



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:50 AM UTC

PDB ID : 7ALA / pdb_00007ala
Title : human GCH-GFRP inhibitory complex
Authors : Ebenhoch, R.; Nar, H.
Deposited on : 2020-10-06
Resolution : 1.85 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

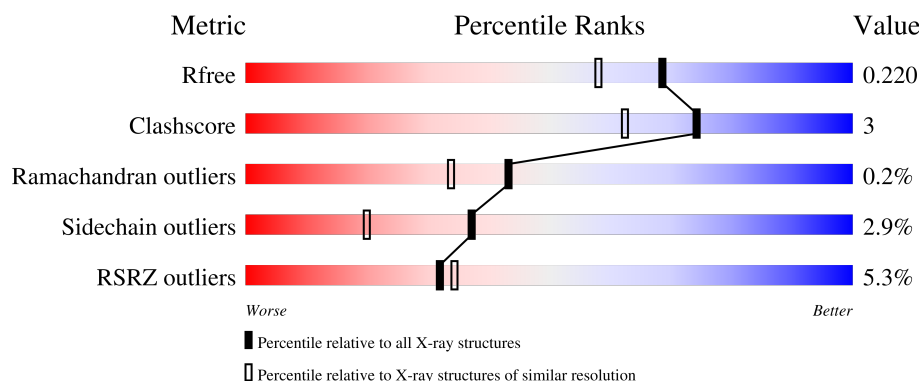
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	209	2% 79% 8% 13%
1	B	209	9% 73% 7% 20%
1	C	209	7% 81% 8% 10%
1	D	209	6% 78% 8% 14%
1	E	209	6% 75% 10% 14%

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Mol	Chain	Length	Quality of chain
2	F	87	% 93% 7%
2	G	87	% 86% 10% .
2	H	87	% 89% 8% .
2	I	87	% 90% 9% .
2	J	87	3% 85% 11% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11408 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 GTP cyclohydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	1	0
			1445	913	250	274	8			
1	B	167	Total	C	N	O	S	0	1	0
			1318	839	233	236	10			
1	C	188	Total	C	N	O	S	0	0	0
			1484	938	257	278	11			
1	D	180	Total	C	N	O	S	0	2	0
			1437	912	252	264	9			
1	E	179	Total	C	N	O	S	0	0	0
			1408	891	248	259	10			

- Molecule 2 is a protein called GTP cyclohydrolase 1 feedback regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	87	Total	C	N	O	S	0	0	0
			698	440	124	128	6			
2	G	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	H	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	I	86	Total	C	N	O	S	0	0	0
			689	435	123	125	6			
2	J	86	Total	C	N	O	S	0	0	0
			694	438	123	127	6			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P30047
F	-1	SER	-	expression tag	UNP P30047
F	0	HIS	-	expression tag	UNP P30047
G	-2	GLY	-	expression tag	UNP P30047
G	-1	SER	-	expression tag	UNP P30047

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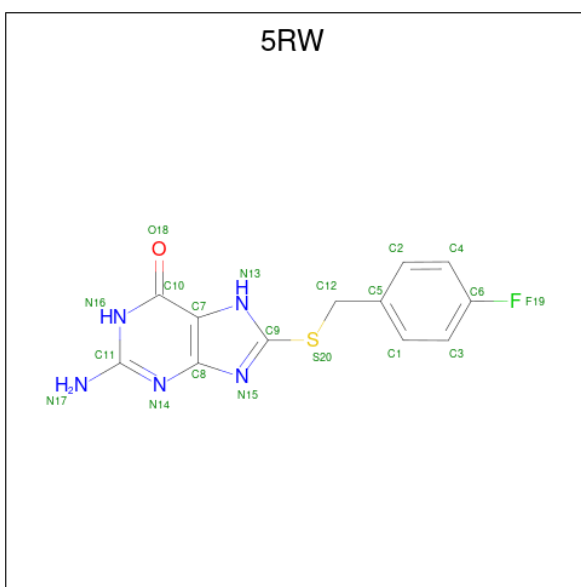
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP P30047
H	-2	GLY	-	expression tag	UNP P30047
H	-1	SER	-	expression tag	UNP P30047
H	0	HIS	-	expression tag	UNP P30047
I	-2	GLY	-	expression tag	UNP P30047
I	-1	SER	-	expression tag	UNP P30047
I	0	HIS	-	expression tag	UNP P30047
J	-2	GLY	-	expression tag	UNP P30047
J	-1	SER	-	expression tag	UNP P30047
J	0	HIS	-	expression tag	UNP P30047

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0

- Molecule 4 is 2-azanyl-8-[(4-fluorophenyl)methylsulfanyl]-1,7-dihydropurin-6-one (CCD ID: 5RW) (formula: C₁₂H₁₀FN₅OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			20	12	1	5	1	1		
4	B	1	Total	C	F	N	O	S	0	0
			20	12	1	5	1	1		
4	C	1	Total	C	F	N	O	S	0	0
			20	12	1	5	1	1		
4	D	1	Total	C	F	N	O	S	0	0
			20	12	1	5	1	1		
4	E	1	Total	C	F	N	O	S	0	0
			20	12	1	5	1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Na	0	0
			1	1		
5	G	1	Total	Na	0	0
			1	1		
5	H	1	Total	Na	0	0
			1	1		
5	I	1	Total	Na	0	0
			1	1		
5	J	1	Total	Na	0	0
			1	1		

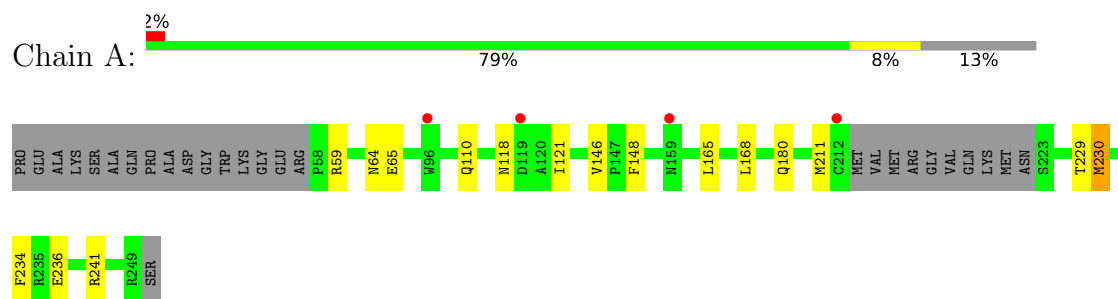
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total 76	O 76	0	0
6	B	61	Total 61	O 61	0	0
6	C	82	Total 82	O 82	0	0
6	D	98	Total 98	O 98	0	0
6	E	85	Total 85	O 85	0	0
6	F	81	Total 81	O 81	0	0
6	G	82	Total 82	O 82	0	0
6	H	64	Total 64	O 64	0	0
6	I	62	Total 62	O 62	0	0
6	J	78	Total 78	O 78	0	0

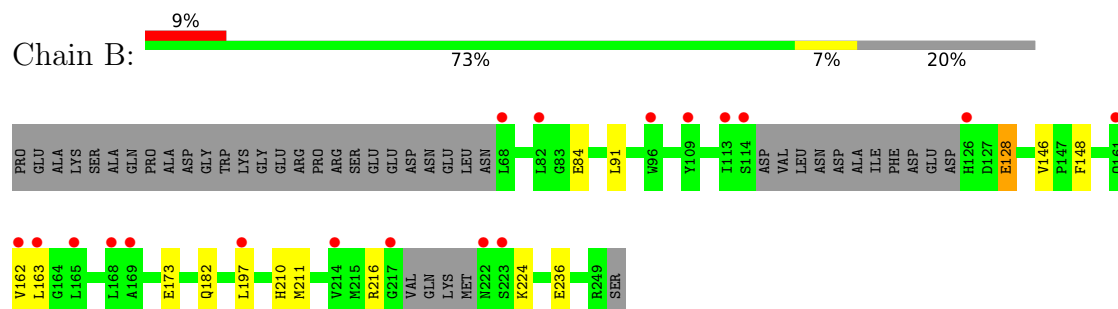
3 Residue-property plots [i](#)

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

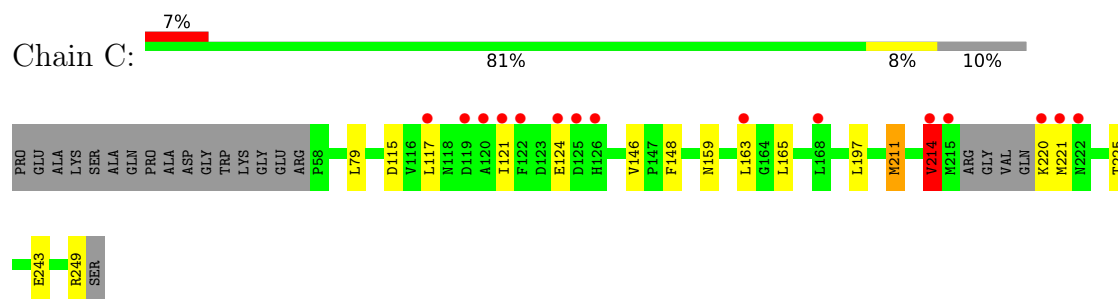
• Molecule 1: GTP cyclohydrolase 1



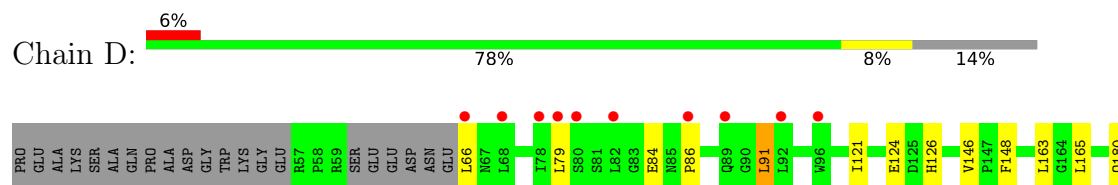
• Molecule 1: GTP cyclohydrolase 1

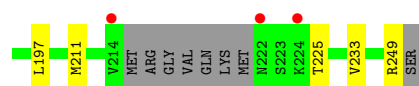


• Molecule 1: GTP cyclohydrolase 1

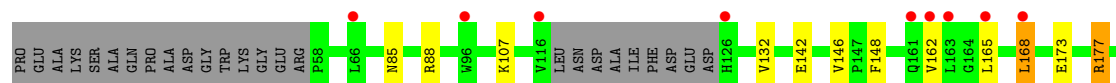
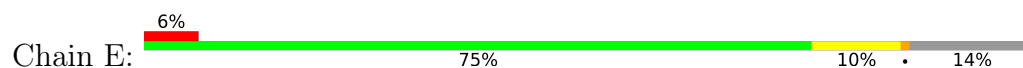


• Molecule 1: GTP cyclohydrolase 1

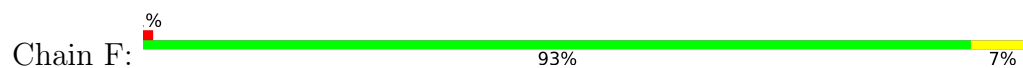




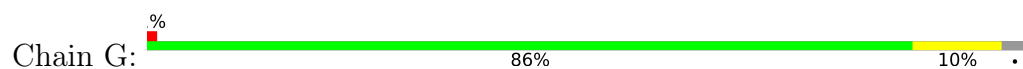
- Molecule 1: GTP cyclohydrolase 1



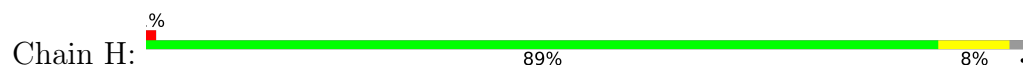
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



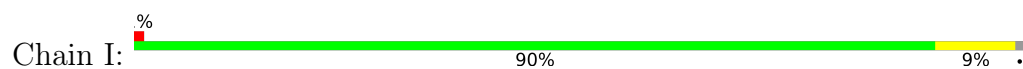
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



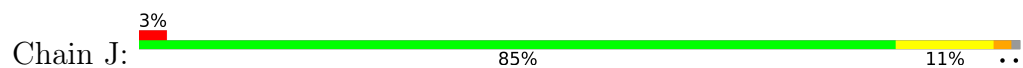
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

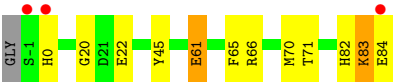


- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.75Å 114.01Å 113.83Å 90.00° 130.34° 90.00°	Depositor
Resolution (Å)	39.74 – 1.85 39.74 – 1.85	Depositor EDS
% Data completeness (in resolution range)	50.1 (39.74-1.85) 50.1 (39.74-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.185 , 0.220 0.189 , 0.220	Depositor DCC
R_{free} test set	2766 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11408	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: 5RW, ZN, NA

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	0.73	1/1469 (0.1%)	1.02	3/1985 (0.2%)
1	B	0.68	0/1339	1.04	2/1805 (0.1%)
1	C	0.75	0/1508	1.05	4/2035 (0.2%)
1	D	0.73	0/1460	1.02	2/1972 (0.1%)
1	E	0.73	0/1430	1.06	2/1928 (0.1%)
2	F	0.71	0/713	0.98	1/962 (0.1%)
2	G	0.74	0/692	0.96	1/934 (0.1%)
2	H	0.70	0/692	0.95	1/934 (0.1%)
2	I	0.73	1/704 (0.1%)	1.01	2/950 (0.2%)
2	J	0.72	0/709	0.97	1/957 (0.1%)
All	All	0.72	2/10716 (0.0%)	1.02	19/14462 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	MET	SD-CE	-7.42	1.61	1.79
2	I	10	ILE	CA-C	5.16	1.58	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	VAL	CA-C-N	6.87	134.06	121.70
1	C	214	VAL	C-N-CA	6.87	134.06	121.70
1	E	148	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	148	PHE	CA-CB-CG	6.40	120.20	113.80
1	D	148	PHE	CA-CB-CG	6.03	119.83	113.80
1	B	148	PHE	CA-CB-CG	5.94	119.74	113.80
1	B	236	GLU	N-CA-C	5.71	117.59	111.36
1	C	148	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	115	ASP	CA-CB-CG	5.58	118.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	20	GLY	N-CA-C	5.32	118.48	110.18
1	D	180	GLN	N-CA-C	5.31	117.48	109.41
2	J	20	GLY	N-CA-C	5.29	118.44	110.18
2	I	20	GLY	N-CA-C	5.15	118.22	110.18
2	I	10	ILE	CB-CA-C	5.14	119.07	111.26
2	F	20	GLY	N-CA-C	5.13	117.97	110.38
1	E	236	GLU	N-CA-C	5.12	117.99	111.69
1	A	180	GLN	N-CA-C	5.09	116.73	109.14
2	H	20	GLY	N-CA-C	5.07	118.08	110.18
1	A	236	GLU	N-CA-C	5.05	117.90	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1445	0	1455	7	0
1	B	1318	0	1362	7	0
1	C	1484	0	1505	7	0
1	D	1437	0	1465	11	0
1	E	1408	0	1441	9	0
2	F	698	0	694	7	0
2	G	678	0	679	5	0
2	H	678	0	679	4	0
2	I	689	0	689	8	0
2	J	694	0	691	10	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
4	A	20	0	0	0	0
4	B	20	0	0	0	0
4	C	20	0	0	1	0
4	D	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	20	0	0	1	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	A	76	0	0	1	0
6	B	61	0	0	0	0
6	C	82	0	0	0	0
6	D	98	0	0	1	0
6	E	85	0	0	0	0
6	F	81	0	0	0	0
6	G	82	0	0	0	0
6	H	64	0	0	1	0
6	I	62	0	0	0	0
6	J	78	0	0	1	0
All	All	11408	0	10660	66	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 3.

All (66) 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:A:230:MET:HE2	1:A:241:ARG:HG3	1.38	1.05
1:A:230:MET:HE3	1:A:234:PHE:HB3	1.58	0.84
2:G:22:GLU:HG2	2:G:45:TYR:HB2	1.69	0.74
2:I:22:GLU:HG2	2:I:45:TYR:HB2	1.70	0.73
2:F:22:GLU:HG2	2:F:45:TYR:HB2	1.71	0.72
2:H:22:GLU:HG2	2:H:45:TYR:HB2	1.71	0.71
2:F:66:ARG:HH22	2:F:82:HIS:CD2	2.08	0.71
2:J:22:GLU:HG2	2:J:45:TYR:HB2	1.72	0.70
1:C:146:VAL:HG12	1:C:211:MET:HB2	1.75	0.69
2:I:66:ARG:NH2	2:I:82:HIS:HD2	1.91	0.69
1:A:59:ARG:HD3	1:A:64:ASN:OD1	1.95	0.66
1:E:146:VAL:HG21	1:E:212:CYS:HB3	1.77	0.64
2:I:66:ARG:HH22	2:I:82:HIS:HD2	1.45	0.63
1:B:146:VAL:HG12	1:B:211:MET:HB2	1.80	0.63
1:E:107:LYS:HE3	1:E:177:ARG:HD3	1.79	0.63
2:J:82:HIS:HD2	2:J:84:GLU:HG3	1.61	0.62
1:D:163:LEU:HB2	1:D:197:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:VAL:HG12	1:D:211:MET:HB2	1.81	0.61
2:H:27:GLU:OE1	2:H:63:ARG:NH2	2.32	0.59
2:F:66:ARG:NH2	2:F:82:HIS:CD2	2.70	0.59
1:D:84:GLU:HG3	1:D:91:LEU:CD2	2.32	0.58
1:A:146:VAL:HG12	1:A:211:MET:HB2	1.84	0.58
1:B:84:GLU:HG3	1:B:91:LEU:CD1	2.35	0.57
1:C:146:VAL:CG1	1:C:211:MET:HB2	2.34	0.57
2:I:66:ARG:HH22	2:I:82:HIS:CD2	2.24	0.56
1:E:146:VAL:CG2	1:E:212:CYS:HB3	2.35	0.56
1:E:142:GLU:OE2	1:E:184:ARG:NH2	2.36	0.55
2:I:66:ARG:NH2	2:I:82:HIS:CD2	2.74	0.55
1:D:233:VAL:HG21	6:D:414:HOH:O	2.07	0.55
2:J:82:HIS:HD2	2:J:84:GLU:CG	2.21	0.53
1:C:163:LEU:HB2	1:C:197:LEU:HD11	1.91	0.53
1:B:146:VAL:CG1	1:B:211:MET:HB2	2.39	0.52
1:A:59:ARG:O	1:A:110:GLN:HB2	2.08	0.51
1:B:84:GLU:CG	1:B:91:LEU:HD11	2.39	0.51
1:C:225:THR:HG21	1:D:165:LEU:CD1	2.41	0.51
2:J:61:GLU:HG3	6:J:230:HOH:O	2.12	0.50
1:D:84:GLU:HG3	1:D:91:LEU:HD21	1.92	0.49
2:I:82:HIS:HE1	2:J:61:GLU:OE2	1.95	0.49
2:J:65:PHE:CZ	2:J:83:LYS:HD3	2.48	0.49
1:B:163:LEU:HB2	1:B:197:LEU:HD11	1.94	0.48
2:F:66:ARG:HH12	2:F:82:HIS:HD2	1.62	0.48
1:C:214:VAL:HG22	1:C:221:MET:HA	1.95	0.47
2:F:66:ARG:NH1	2:F:82:HIS:HD2	2.12	0.47
1:A:229:THR:OG1	1:B:128:GLU:HG2	2.14	0.47
2:I:71:THR:HG22	2:J:70:MET:HE3	1.96	0.46
2:J:82:HIS:CD2	2:J:84:GLU:HG3	2.47	0.46
2:G:65:PHE:CZ	2:G:83:LYS:HD3	2.49	0.46
2:F:70:MET:HE3	2:J:71:THR:HG22	1.99	0.45
1:C:225:THR:HG21	1:D:165:LEU:HD11	1.99	0.45
2:G:82:HIS:HD2	2:G:84:GLU:HB3	1.81	0.45
2:G:84:GLU:OE2	2:H:66:ARG:NH2	2.38	0.45
1:D:86:PRO:HA	1:D:91:LEU:HD23	1.99	0.44
1:E:132:VAL:HG21	1:E:168:LEU:HD11	1.98	0.44
1:D:225:THR:HG21	1:E:165:LEU:HD21	1.99	0.44
2:F:66:ARG:NH2	2:F:82:HIS:HD2	2.14	0.43
2:J:66:ARG:HB3	2:J:84:GLU:HB2	2.00	0.43
1:E:85:ASN:O	1:E:88:ARG:HG2	2.18	0.43
1:A:118:ASN:HB2	6:A:455:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:OE1	1:B:210:HIS:HE1	2.03	0.42
1:E:243:GLU:OE1	4:E:302:5RW:N16	2.52	0.42
1:D:124:GLU:OE2	1:D:126:HIS:HE1	2.04	0.41
1:E:182:GLN:OE1	1:E:210:HIS:HE1	2.04	0.41
2:G:18:MET:HB3	6:H:212:HOH:O	2.20	0.40
2:H:71:THR:HG22	2:I:70:MET:HE3	2.04	0.40
1:C:243:GLU:OE1	4:C:302:5RW:N16	2.55	0.40
1:D:124:GLU:OE2	1:D:126:HIS:CE1	2.74	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	A	179/209 (86%)	176 (98%)	3 (2%)	0	100	100
1	B	162/209 (78%)	160 (99%)	2 (1%)	0	100	100
1	C	184/209 (88%)	181 (98%)	3 (2%)	0	100	100
1	D	176/209 (84%)	174 (99%)	2 (1%)	0	100	100
1	E	173/209 (83%)	169 (98%)	2 (1%)	2 (1%)	10	3
2	F	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
2	G	82/87 (94%)	81 (99%)	1 (1%)	0	100	100
2	H	82/87 (94%)	81 (99%)	1 (1%)	0	100	100
2	I	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
2	J	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
All	All	1291/1480 (87%)	1271 (98%)	18 (1%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	216	ARG
1	E	217	GLY

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	161/181 (89%)	157 (98%)	4 (2%)	42	24
1	B	146/181 (81%)	141 (97%)	5 (3%)	32	15
1	C	166/181 (92%)	156 (94%)	10 (6%)	17	4
1	D	160/181 (88%)	155 (97%)	5 (3%)	35	18
1	E	157/181 (87%)	151 (96%)	6 (4%)	29	12
2	F	77/77 (100%)	77 (100%)	0	100	100
2	G	75/77 (97%)	74 (99%)	1 (1%)	61	47
2	H	75/77 (97%)	75 (100%)	0	100	100
2	I	76/77 (99%)	76 (100%)	0	100	100
2	J	77/77 (100%)	74 (96%)	3 (4%)	28	11
All	All	1170/1290 (91%)	1136 (97%)	34 (3%)	37	20

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	121	ILE
1	A	165	LEU
1	A	168	LEU
1	B	128	GLU
1	B	162	VAL
1	B	173	GLU
1	B	216	ARG
1	B	224	LYS
1	C	79	LEU
1	C	117	LEU
1	C	121	ILE

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Mol	Chain	Res	Type
1	C	124	GLU
1	C	159	ASN
1	C	165	LEU
1	C	211	MET
1	C	214	VAL
1	C	220	LYS
1	C	249	ARG
1	D	66	LEU
1	D	79	LEU
1	D	91	LEU
1	D	121	ILE
1	D	249	ARG
1	E	162	VAL
1	E	168	LEU
1	E	173	GLU
1	E	177	ARG
1	E	197	LEU
1	E	218	VAL
2	G	61	GLU
2	J	0	HIS
2	J	61	GLU
2	J	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	180	GLN
1	A	210	HIS
1	B	180	GLN
1	B	188	GLN
1	B	210	HIS
1	B	222	ASN
1	C	70	ASN
1	C	210	HIS
1	C	222	ASN
1	D	67	ASN
1	D	70	ASN
1	D	126	HIS
1	D	180	GLN
1	D	188	GLN
1	D	210	HIS

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Mol	Chain	Res	Type
1	E	67	ASN
1	E	70	ASN
1	E	180	GLN
1	E	188	GLN
1	E	210	HIS
2	F	9	GLN
2	F	82	HIS
2	G	9	GLN
2	G	23	GLN
2	G	30	GLN
2	G	82	HIS
2	H	9	GLN
2	H	23	GLN
2	H	43	ASN
2	H	82	HIS
2	I	82	HIS
2	J	9	GLN
2	J	23	GLN
2	J	82	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 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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	5RW	A	302	-	21,22,22	1.37	3 (14%)	25,31,31	3.25	9 (36%)
4	5RW	C	302	-	21,22,22	1.51	3 (14%)	25,31,31	3.11	10 (40%)
4	5RW	B	302	-	21,22,22	1.48	3 (14%)	25,31,31	3.14	9 (36%)
4	5RW	D	302	-	21,22,22	1.45	3 (14%)	25,31,31	2.98	8 (32%)
4	5RW	E	302	-	21,22,22	1.64	3 (14%)	25,31,31	3.08	7 (28%)

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
4	5RW	A	302	-	-	0/5/5/5	0/3/3/3
4	5RW	C	302	-	-	0/5/5/5	0/3/3/3
4	5RW	B	302	-	-	2/5/5/5	0/3/3/3
4	5RW	D	302	-	-	2/5/5/5	0/3/3/3
4	5RW	E	302	-	-	0/5/5/5	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	302	5RW	O18-C10	5.49	1.34	1.23
4	C	302	5RW	O18-C10	4.45	1.32	1.23
4	D	302	5RW	O18-C10	4.18	1.31	1.23
4	B	302	5RW	O18-C10	4.01	1.31	1.23
4	A	302	5RW	O18-C10	3.75	1.30	1.23
4	D	302	5RW	C9-N13	-3.54	1.27	1.36
4	C	302	5RW	C9-N13	-3.53	1.27	1.36
4	B	302	5RW	C9-N15	3.49	1.36	1.31
4	A	302	5RW	C9-N13	-3.38	1.28	1.36
4	E	302	5RW	C9-N15	3.29	1.36	1.31
4	E	302	5RW	C9-N13	-3.25	1.28	1.36
4	B	302	5RW	C9-N13	-3.24	1.28	1.36
4	C	302	5RW	C9-N15	3.18	1.36	1.31
4	D	302	5RW	C9-N15	3.13	1.36	1.31
4	A	302	5RW	C9-N15	3.10	1.36	1.31

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	5RW	C10-C7-C8	-12.51	113.08	121.61
4	E	302	5RW	C10-C7-C8	-12.29	113.23	121.61
4	C	302	5RW	C10-C7-C8	-12.10	113.36	121.61
4	D	302	5RW	C10-C7-C8	-11.79	113.57	121.61
4	B	302	5RW	C10-C7-C8	-11.73	113.61	121.61
4	B	302	5RW	C5-C12-S20	5.37	130.16	111.04
4	D	302	5RW	C11-N16-C10	-4.96	116.12	125.11
4	A	302	5RW	C11-N16-C10	-4.82	116.37	125.11
4	B	302	5RW	C11-N16-C10	-4.78	116.44	125.11
4	E	302	5RW	C11-N16-C10	-4.77	116.46	125.11
4	C	302	5RW	C11-N16-C10	-4.74	116.52	125.11
4	A	302	5RW	C7-C10-N16	3.96	122.99	112.13
4	B	302	5RW	C7-C10-N16	3.95	122.99	112.13
4	C	302	5RW	C7-C10-N16	3.95	122.97	112.13
4	D	302	5RW	C7-C10-N16	3.88	122.78	112.13
4	E	302	5RW	C7-C10-N16	3.81	122.60	112.13
4	E	302	5RW	C10-C7-N13	3.78	138.88	131.54
4	A	302	5RW	C10-C7-N13	3.74	138.79	131.54
4	D	302	5RW	C10-C7-N13	3.54	138.40	131.54
4	C	302	5RW	C10-C7-N13	3.51	138.35	131.54
4	A	302	5RW	C5-C12-S20	3.45	123.34	111.04
4	B	302	5RW	C10-C7-N13	3.43	138.19	131.54
4	C	302	5RW	C5-C12-S20	-3.39	98.95	111.04
4	A	302	5RW	S20-C9-N15	-3.16	118.49	125.97
4	A	302	5RW	S20-C9-N13	3.16	129.21	120.61
4	C	302	5RW	O18-C10-N16	-2.87	114.71	120.11
4	E	302	5RW	S20-C9-N13	2.81	128.26	120.61
4	E	302	5RW	S20-C9-N15	-2.73	119.51	125.97
4	A	302	5RW	O18-C10-N16	-2.69	115.06	120.11
4	E	302	5RW	O18-C10-C7	-2.65	120.88	127.26
4	B	302	5RW	O18-C10-N16	-2.63	115.17	120.11
4	C	302	5RW	S20-C9-N13	2.55	127.55	120.61
4	D	302	5RW	S20-C9-N13	2.54	127.54	120.61
4	C	302	5RW	S20-C9-N15	-2.44	120.21	125.97
4	D	302	5RW	O18-C10-C7	-2.42	121.43	127.26
4	D	302	5RW	S20-C9-N15	-2.41	120.28	125.97
4	D	302	5RW	O18-C10-N16	-2.30	115.79	120.11
4	B	302	5RW	O18-C10-C7	-2.25	121.85	127.26
4	A	302	5RW	O18-C10-C7	-2.22	121.91	127.26
4	B	302	5RW	S20-C9-N13	2.17	126.53	120.61
4	C	302	5RW	O18-C10-C7	-2.11	122.17	127.26
4	B	302	5RW	N15-C8-N14	2.07	128.19	125.33
4	C	302	5RW	N15-C8-N14	2.07	128.18	125.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

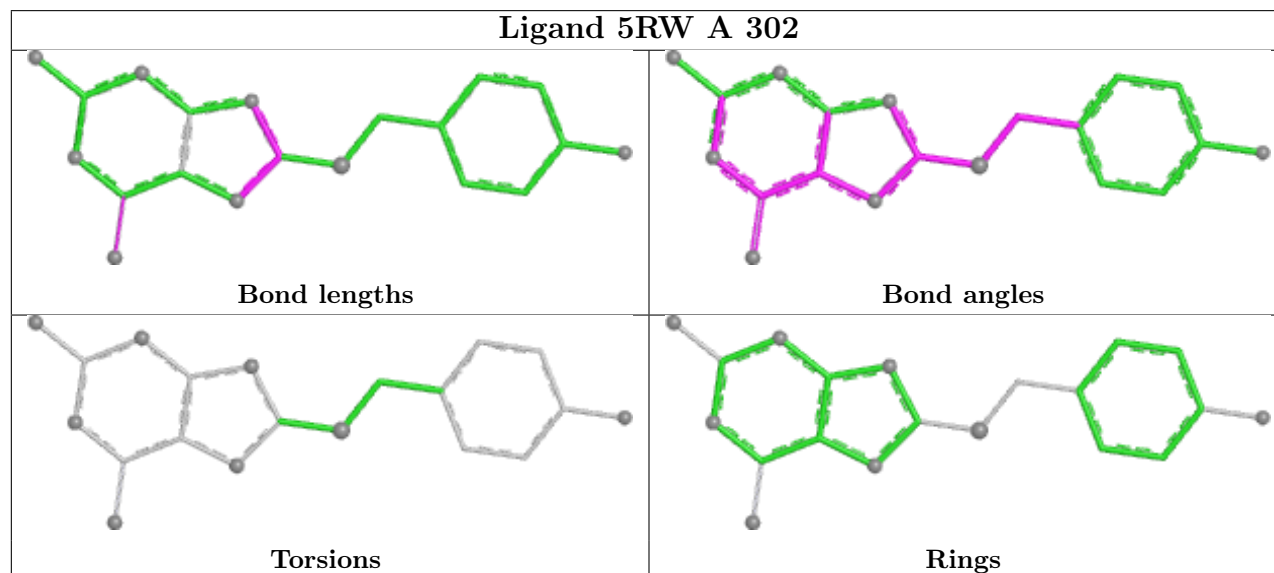
Mol	Chain	Res	Type	Atoms
4	B	302	5RW	S20-C12-C5-C1
4	B	302	5RW	S20-C12-C5-C2
4	D	302	5RW	S20-C12-C5-C1
4	D	302	5RW	S20-C12-C5-C2

There are no ring outliers.

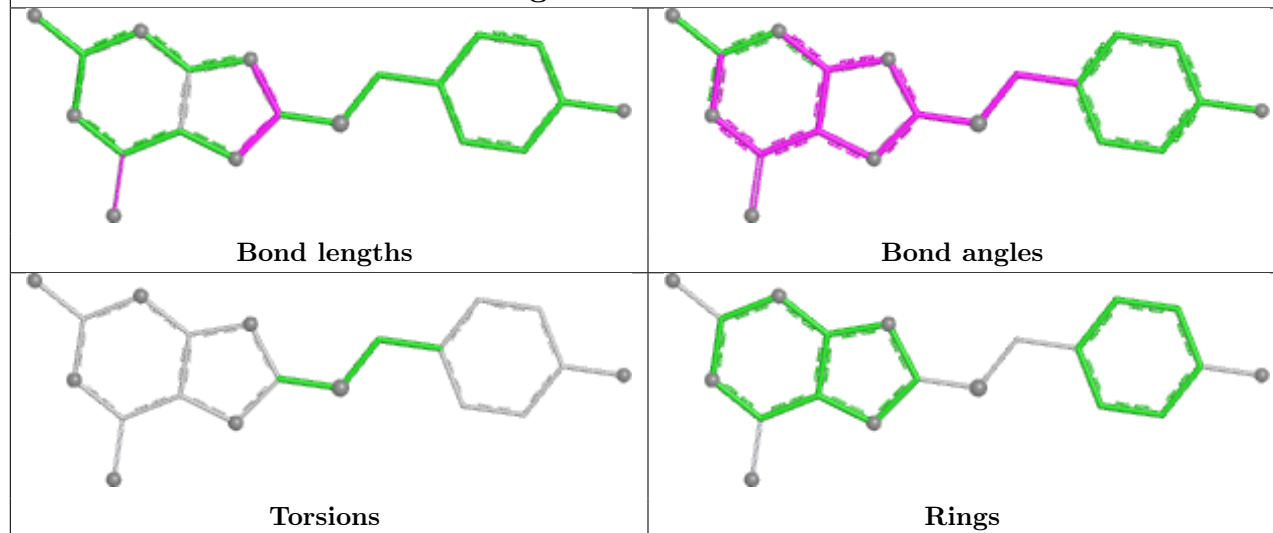
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	5RW	1	0
4	E	302	5RW	1	0

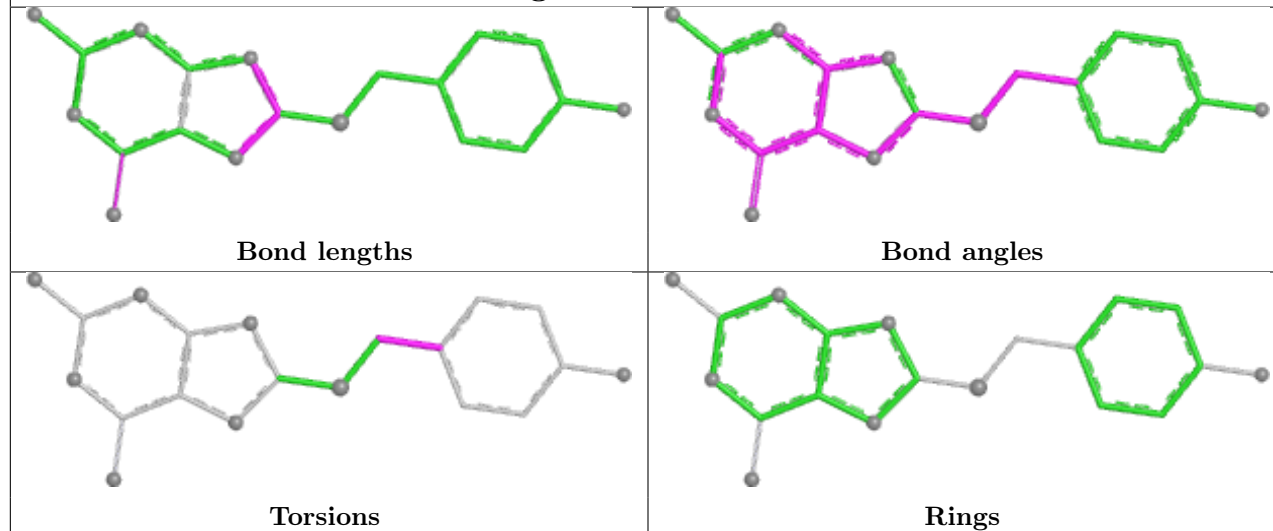
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



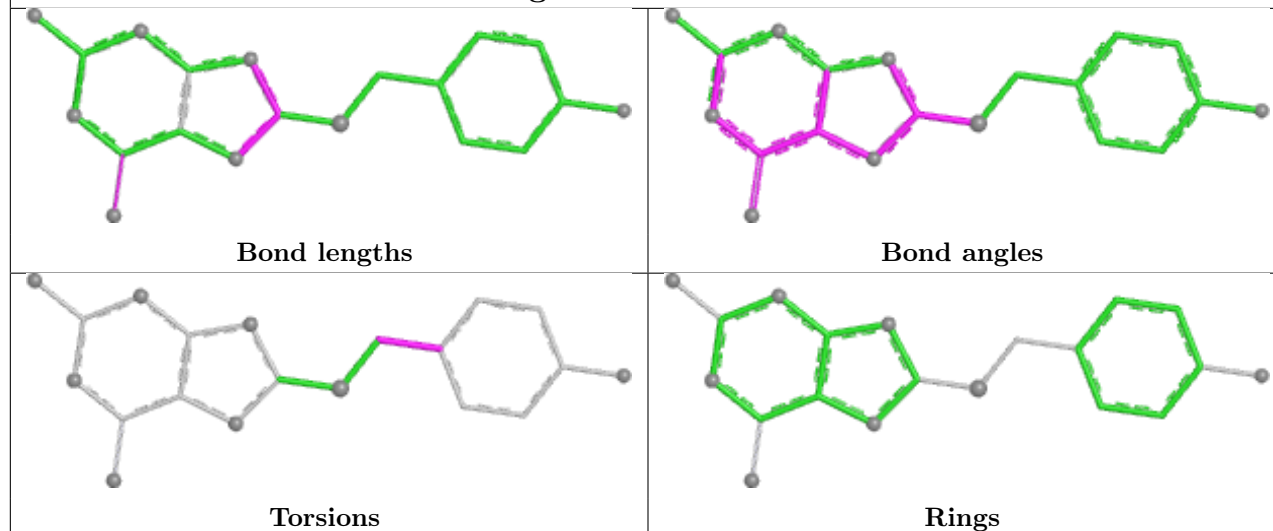
Ligand 5RW C 302

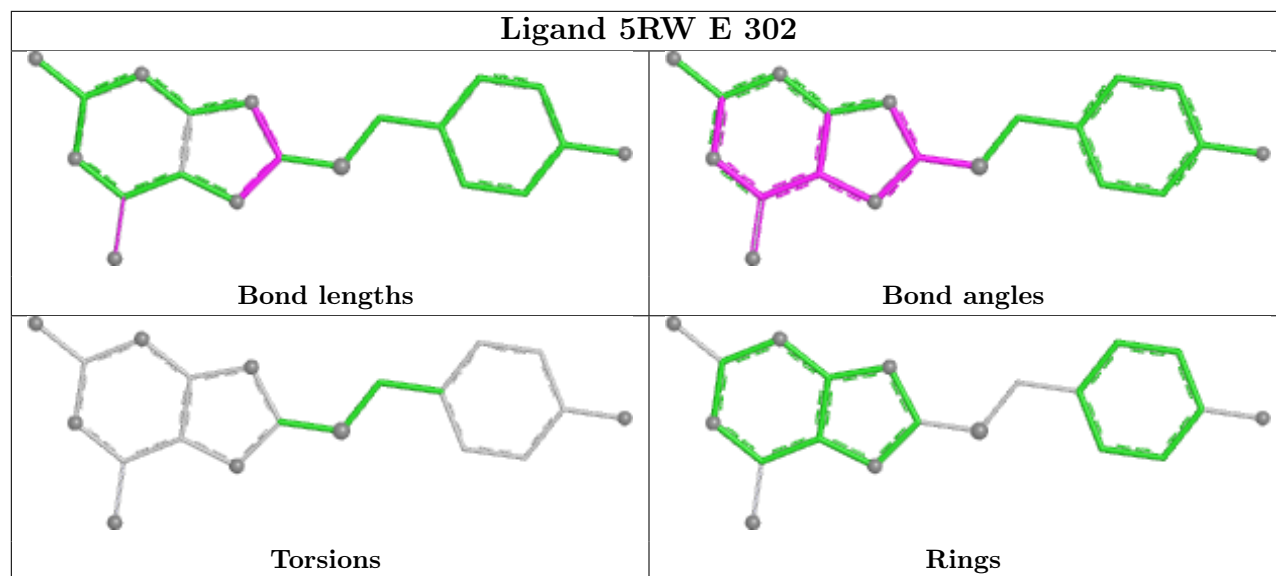


Ligand 5RW B 302



Ligand 5RW D 302





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	182/209 (87%)	0.23	4 (2%) 62 69	17, 40, 60, 77	1 (0%)
1	B	167/209 (79%)	0.69	18 (10%) 11 11	14, 43, 67, 74	1 (0%)
1	C	188/209 (89%)	0.38	15 (7%) 18 19	18, 33, 65, 83	0
1	D	180/209 (86%)	0.37	13 (7%) 21 22	11, 33, 67, 72	2 (1%)
1	E	179/209 (85%)	0.41	13 (7%) 21 22	18, 37, 64, 71	0
2	F	87/87 (100%)	-0.20	1 (1%) 78 84	14, 26, 42, 52	0
2	G	84/87 (96%)	-0.18	1 (1%) 76 82	18, 27, 43, 55	0
2	H	84/87 (96%)	-0.13	1 (1%) 76 82	15, 30, 45, 57	0
2	I	86/87 (98%)	-0.04	1 (1%) 76 82	17, 31, 45, 51	0
2	J	86/87 (98%)	-0.14	3 (3%) 47 51	17, 27, 45, 63	0
All	All	1323/1480 (89%)	0.23	70 (5%) 32 34	11, 33, 62, 83	4 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	218	VAL	5.7
1	C	122	PHE	5.7
1	D	214	VAL	5.7
1	B	165	LEU	5.4
1	C	215	MET	4.7
1	C	214	VAL	4.4
1	D	80	SER	4.3
1	E	116	VAL	4.2
1	C	121	ILE	4.0
1	E	96	TRP	3.8
1	C	124	GLU	3.7
1	B	169	ALA	3.2
1	E	126	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	125	ASP	3.1
1	E	214	VAL	3.1
1	D	66	LEU	3.0
1	B	163	LEU	2.9
1	B	114	SER	2.9
1	D	82	LEU	2.9
1	B	162	VAL	2.9
1	D	222	ASN	2.9
1	A	212	CYS	2.9
1	B	217	GLY	2.9
1	E	217	GLY	2.9
1	E	162	VAL	2.8
1	C	126	HIS	2.8
1	E	161	GLN	2.8
1	B	96	TRP	2.8
1	B	126	HIS	2.8
1	B	214	VAL	2.8
1	B	82	LEU	2.8
1	D	78	ILE	2.8
1	E	165	LEU	2.8
1	C	120	ALA	2.7
1	D	86	PRO	2.7
1	B	113	ILE	2.7
1	B	168	LEU	2.7
2	J	0	HIS	2.7
1	D	68	LEU	2.6
2	H	84	GLU	2.6
2	J	84	GLU	2.6
1	A	159	ASN	2.6
1	B	222	ASN	2.5
1	D	89	GLN	2.5
1	C	220	LYS	2.5
1	C	163	LEU	2.4
1	E	168	LEU	2.4
1	A	96	TRP	2.4
1	D	96	TRP	2.4
1	C	119	ASP	2.4
1	E	163	LEU	2.3
1	B	161	GLN	2.3
1	B	109	TYR	2.3
1	B	68	LEU	2.2
1	B	197	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	79	LEU	2.2
1	C	221	MET	2.2
1	B	223	SER	2.2
2	J	-1	SER	2.2
1	D	92	LEU	2.2
1	D	224	LYS	2.1
1	C	117	LEU	2.1
2	G	84	GLU	2.1
2	I	0	HIS	2.1
1	A	119	ASP	2.1
1	E	216	ARG	2.1
1	C	222	ASN	2.0
1	C	168	LEU	2.0
1	E	66	LEU	2.0
2	F	66	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

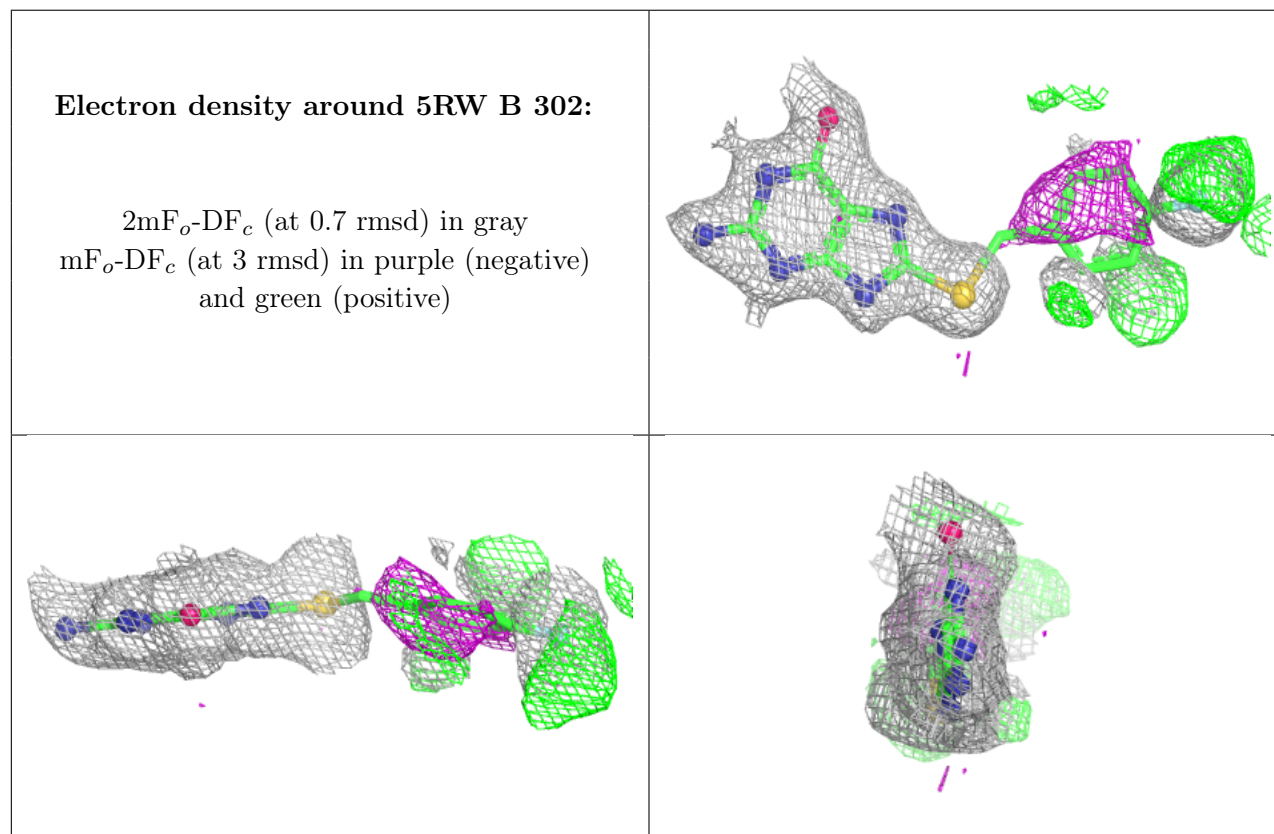
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5RW	B	302	20/20	0.79	0.17	43,47,57,57	0
4	5RW	A	302	20/20	0.88	0.16	38,42,58,59	0
4	5RW	C	302	20/20	0.90	0.13	38,40,56,58	0
4	5RW	D	302	20/20	0.91	0.12	27,34,48,49	0
4	5RW	E	302	20/20	0.91	0.10	30,35,49,50	0
5	NA	H	101	1/1	0.94	0.09	29,29,29,29	0
3	ZN	A	301	1/1	0.96	0.06	69,69,69,69	0
3	ZN	B	301	1/1	0.96	0.07	65,65,65,65	0

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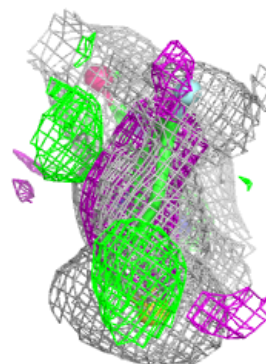
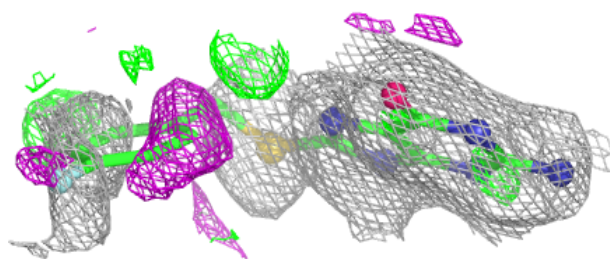
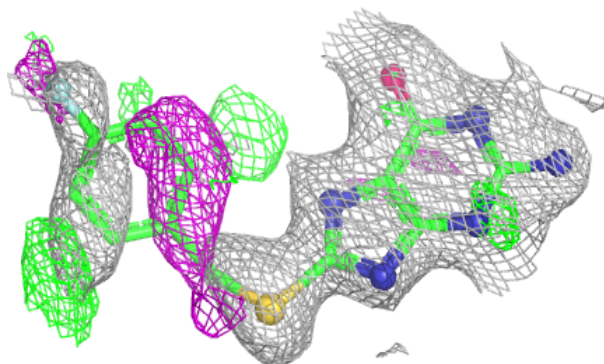
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	I	101	1/1	0.96	0.04	25,25,25,25	0
3	ZN	D	301	1/1	0.97	0.04	60,60,60,60	0
3	ZN	C	301	1/1	0.97	0.04	47,47,47,47	0
5	NA	F	101	1/1	0.98	0.03	21,21,21,21	0
5	NA	J	101	1/1	0.98	0.03	21,21,21,21	0
5	NA	G	101	1/1	0.99	0.02	22,22,22,22	0
3	ZN	E	301	1/1	0.99	0.03	51,51,51,51	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.

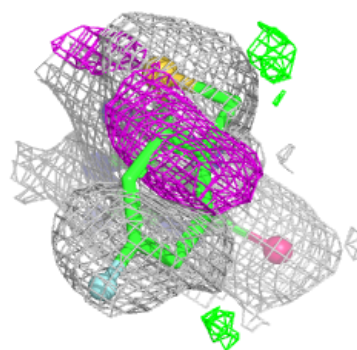
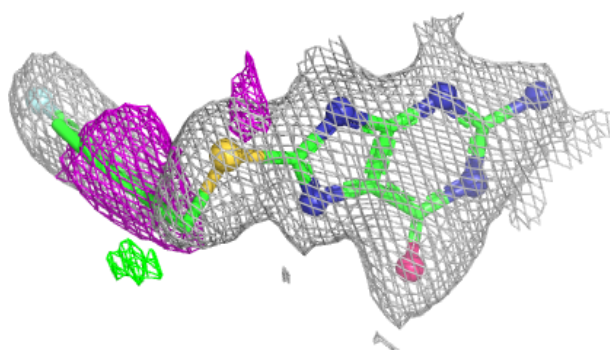
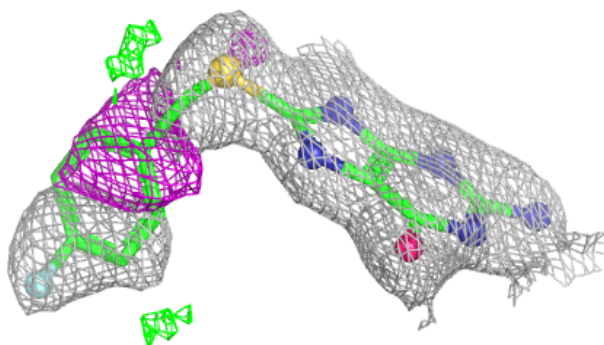


Electron density around 5RW A 302:

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

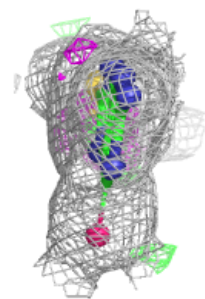
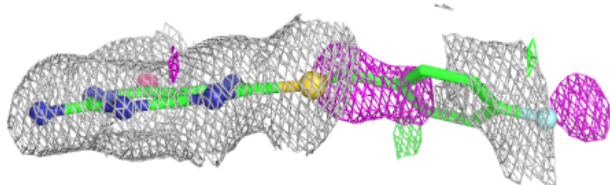
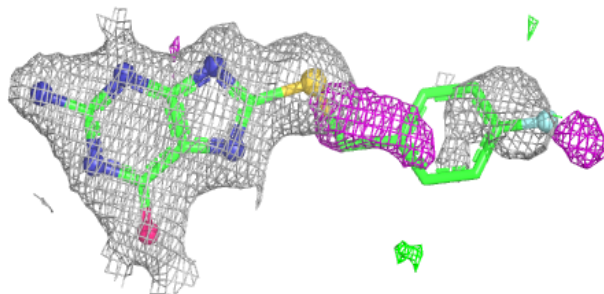
**Electron density around 5RW C 302:**

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

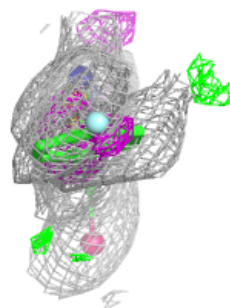
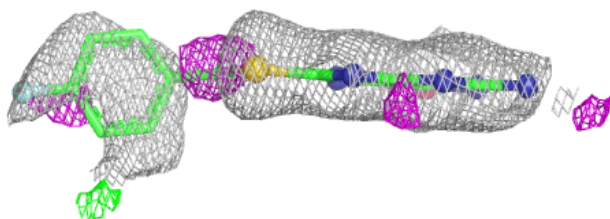
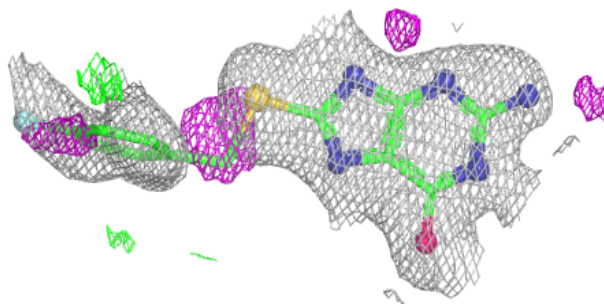


Electron density around 5RW D 302:

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

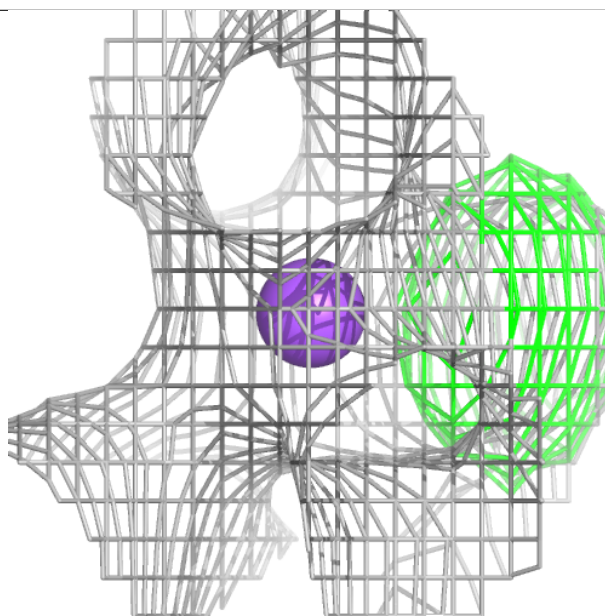
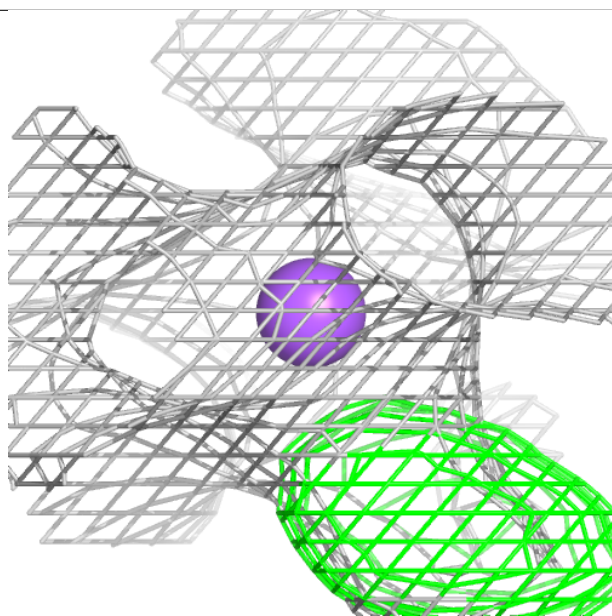
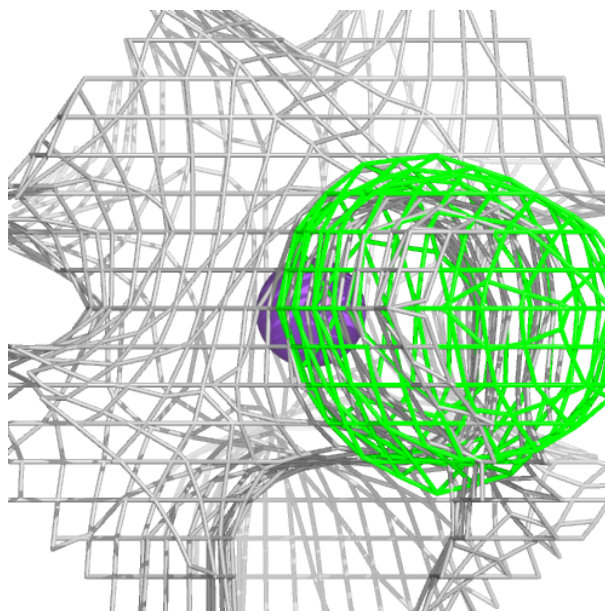
**Electron density around 5RW E 302:**

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



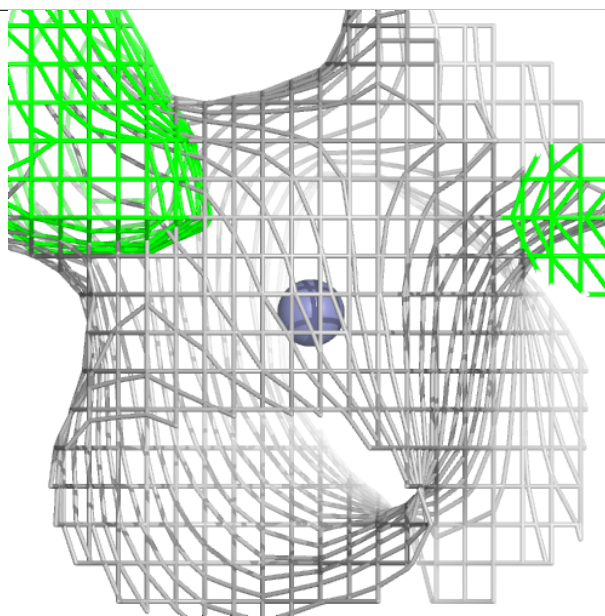
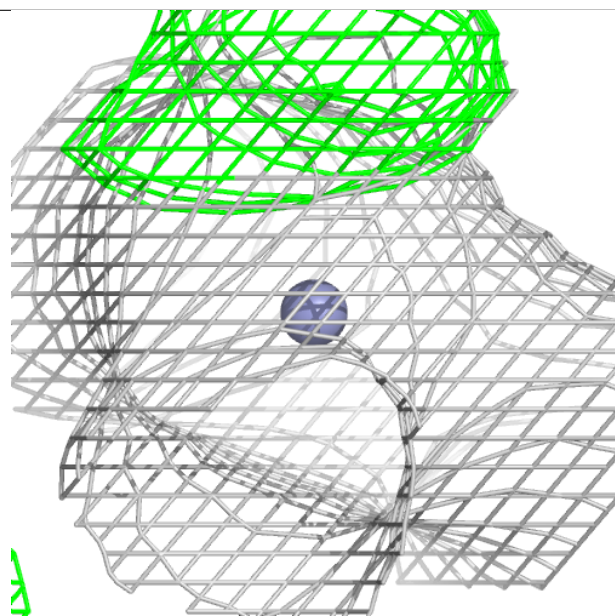
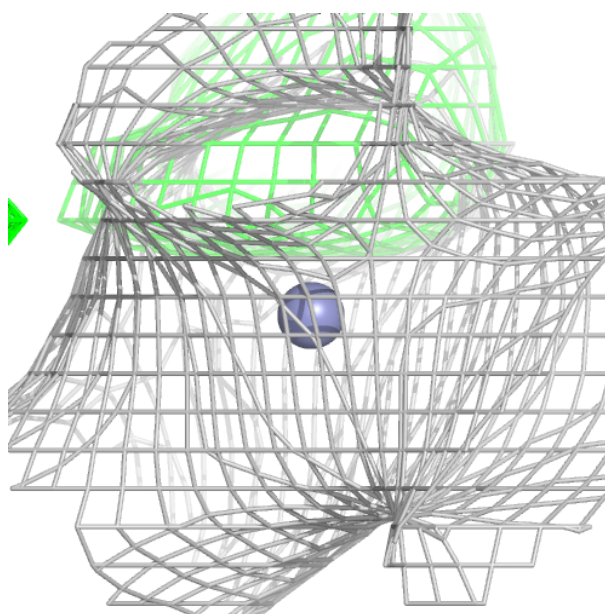
Electron density around NA H 101:

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



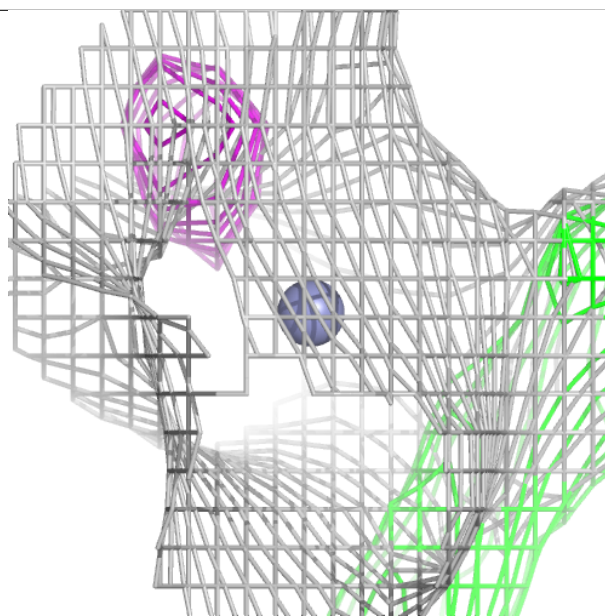
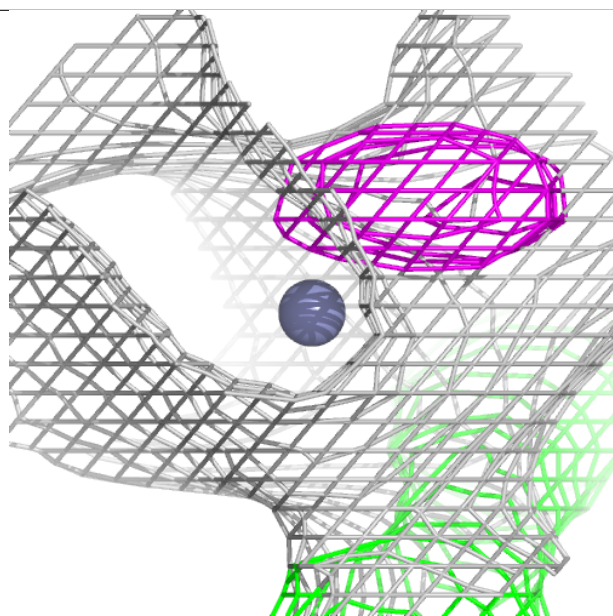
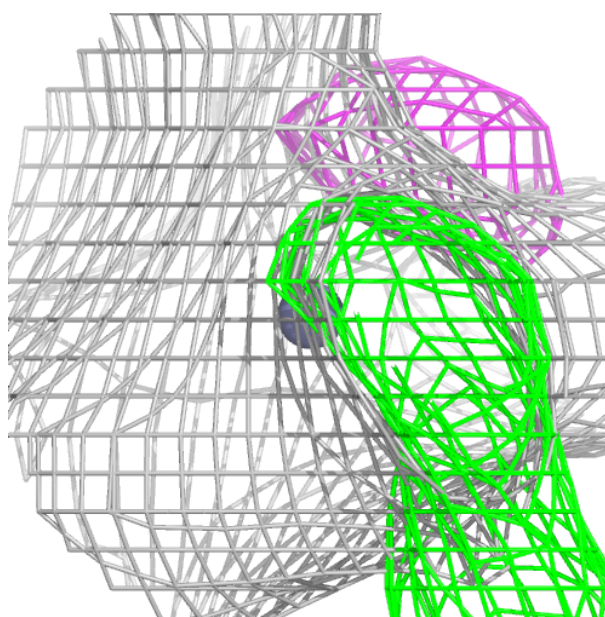
Electron density around ZN A 301:

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



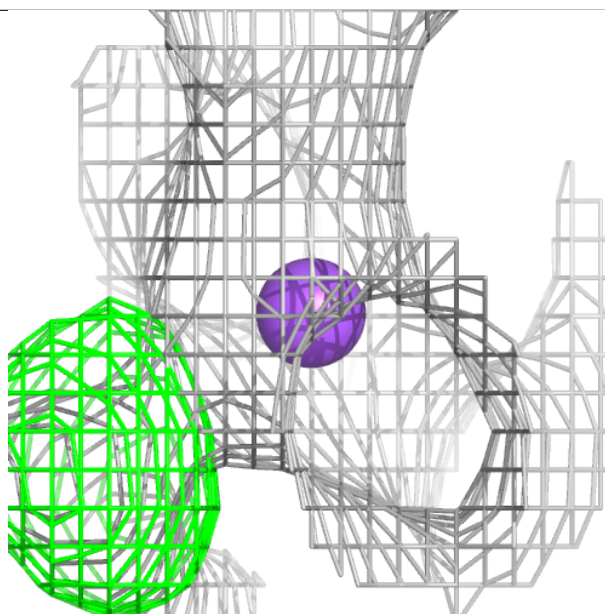
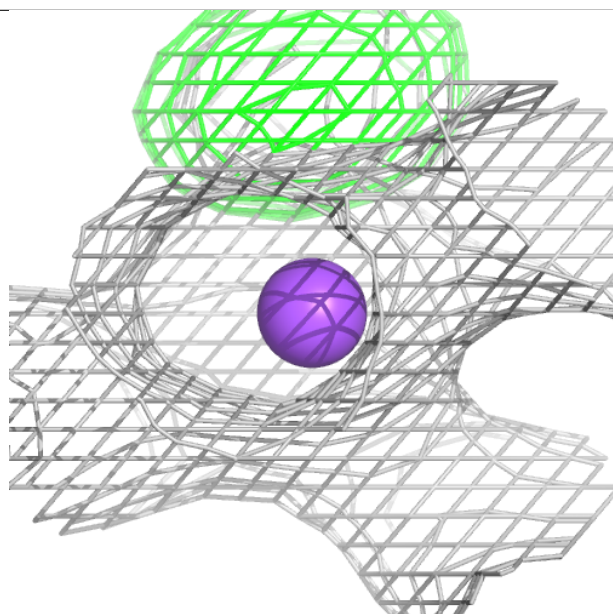
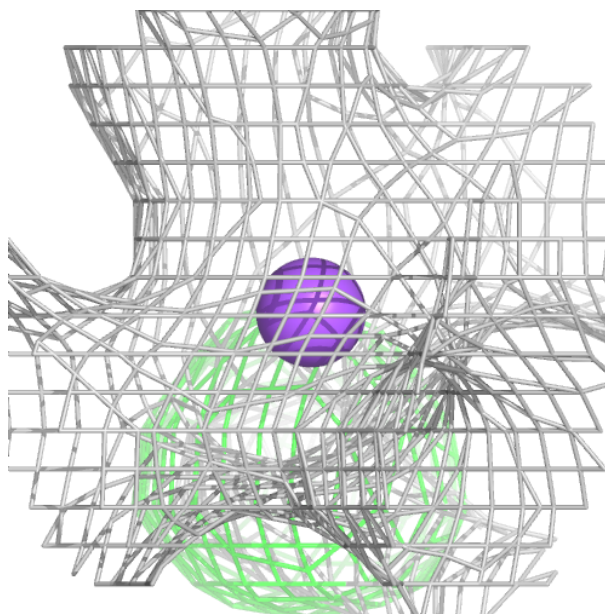
Electron density around ZN B 301:

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



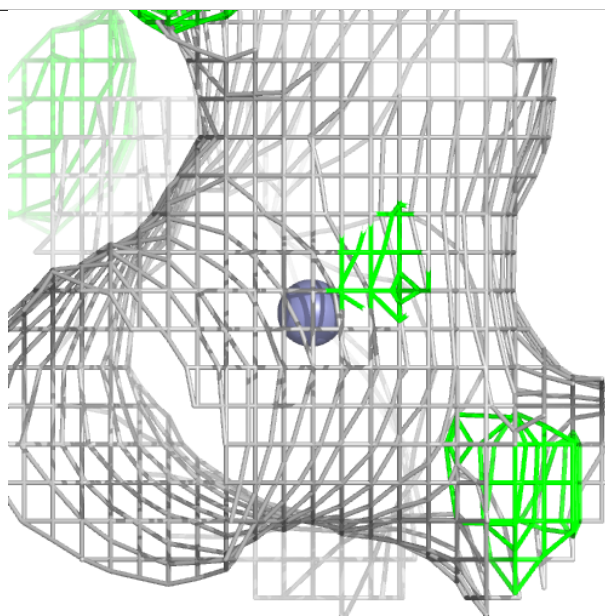
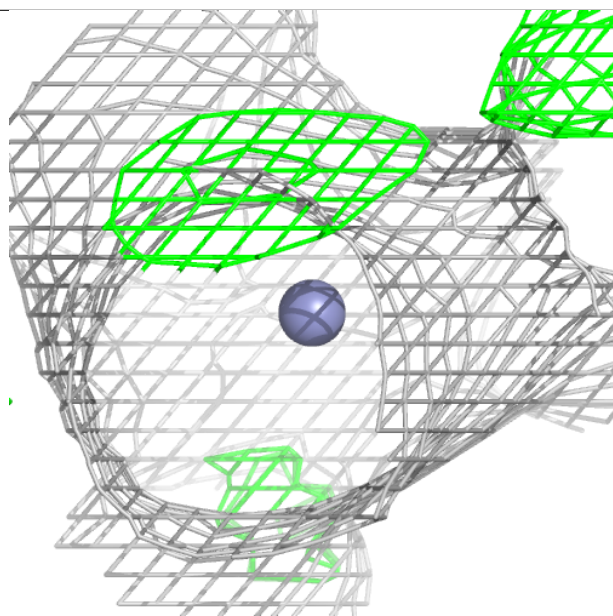
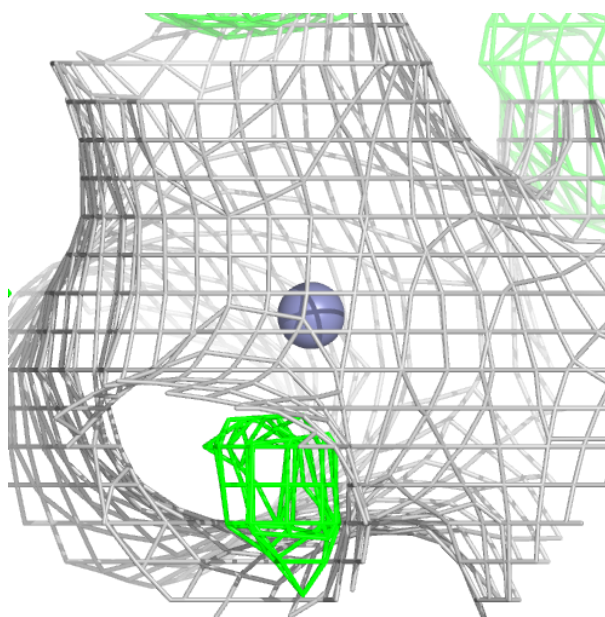
Electron density around NA I 101:

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



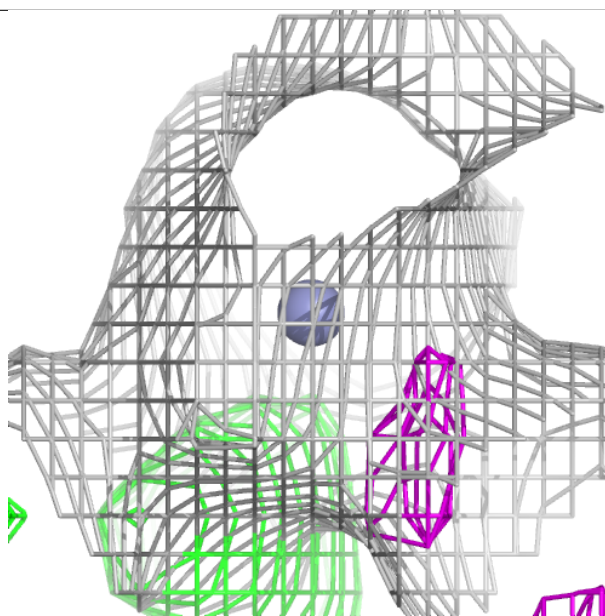
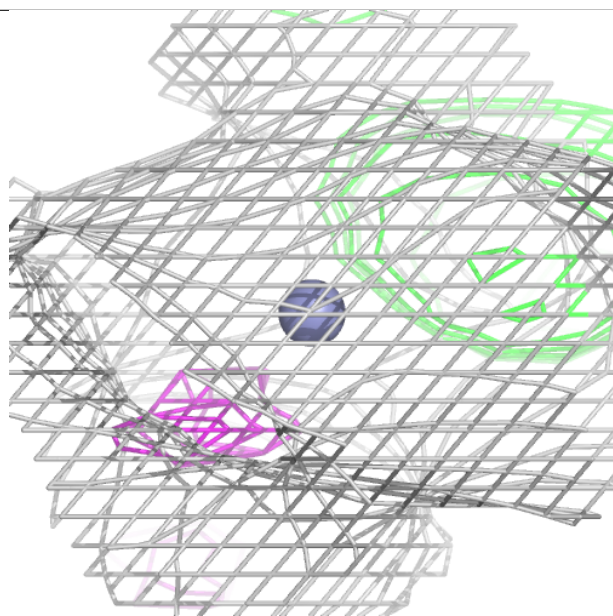
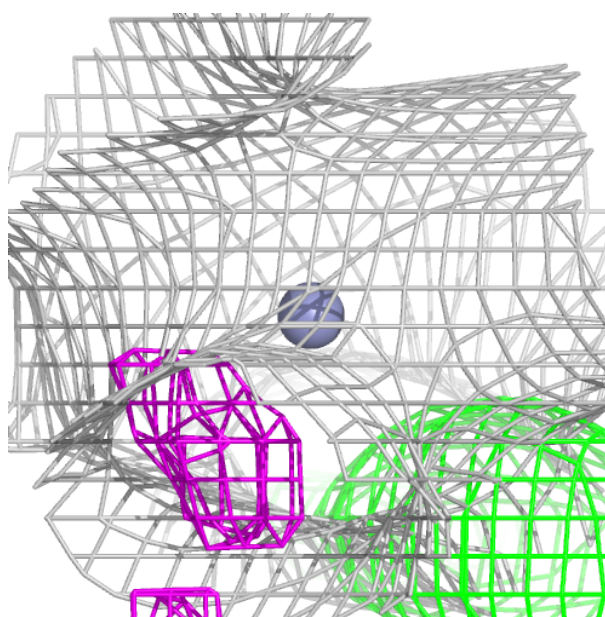
Electron density around ZN D 301:

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



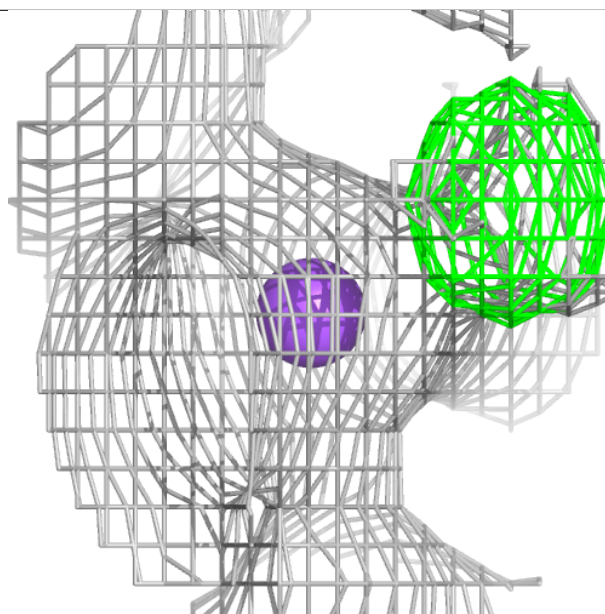
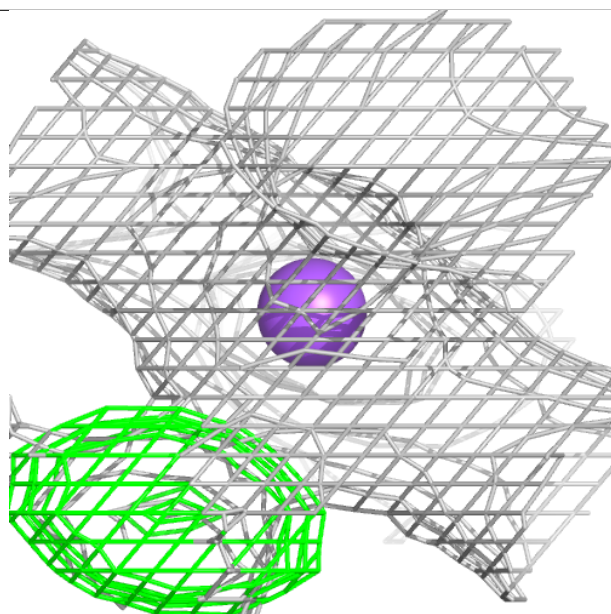
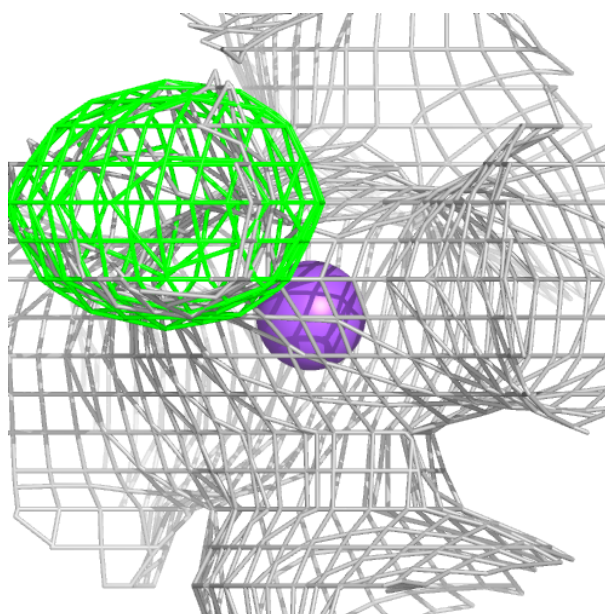
Electron density around ZN C 301:

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



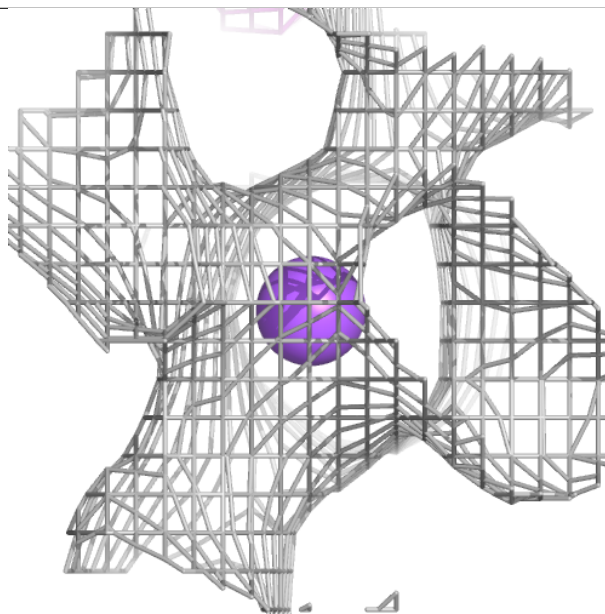
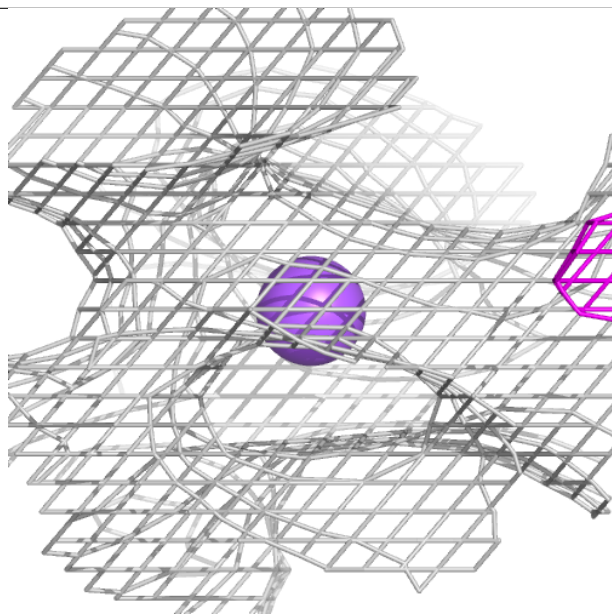
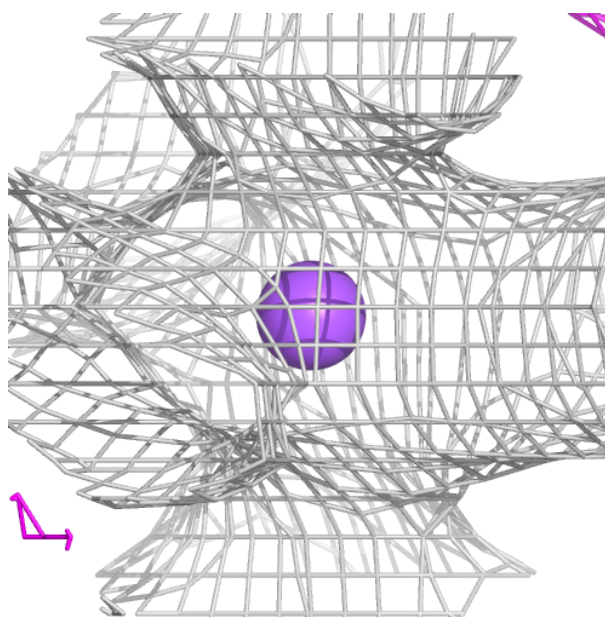
Electron density around NA F 101:

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



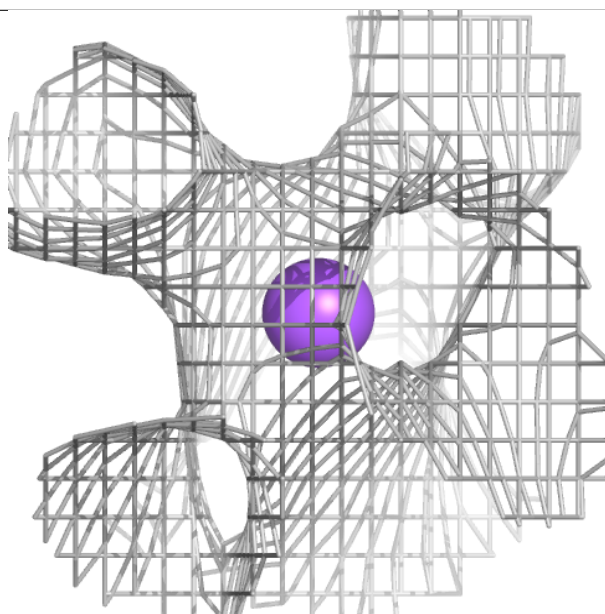
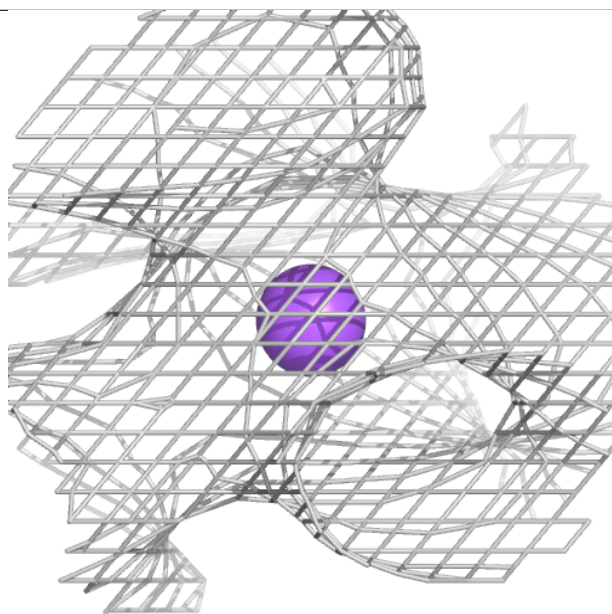
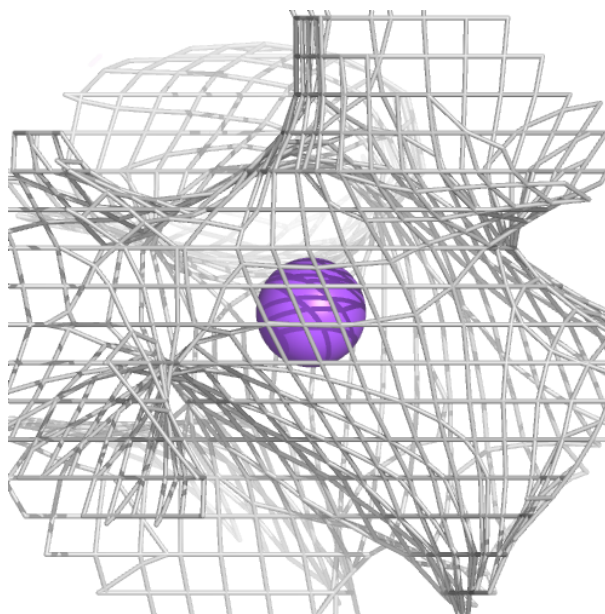
Electron density around NA J 101:

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



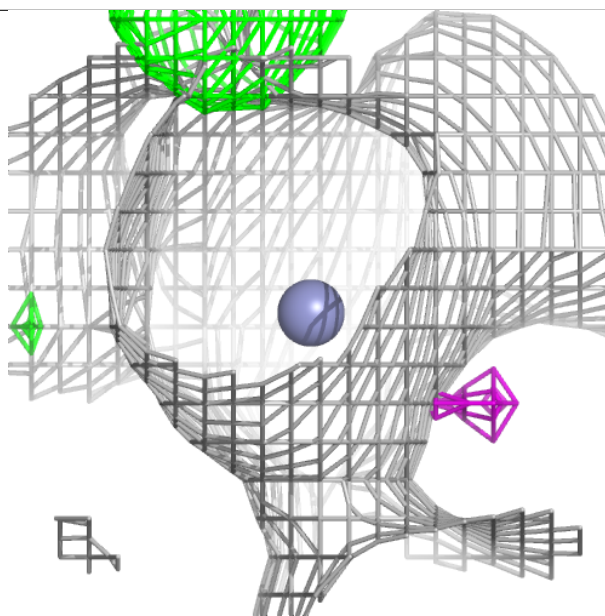
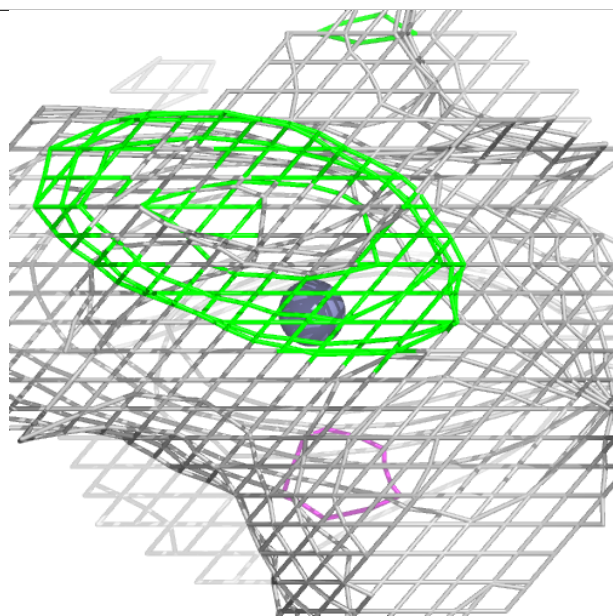
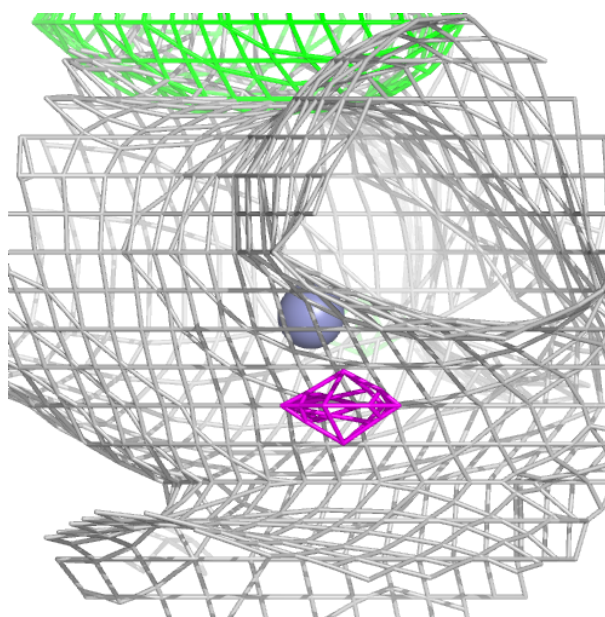
Electron density around NA G 101:

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



Electron density around ZN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.