



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:17 AM UTC

PDB ID : 6S0W / pdb_00006s0w
Title : The crystal structure of kanamycin B dioxygenase (KanJ) from *Streptomyces kanamyceticus* in complex with nickel and kanamycin B sulfate
Authors : Mrugala, B.; Niedzialkowska, E.; Minor, W.; Borowski, T.
Deposited on : 2019-06-18
Resolution : 2.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

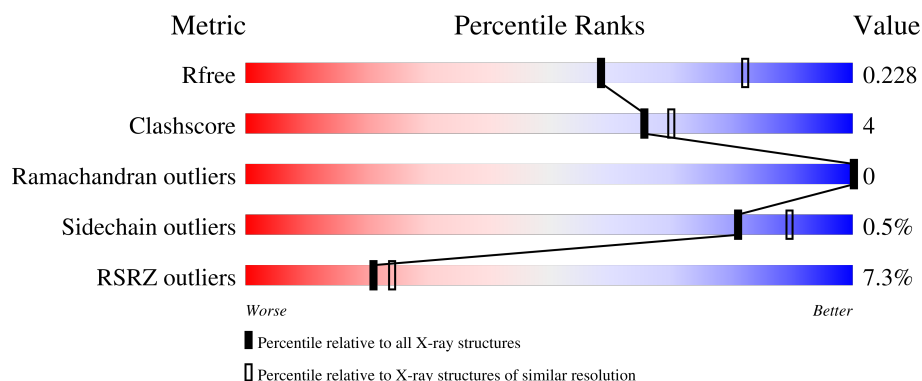
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	288	5% 84% 11% 5%
1	B	288	4% 87% 10% ..
1	C	288	6% 88% 8% .
1	D	288	5% 87% 10% .
1	E	288	17% 86% 9% 5%

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Mol	Chain	Length	Quality of chain
1	F	288	7% 93% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14359 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 Kanamycin B dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2156	1370	379	398	9			
1	B	282	Total	C	N	O	S	0	0	0
			2197	1397	386	405	9			
1	C	277	Total	C	N	O	S	0	1	0
			2169	1378	381	400	10			
1	D	279	Total	C	N	O	S	0	0	0
			2173	1380	382	401	10			
1	E	274	Total	C	N	O	S	0	1	0
			2149	1366	378	396	9			
1	F	283	Total	C	N	O	S	0	0	0
			2202	1402	387	404	9			

There are 18 discrepancies between the modelled and reference sequences:

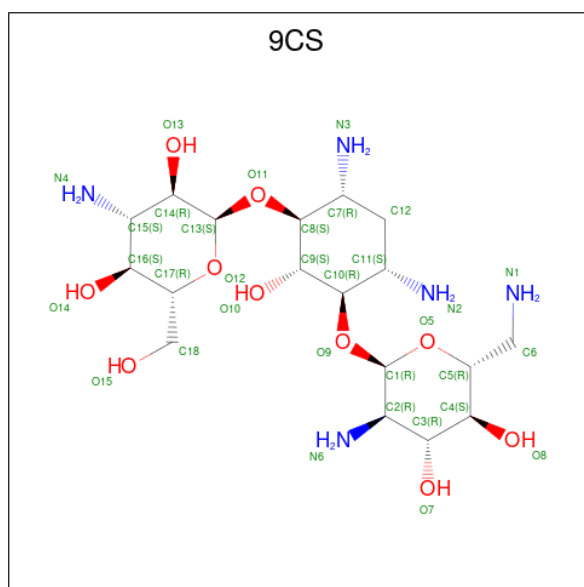
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q6L732
A	-1	ASN	-	expression tag	UNP Q6L732
A	0	ALA	-	expression tag	UNP Q6L732
B	-2	SER	-	expression tag	UNP Q6L732
B	-1	ASN	-	expression tag	UNP Q6L732
B	0	ALA	-	expression tag	UNP Q6L732
C	-2	SER	-	expression tag	UNP Q6L732
C	-1	ASN	-	expression tag	UNP Q6L732
C	0	ALA	-	expression tag	UNP Q6L732
D	-2	SER	-	expression tag	UNP Q6L732
D	-1	ASN	-	expression tag	UNP Q6L732
D	0	ALA	-	expression tag	UNP Q6L732
E	-2	SER	-	expression tag	UNP Q6L732
E	-1	ASN	-	expression tag	UNP Q6L732
E	0	ALA	-	expression tag	UNP Q6L732
F	-2	SER	-	expression tag	UNP Q6L732
F	-1	ASN	-	expression tag	UNP Q6L732

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q6L732

- Molecule 2 is (1R,2S,3S,4R,6S)-4,6-DIAMINO-3-[(3-AMINO-3-DEOXY-ALPHA-D-GLUCOPYRANOSYL)OXY]-2-HYDROXYCYCLOHEXYL 2,6-DIAMINO-2,6-DIDEOXY-ALPHA-D-GLUCOPYRANOSIDE (CCD ID: 9CS) (formula: C₁₈H₃₇N₅O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	18	5	10		
2	B	1	Total	C	N	O	0	0
			33	18	5	10		
2	C	1	Total	C	N	O	0	0
			33	18	5	10		
2	D	1	Total	C	N	O	0	0
			33	18	5	10		
2	E	1	Total	C	N	O	0	0
			33	18	5	10		
2	F	1	Total	C	N	O	0	0
			33	18	5	10		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

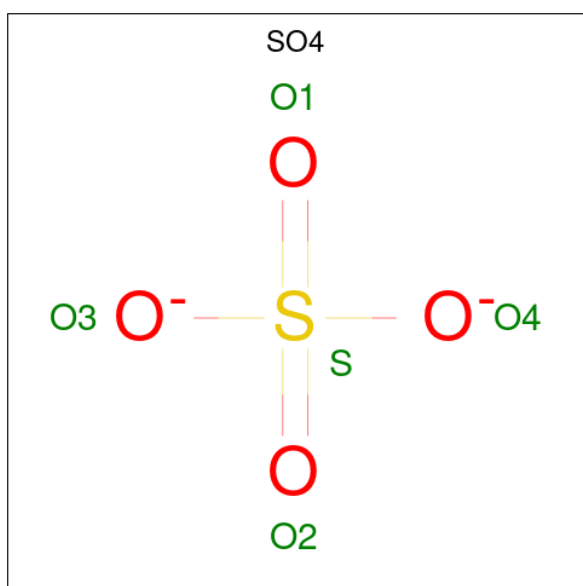
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		
3	F	1	Total	Ni	0	0
			1	1		

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



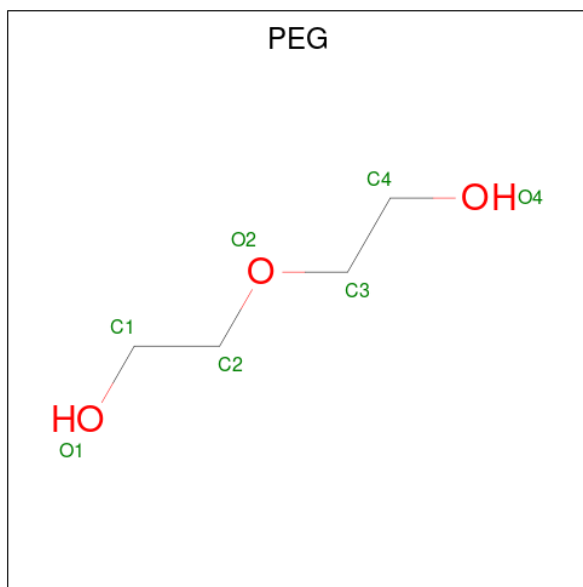
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	4	3		

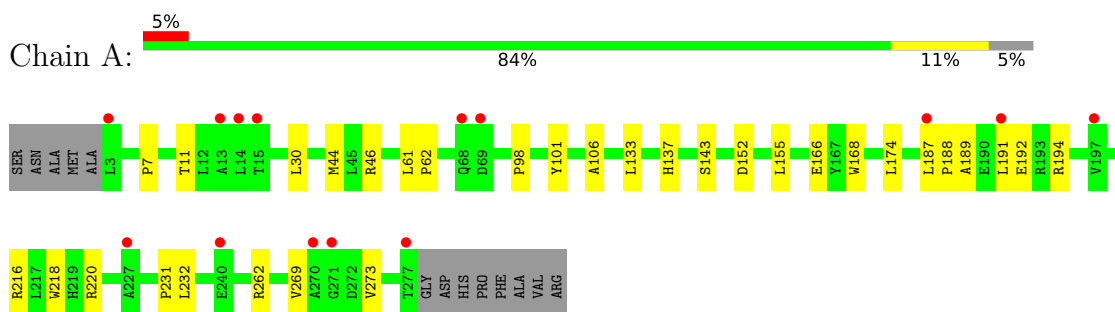
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		
6	B	269	Total	O	0	0
			269	269		
6	C	161	Total	O	0	0
			161	161		
6	D	216	Total	O	0	0
			216	216		
6	E	82	Total	O	0	0
			82	82		
6	F	137	Total	O	0	0
			137	137		

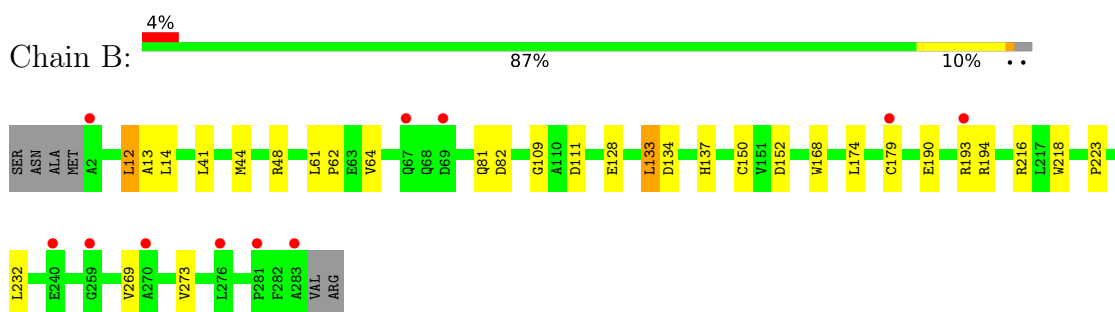
3 Residue-property plots [i](#)

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.

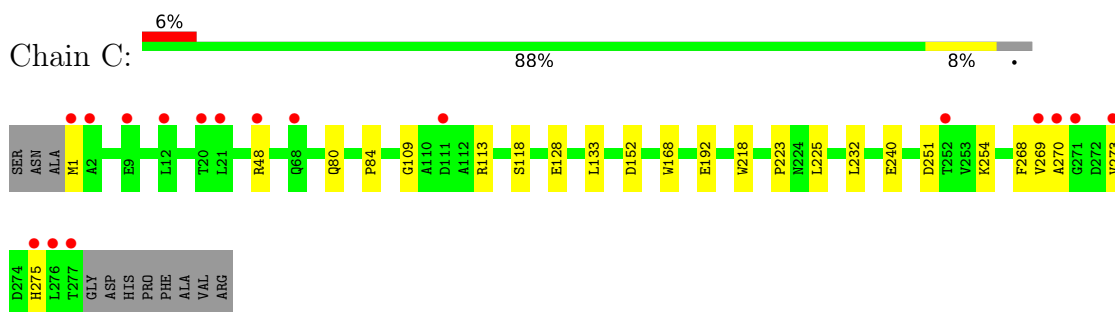
- Molecule 1: Kanamycin B dioxygenase



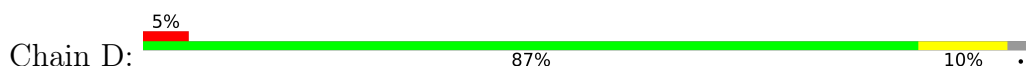
- Molecule 1: Kanamycin B dioxygenase

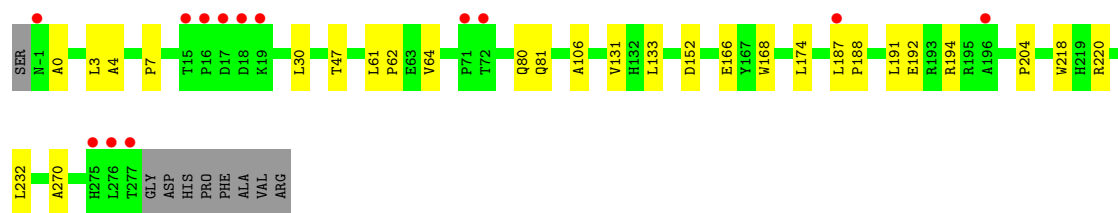


- Molecule 1: Kanamycin B dioxygenase

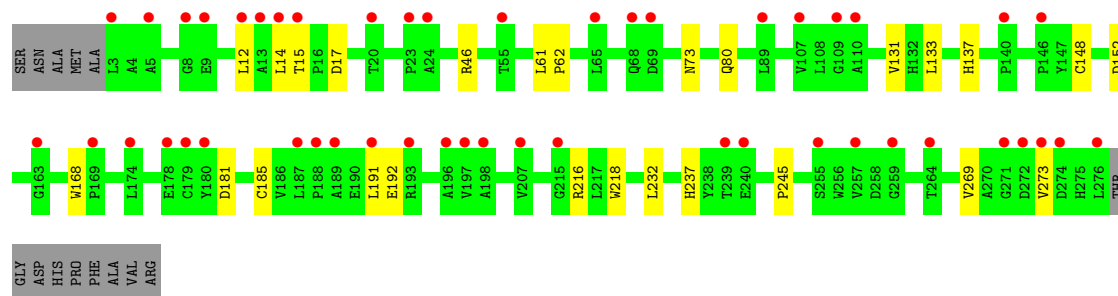
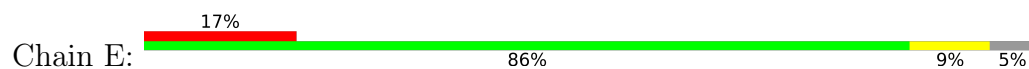


- Molecule 1: Kanamycin B dioxygenase

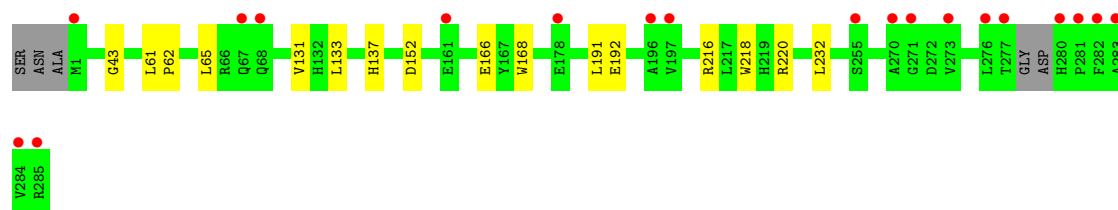




● Molecule 1: Kanamycin B dioxygenase



● Molecule 1: Kanamycin B dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.44Å 186.06Å 110.17Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	44.22 – 2.36 44.22 – 2.36	Depositor EDS
% Data completeness (in resolution range)	95.1 (44.22-2.36) 95.5 (44.22-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.185 , 0.225 0.191 , 0.228	Depositor DCC
R_{free} test set	3946 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14359	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: PEG, SO4, 9CS, NI

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	0.96	0/2222	1.20	2/3057 (0.1%)
1	B	1.00	0/2266	1.20	1/3118 (0.0%)
1	C	0.97	0/2235	1.18	3/3074 (0.1%)
1	D	0.97	0/2239	1.21	0/3080
1	E	0.96	0/2215	1.20	1/3047 (0.0%)
1	F	0.96	0/2270	1.23	0/3123
All	All	0.97	0/13447	1.20	7/18499 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	GLY	CA-C-O	-5.43	118.49	122.23
1	C	109	GLY	CA-C-O	-5.32	118.56	122.23
1	E	245	PRO	N-CA-CB	5.09	105.87	103.22
1	A	46	ARG	CA-C-N	5.05	127.30	120.38
1	A	46	ARG	C-N-CA	5.05	127.30	120.38
1	C	1	MET	CA-C-N	5.02	128.60	121.42
1	C	1	MET	C-N-CA	5.02	128.60	121.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2156	0	2106	25	0
1	B	2197	0	2139	20	0
1	C	2169	0	2123	13	0
1	D	2173	0	2127	19	0
1	E	2149	0	2099	18	0
1	F	2202	0	2147	9	0
2	A	33	0	37	0	0
2	B	33	0	37	3	0
2	C	33	0	37	0	0
2	D	33	0	37	1	0
2	E	33	0	37	0	0
2	F	33	0	37	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
4	E	15	0	0	0	0
4	F	25	0	0	0	0
5	D	7	0	10	1	0
6	A	142	0	0	0	0
6	B	269	0	0	2	0
6	C	161	0	0	0	0
6	D	216	0	0	0	0
6	E	82	0	0	0	0
6	F	137	0	0	1	0
All	All	14359	0	12973	99	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 4.

All (99) 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:C:251:ASP:OD2	1:C:270:ALA:HA	1.78	0.83
1:D:187:LEU:HD12	1:D:188:PRO:HD2	1.67	0.76
1:A:187:LEU:HD23	1:A:189:ALA:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:ASN:HD21	1:E:80[B]:GLN:HG2	1.57	0.69
1:F:166:GLU:HB3	1:F:220:ARG:HG3	1.79	0.65
1:B:269:VAL:CG2	1:B:273:VAL:HG22	2.31	0.60
1:A:152:ASP:HB3	1:A:232:LEU:HD11	1.83	0.59
1:B:133:LEU:HD12	1:B:133:LEU:O	2.04	0.58
1:F:192:GLU:HA	1:F:192:GLU:OE1	2.03	0.58
1:A:188:PRO:HG2	1:E:15:THR:HG22	1.86	0.57
1:B:152:ASP:HB3	1:B:232:LEU:HD11	1.86	0.57
1:C:269:VAL:CG2	1:C:273:VAL:HG22	2.34	0.57
1:E:192:GLU:HA	1:E:192:GLU:OE1	2.05	0.57
1:B:190:GLU:OE1	1:B:193:ARG:NH1	2.27	0.56
1:A:192:GLU:HA	1:A:192:GLU:OE1	2.05	0.55
1:A:101:TYR:CD2	1:A:262:ARG:HB3	2.42	0.54
1:E:131:VAL:HB	1:E:191:LEU:HD11	1.90	0.53
1:B:269:VAL:HG21	1:B:273:VAL:HG22	1.89	0.53
1:D:168:TRP:CH2	1:D:191:LEU:HD22	2.44	0.53
1:D:192:GLU:OE1	1:D:192:GLU:HA	2.09	0.53
2:B:301:9CS:O10	2:B:301:9CS:H1	2.09	0.53
1:E:73:ASN:ND2	1:E:80[B]:GLN:HG2	2.24	0.52
1:A:269:VAL:CG2	1:A:273:VAL:HG22	2.41	0.51
1:B:168:TRP:HB2	1:B:218:TRP:HB2	1.93	0.51
1:E:181:ASP:OD2	1:E:185:CYS:HB2	2.11	0.51
1:D:166:GLU:HB3	1:D:220:ARG:HG3	1.92	0.51
1:D:64:VAL:HG21	1:D:81:GLN:HG3	1.92	0.50
1:A:7:PRO:O	1:A:11:THR:OG1	2.20	0.50
1:D:3:LEU:CD1	1:D:7:PRO:HG3	2.42	0.50
1:E:269:VAL:CG2	1:E:273:VAL:HG22	2.42	0.50
1:A:269:VAL:HG21	1:A:273:VAL:HG22	1.94	0.49
1:E:17:ASP:OD1	1:E:46:ARG:NH2	2.46	0.49
1:B:111:ASP:HB2	6:B:498:HOH:O	2.13	0.49
1:D:174:LEU:HD11	1:D:194:ARG:HD3	1.93	0.49
1:E:131:VAL:HG11	1:E:191:LEU:HD21	1.94	0.48
1:B:82:ASP:HB3	6:B:426:HOH:O	2.13	0.48
1:A:137:HIS:CE1	1:A:216:ARG:HD2	2.49	0.48
1:B:174:LEU:HD11	1:B:194:ARG:HD3	1.96	0.48
1:B:179:CYS:SG	1:B:190:GLU:HG2	2.53	0.48
1:A:168:TRP:CH2	1:A:191:LEU:HD22	2.48	0.47
1:A:187:LEU:HG	1:A:188:PRO:HD2	1.97	0.47
1:D:4:ALA:O	1:D:204:PRO:HG2	2.13	0.47
1:A:168:TRP:HB2	1:A:218:TRP:HB2	1.97	0.47
1:E:137:HIS:CE1	1:E:216:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:TRP:HB2	1:C:218:TRP:HB2	1.96	0.47
1:F:168:TRP:HB2	1:F:218:TRP:HB2	1.97	0.47
1:E:168:TRP:HB2	1:E:218:TRP:HB2	1.97	0.46
1:A:187:LEU:HD23	1:A:189:ALA:N	2.26	0.46
1:C:269:VAL:HG21	1:C:273:VAL:HG22	1.97	0.46
1:B:12:LEU:HD12	1:B:13:ALA:N	2.31	0.46
1:B:48:ARG:NH1	1:C:48:ARG:HG3	2.30	0.46
1:C:225:LEU:O	1:D:62:PRO:HA	2.16	0.46
1:C:128:GLU:HG2	1:C:223:PRO:HD3	1.97	0.45
1:A:44:MET:HE3	1:A:44:MET:HB3	1.82	0.45
1:D:47:THR:H	5:D:306:PEG:C1	2.30	0.45
1:A:174:LEU:HD11	1:A:194:ARG:HD3	1.99	0.45
1:D:61:LEU:HB3	1:D:62:PRO:HD3	1.99	0.45
1:B:64:VAL:HG21	1:B:81:GLN:HG3	1.99	0.44
1:B:150:CYS:SG	2:B:301:9CS:N1	2.90	0.44
1:C:84:PRO:HA	1:C:275:HIS:CE1	2.52	0.44
1:A:166:GLU:HB3	1:A:220:ARG:HG3	2.00	0.44
1:A:101:TYR:CG	1:A:262:ARG:HB3	2.52	0.44
1:D:0:ALA:HB2	1:D:166:GLU:OE1	2.17	0.44
1:C:192:GLU:HB3	1:F:65:LEU:HD13	2.00	0.43
1:C:152:ASP:HB3	1:C:232:LEU:HD11	2.01	0.43
1:E:269:VAL:HG21	1:E:273:VAL:HG22	2.01	0.43
1:A:98:PRO:HB3	1:A:262:ARG:NH2	2.33	0.43
1:E:12:LEU:HD23	1:E:14:LEU:HG	2.01	0.43
1:D:80:GLN:NE2	2:D:301:9CS:O7	2.52	0.42
1:A:30:LEU:HD11	1:A:106:ALA:HB1	2.01	0.42
1:D:168:TRP:HB2	1:D:218:TRP:HB2	2.01	0.42
1:C:80[B]:GLN:NE2	1:C:118:SER:OG	2.52	0.42
1:A:188:PRO:HG2	1:E:15:THR:CG2	2.49	0.42
1:D:152:ASP:HB3	1:D:232:LEU:HD11	2.02	0.42
1:F:137:HIS:CE1	1:F:216:ARG:HD2	2.55	0.42
1:C:254:LYS:HA	1:C:268:PHE:CE2	2.55	0.42
1:E:61:LEU:HB3	1:E:62:PRO:HD3	2.00	0.42
1:B:14:LEU:HD12	1:B:44:MET:SD	2.60	0.42
1:F:152:ASP:HB3	1:F:232:LEU:HD11	2.01	0.42
1:D:61:LEU:N	1:D:62:PRO:CD	2.83	0.42
1:F:43:GLY:HA2	6:F:500:HOH:O	2.18	0.42
1:B:12:LEU:HB3	1:B:41:LEU:HD23	2.02	0.42
1:B:137:HIS:CE1	1:B:216:ARG:HD2	2.55	0.41
1:A:61:LEU:HB3	1:A:62:PRO:HD3	2.02	0.41
1:E:168:TRP:CH2	1:E:191:LEU:HD22	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HB2	1:A:231:PRO:HG2	2.01	0.41
1:C:113:ARG:HD3	1:C:240:GLU:HA	2.02	0.41
1:B:61:LEU:N	1:B:62:PRO:CD	2.84	0.41
1:F:61:LEU:HB3	1:F:62:PRO:HD3	2.02	0.41
1:A:143:SER:OG	1:D:270:ALA:HB1	2.21	0.41
1:B:128:GLU:HG3	1:B:223:PRO:HD3	2.02	0.41
1:D:30:LEU:HD11	1:D:106:ALA:HB1	2.01	0.41
1:E:148:CYS:HA	1:E:237:HIS:O	2.21	0.41
1:F:131:VAL:HG11	1:F:191:LEU:HD21	2.03	0.41
1:B:134:ASP:OD2	2:B:301:9CS:N1	2.50	0.40
1:D:131:VAL:HG11	1:D:191:LEU:HD21	2.03	0.40
1:E:152:ASP:HB3	1:E:232:LEU:HD11	2.02	0.40
1:A:187:LEU:HG	1:A:188:PRO:CD	2.51	0.40
1:A:61:LEU:N	1:A:62:PRO:CD	2.85	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	274/288 (95%)	269 (98%)	5 (2%)	0	100	100
1	B	280/288 (97%)	276 (99%)	4 (1%)	0	100	100
1	C	276/288 (96%)	271 (98%)	5 (2%)	0	100	100
1	D	277/288 (96%)	273 (99%)	4 (1%)	0	100	100
1	E	273/288 (95%)	269 (98%)	4 (2%)	0	100	100
1	F	279/288 (97%)	275 (99%)	4 (1%)	0	100	100
All	All	1659/1728 (96%)	1633 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/248 (97%)	239 (100%)	1 (0%)	84	91
1	B	243/248 (98%)	241 (99%)	2 (1%)	73	84
1	C	241/248 (97%)	240 (100%)	1 (0%)	84	91
1	D	241/248 (97%)	240 (100%)	1 (0%)	84	91
1	E	239/248 (96%)	238 (100%)	1 (0%)	84	91
1	F	243/248 (98%)	242 (100%)	1 (0%)	84	91
All	All	1447/1488 (97%)	1440 (100%)	7 (0%)	81	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
1	B	12	LEU
1	B	133	LEU
1	C	133	LEU
1	D	133	LEU
1	E	133	LEU
1	F	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	67	GLN
1	A	73	ASN
1	A	105	HIS
1	B	52	GLN
1	B	67	GLN
1	B	105	HIS
1	B	248	GLN
1	C	52	GLN
1	C	73	ASN

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Mol	Chain	Res	Type
1	C	114	ASN
1	C	127	HIS
1	C	137	HIS
1	C	248	GLN
1	D	52	GLN
1	D	67	GLN
1	D	73	ASN
1	D	80	GLN
1	D	120	ASN
1	D	137	HIS
1	E	52	GLN
1	E	73	ASN
1	E	114	ASN
1	E	120	ASN
1	F	52	GLN
1	F	127	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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
2	9CS	C	301	-	34,35,35	0.49	0	47,52,52	0.78	0
4	SO4	F	307	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	C	303	-	4,4,4	0.32	0	6,6,6	0.10	0
5	PEG	D	306	-	6,6,6	0.18	0	5,5,5	0.10	0
2	9CS	E	301	-	34,35,35	0.42	0	47,52,52	0.78	0
2	9CS	B	301	-	34,35,35	0.34	0	47,52,52	0.78	1 (2%)
4	SO4	C	305	-	4,4,4	0.33	0	6,6,6	0.08	0
2	9CS	A	301	-	34,35,35	0.34	0	47,52,52	0.76	0
4	SO4	A	304	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	F	303	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	E	304	-	4,4,4	0.34	0	6,6,6	0.06	0
4	SO4	D	305	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	E	303	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	B	305	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	D	304	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	B	303	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	F	304	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	E	305	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	C	304	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	F	305	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	B	304	-	4,4,4	0.34	0	6,6,6	0.04	0
2	9CS	D	301	-	34,35,35	0.42	0	47,52,52	0.55	0
4	SO4	F	306	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	D	303	-	4,4,4	0.33	0	6,6,6	0.07	0
2	9CS	F	301	-	34,35,35	0.51	1 (2%)	47,52,52	0.67	0
4	SO4	A	303	-	4,4,4	0.33	0	6,6,6	0.05	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
2	9CS	C	301	-	-	2/12/72/72	0/3/3/3
2	9CS	D	301	-	-	3/12/72/72	0/3/3/3
5	PEG	D	306	-	-	1/4/4/4	-
2	9CS	E	301	-	-	2/12/72/72	0/3/3/3
2	9CS	B	301	-	-	3/12/72/72	0/3/3/3
2	9CS	F	301	-	-	4/12/72/72	0/3/3/3
2	9CS	A	301	-	-	2/12/72/72	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	9CS	C1-C2	-2.21	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	9CS	O5-C5-C6	2.59	111.05	106.07

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	9CS	C4-C5-C6-N1
2	B	301	9CS	O5-C5-C6-N1
2	C	301	9CS	C4-C5-C6-N1
2	C	301	9CS	O5-C5-C6-N1
2	D	301	9CS	C4-C5-C6-N1
2	D	301	9CS	O5-C5-C6-N1
2	E	301	9CS	C4-C5-C6-N1
2	F	301	9CS	C4-C5-C6-N1
2	F	301	9CS	O5-C5-C6-N1
2	F	301	9CS	C16-C17-C18-O15
2	A	301	9CS	O12-C17-C18-O15
2	F	301	9CS	O12-C17-C18-O15
2	A	301	9CS	C16-C17-C18-O15
2	B	301	9CS	C9-C10-O9-C1
2	E	301	9CS	O5-C5-C6-N1
5	D	306	PEG	C4-C3-O2-C2
2	D	301	9CS	C16-C17-C18-O15

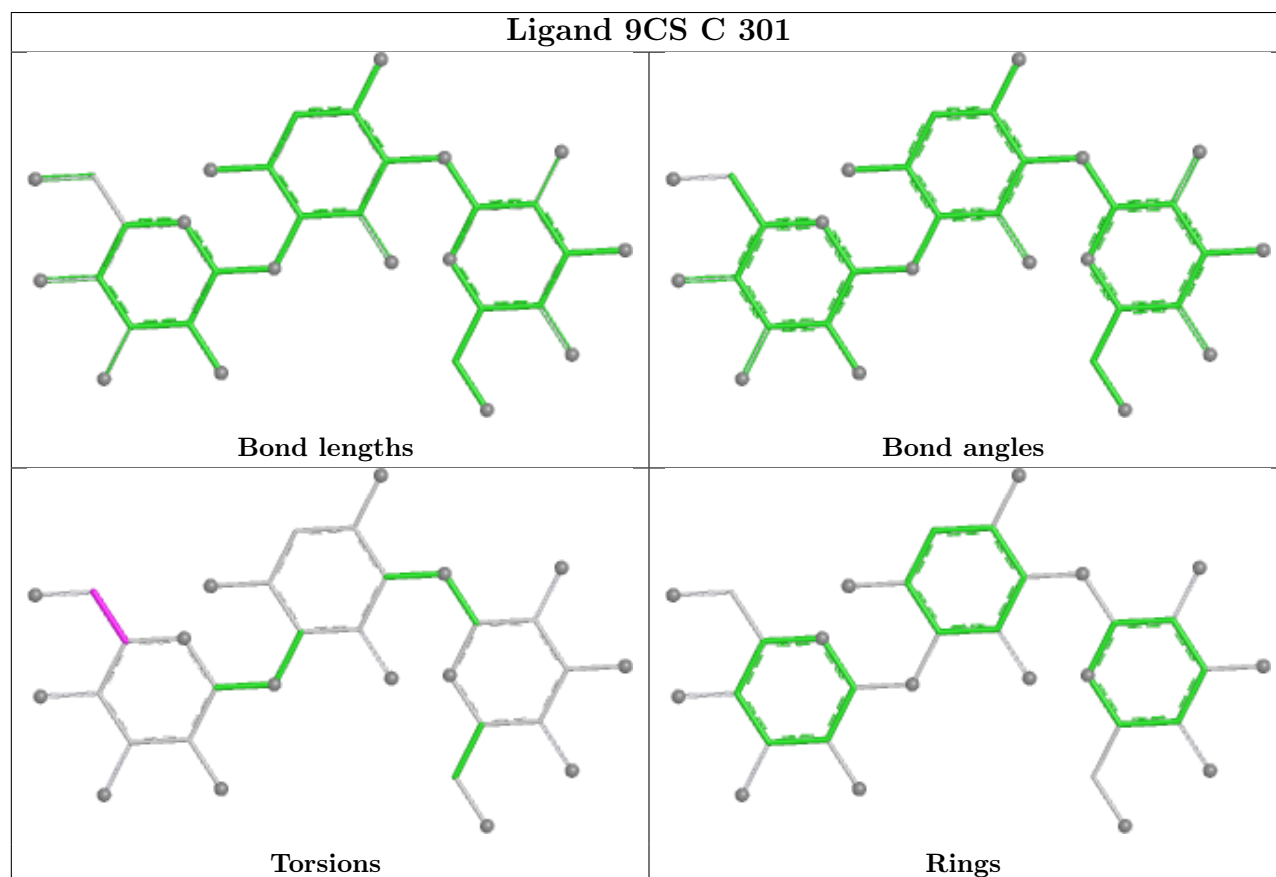
There are no ring outliers.

3 monomers are involved in 5 short contacts:

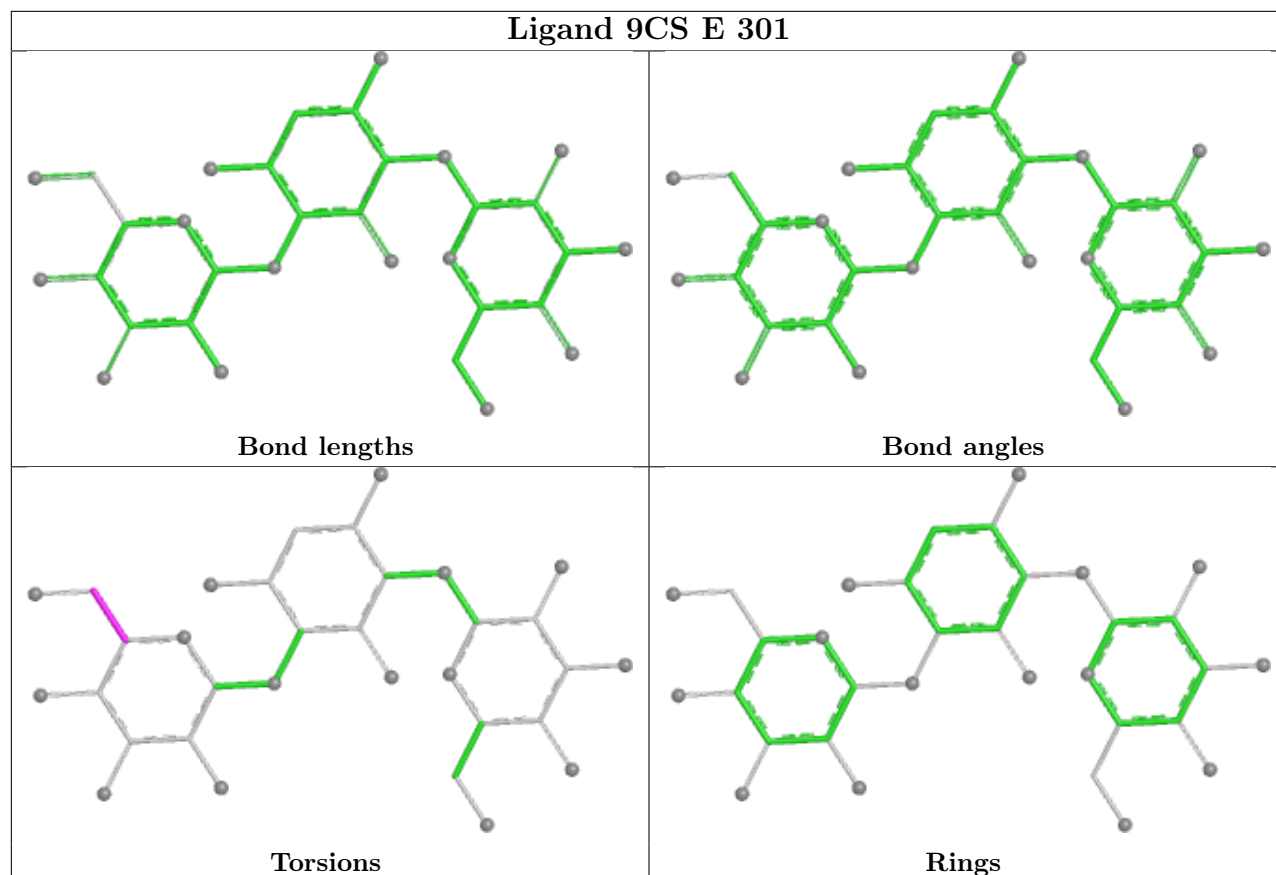
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	306	PEG	1	0
2	B	301	9CS	3	0
2	D	301	9CS	1	0

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

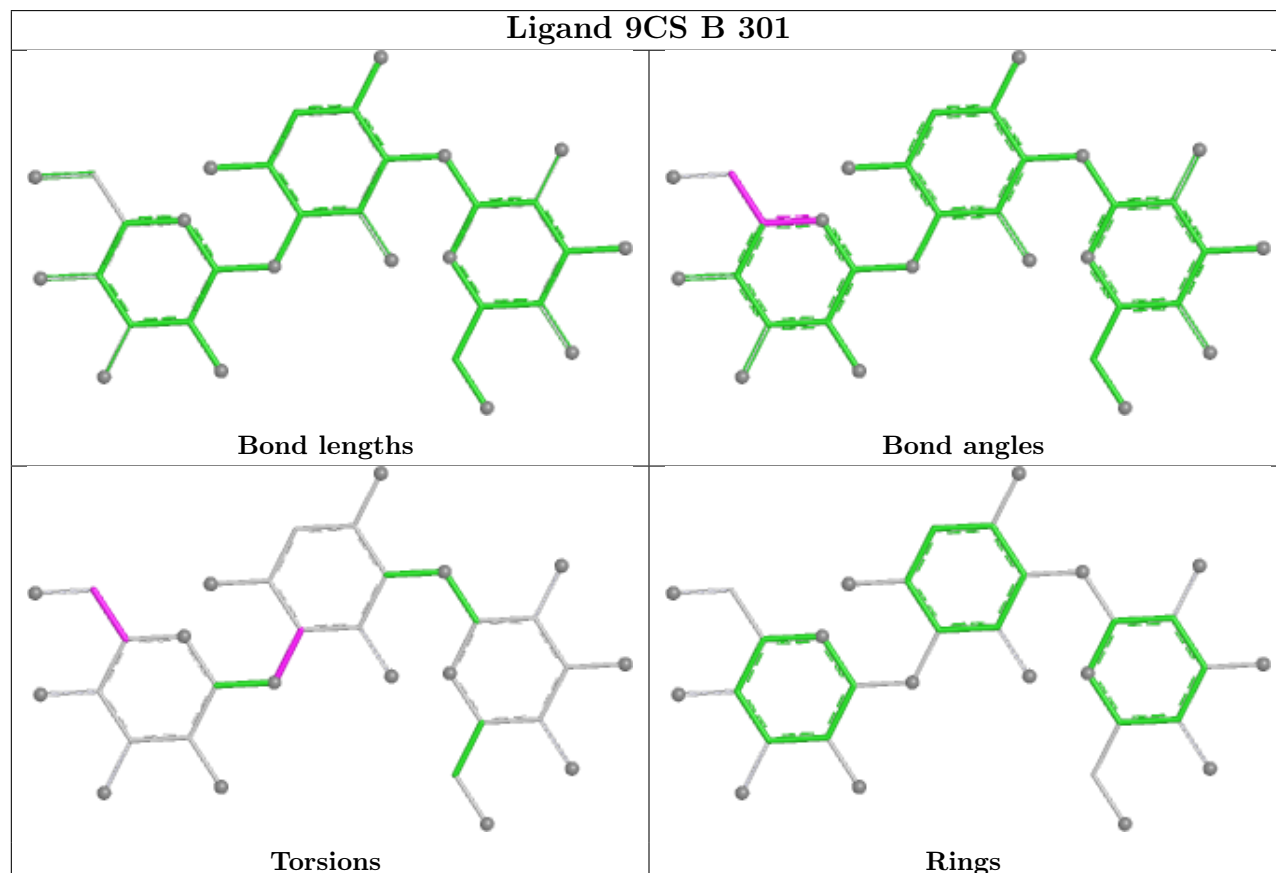
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



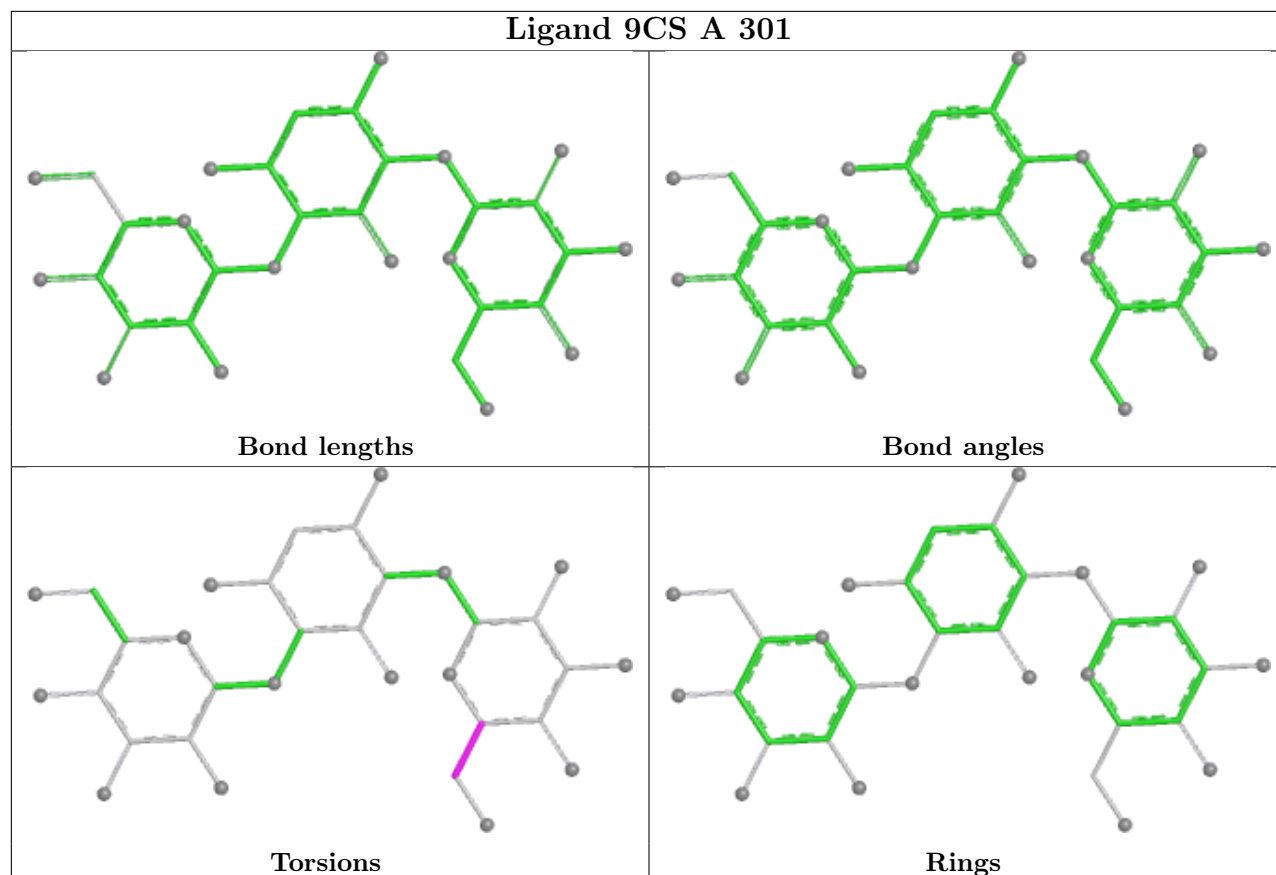
Ligand 9CS E 301



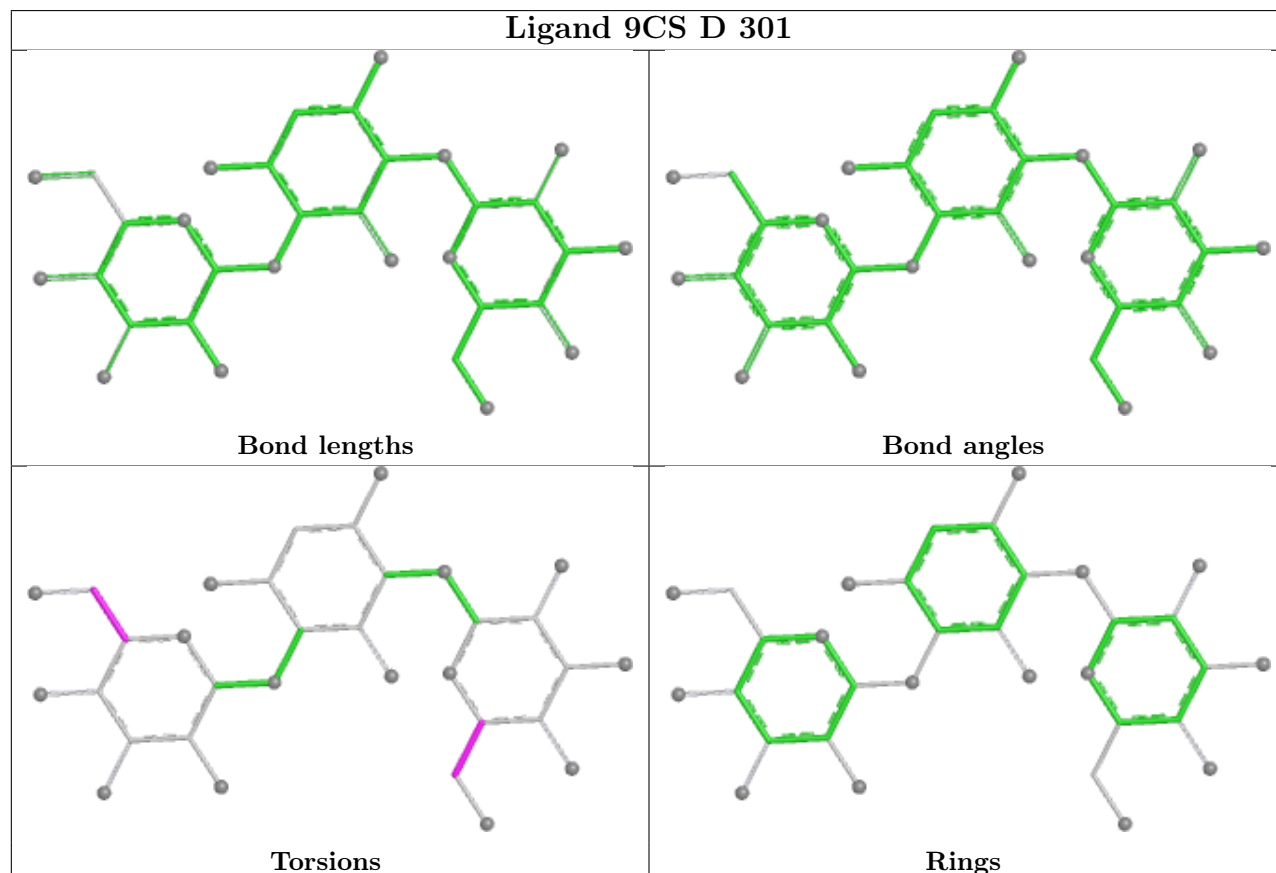
Ligand 9CS B 301

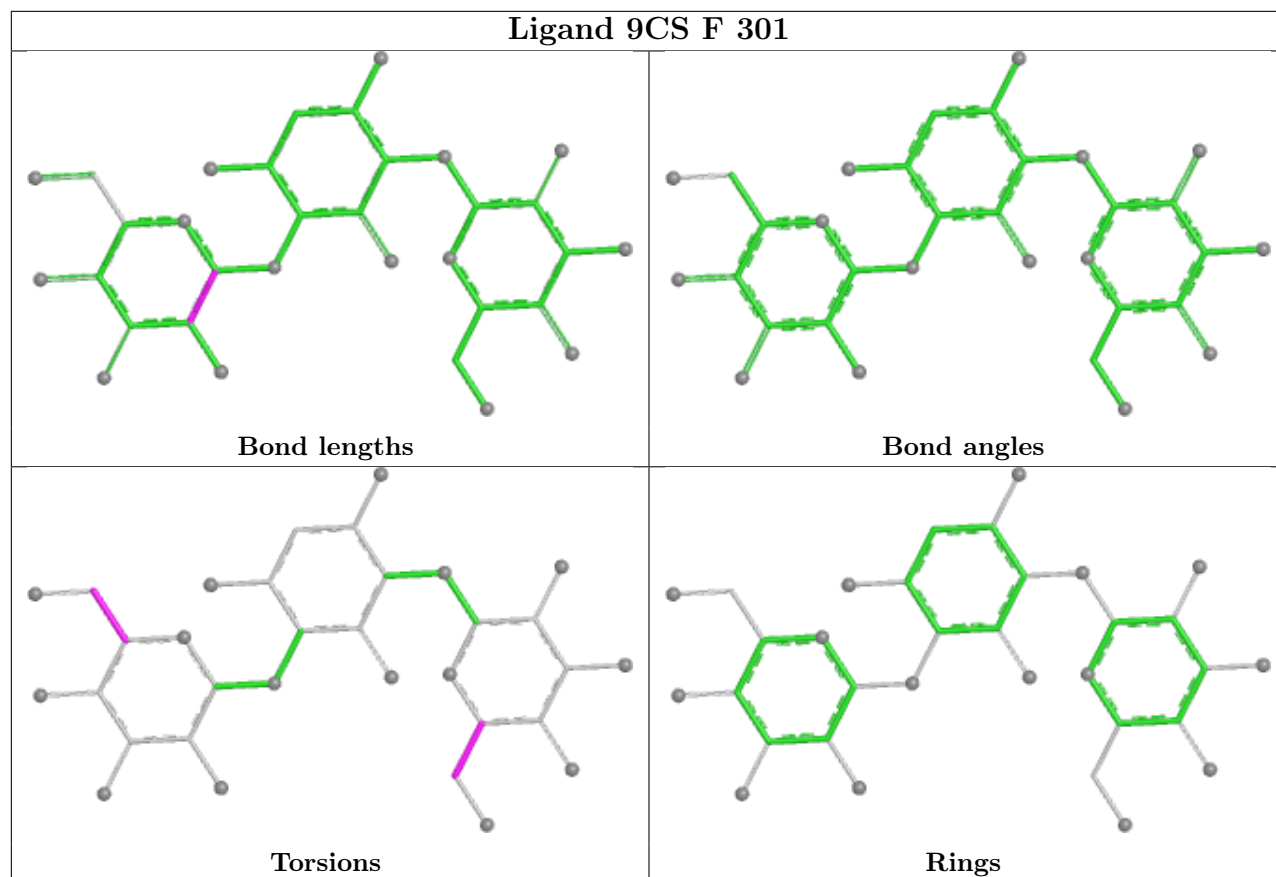


Ligand 9CS A 301



Ligand 9CS D 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	275/288 (95%)	0.64	14 (5%)	33 39	25, 62, 98, 112	2 (0%)
1	B	282/288 (97%)	0.31	11 (3%)	43 49	31, 46, 77, 106	1 (0%)
1	C	277/288 (96%)	0.62	17 (6%)	27 31	27, 62, 106, 141	1 (0%)
1	D	279/288 (96%)	0.35	13 (4%)	36 42	36, 50, 79, 118	0
1	E	274/288 (95%)	1.37	48 (17%)	4 4	30, 78, 117, 145	1 (0%)
1	F	283/288 (98%)	0.69	19 (6%)	24 27	36, 63, 103, 124	1 (0%)
All	All	1670/1728 (96%)	0.66	122 (7%)	21 24	25, 59, 103, 145	6 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	282	PHE	5.8
1	E	189	ALA	4.6
1	F	281	PRO	4.4
1	F	284	VAL	4.4
1	F	271	GLY	3.9
1	E	207	VAL	3.8
1	E	179	CYS	3.7
1	E	276	LEU	3.7
1	B	276	LEU	3.6
1	D	187	LEU	3.6
1	B	259	GLY	3.5
1	F	196	ALA	3.5
1	F	1	MET	3.5
1	B	2	ALA	3.5
1	C	252	THR	3.5
1	C	276	LEU	3.4
1	D	277	THR	3.4
1	E	187	LEU	3.3
1	E	197	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	283	ALA	3.3
1	E	69	ASP	3.3
1	B	179	CYS	3.3
1	A	277	THR	3.3
1	D	276	LEU	3.3
1	F	285	ARG	3.2
1	B	281	PRO	3.2
1	D	15	THR	3.2
1	F	280	HIS	3.1
1	E	196	ALA	3.1
1	C	12	LEU	3.1
1	A	187	LEU	3.0
1	A	3	LEU	3.0
1	E	3	LEU	2.9
1	F	276	LEU	2.9
1	E	264	THR	2.9
1	B	283	ALA	2.8
1	F	277	THR	2.8
1	C	277	THR	2.8
1	E	15	THR	2.7
1	D	17	ASP	2.7
1	D	-1	ASN	2.7
1	E	240	GLU	2.7
1	B	69	ASP	2.7
1	E	13	ALA	2.6
1	C	68	GLN	2.6
1	A	15	THR	2.6
1	E	8	GLY	2.6
1	E	188	PRO	2.6
1	D	196	ALA	2.6
1	F	270	ALA	2.6
1	E	272	ASP	2.6
1	B	240	GLU	2.5
1	E	259	GLY	2.5
1	C	269	VAL	2.5
1	E	274	ASP	2.5
1	E	20	THR	2.5
1	E	239	THR	2.5
1	E	255	SER	2.5
1	E	273	VAL	2.5
1	E	180	TYR	2.5
1	C	21	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.5
1	E	198	ALA	2.5
1	A	13	ALA	2.4
1	A	227	ALA	2.4
1	E	24	ALA	2.4
1	E	140	PRO	2.4
1	E	23	PRO	2.4
1	E	55	THR	2.4
1	C	48	ARG	2.4
1	F	67	GLN	2.4
1	A	69	ASP	2.4
1	D	72	THR	2.4
1	C	273	VAL	2.4
1	E	107	VAL	2.4
1	E	193	ARG	2.4
1	A	68	GLN	2.4
1	C	111	ASP	2.3
1	E	271	GLY	2.3
1	E	12	LEU	2.3
1	E	178	GLU	2.3
1	A	270	ALA	2.3
1	C	275	HIS	2.3
1	E	9	GLU	2.3
1	E	163	GLY	2.3
1	E	215	GLY	2.3
1	E	5	ALA	2.3
1	D	18	ASP	2.3
1	E	65	LEU	2.2
1	D	16	PRO	2.2
1	E	89	LEU	2.2
1	E	14	LEU	2.2
1	D	19	LYS	2.2
1	F	197	VAL	2.2
1	E	169	PRO	2.2
1	F	68	GLN	2.2
1	A	14	LEU	2.1
1	E	174	LEU	2.1
1	E	191	LEU	2.1
1	F	273	VAL	2.1
1	D	71	PRO	2.1
1	C	271	GLY	2.1
1	E	109	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	2.1
1	C	20	THR	2.1
1	A	197	VAL	2.1
1	E	257	VAL	2.1
1	A	271	GLY	2.1
1	F	178	GLU	2.1
1	E	146	PRO	2.1
1	F	255	SER	2.1
1	B	270	ALA	2.1
1	A	191	LEU	2.1
1	B	67	GLN	2.1
1	B	193	ARG	2.1
1	C	9	GLU	2.0
1	C	270	ALA	2.0
1	E	110	ALA	2.0
1	E	68	GLN	2.0
1	A	240	GLU	2.0
1	F	161	GLU	2.0
1	D	275	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	E	305	5/5	0.45	0.15	144,146,147,148	0
4	SO4	F	305	5/5	0.58	0.20	113,126,129,129	0
4	SO4	B	305	5/5	0.59	0.19	125,130,139,140	0
4	SO4	F	307	5/5	0.61	0.14	124,125,134,135	0

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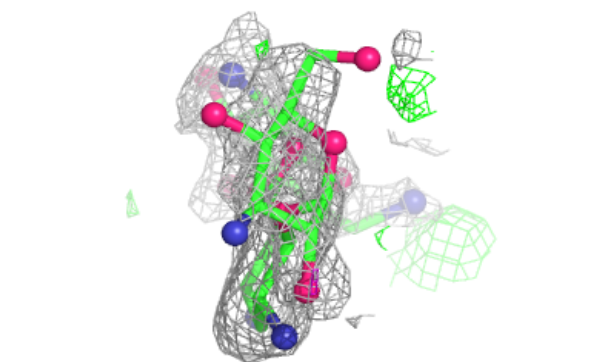
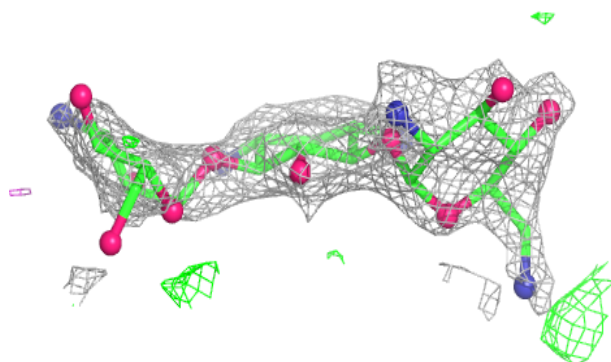
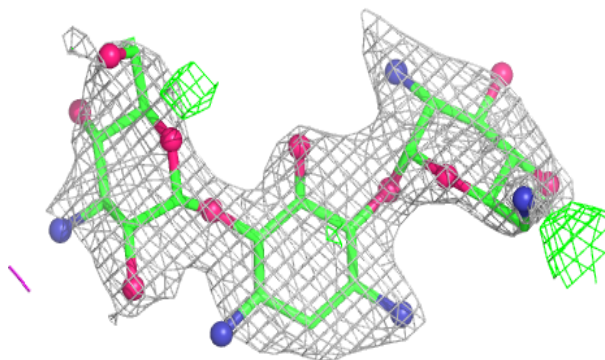
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	304	5/5	0.66	0.14	100,109,113,113	0
4	SO4	F	306	5/5	0.70	0.12	138,141,142,144	0
4	SO4	C	304	5/5	0.75	0.12	92,92,101,102	0
4	SO4	E	304	5/5	0.75	0.11	109,112,115,116	0
4	SO4	D	305	5/5	0.76	0.14	104,105,109,112	0
5	PEG	D	306	7/7	0.76	0.24	78,86,96,96	0
4	SO4	C	305	5/5	0.78	0.18	120,133,133,134	0
4	SO4	B	304	5/5	0.81	0.13	86,91,93,93	0
2	9CS	E	301	33/33	0.83	0.19	57,61,72,73	33
2	9CS	B	301	33/33	0.85	0.21	48,55,68,70	33
4	SO4	F	304	5/5	0.87	0.10	89,89,97,101	0
4	SO4	A	304	5/5	0.88	0.09	93,95,100,102	0
4	SO4	E	303	5/5	0.88	0.15	92,93,95,96	0
2	9CS	C	301	33/33	0.88	0.16	61,65,69,72	33
2	9CS	A	301	33/33	0.89	0.19	51,60,65,68	33
2	9CS	D	301	33/33	0.89	0.15	60,68,79,80	7
4	SO4	F	303	5/5	0.92	0.15	71,77,82,84	0
2	9CS	F	301	33/33	0.92	0.12	37,42,46,48	33
4	SO4	D	303	5/5	0.95	0.17	64,70,74,75	0
4	SO4	A	303	5/5	0.95	0.13	65,69,74,76	0
4	SO4	C	303	5/5	0.95	0.14	56,61,69,69	0
4	SO4	B	303	5/5	0.96	0.13	56,59,66,69	0
3	NI	A	302	1/1	0.99	0.04	44,44,44,44	0
3	NI	D	302	1/1	0.99	0.03	38,38,38,38	0
3	NI	E	302	1/1	0.99	0.05	51,51,51,51	0
3	NI	F	302	1/1	0.99	0.03	41,41,41,41	0
3	NI	C	302	1/1	1.00	0.02	40,40,40,40	0
3	NI	B	302	1/1	1.00	0.02	30,30,30,30	1

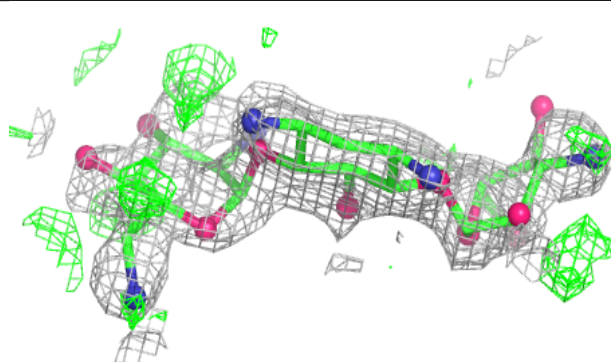
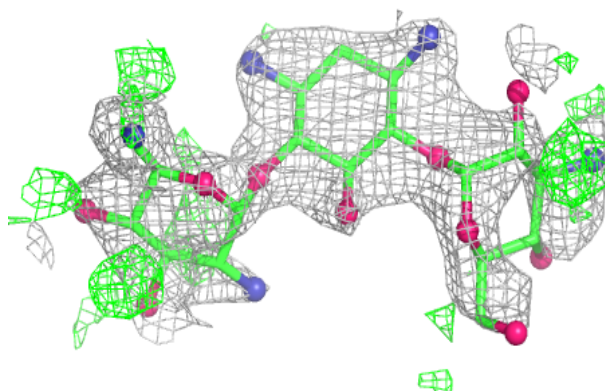
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9CS E 301:

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

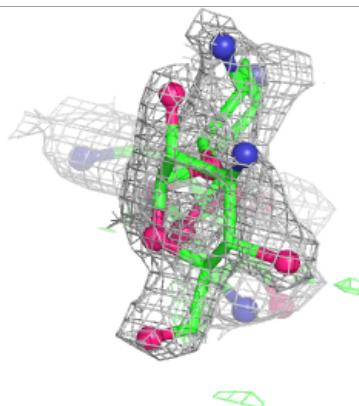
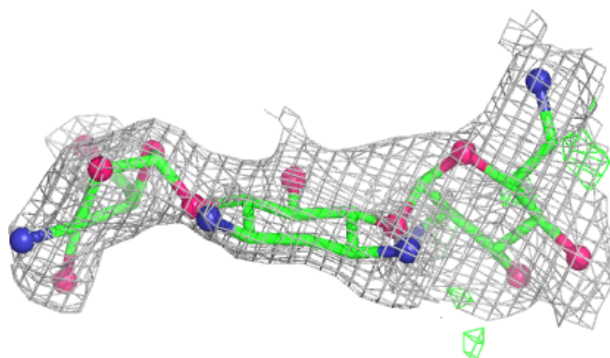
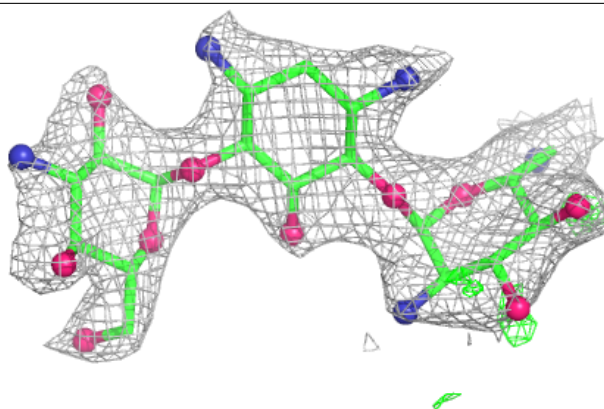
**Electron density around 9CS B 301:**

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

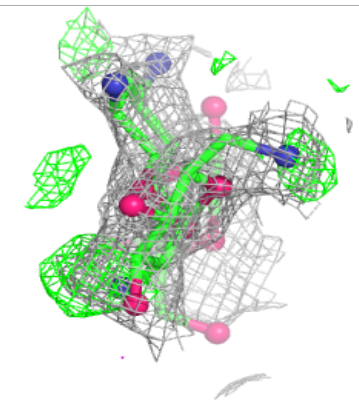
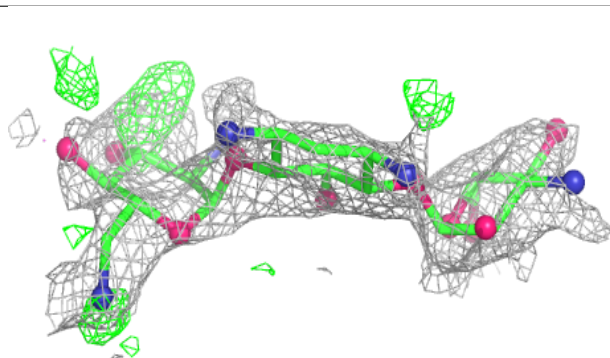
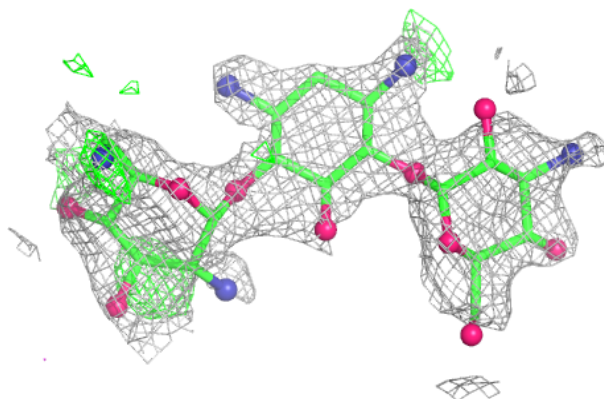


Electron density around 9CS C 301:

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

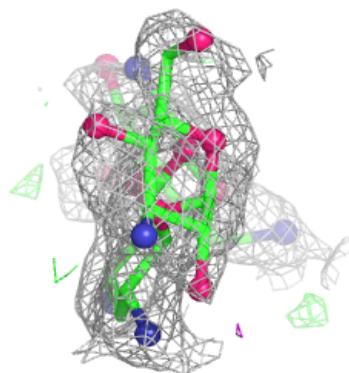
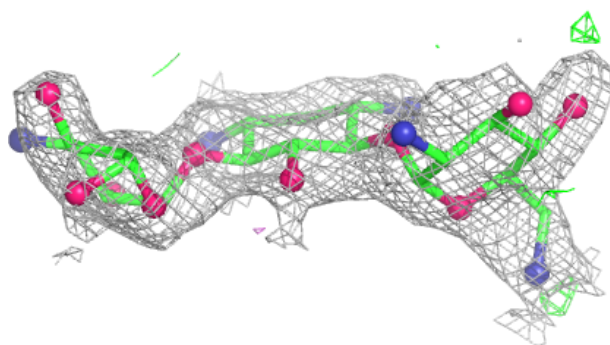
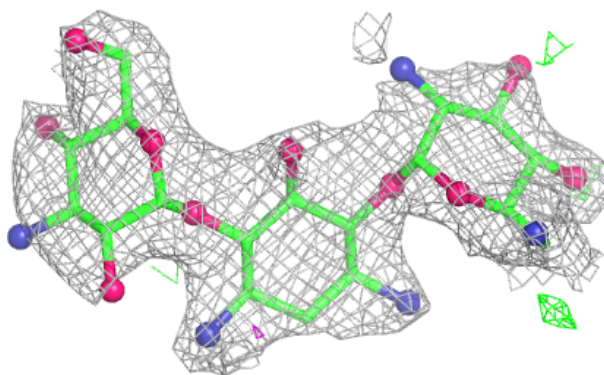
**Electron density around 9CS A 301:**

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

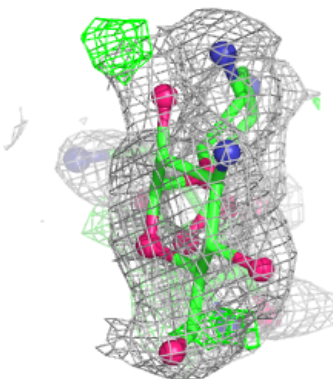
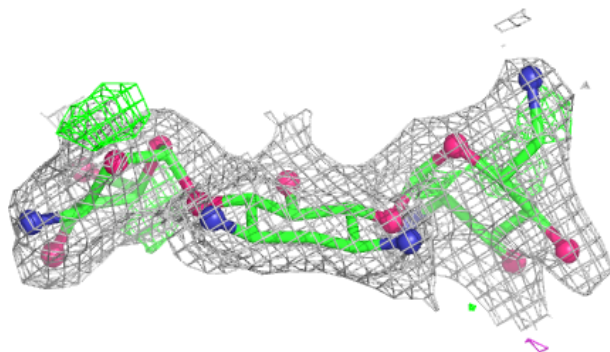
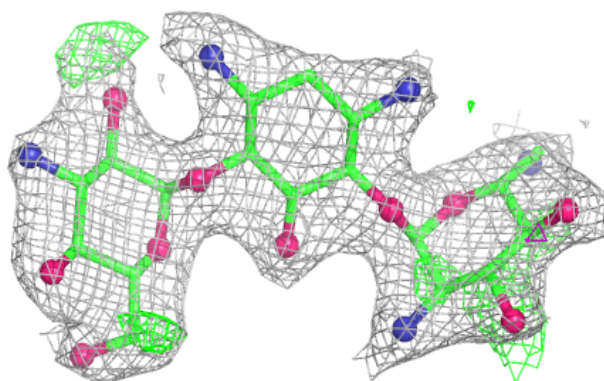


Electron density around 9CS D 301:

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

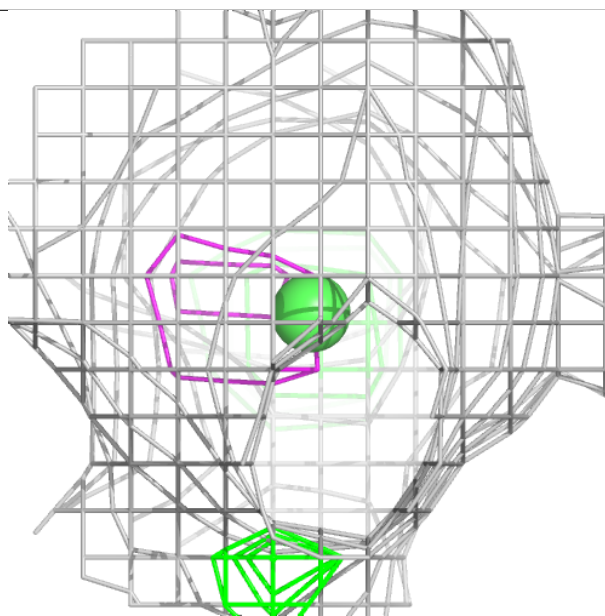
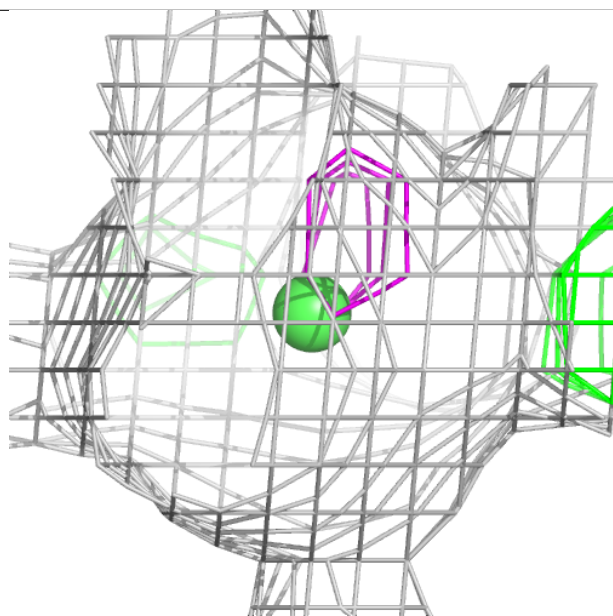
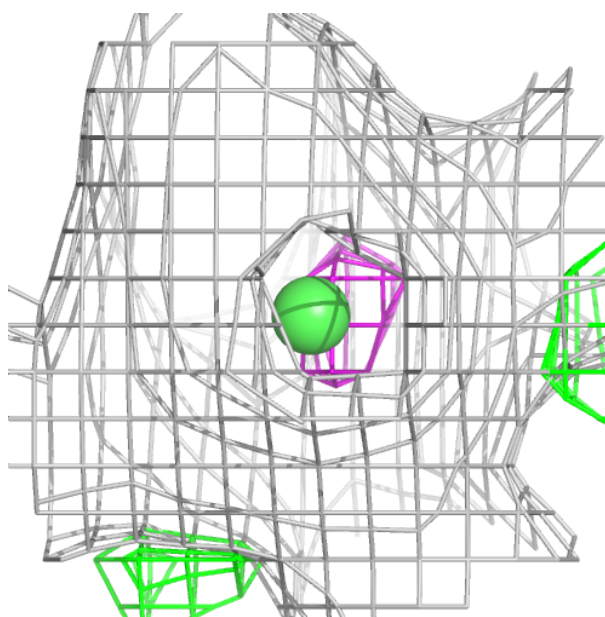
**Electron density around 9CS F 301:**

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



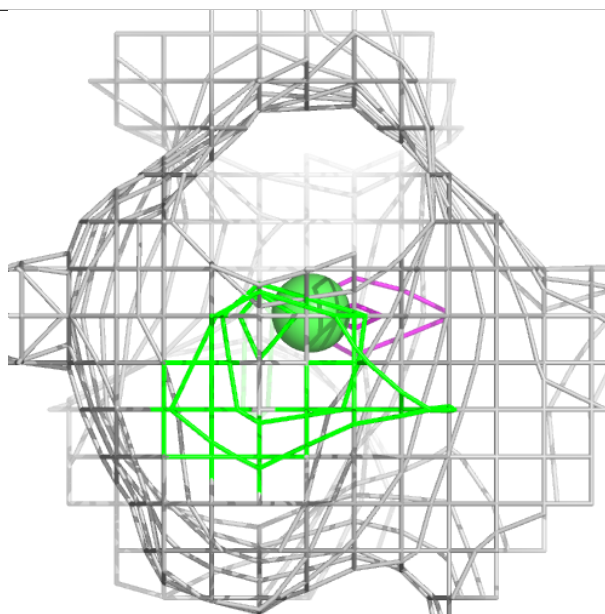
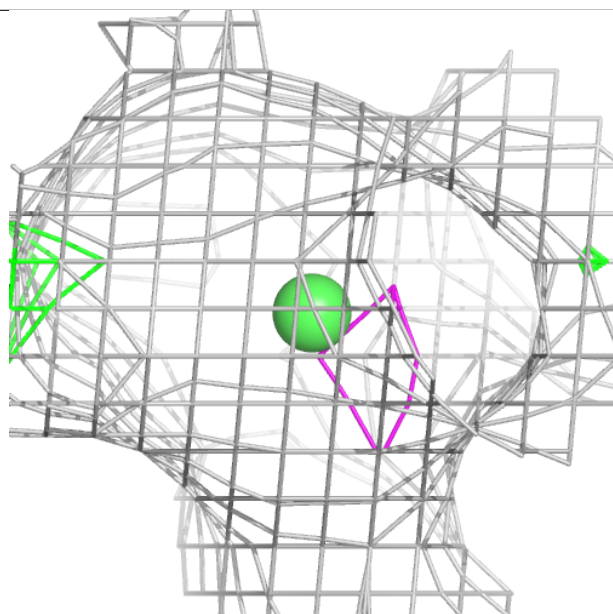
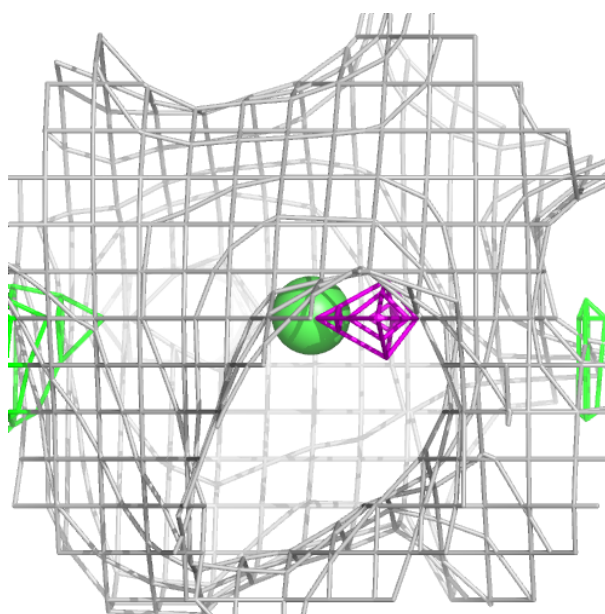
Electron density around NI A 302:

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



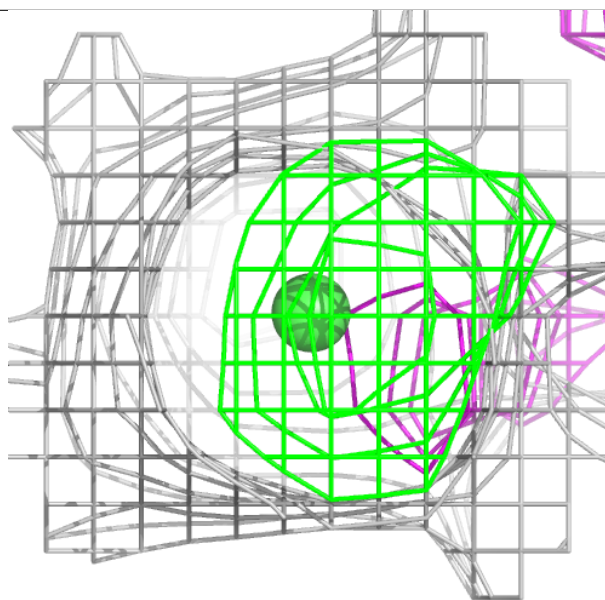
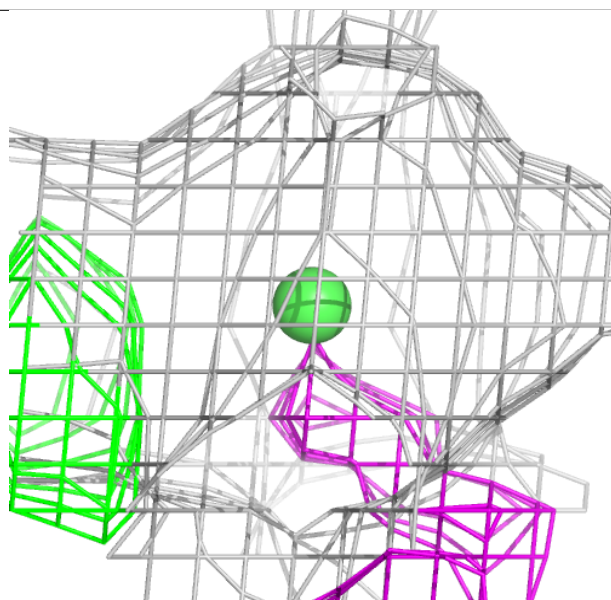
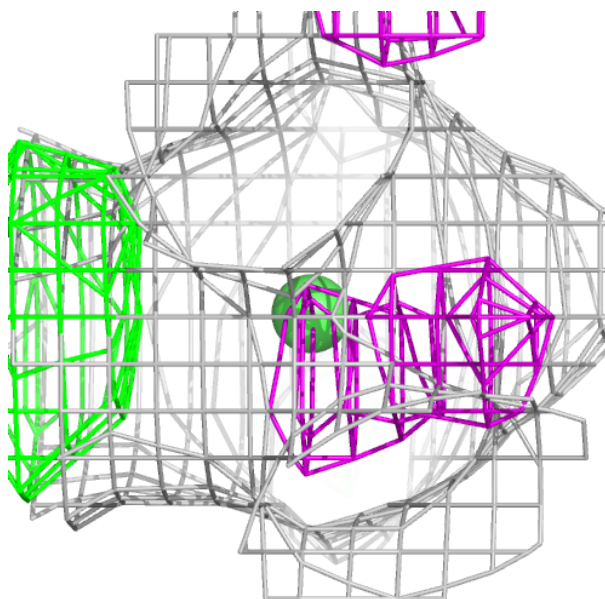
Electron density around NI D 302:

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



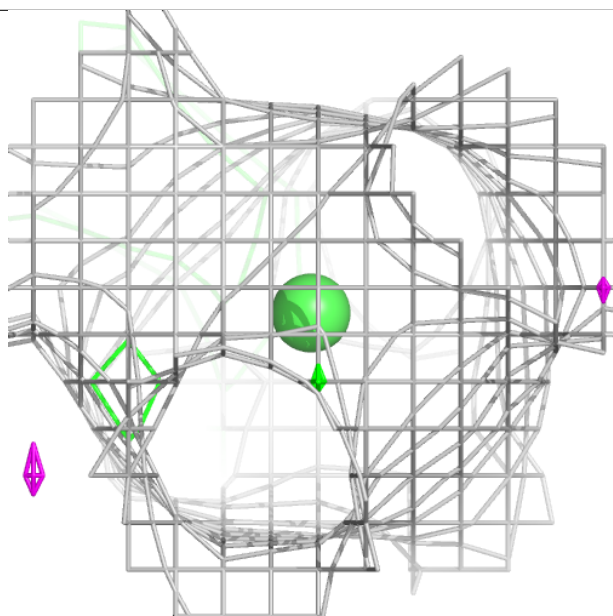
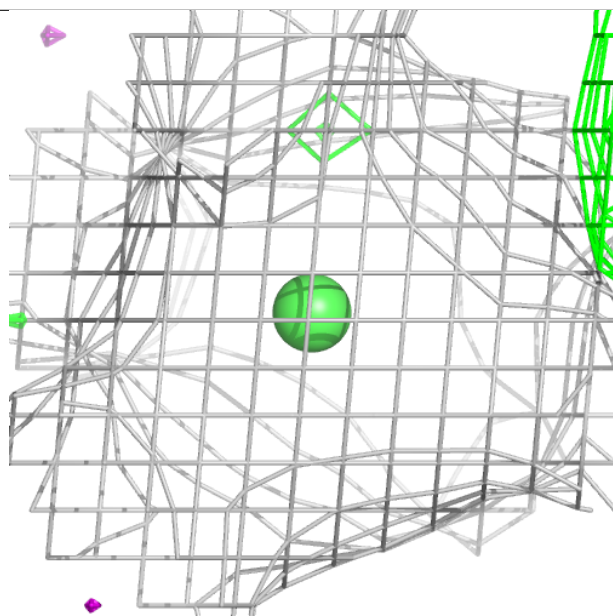
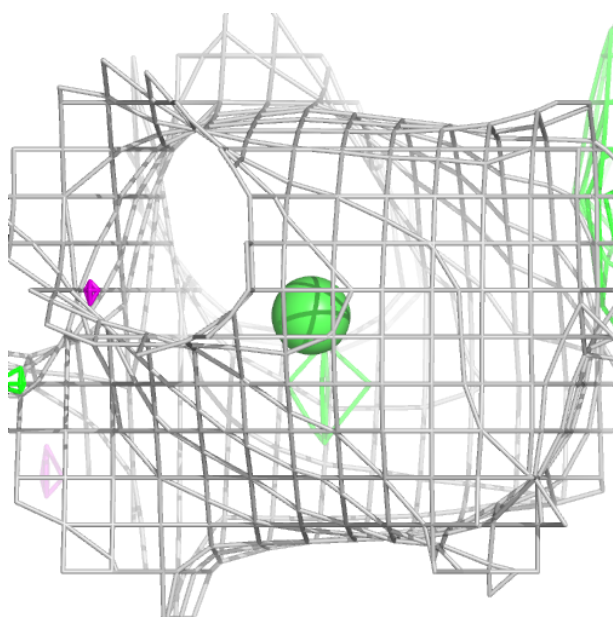
Electron density around NI E 302:

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



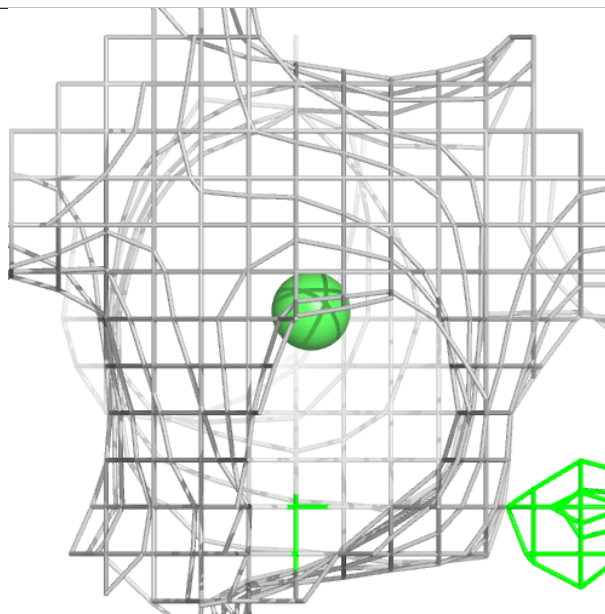
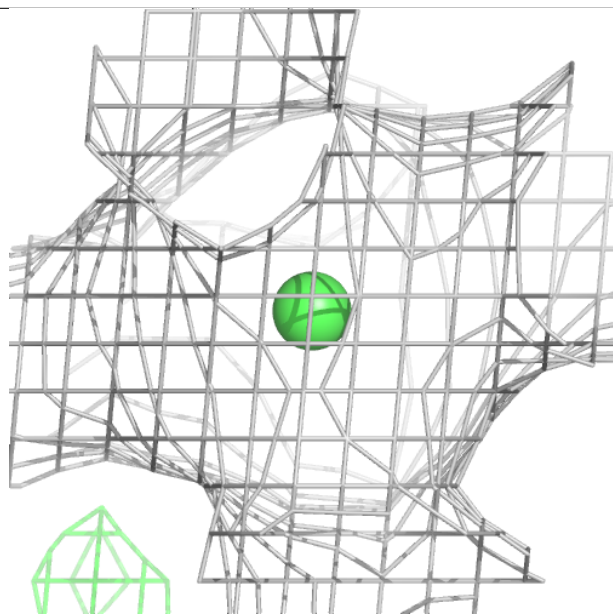
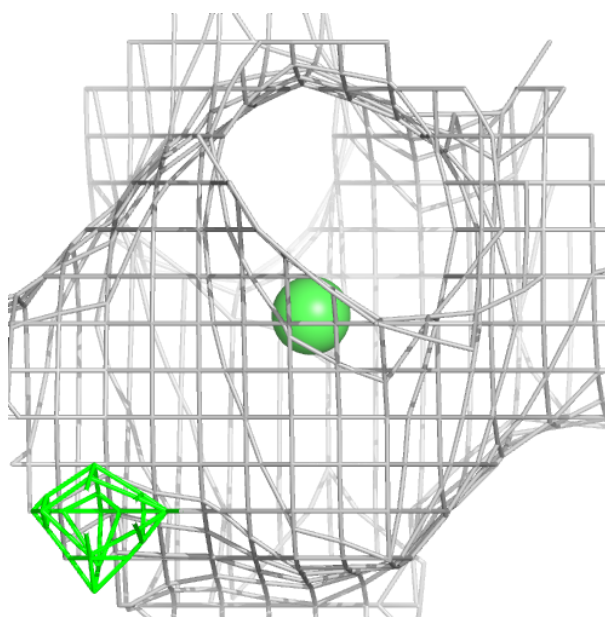
Electron density around NI F 302:

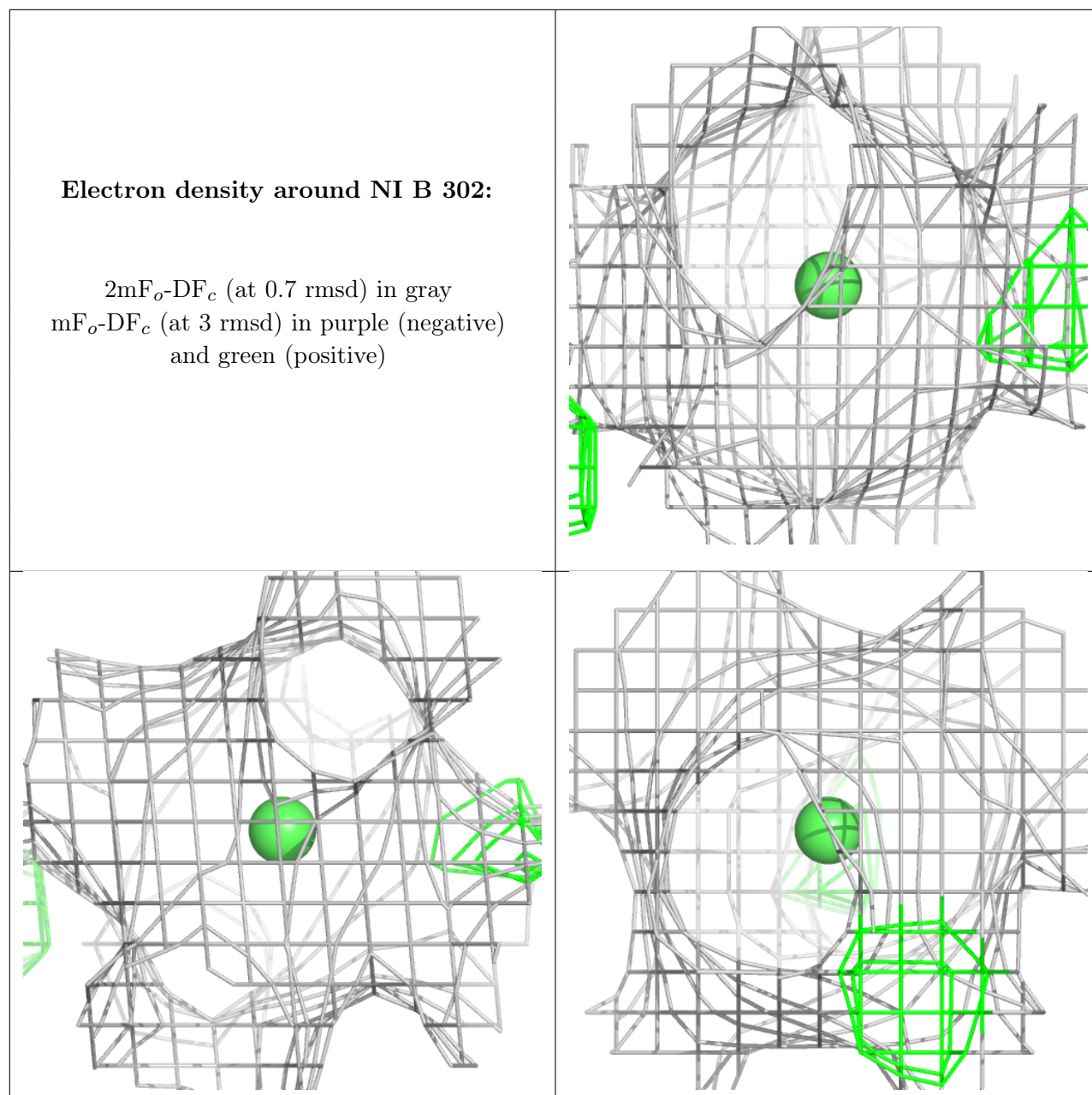
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI C 302:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.