF	C14-C15-C16-C17
2	BBB	201	8IF	C13-C14-C15-C16
2	DDD	201	8IF	C13-C14-C15-C16
2	AAA	201	8IF	C13-C14-C15-C16
3	CCC	201	EPE	N4-C7-C8-O8
2	DDD	201	8IF	C15-C16-C17-C18
2	DDD	201	8IF	C12-C11-C9-C8
2	BBB	201	8IF	C4-C5-C6-C8
3	CCC	201	EPE	C10-C9-N1-C2
3	CCC	201	EPE	C10-C9-N1-C6
3	DDD	202	EPE	C10-C9-N1-C6
2	BBB	201	8IF	C15-C16-C17-C18
3	CCC	201	EPE	C9-C10-S-O2S
3	DDD	202	EPE	C9-C10-S-O1S
2	DDD	201	8IF	C6-C8-C9-C10
2	BBB	201	8IF	C12-C13-C14-C15
2	BBB	201	8IF	C4-C5-C6-C7
2	DDD	201	8IF	C4-C5-C6-C7
2	DDD	201	8IF	C9-C11-C12-C13
2	DDD	201	8IF	C4-C5-C6-C8
2	AAA	201	8IF	C15-C16-C17-C18
2	AAA	201	8IF	C7-C6-C8-C9
2	BBB	201	8IF	C7-C6-C8-C9
2	AAA	201	8IF	C19-C4-C5-C6
2	AAA	201	8IF	C6-C8-C9-C11
2	BBB	201	8IF	C4-C19-O5-C20
2	DDD	201	8IF	O4-C11-C12-C13
2	DDD	201	8IF	O4-C11-C9-C8
3	DDD	202	EPE	S-C10-C9-N1
2	BBB	201	8IF	C19-C4-C5-O3
2	BBB	201	8IF	O3-C5-C6-C8

There are no ring outliers.

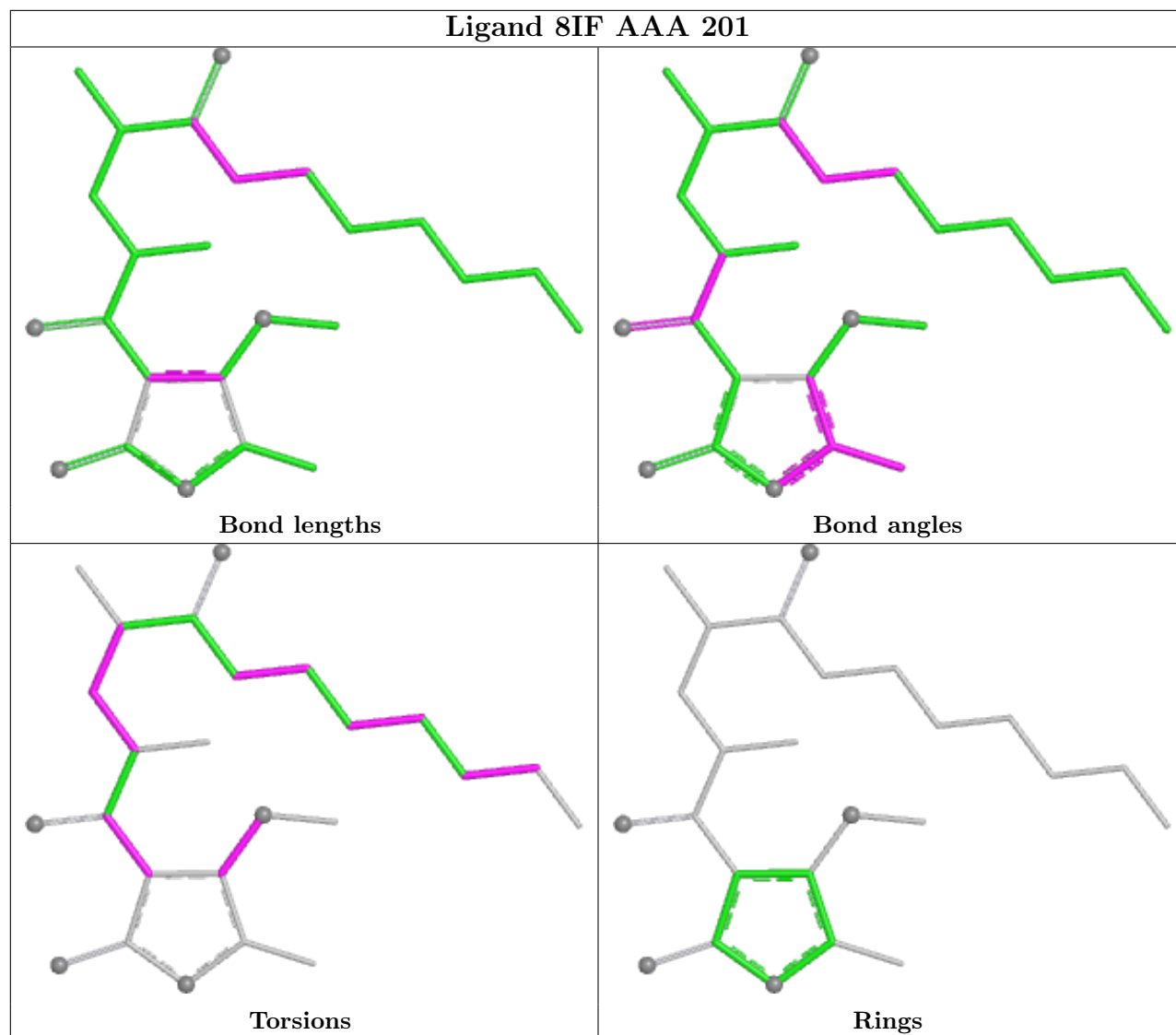
4 monomers are involved in 40 short contacts:

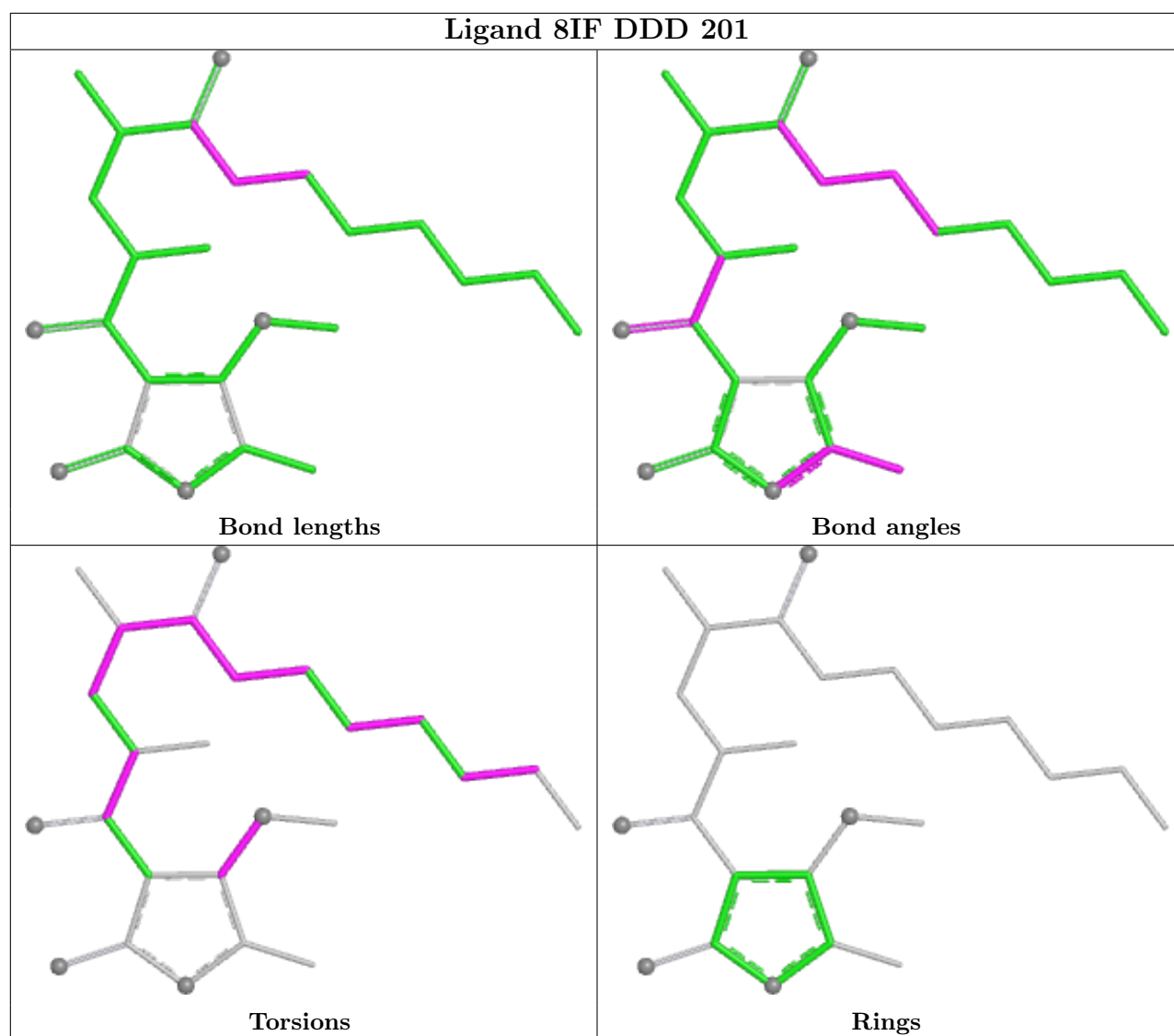
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	201	8IF	22	0
2	AAA	201	8IF	10	0
3	CCC	201	EPE	3	0
2	DDD	201	8IF	5	0

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



Ligand 8IF AAA 201





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 [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	136/160 (85%)	-0.19	0	100 100	37, 45, 62, 87	0
1	BBB	136/160 (85%)	-0.20	0	100 100	37, 46, 63, 70	0
1	CCC	133/160 (83%)	-0.20	0	100 100	40, 53, 71, 94	0
1	DDD	132/160 (82%)	-0.08	1 (0%)	86 90	42, 55, 78, 91	0
All	All	537/640 (83%)	-0.17	1 (0%)	95 97	37, 50, 69, 94	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	141	GLU	4.5

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 monosaccharides 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.

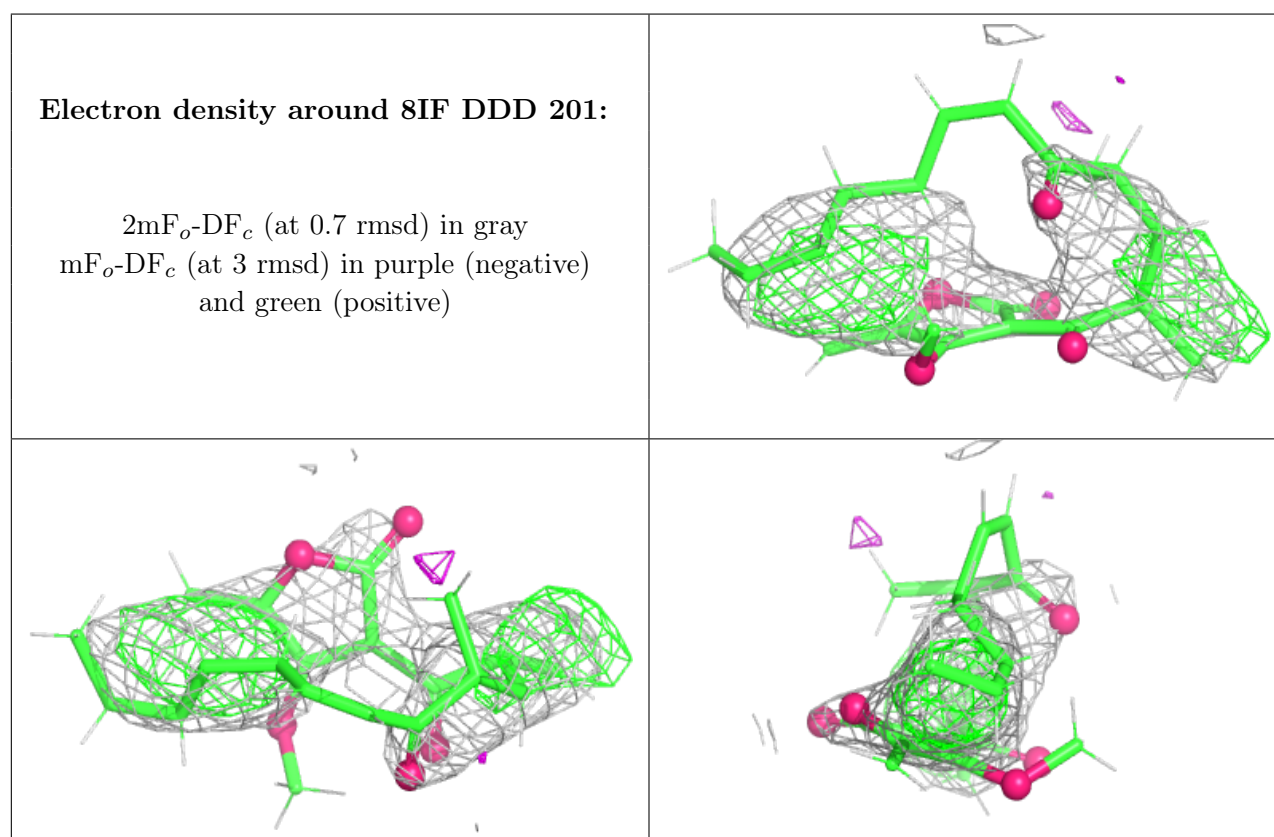
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8IF	DDD	201	25/25	0.76	0.47	67,77,100,100	53

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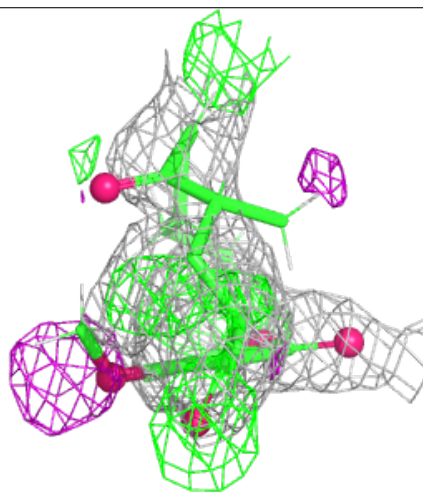
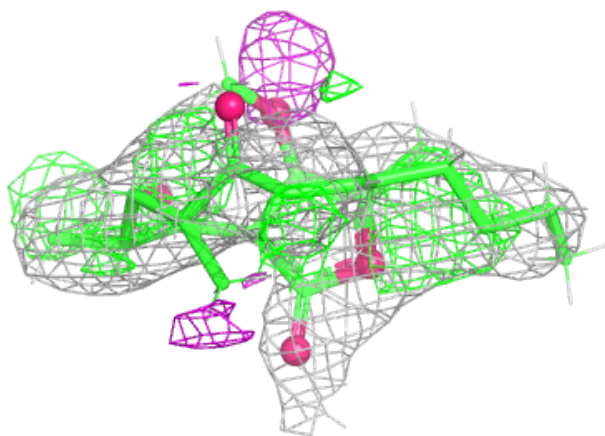
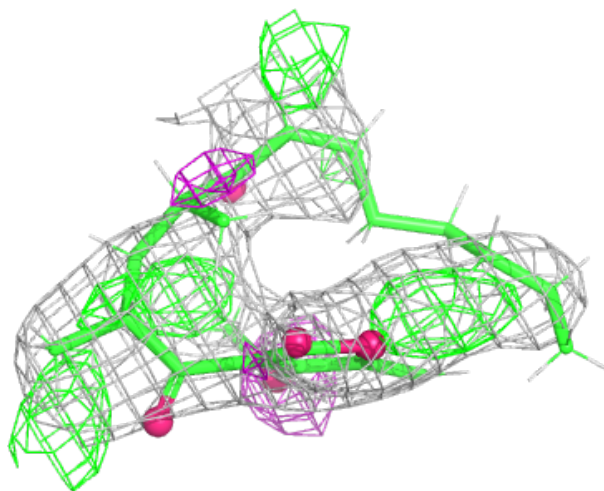
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	8IF	AAA	201	25/25	0.78	0.31	57,78,89,94	53
2	8IF	BBB	201	25/25	0.79	0.30	50,61,80,80	53
3	EPE	DDD	202	15/15	0.80	0.20	77,98,116,148	1
3	EPE	CCC	201	15/15	0.87	0.18	74,81,105,117	1
3	EPE	CCC	202	15/15	0.92	0.12	63,68,85,86	1

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.



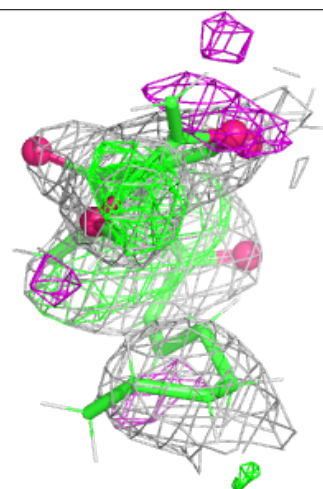
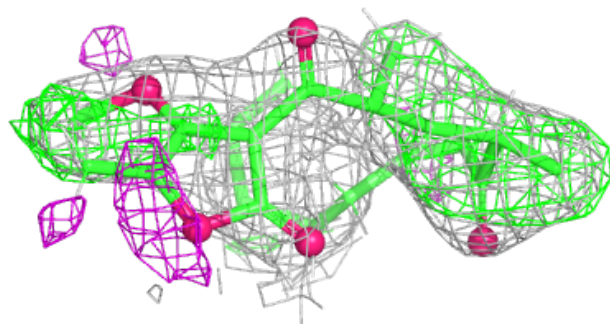
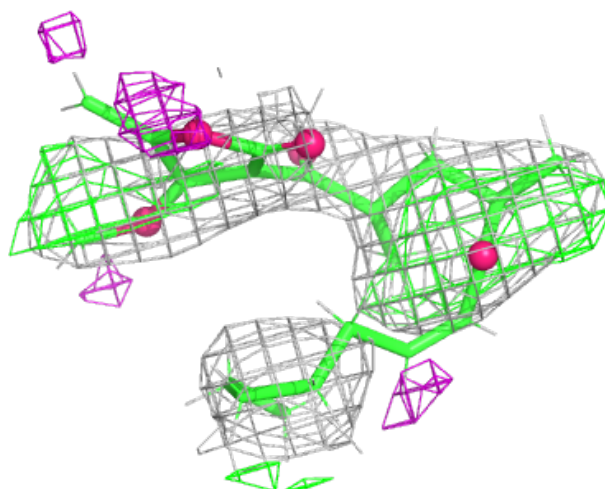
Electron density around 8IF AAA 201:

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



Electron density around 8IF BBB 201:

$2mF_o-DF_c$ (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.