



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 12:34 PM EDT

PDB ID : 8TCC
Title : GTP Cyclohydrolase-IB with dehydrocostus lactone
Authors : McWhorter, K.L.; Amaya Lopez, C.Y.; Davis, K.M.
Deposited on : 2023-06-30
Resolution : 3.10 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

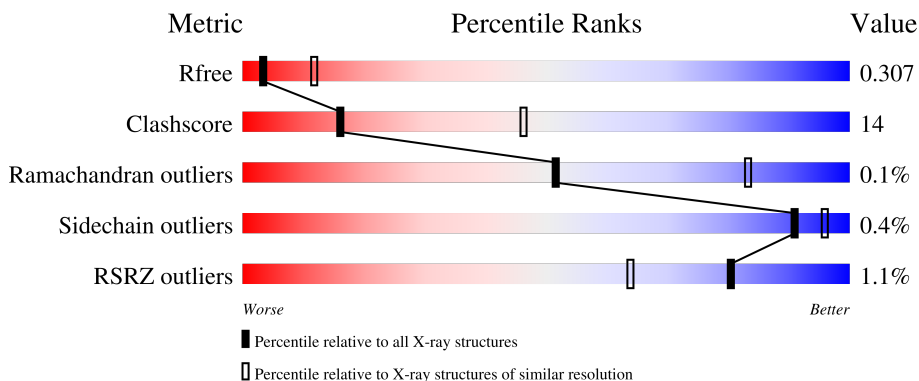
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	303	
1	B	303	
1	C	303	
1	D	303	

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
5	ZS9	C	301	X	-	-	-
5	ZS9	D	301[A]	X	-	-	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 6801 atoms, of which 12 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 GTP cyclohydrolase FolE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	Total 1564	C 994	N 270	O 293	S 7	0	0	0
1	B	245	Total 1707	C 1075	N 294	O 333	S 5	0	2	0
1	C	246	Total 1729	C 1091	N 296	O 337	S 5	0	0	0
1	D	244	Total 1684	C 1064	N 293	O 322	S 5	0	1	0

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP A0A069BB45
A	-32	GLY	-	expression tag	UNP A0A069BB45
A	-31	SER	-	expression tag	UNP A0A069BB45
A	-30	SER	-	expression tag	UNP A0A069BB45
A	-29	HIS	-	expression tag	UNP A0A069BB45
A	-28	HIS	-	expression tag	UNP A0A069BB45
A	-27	HIS	-	expression tag	UNP A0A069BB45
A	-26	HIS	-	expression tag	UNP A0A069BB45
A	-25	HIS	-	expression tag	UNP A0A069BB45
A	-24	HIS	-	expression tag	UNP A0A069BB45
A	-23	SER	-	expression tag	UNP A0A069BB45
A	-22	SER	-	expression tag	UNP A0A069BB45
A	-21	GLY	-	expression tag	UNP A0A069BB45
A	-20	LEU	-	expression tag	UNP A0A069BB45
A	-19	VAL	-	expression tag	UNP A0A069BB45
A	-18	PRO	-	expression tag	UNP A0A069BB45
A	-17	ARG	-	expression tag	UNP A0A069BB45
A	-16	GLY	-	expression tag	UNP A0A069BB45
A	-15	SER	-	expression tag	UNP A0A069BB45
A	-14	HIS	-	expression tag	UNP A0A069BB45
A	-13	MET	-	expression tag	UNP A0A069BB45

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP A0A069BB45
A	-11	SER	-	expression tag	UNP A0A069BB45
A	-10	MET	-	expression tag	UNP A0A069BB45
A	-9	THR	-	expression tag	UNP A0A069BB45
A	-8	GLY	-	expression tag	UNP A0A069BB45
A	-7	GLY	-	expression tag	UNP A0A069BB45
A	-6	GLN	-	expression tag	UNP A0A069BB45
A	-5	GLN	-	expression tag	UNP A0A069BB45
A	-4	MET	-	expression tag	UNP A0A069BB45
A	-3	GLY	-	expression tag	UNP A0A069BB45
A	-2	ARG	-	expression tag	UNP A0A069BB45
A	-1	GLY	-	expression tag	UNP A0A069BB45
A	0	SER	-	expression tag	UNP A0A069BB45
B	-33	MET	-	initiating methionine	UNP A0A069BB45
B	-32	GLY	-	expression tag	UNP A0A069BB45
B	-31	SER	-	expression tag	UNP A0A069BB45
B	-30	SER	-	expression tag	UNP A0A069BB45
B	-29	HIS	-	expression tag	UNP A0A069BB45
B	-28	HIS	-	expression tag	UNP A0A069BB45
B	-27	HIS	-	expression tag	UNP A0A069BB45
B	-26	HIS	-	expression tag	UNP A0A069BB45
B	-25	HIS	-	expression tag	UNP A0A069BB45
B	-24	HIS	-	expression tag	UNP A0A069BB45
B	-23	SER	-	expression tag	UNP A0A069BB45
B	-22	SER	-	expression tag	UNP A0A069BB45
B	-21	GLY	-	expression tag	UNP A0A069BB45
B	-20	LEU	-	expression tag	UNP A0A069BB45
B	-19	VAL	-	expression tag	UNP A0A069BB45
B	-18	PRO	-	expression tag	UNP A0A069BB45
B	-17	ARG	-	expression tag	UNP A0A069BB45
B	-16	GLY	-	expression tag	UNP A0A069BB45
B	-15	SER	-	expression tag	UNP A0A069BB45
B	-14	HIS	-	expression tag	UNP A0A069BB45
B	-13	MET	-	expression tag	UNP A0A069BB45
B	-12	ALA	-	expression tag	UNP A0A069BB45
B	-11	SER	-	expression tag	UNP A0A069BB45
B	-10	MET	-	expression tag	UNP A0A069BB45
B	-9	THR	-	expression tag	UNP A0A069BB45
B	-8	GLY	-	expression tag	UNP A0A069BB45
B	-7	GLY	-	expression tag	UNP A0A069BB45
B	-6	GLN	-	expression tag	UNP A0A069BB45
B	-5	GLN	-	expression tag	UNP A0A069BB45

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	expression tag	UNP A0A069BB45
B	-3	GLY	-	expression tag	UNP A0A069BB45
B	-2	ARG	-	expression tag	UNP A0A069BB45
B	-1	GLY	-	expression tag	UNP A0A069BB45
B	0	SER	-	expression tag	UNP A0A069BB45
C	-33	MET	-	initiating methionine	UNP A0A069BB45
C	-32	GLY	-	expression tag	UNP A0A069BB45
C	-31	SER	-	expression tag	UNP A0A069BB45
C	-30	SER	-	expression tag	UNP A0A069BB45
C	-29	HIS	-	expression tag	UNP A0A069BB45
C	-28	HIS	-	expression tag	UNP A0A069BB45
C	-27	HIS	-	expression tag	UNP A0A069BB45
C	-26	HIS	-	expression tag	UNP A0A069BB45
C	-25	HIS	-	expression tag	UNP A0A069BB45
C	-24	HIS	-	expression tag	UNP A0A069BB45
C	-23	SER	-	expression tag	UNP A0A069BB45
C	-22	SER	-	expression tag	UNP A0A069BB45
C	-21	GLY	-	expression tag	UNP A0A069BB45
C	-20	LEU	-	expression tag	UNP A0A069BB45
C	-19	VAL	-	expression tag	UNP A0A069BB45
C	-18	PRO	-	expression tag	UNP A0A069BB45
C	-17	ARG	-	expression tag	UNP A0A069BB45
C	-16	GLY	-	expression tag	UNP A0A069BB45
C	-15	SER	-	expression tag	UNP A0A069BB45
C	-14	HIS	-	expression tag	UNP A0A069BB45
C	-13	MET	-	expression tag	UNP A0A069BB45
C	-12	ALA	-	expression tag	UNP A0A069BB45
C	-11	SER	-	expression tag	UNP A0A069BB45
C	-10	MET	-	expression tag	UNP A0A069BB45
C	-9	THR	-	expression tag	UNP A0A069BB45
C	-8	GLY	-	expression tag	UNP A0A069BB45
C	-7	GLY	-	expression tag	UNP A0A069BB45
C	-6	GLN	-	expression tag	UNP A0A069BB45
C	-5	GLN	-	expression tag	UNP A0A069BB45
C	-4	MET	-	expression tag	UNP A0A069BB45
C	-3	GLY	-	expression tag	UNP A0A069BB45
C	-2	ARG	-	expression tag	UNP A0A069BB45
C	-1	GLY	-	expression tag	UNP A0A069BB45
C	0	SER	-	expression tag	UNP A0A069BB45
D	-33	MET	-	initiating methionine	UNP A0A069BB45
D	-32	GLY	-	expression tag	UNP A0A069BB45
D	-31	SER	-	expression tag	UNP A0A069BB45

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	SER	-	expression tag	UNP A0A069BB45
D	-29	HIS	-	expression tag	UNP A0A069BB45
D	-28	HIS	-	expression tag	UNP A0A069BB45
D	-27	HIS	-	expression tag	UNP A0A069BB45
D	-26	HIS	-	expression tag	UNP A0A069BB45
D	-25	HIS	-	expression tag	UNP A0A069BB45
D	-24	HIS	-	expression tag	UNP A0A069BB45
D	-23	SER	-	expression tag	UNP A0A069BB45
D	-22	SER	-	expression tag	UNP A0A069BB45
D	-21	GLY	-	expression tag	UNP A0A069BB45
D	-20	LEU	-	expression tag	UNP A0A069BB45
D	-19	VAL	-	expression tag	UNP A0A069BB45
D	-18	PRO	-	expression tag	UNP A0A069BB45
D	-17	ARG	-	expression tag	UNP A0A069BB45
D	-16	GLY	-	expression tag	UNP A0A069BB45
D	-15	SER	-	expression tag	UNP A0A069BB45
D	-14	HIS	-	expression tag	UNP A0A069BB45
D	-13	MET	-	expression tag	UNP A0A069BB45
D	-12	ALA	-	expression tag	UNP A0A069BB45
D	-11	SER	-	expression tag	UNP A0A069BB45
D	-10	MET	-	expression tag	UNP A0A069BB45
D	-9	THR	-	expression tag	UNP A0A069BB45
D	-8	GLY	-	expression tag	UNP A0A069BB45
D	-7	GLY	-	expression tag	UNP A0A069BB45
D	-6	GLN	-	expression tag	UNP A0A069BB45
D	-5	GLN	-	expression tag	UNP A0A069BB45
D	-4	MET	-	expression tag	UNP A0A069BB45
D	-3	GLY	-	expression tag	UNP A0A069BB45
D	-2	ARG	-	expression tag	UNP A0A069BB45
D	-1	GLY	-	expression tag	UNP A0A069BB45
D	0	SER	-	expression tag	UNP A0A069BB45

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

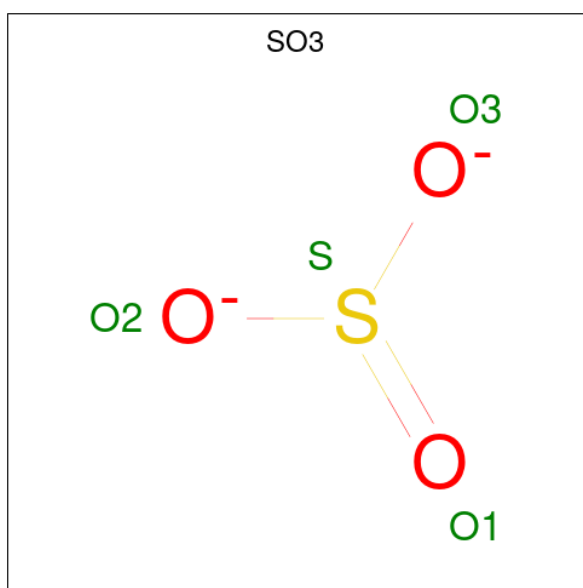
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

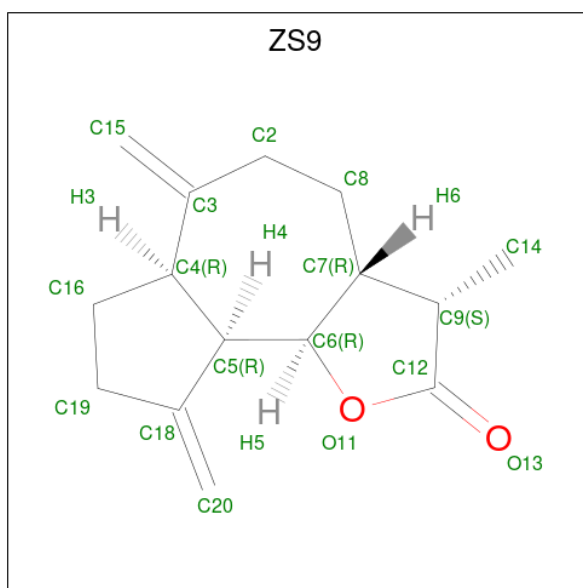
- Molecule 4 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total	O	S	0	1
			4	3	1		

- Molecule 5 is dehydrocostus lactone, bound form (three-letter code: ZS9) (formula: C₁₅H₂₀O₂)

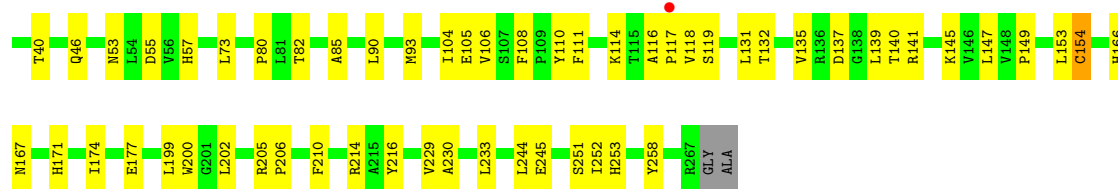
(labeled as "Ligand of Interest" by depositor).



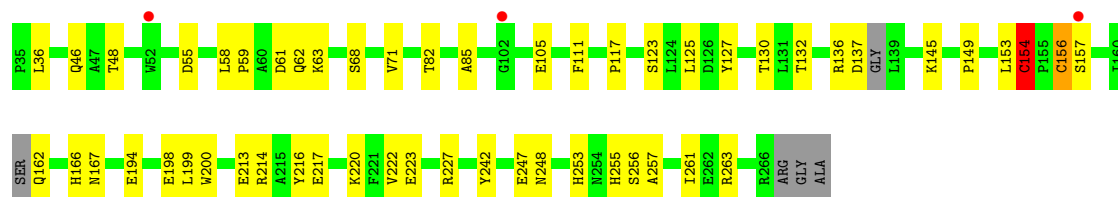
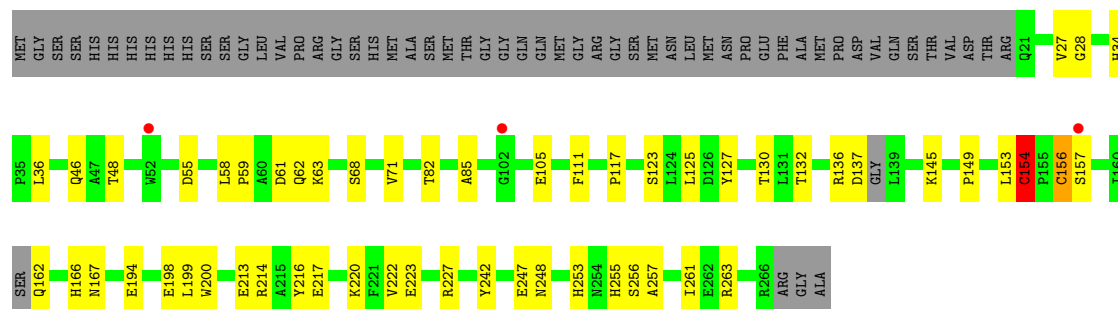
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 17 15 2	0	1
5	C	1	Total C O 17 15 2	0	0
5	D	1	Total C O 17 15 2	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0
6	B	10	Total O 10 10	0	0
6	C	13	Total O 13 13	0	0
6	D	12	Total O 12 12	0	0



● Molecule 1: GTP cyclohydrolase FolE2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.31Å 71.32Å 193.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.16 – 3.10 48.25 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.16-3.10) 96.9 (48.25-3.10)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.288 , 0.312 0.288 , 0.307	Depositor DCC
R_{free} test set	875 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtrriage
Anisotropy	0.638	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 100.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.029 for k,h,-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6801	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: MN, SNC, SO3, ZS9, EDO

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	0.45	0/1581	0.65	0/2171
1	B	0.43	1/1734 (0.1%)	0.66	3/2383 (0.1%)
1	C	0.48	1/1755 (0.1%)	0.68	1/2413 (0.0%)
1	D	0.48	2/1709 (0.1%)	0.73	3/2339 (0.1%)
All	All	0.46	4/6779 (0.1%)	0.68	7/9306 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	154[A]	CYS	N-CA	-6.98	1.32	1.46
1	D	153	LEU	C-N	6.81	1.49	1.34
1	B	154[A]	CYS	N-CA	-5.86	1.34	1.46
1	C	154	CYS	N-CA	-5.68	1.34	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154[A]	CYS	N-CA-CB	13.10	134.18	110.60
1	D	154[A]	CYS	N-CA-CB	12.62	133.31	110.60
1	D	153	LEU	O-C-N	11.15	140.54	122.70
1	C	154	CYS	N-CA-CB	9.56	127.80	110.60
1	D	153	LEU	CA-C-N	-8.05	99.49	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154[A]	CYS	CA-CB-SG	5.68	124.23	114.00
1	B	153	LEU	O-C-N	5.63	131.71	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	154[A]	CYS	CA

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	1564	0	1311	53	0
1	B	1707	0	1499	56	0
1	C	1729	0	1511	44	0
1	D	1684	0	1433	47	0
2	A	1	0	0	0	0
3	A	4	6	6	0	0
3	D	4	6	6	0	0
4	A	4	0	0	0	0
5	B	17	0	0	1	0
5	C	17	0	0	1	0
5	D	17	0	0	2	0
6	A	6	0	0	0	0
6	B	10	0	0	0	0
6	C	13	0	0	0	0
6	D	12	0	0	0	0
All	All	6789	12	5766	181	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 14.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154[A]:CYS:SG	1:B:166:HIS:NE2	2.37	0.98
1:C:154:CYS:HB3	1:C:166:HIS:NE2	1.92	0.84
1:B:58:LEU:HD13	1:B:65:THR:HG23	1.64	0.79
1:A:113:ASN:HA	1:A:124:LEU:HD23	1.63	0.79
1:B:36:LEU:CD2	1:B:48:THR:HG23	2.13	0.78
1:A:113:ASN:HB2	1:A:124:LEU:HD21	1.66	0.78
1:B:36:LEU:HD21	1:B:48:THR:HG23	1.64	0.78
1:A:212:THR:HG21	1:B:157:SER:OG	1.83	0.77
1:A:226:VAL:HG11	1:A:259:ALA:HB3	1.69	0.74
1:A:101:ALA:HA	1:A:135:VAL:O	1.88	0.73
1:B:156:SNC:O	1:B:160:ILE:HG23	1.89	0.72
1:C:167:ASN:OD1	1:D:167:ASN:O	2.08	0.72
1:C:153:LEU:HD12	1:C:167:ASN:HB3	1.75	0.69
1:C:90:LEU:HD21	1:C:135:VAL:HG23	1.73	0.69
1:A:124:LEU:HD12	1:D:34:HIS:CE1	2.28	0.68
1:B:182:VAL:HG22	1:B:238:ARG:HE	1.58	0.68
1:D:166:HIS:NE2	5:D:301[A]:ZS9:C9	2.58	0.67
1:C:90:LEU:HD23	1:C:140:THR:HG23	1.78	0.65
1:B:166:HIS:NE2	5:B:301[A]:ZS9:C14	2.59	0.65
1:D:27:VAL:CG1	1:D:58:LEU:HD13	2.26	0.64
1:A:90:LEU:HA	1:A:104:ILE:HD11	1.78	0.64
1:C:53:ASN:HB2	1:C:105:GLU:HG3	1.79	0.64
1:B:176:ALA:HB1	1:B:239:ILE:HG23	1.80	0.63
1:C:245:GLU:OE1	1:C:258:TYR:OH	2.16	0.62
1:C:210:PHE:O	1:C:214:ARG:HG2	1.99	0.62
1:A:199:LEU:HD23	1:B:253:HIS:C	2.20	0.62
1:D:46:GLN:HE22	1:D:111:PHE:HB2	1.65	0.62
1:C:82:THR:H	1:C:85:ALA:HB3	1.65	0.62
1:D:198:GLU:HG2	1:D:214:ARG:HH22	1.65	0.61
1:C:90:LEU:CD2	1:C:135:VAL:HG23	2.29	0.61
1:A:214:ARG:NE	1:A:214:ARG:HA	2.16	0.61
1:A:113:ASN:CA	1:A:124:LEU:HD23	2.31	0.61
1:A:67:MET:HA	1:A:70:PHE:HD2	1.66	0.60
1:C:80:PRO:O	1:C:82:THR:HG23	2.02	0.60
1:B:90:LEU:HG	1:B:135:VAL:HG23	1.83	0.59
1:D:36:LEU:HD21	1:D:48:THR:HG23	1.83	0.59
1:D:166:HIS:NE2	5:D:301[A]:ZS9:C12	2.65	0.59
1:A:214:ARG:HA	1:A:214:ARG:HE	1.66	0.59
1:C:205:ARG:N	1:C:206:PRO:HD2	2.17	0.59
1:D:82:THR:H	1:D:85:ALA:HB3	1.68	0.59
1:C:108:PHE:HE1	1:C:131:LEU:HG	1.67	0.59
1:A:116:ALA:HB2	1:A:121:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:GLY:HA3	1:D:55:ASP:HA	1.85	0.58
1:A:113:ASN:HB2	1:A:124:LEU:CD2	2.32	0.58
1:A:82:THR:H	1:A:85:ALA:HB3	1.68	0.57
1:B:59:PRO:HB2	1:B:61:ASP:OD1	2.04	0.57
1:C:53:ASN:HB2	1:C:105:GLU:CG	2.34	0.57
1:C:167:ASN:OD1	1:D:167:ASN:N	2.31	0.56
1:B:247:GLU:HA	1:B:257:ALA:O	2.05	0.56
1:C:252:ILE:HG13	1:C:253:HIS:CD2	2.40	0.56
1:C:116:ALA:HB3	1:C:119:SER:OG	2.06	0.56
1:D:136:ARG:O	1:D:137:ASP:C	2.43	0.56
1:C:230:ALA:HA	1:C:233:LEU:HD12	1.87	0.56
1:C:229:VAL:HB	1:C:244:LEU:HD21	1.87	0.55
1:C:153:LEU:HD22	1:C:216:TYR:HA	1.87	0.55
1:B:58:LEU:HD13	1:B:65:THR:CG2	2.34	0.55
1:B:156:SNC:O	1:B:160:ILE:CG2	2.55	0.54
1:B:179:ALA:HB2	1:B:240:VAL:HG13	1.89	0.54
1:B:90:LEU:O	1:B:94:LEU:HD23	2.08	0.54
1:A:174:ILE:HG12	1:A:244:LEU:HD13	1.89	0.54
1:B:38:VAL:HG13	1:B:46:GLN:HB3	1.89	0.54
1:A:90:LEU:HA	1:A:104:ILE:CD1	2.37	0.54
1:C:154:CYS:HB3	1:C:166:HIS:CD2	2.42	0.53
1:D:59:PRO:HB2	1:D:61:ASP:OD1	2.08	0.53
1:A:82:THR:O	1:A:83:ALA:C	2.46	0.53
1:B:157:SER:CB	1:B:166:HIS:HD2	2.22	0.53
1:A:111:PHE:HA	1:A:125:LEU:O	2.08	0.52
1:B:147:LEU:HD12	1:B:173:THR:OG1	2.10	0.52
1:C:25:GLN:HA	1:C:57:HIS:ND1	2.25	0.52
1:D:27:VAL:HG11	1:D:58:LEU:HD13	1.92	0.52
1:A:245:GLU:HA	1:A:259:ALA:O	2.10	0.51
1:C:28:GLY:HA3	1:C:55:ASP:HA	1.93	0.51
1:C:149:PRO:HB2	1:C:199:LEU:HD12	1.92	0.51
1:A:75:GLU:HG2	1:D:123:SER:HA	1.91	0.51
1:C:46:GLN:HE22	1:C:111:PHE:H	1.58	0.51
1:A:182:VAL:HG13	1:A:238:ARG:NH2	2.25	0.51
1:A:127:TYR:CD2	1:A:149:PRO:HD2	2.45	0.51
1:B:245:GLU:HG2	1:B:260:LEU:HD12	1.91	0.51
1:A:56:VAL:HG22	1:A:70:PHE:HZ	1.75	0.51
1:A:210:PHE:HE1	1:A:214:ARG:HH11	1.57	0.51
1:D:149:PRO:HB2	1:D:199:LEU:HD12	1.92	0.51
1:A:38:VAL:HG12	1:A:39:ARG:N	2.26	0.50
1:C:141:ARG:HE	1:C:177:GLU:CD	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:O	1:B:155:PRO:HD3	2.11	0.50
1:B:157:SER:HB2	1:B:166:HIS:HD2	1.76	0.50
1:D:105:GLU:HG3	1:D:132:THR:HG23	1.93	0.50
1:A:25:GLN:HA	1:A:57:HIS:ND1	2.27	0.49
1:B:156:SNC:O	1:B:160:ILE:HG12	2.12	0.49
1:B:168:GLN:HG3	1:B:248:ASN:O	2.12	0.49
1:D:247:GLU:HG2	1:D:256:SER:HB3	1.94	0.49
1:B:32:VAL:HG22	1:D:255:HIS:CB	2.42	0.49
1:D:198:GLU:HG2	1:D:214:ARG:NH2	2.27	0.49
1:B:216:TYR:O	1:B:219:PRO:HD3	2.13	0.49
1:B:149:PRO:HB2	1:B:199:LEU:HD12	1.95	0.48
1:B:227:ARG:NH2	1:D:63:LYS:HA	2.28	0.48
1:A:226:VAL:HG11	1:A:259:ALA:CB	2.40	0.48
1:B:56:VAL:HG22	1:B:70:PHE:HZ	1.78	0.48
1:D:253:HIS:HB3	1:D:255:HIS:CD2	2.48	0.48
1:B:182:VAL:HG22	1:B:238:ARG:NE	2.28	0.48
1:A:188:ILE:O	1:A:192:GLU:HG3	2.13	0.48
1:C:167:ASN:CG	1:D:167:ASN:H	2.16	0.48
1:D:213:GLU:O	1:D:217:GLU:HG3	2.14	0.48
1:A:67:MET:HA	1:A:70:PHE:CD2	2.48	0.48
1:B:25:GLN:OE1	1:D:261:ILE:HA	2.14	0.48
1:C:251:SER:O	1:D:199:LEU:HD21	2.14	0.48
1:B:71:VAL:HB	1:C:202:LEU:HD13	1.96	0.47
1:B:145:LYS:HG3	1:B:175:ASP:HB2	1.95	0.47
1:B:154[A]:CYS:SG	1:B:166:HIS:CD2	3.06	0.47
1:B:194:GLU:HG2	1:B:232:ARG:NE	2.28	0.47
1:A:208:GLU:O	1:A:211:VAL:HG22	2.14	0.47
1:A:245:GLU:HB3	1:A:258:TYR:CE1	2.49	0.47
1:B:32:VAL:HG22	1:D:255:HIS:HB3	1.97	0.47
1:A:205:ARG:N	1:A:206:PRO:CD	2.78	0.47
1:B:115:THR:HG23	1:B:120:GLY:HA2	1.96	0.47
1:B:171:HIS:CG	1:B:249:PHE:HE2	2.32	0.47
1:B:145:LYS:HE2	1:B:173:THR:HG21	1.96	0.47
1:C:73:LEU:HD21	1:C:93:MET:HA	1.97	0.47
1:A:113:ASN:CB	1:A:124:LEU:HD21	2.43	0.46
1:A:225:LEU:C	1:A:225:LEU:HD23	2.35	0.46
1:A:168:GLN:OE1	1:A:168:GLN:N	2.31	0.46
1:C:153:LEU:CD2	1:C:216:TYR:HA	2.45	0.46
1:A:202:LEU:CD1	1:D:68:SER:HB2	2.45	0.46
1:A:113:ASN:CB	1:A:124:LEU:CD2	2.94	0.46
1:A:53:ASN:HB2	1:A:105:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:GLU:O	1:D:220:LYS:NZ	2.43	0.45
1:C:114:LYS:HB3	1:C:200:TRP:HE1	1.82	0.45
1:B:41:ALA:HB2	1:B:185:GLU:OE1	2.16	0.45
1:D:125:LEU:HD23	1:D:127:TYR:CZ	2.51	0.45
1:A:202:LEU:HB2	1:D:71:VAL:CG1	2.47	0.45
1:B:68:SER:O	1:B:69:ARG:C	2.56	0.45
1:D:162:GLN:O	1:D:216:TYR:OH	2.33	0.45
1:B:61:ASP:OD1	1:B:62:GLN:N	2.50	0.44
1:B:111:PHE:HA	1:B:125:LEU:O	2.18	0.44
1:B:36:LEU:HD23	1:B:48:THR:HG23	1.97	0.44
1:B:25:GLN:O	1:B:57:HIS:HA	2.18	0.44
1:C:104:ILE:O	1:C:132:THR:HA	2.16	0.44
1:B:45:THR:HG22	1:B:46:GLN:N	2.33	0.44
1:B:182:VAL:HG13	1:B:238:ARG:HH21	1.83	0.44
1:B:198:GLU:HG3	1:B:200:TRP:CH2	2.53	0.44
1:C:137:ASP:O	1:C:139:LEU:HG	2.16	0.44
1:D:117:PRO:HG3	1:D:200:TRP:CH2	2.53	0.44
1:C:252:ILE:HG13	1:C:253:HIS:NE2	2.32	0.44
1:D:248:ASN:HB2	1:D:257:ALA:HB3	2.00	0.44
1:B:221:PHE:HB2	1:B:224:ASP:OD2	2.17	0.44
1:C:118:VAL:CB	1:C:206:PRO:HB2	2.48	0.44
1:B:81:LEU:HD11	1:B:86:PHE:HD1	1.82	0.44
1:D:222:VAL:HG12	1:D:223:GLU:OE1	2.18	0.43
1:C:147:LEU:HD11	1:C:171:HIS:HB3	2.00	0.43
1:A:90:LEU:HD13	1:A:104:ILE:HG13	2.00	0.43
1:D:130:THR:HB	1:D:145:LYS:HB2	2.01	0.43
1:A:226:VAL:CG2	1:A:227:ARG:N	2.80	0.43
1:D:154[A]:CYS:SG	1:D:166:HIS:NE2	2.91	0.43
1:B:244:LEU:O	1:B:260:LEU:HA	2.18	0.43
1:C:252:ILE:C	1:D:199:LEU:HD22	2.39	0.43
1:A:226:VAL:HG23	1:A:227:ARG:N	2.33	0.43
1:D:154[A]:CYS:HB3	1:D:166:HIS:NE2	2.34	0.43
1:C:40:THR:HG22	1:C:110:TYR:OH	2.19	0.42
1:D:154[A]:CYS:SG	1:D:156:SNC:N	2.92	0.42
1:C:114:LYS:HB3	1:C:200:TRP:NE1	2.34	0.42
1:A:113:ASN:CA	1:A:124:LEU:CD2	2.98	0.42
1:A:124:LEU:HD12	1:D:34:HIS:HE1	1.83	0.42
1:D:247:GLU:HA	1:D:257:ALA:O	2.20	0.42
1:A:157:SER:O	1:A:158:LYS:CB	2.67	0.42
1:A:129:VAL:HG11	1:A:184:VAL:HG11	2.01	0.42
1:A:250:GLU:HB3	1:A:253:HIS:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:CG1	1:A:39:ARG:N	2.83	0.41
1:A:208:GLU:HA	1:A:211:VAL:HG22	2.03	0.41
1:C:117:PRO:HB3	1:C:210:PHE:CD1	2.55	0.41
1:B:213:GLU:O	1:B:217:GLU:N	2.42	0.41
1:D:242:TYR:CZ	1:D:263:ARG:HB2	2.55	0.41
1:B:48:THR:OG1	1:B:49:VAL:N	2.54	0.41
1:D:157:SER:HB2	1:D:166:HIS:HD2	1.86	0.41
1:B:223:GLU:O	1:B:227:ARG:HG3	2.21	0.41
1:B:22:MET:O	1:D:227:ARG:NH1	2.54	0.41
1:C:145:LYS:HA	1:C:174:ILE:O	2.21	0.41
1:A:202:LEU:HB2	1:D:71:VAL:HG12	2.02	0.40
1:A:154:CYS:HA	1:A:155:PRO:HD3	1.92	0.40
1:C:106:VAL:CG1	1:C:131:LEU:HB2	2.51	0.40
1:A:210:PHE:CZ	1:A:214:ARG:HG3	2.57	0.40
1:C:252:ILE:HD11	5:C:301:ZS9:C6	2.52	0.40
1:D:59:PRO:HD2	1:D:62:GLN:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/303 (72%)	208 (95%)	10 (5%)	1 (0%)	29	64
1	B	241/303 (80%)	230 (95%)	11 (5%)	0	100	100
1	C	243/303 (80%)	230 (95%)	13 (5%)	0	100	100
1	D	237/303 (78%)	228 (96%)	9 (4%)	0	100	100
All	All	940/1212 (78%)	896 (95%)	43 (5%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	PRO

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	123/254 (48%)	123 (100%)	0	100	100
1	B	151/254 (59%)	150 (99%)	1 (1%)	84	93
1	C	152/254 (60%)	152 (100%)	0	100	100
1	D	136/254 (54%)	135 (99%)	1 (1%)	84	93
All	All	562/1016 (55%)	560 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	154[A]	CYS
1	D	154[A]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	34	HIS
1	D	46	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	SNC	C	156	1	4,7,8	0.60	0	1,7,9	1.49	0
1	SNC	D	156	1	3,4,8	0.64	0	2,4,9	1.54	1 (50%)
1	SNC	B	156	1	3,4,8	0.54	0	2,4,9	1.48	0
1	SNC	A	156	1	4,7,8	0.61	0	1,7,9	1.29	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
1	SNC	C	156	1	-	0/0/6/8	-
1	SNC	D	156	1	-	0/0/2/8	-
1	SNC	B	156	1	-	0/0/2/8	-
1	SNC	A	156	1	-	0/0/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	SNC	O-C-CA	-2.06	117.78	124.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	156	SNC	1	0
1	B	156	SNC	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO3	A	303[B]	2	1,3,3	0.19	0	0,3,3	-	-
3	EDO	D	302	-	3,3,3	0.13	0	2,2,2	0.08	0
5	ZS9	D	301[A]	1	19,19,19	1.66	4 (21%)	27,29,29	2.83	11 (40%)
5	ZS9	B	301[A]	1	19,19,19	1.41	2 (10%)	27,29,29	3.19	12 (44%)
5	ZS9	C	301	1	19,19,19	1.69	2 (10%)	27,29,29	3.21	12 (44%)
3	EDO	A	302	-	3,3,3	0.10	0	2,2,2	0.10	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	EDO	D	302	-	-	0/1/1/1	-
5	ZS9	D	301[A]	1	2/2/8/8	-	0/3/3/3
5	ZS9	B	301[A]	1	-	-	0/3/3/3
5	ZS9	C	301	1	2/2/8/8	-	0/3/3/3
3	EDO	A	302	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	ZS9	O11-C6	-4.99	1.39	1.46
5	D	301[A]	ZS9	O11-C6	-4.34	1.40	1.46
5	B	301[A]	ZS9	O11-C6	-3.82	1.41	1.46
5	C	301	ZS9	C9-C12	-3.81	1.44	1.51
5	B	301[A]	ZS9	C9-C12	-2.63	1.46	1.51
5	D	301[A]	ZS9	C5-C18	-2.48	1.47	1.52
5	D	301[A]	ZS9	C14-C9	-2.40	1.48	1.53
5	D	301[A]	ZS9	C9-C12	-2.16	1.47	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	ZS9	C19-C18-C20	-9.68	115.50	125.51
5	B	301[A]	ZS9	C19-C18-C20	-9.00	116.21	125.51
5	D	301[A]	ZS9	C19-C18-C20	-7.02	118.25	125.51
5	D	301[A]	ZS9	C2-C3-C15	-6.21	111.44	120.77
5	C	301	ZS9	C2-C3-C15	-6.18	111.50	120.77
5	B	301[A]	ZS9	C8-C2-C3	5.88	124.55	114.71
5	B	301[A]	ZS9	C14-C9-C7	-5.55	106.17	116.68
5	B	301[A]	ZS9	O11-C6-C5	5.06	116.23	108.50
5	B	301[A]	ZS9	C2-C3-C15	-4.81	113.55	120.77
5	C	301	ZS9	C8-C7-C6	-4.81	107.02	114.21
5	C	301	ZS9	O11-C6-C5	4.55	115.45	108.50
5	C	301	ZS9	C8-C2-C3	4.31	121.92	114.71
5	C	301	ZS9	C7-C9-C12	-4.23	95.91	101.97
5	D	301[A]	ZS9	C16-C4-C3	4.14	122.49	115.63
5	D	301[A]	ZS9	C19-C18-C5	3.92	111.35	108.57
5	D	301[A]	ZS9	O11-C6-C5	3.88	114.43	108.50
5	C	301	ZS9	C5-C18-C20	3.80	132.07	126.35
5	D	301[A]	ZS9	C5-C6-C7	3.62	122.86	116.39
5	D	301[A]	ZS9	C5-C4-C3	3.49	124.08	114.95
5	C	301	ZS9	C16-C4-C3	3.47	121.39	115.63
5	D	301[A]	ZS9	C4-C5-C6	3.46	120.80	113.44
5	B	301[A]	ZS9	C4-C5-C6	-3.42	106.15	113.44
5	D	301[A]	ZS9	O11-C12-O13	-2.86	117.69	121.29
5	C	301	ZS9	C4-C5-C6	-2.77	107.53	113.44
5	B	301[A]	ZS9	C14-C9-C12	-2.77	107.14	112.50
5	B	301[A]	ZS9	C7-C9-C12	-2.75	98.03	101.97
5	B	301[A]	ZS9	C19-C18-C5	2.70	110.48	108.57
5	B	301[A]	ZS9	C16-C4-C3	2.66	120.04	115.63
5	C	301	ZS9	C5-C6-C7	-2.63	111.69	116.39
5	D	301[A]	ZS9	C14-C9-C7	-2.54	111.88	116.68
5	C	301	ZS9	C14-C9-C12	-2.52	107.63	112.50
5	B	301[A]	ZS9	O11-C12-O13	-2.48	118.17	121.29
5	C	301	ZS9	C6-O11-C12	-2.43	106.43	109.87
5	B	301[A]	ZS9	C16-C4-C5	2.18	107.75	103.30
5	D	301[A]	ZS9	C16-C4-C5	2.16	107.71	103.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	301	ZS9	C7
5	C	301	ZS9	C5
5	D	301[A]	ZS9	C6

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Mol	Chain	Res	Type	Atom
5	D	301[A]	ZS9	C9

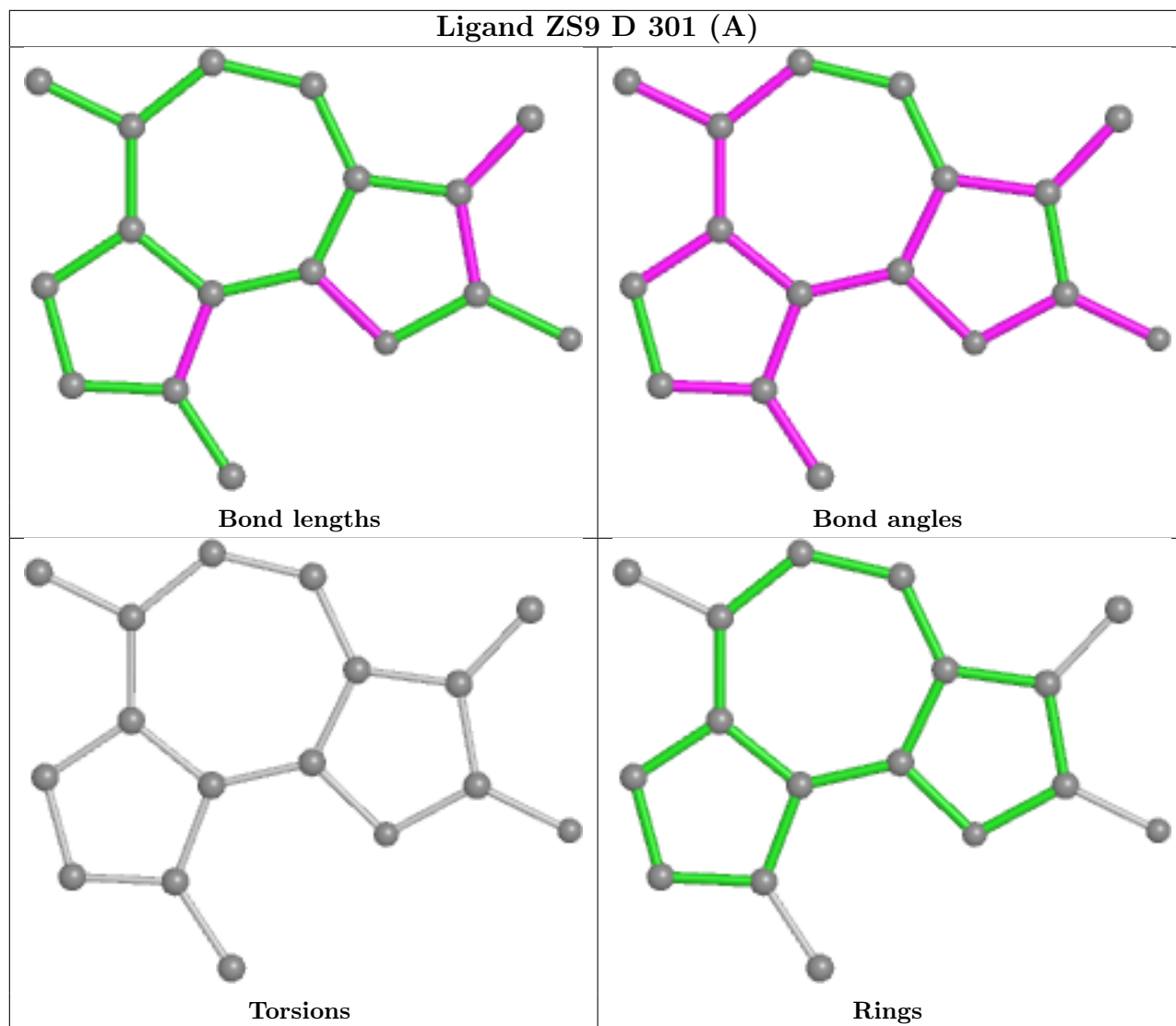
There are no torsion outliers.

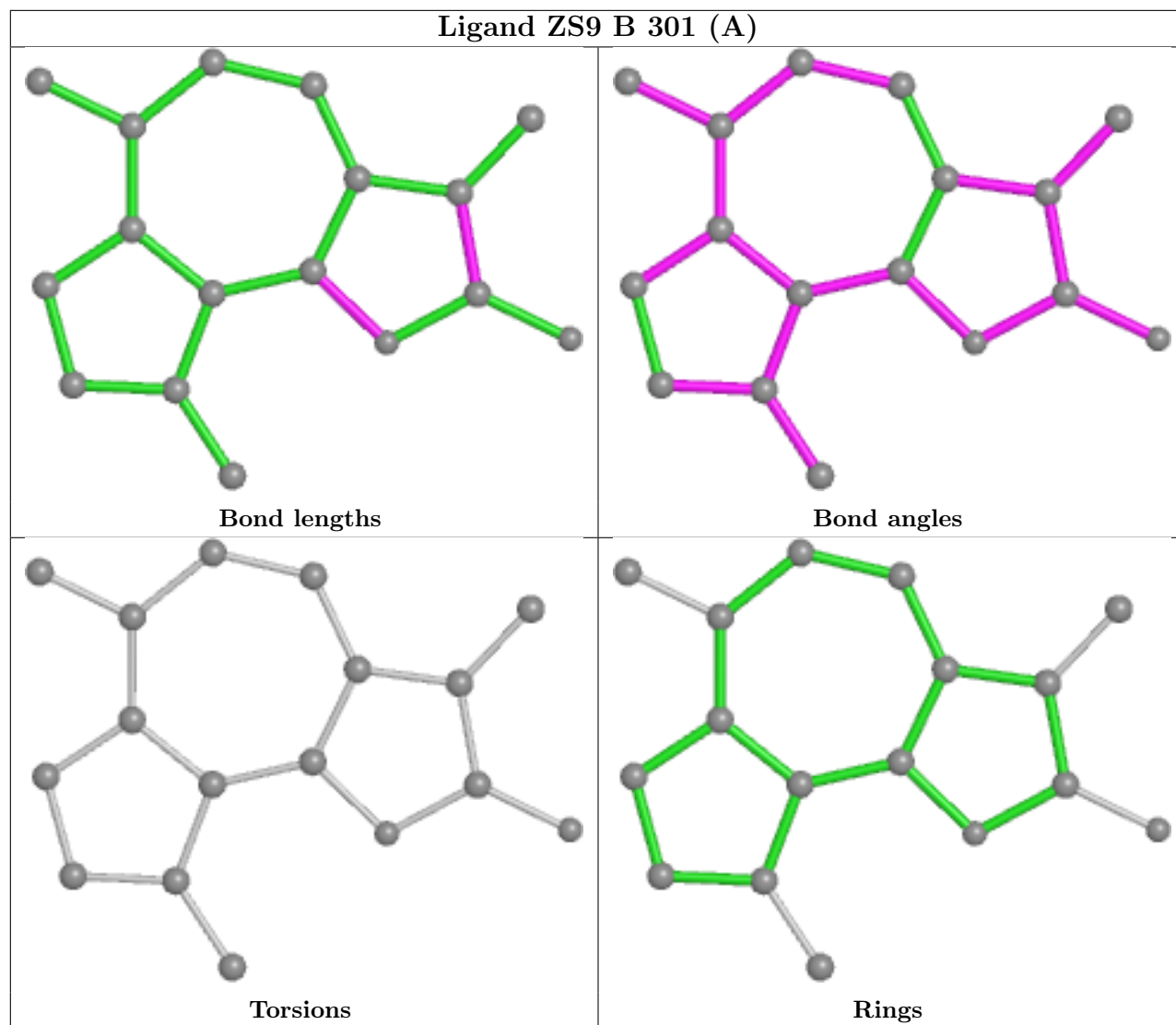
There are no ring outliers.

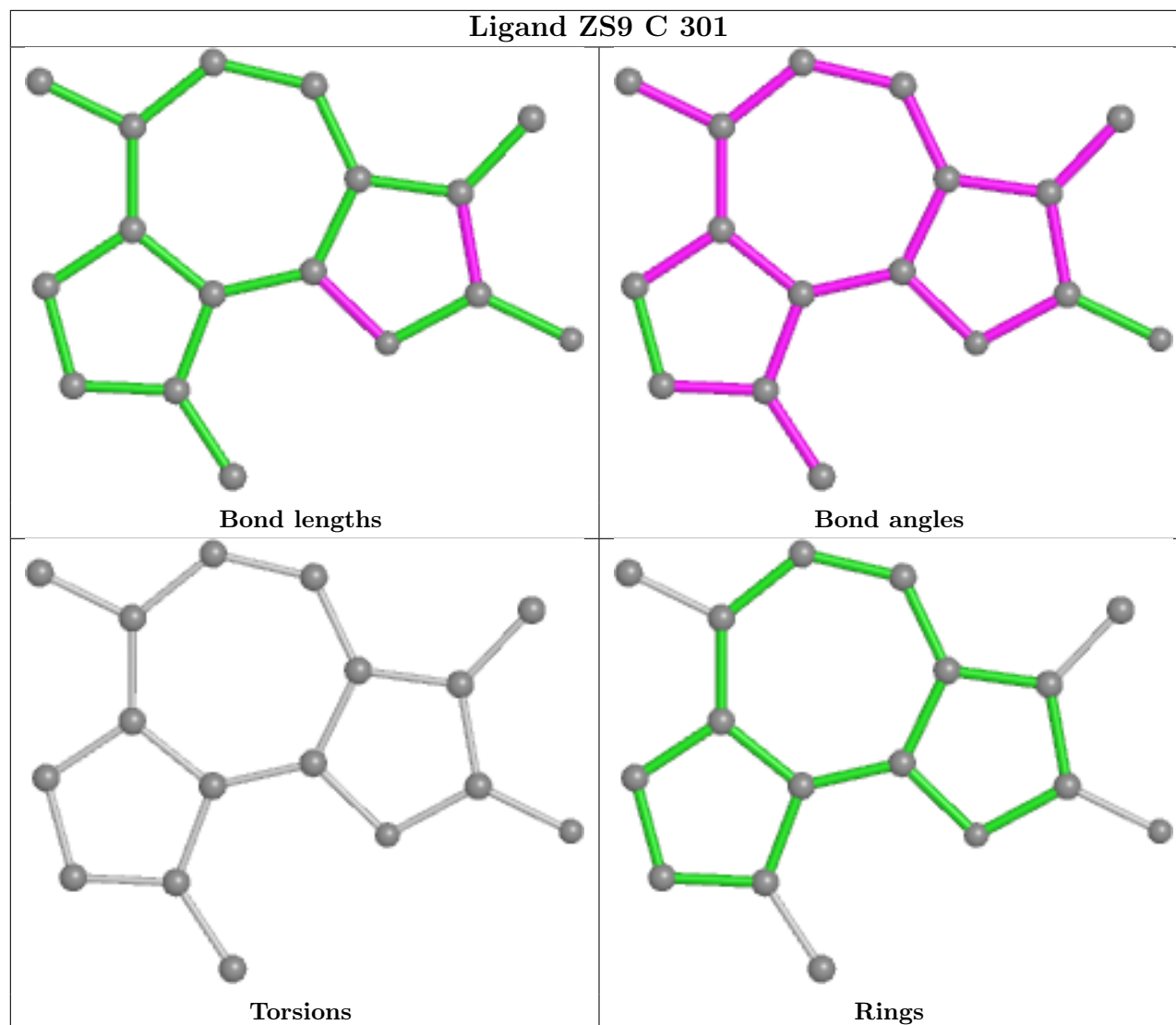
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	301[A]	ZS9	2	0
5	B	301[A]	ZS9	1	0
5	C	301	ZS9	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	A	231/303 (76%)	0.10	3 (1%) 77 59	32, 54, 74, 96	0
1	B	244/303 (80%)	-0.00	4 (1%) 72 51	25, 46, 67, 85	0
1	C	245/303 (80%)	0.04	1 (0%) 92 84	29, 48, 71, 97	0
1	D	243/303 (80%)	0.09	3 (1%) 79 61	29, 54, 76, 100	0
All	All	963/1212 (79%)	0.06	11 (1%) 80 64	25, 50, 73, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	GLY	2.9
1	B	165	ALA	2.9
1	B	252	ILE	2.7
1	D	157	SER	2.6
1	B	164	GLY	2.5
1	A	161	SER	2.3
1	B	168	GLN	2.2
1	D	52	TRP	2.1
1	A	120	GLY	2.1
1	A	181	ASP	2.1
1	C	117	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SNC	B	156	5/9	0.84	0.20	64,66,69,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SNC	D	156	5/9	0.86	0.37	55,57,65,70	0
1	SNC	A	156	8/9	0.88	0.22	53,61,74,80	0
1	SNC	C	156	8/9	0.90	0.27	47,56,66,72	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

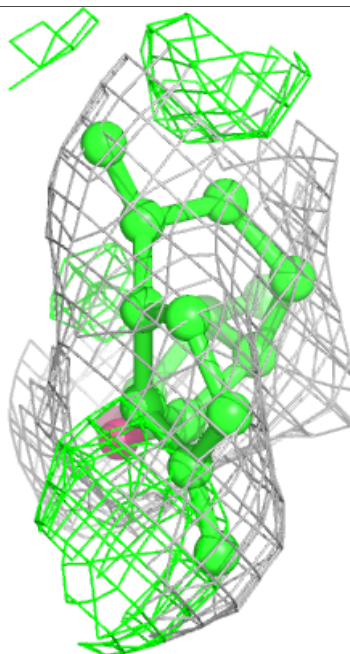
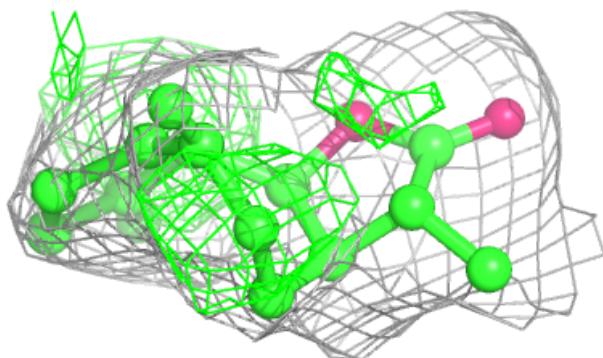
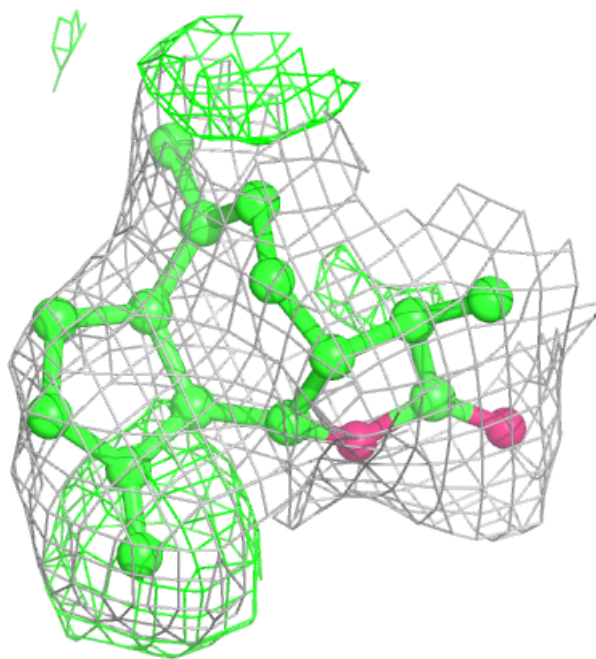
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	A	301	1/1	0.81	0.13	59,59,59,59	0
5	ZS9	D	301[A]	17/17	0.81	0.26	34,42,51,54	0
5	ZS9	C	301	17/17	0.84	0.31	31,39,49,54	0
5	ZS9	B	301[A]	17/17	0.86	0.24	40,51,61,61	0
3	EDO	A	302	4/4	0.87	0.28	40,52,62,62	0
3	EDO	D	302	4/4	0.92	0.15	36,46,51,61	0
4	SO3	A	303[B]	4/4	0.96	0.14	44,46,50,55	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.

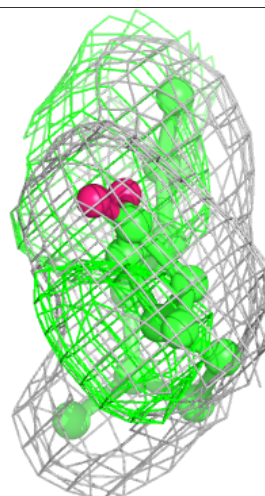
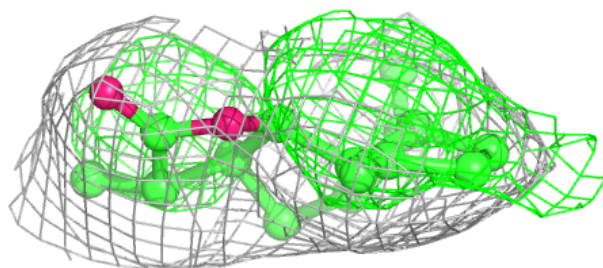
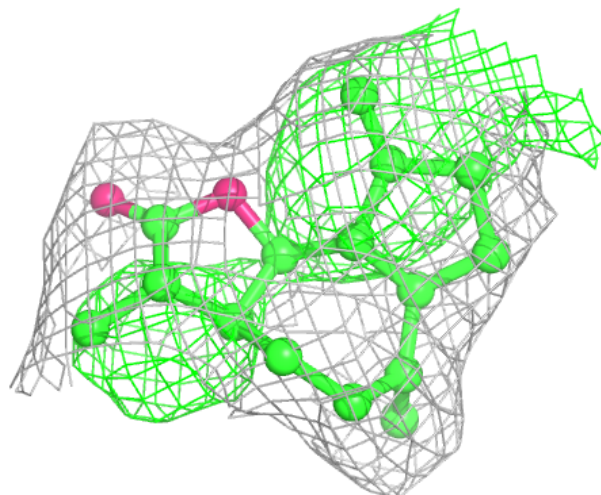
Electron density around ZS9 D 301 (A):

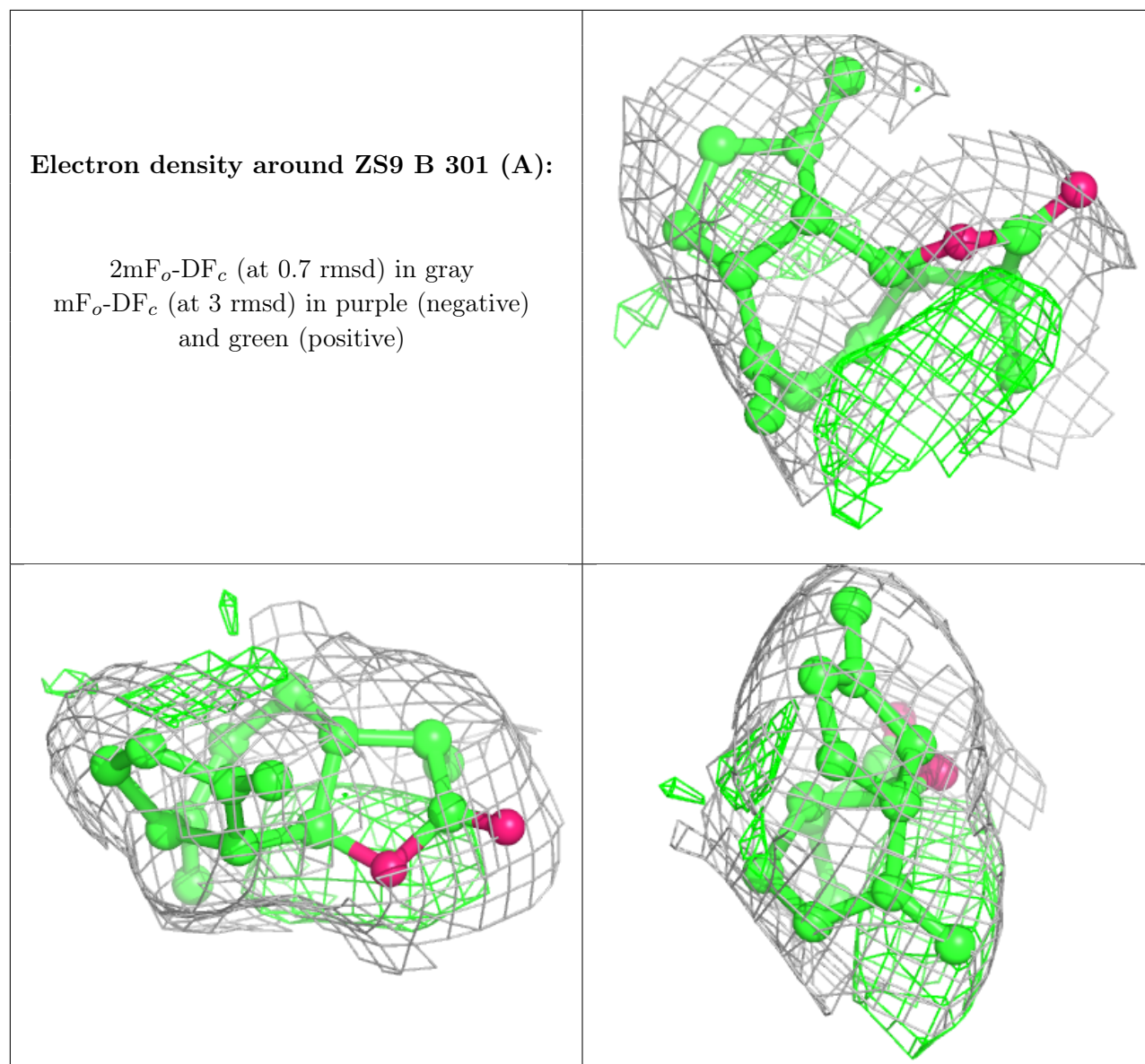
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZS9 C 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.