Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 11:22 PM JST

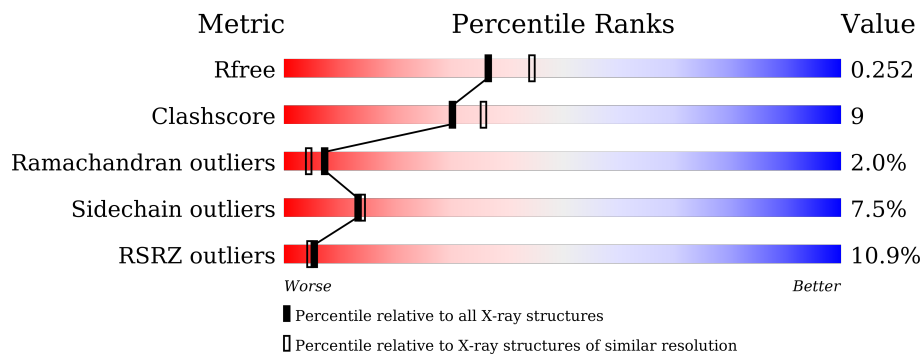|		
PDB ID	:	6K6T
Title	:	Crystal structure of a standalone versatile EAL protein from Vibrio cholerae O395 - c-di-IMP bound form
Authors	:	Yadav, M.; Pal, K.; Sen, U.
Deposited on	:	2019-06-04
Resolution	:	2.20 Å(reported)

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 2.20 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		9
Ramachandran outliers		2.0%
Sidechain outliers		7.5%
RSRZ outliers		10.9%

Worse ▐ Better

▐ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	257	11% / 74% 16% • 8%
1	B	257	11% / 70% 17% 5% • 8%
1	C	257	8% / 71% 17% • 8%
1	D	257	10% / 74% 15% • 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8196 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 EAL domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1894	1215	315	354	10			
1	B	237	Total	C	N	O	S	0	0	0
			1894	1215	315	354	10			
1	C	237	Total	C	N	O	S	0	0	0
			1894	1215	315	354	10			
1	D	237	Total	C	N	O	S	0	0	0
			1894	1215	315	354	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	CYS	engineered mutation	UNP A0A0H3AJ04
B	15	SER	CYS	engineered mutation	UNP A0A0H3AJ04
C	15	SER	CYS	engineered mutation	UNP A0A0H3AJ04
D	15	SER	CYS	engineered mutation	UNP A0A0H3AJ04

- Molecule 2 is 9-[(1R,6R,8R,9S,10R,15S,17R,18S)-3,9,12,18-tetrakis(oxidanyl)-3,12-bis(oxidanylidene)-17-(6-oxidanylidene-3H-purin-9-yl)-2,4,7,11,13,16-hexaoxa-3l^{5},12l^{5}-diphosphatricyclo[13.3.0.0^{6,10}]octadecan-8-yl]-3H-purin-6-one (three-letter code: C2I) (formula: $C_{20}H_{22}N_8O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).
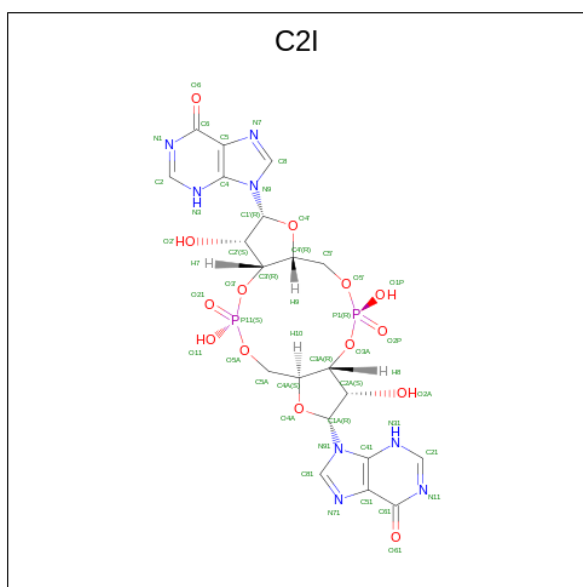
C2I

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	20	8	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	20	8	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	20	8	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	20	8	14	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	110	Total 110	O 110	0	0
4	C	110	Total 110	O 110	0	0
4	D	108	Total 108	O 108	0	0

3 Residue-property plots ⓘ

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: EAL domain protein

Chain A:

- Molecule 1: EAL domain protein

Chain B:

- Molecule 1: EAL domain protein

Chain C:

- Molecule 1: EAL domain protein

Chain D:

10%

74% 15% · 8%

MET HIS ILE ILE PRO VAL ALA SER ASP PRO LYS THR CYS SER SER GLY VAL ASN GLU ASN S21 L22 D23 F24 I41 V48 R49 G50 L51 Y57 S58 D66 Y69 C75 L82 N99 A100 I101 Y102 V103 P104 E105 R106 C107 I108 R109 Y118 Q119 I122 E123

T130 E131 A132 E133 R134 V135 E136 D137 V138 N139 H140 I141 K142 R143 I144 K149 S150 L151 G163 Y164 Q174 V178 K179 V180 I185 Q192 M198 K203 L204 I210 F223 A228 A229 V250 E253 F254 S255 E256 A257

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wwPDB
PROTEIN DATA BANK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.45Å 42.54Å 155.04Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	51.11 – 2.20 51.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (51.11-2.20) 92.3 (51.11-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.197 , 0.252 0.198 , 0.252	Depositor DCC
R_{free} test set	1996 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	1.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.7	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8196	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6653e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: C2I, CA

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	0.49	0/1933	0.63	0/2611
1	B	0.58	0/1933	0.67	0/2611
1	C	0.55	0/1933	0.64	0/2611
1	D	0.50	0/1933	0.66	0/2611
All	All	0.53	0/7732	0.65	0/10444

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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	1894	0	1870	31	0
1	B	1894	0	1870	43	0
1	C	1894	0	1869	30	0
1	D	1894	0	1869	36	0
2	A	44	0	0	3	0
2	B	44	0	0	0	0
2	C	44	0	0	1	0
2	D	44	0	0	4	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	108	0	0	6	0
4	B	110	0	0	3	0
4	C	110	0	0	4	0
4	D	108	0	0	3	0
All	All	8196	0	7478	141	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 9.

All (141) 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:102:TYR:HA	1:B:140:HIS:HE1	1.22	1.00
1:B:102:TYR:HA	1:B:140:HIS:CE1	2.00	0.96
1:C:25:ASP:HB3	1:C:51:LEU:HD21	1.63	0.81
1:B:157:ILE:HG23	1:B:178:VAL:HG22	1.65	0.77
1:D:101:ILE:HG23	1:D:144:ILE:HD11	1.66	0.76
1:A:22:LEU:HD22	1:A:74:MET:HG3	1.70	0.74
1:B:102:TYR:CA	1:B:140:HIS:CE1	2.71	0.74
1:B:102:TYR:CA	1:B:140:HIS:HE1	2.00	0.73
1:C:130:THR:HG22	1:C:158:ASP:HB3	1.71	0.72
1:B:157:ILE:HD11	1:B:165:SER:HB3	1.71	0.72
1:B:102:TYR:N	1:B:140:HIS:CE1	2.58	0.70
1:A:178:VAL:HG23	1:A:210:ILE:HG21	1.73	0.69
1:B:101:ILE:O	1:B:103:VAL:N	2.26	0.68
1:B:178:VAL:HG23	1:B:210:ILE:HG21	1.74	0.68
1:B:131:GLU:OE1	1:B:141:ILE:HG21	1.94	0.67
1:B:102:TYR:H	1:B:140:HIS:CE1	2.13	0.67
1:D:109:ARG:HH11	1:D:109:ARG:HG2	1.60	0.66
1:D:136:GLU:O	1:D:136:GLU:HG3	1.97	0.65
1:C:215:GLU:OE1	4:C:601:HOH:O	2.14	0.65
1:C:252:PRO:O	1:C:256:GLU:HG3	1.98	0.64
1:B:134:ARG:HD3	1:B:134:ARG:H	1.62	0.63
1:C:109:ARG:HD3	1:C:113:GLU:OE2	1.97	0.63
1:D:101:ILE:HG23	1:D:144:ILE:CD1	2.29	0.63
1:C:50:GLY:HA3	1:C:54:GLU:HG2	1.81	0.63
1:A:199:LYS:NZ	4:A:605:HOH:O	2.32	0.62
1:A:180:VAL:HG11	1:A:198:MET:HE1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ILE:HD11	1:D:250:VAL:HG21	1.83	0.61
1:A:65:GLU:HA	1:A:68:ARG:HG3	1.82	0.61
1:A:99:ASN:OD1	1:A:99:ASN:N	2.27	0.61
1:D:135:VAL:O	1:D:135:VAL:HG22	2.01	0.60
1:A:105:GLU:HB2	1:A:147:TYR:CE2	2.36	0.59
1:B:131:GLU:HG3	1:B:134:ARG:HG3	1.84	0.59
1:C:135:VAL:HG11	1:C:138:VAL:HG23	1.84	0.59
1:C:101:ILE:O	1:C:140:HIS:NE2	2.28	0.59
1:C:131:GLU:OE2	1:C:135:VAL:HG12	2.02	0.59
1:C:149:LYS:NZ	4:C:609:HOH:O	2.36	0.58
1:C:162:SER:O	1:C:164:TYR:N	2.37	0.58
1:D:123:GLU:H	1:D:123:GLU:CD	2.06	0.58
2:D:501:C2I:O2P	2:D:501:C2I:O2A	2.22	0.58
1:C:37:ARG:NH1	4:C:605:HOH:O	2.34	0.57
1:B:180:VAL:HG11	1:B:198:MET:HE1	1.85	0.57
1:B:136:GLU:O	1:B:136:GLU:HG3	2.04	0.57
1:D:101:ILE:HG22	1:D:140:HIS:NE2	2.21	0.56
1:C:64:ASN:H	1:C:67:ASN:HB2	1.70	0.56
1:D:118:TYR:O	1:D:119:GLN:HG2	2.05	0.56
1:D:180:VAL:HG11	1:D:198:MET:HE1	1.88	0.56
1:B:131:GLU:HB2	1:B:169:LEU:HD11	1.88	0.56
1:C:103:VAL:C	1:C:105:GLU:H	2.09	0.55
1:A:168:ASN:ND2	4:A:608:HOH:O	2.34	0.55
1:B:139:ASN:O	1:B:143:ARG:N	2.36	0.55
1:A:130:THR:HG22	1:A:158:ASP:HB3	1.87	0.54
1:C:22:LEU:HG	1:C:23:ASP:H	1.71	0.54
1:D:103:VAL:N	1:D:104:PRO:HD3	2.22	0.54
1:A:134:ARG:HH12	1:A:137:ASP:HB3	1.73	0.54
1:A:256:GLU:HG2	1:A:257:ALA:N	2.21	0.54
1:B:73:GLN:HE21	1:B:73:GLN:HA	1.71	0.54
1:A:134:ARG:CZ	1:A:134:ARG:HB2	2.25	0.54
1:B:106:ARG:NH2	4:B:612:HOH:O	2.42	0.53
1:D:41:ILE:HD11	1:D:250:VAL:CG2	2.39	0.52
1:D:192:GLN:NE2	4:D:610:HOH:O	2.43	0.51
2:A:501:C2I:O2A	2:A:501:C2I:O2P	2.29	0.51
1:B:195:GLN:HG2	1:B:225:TRP:CZ2	2.47	0.50
1:A:165:SER:N	4:A:613:HOH:O	2.44	0.50
1:D:49:ARG:NH2	2:D:501:C2I:O11	2.37	0.50
1:B:101:ILE:C	1:B:103:VAL:H	2.15	0.49
1:D:138:VAL:O	1:D:142:LYS:N	2.37	0.49
1:A:121:PRO:HA	4:A:632:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HD2	1:A:232:GLU:CD	2.33	0.48
1:B:102:TYR:N	1:B:140:HIS:NE2	2.58	0.48
1:C:178:VAL:HG23	1:C:210:ILE:HG21	1.95	0.48
1:D:48:VAL:HG13	2:D:501:C2I:O61	2.13	0.48
1:D:48:VAL:O	1:D:49:ARG:NH2	2.44	0.48
1:D:48:VAL:HG22	2:D:501:C2I:N71	2.28	0.48
1:A:68:ARG:HD3	1:A:99:ASN:O	2.14	0.48
1:C:49:ARG:NH2	2:C:501:C2I:O11	2.45	0.48
1:B:52:ASN:HB2	1:B:54:GLU:OE1	2.14	0.48
1:D:109:ARG:HG2	1:D:109:ARG:NH1	2.29	0.48
1:A:203:LYS:NZ	1:A:207:ASP:OD1	2.45	0.47
1:C:254:PHE:HA	4:C:659:HOH:O	2.15	0.47
1:D:101:ILE:HG22	1:D:140:HIS:CE1	2.49	0.47
1:A:37:ARG:HD2	1:A:232:GLU:OE2	2.15	0.47
1:B:131:GLU:CG	1:B:134:ARG:HG3	2.45	0.46
1:A:97:LEU:HD12	1:A:98:PRO:HD2	1.98	0.46
1:B:122:ILE:HG22	4:B:655:HOH:O	2.15	0.46
1:B:215:GLU:OE2	4:B:601:HOH:O	2.20	0.46
1:B:139:ASN:HA	1:B:142:LYS:HB3	1.97	0.46
1:A:136:GLU:O	1:A:136:GLU:HG3	2.16	0.46
1:B:50:GLY:HA3	1:B:54:GLU:CG	2.47	0.45
1:B:223:PHE:CZ	1:B:254:PHE:HB2	2.51	0.45
1:C:138:VAL:HG21	1:C:169:LEU:HD23	1.99	0.45
1:C:173:PHE:C	1:C:174:GLN:NE2	2.70	0.45
1:A:164:TYR:N	4:A:613:HOH:O	2.50	0.45
1:D:178:VAL:HG23	1:D:210:ILE:HG21	1.99	0.45
1:B:157:ILE:CG2	1:B:178:VAL:HG22	2.41	0.45
1:A:142:LYS:NZ	1:A:146:GLU:OE2	2.33	0.44
1:D:134:ARG:O	1:D:134:ARG:HG3	2.17	0.44
1:A:199:LYS:HD3	4:D:602:HOH:O	2.17	0.44
1:B:109:ARG:HD2	1:B:113:GLU:OE2	2.17	0.44
1:A:63:VAL:HA	1:A:67:ASN:HD22	1.83	0.44
4:A:605:HOH:O	1:D:203:LYS:HE3	2.18	0.44
1:C:149:LYS:HE3	1:C:175:THR:HA	2.00	0.44
1:D:104:PRO:HB2	1:D:107:CYS:SG	2.57	0.44
1:C:195:GLN:HG2	1:C:225:TRP:CZ2	2.52	0.43
1:B:109:ARG:CD	1:B:113:GLU:OE2	2.65	0.43
1:C:50:GLY:HA3	1:C:54:GLU:CG	2.48	0.43
1:C:229:ALA:HA	1:D:229:ALA:HA	2.00	0.43
1:B:63:VAL:HA	1:B:67:ASN:HD22	1.82	0.43
1:B:203:LYS:NZ	1:B:207:ASP:OD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LYS:HB2	1:D:149:LYS:HE2	1.64	0.43
1:A:133:GLU:HG2	1:A:134:ARG:H	1.83	0.43
1:C:185:ILE:HD13	1:C:215:GLU:O	2.18	0.43
1:A:37:ARG:HB2	1:A:232:GLU:HG2	2.01	0.43
1:A:49:ARG:NH2	2:A:501:C2I:O11	2.45	0.43
1:C:69:TYR:OH	1:C:107:CYS:HB2	2.18	0.43
1:D:228:ALA:O	4:D:601:HOH:O	2.22	0.43
1:B:157:ILE:HG22	1:B:175:THR:OG1	2.19	0.42
1:A:126:MET:HA	1:A:154:GLN:O	2.19	0.42
1:B:256:GLU:HB2	1:B:257:ALA:H	1.60	0.42
1:D:101:ILE:O	1:D:140:HIS:NE2	2.51	0.42
1:D:174:GLN:HB3	1:D:210:ILE:HD11	2.01	0.42
1:B:65:GLU:HA	1:B:68:ARG:NE	2.35	0.42
1:C:72:ASP:OD2	1:C:76:ARG:NE	2.53	0.42
1:D:21:SER:HB2	1:D:22:LEU:H	1.74	0.42
1:A:48:VAL:HG22	2:A:501:C2I:N71	2.34	0.42
1:B:149:LYS:HE3	1:B:149:LYS:HB2	1.78	0.42
1:C:27:THR:OG1	1:C:28:MET:N	2.50	0.42
1:D:137:ASP:HB3	1:D:140:HIS:HB3	2.01	0.42
1:D:101:ILE:HD13	1:D:141:ILE:HG13	2.02	0.41
1:B:137:ASP:OD1	1:B:138:VAL:N	2.53	0.41
1:A:76:ARG:HH11	1:A:76:ARG:HD3	1.67	0.41
1:C:117:ARG:HD2	1:C:118:TYR:CE2	2.55	0.41
1:B:50:GLY:HA3	1:B:54:GLU:HG2	2.03	0.41
1:D:51:LEU:HA	1:D:51:LEU:HD12	1.81	0.41
1:B:104:PRO:C	1:B:106:ARG:H	2.23	0.41
1:D:118:TYR:C	1:D:119:GLN:HG2	2.42	0.41
1:B:37:ARG:HB2	1:B:232:GLU:HG2	2.02	0.40
1:C:135:VAL:HG21	1:C:138:VAL:HA	2.03	0.40
1:A:51:LEU:HD12	1:A:51:LEU:HA	1.91	0.40
1:D:122:ILE:HD12	1:D:151:LEU:O	2.20	0.40
1:B:100:ALA:HB1	1:B:103:VAL:HG11	2.04	0.40
1:D:82:LEU:HA	1:D:82:LEU:HD23	1.80	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	235/257 (91%)	223 (95%)	9 (4%)	3 (1%)	12	9
1	B	235/257 (91%)	215 (92%)	14 (6%)	6 (3%)	5	3
1	C	235/257 (91%)	218 (93%)	11 (5%)	6 (3%)	5	3
1	D	235/257 (91%)	222 (94%)	9 (4%)	4 (2%)	9	6
All	All	940/1028 (91%)	878 (93%)	43 (5%)	19 (2%)	7	4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	B	102	TYR
1	B	137	ASP
1	B	138	VAL
1	C	163	GLY
1	D	136	GLU
1	D	138	VAL
1	A	134	ARG
1	D	135	VAL
1	C	132	ALA
1	D	104	PRO
1	A	132	ALA
1	C	103	VAL
1	B	103	VAL
1	B	254	PHE
1	C	22	LEU
1	C	105	GLU
1	B	135	VAL
1	C	104	PRO

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	203/222 (91%)	193 (95%)	10 (5%)	25	31
1	B	203/222 (91%)	180 (89%)	23 (11%)	6	5
1	C	203/222 (91%)	190 (94%)	13 (6%)	17	20
1	D	203/222 (91%)	188 (93%)	15 (7%)	13	14
All	All	812/888 (91%)	751 (92%)	61 (8%)	13	14

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	57	TYR
1	A	99	ASN
1	A	101	ILE
1	A	106	ARG
1	A	130	THR
1	A	134	ARG
1	A	196	SER
1	A	223	PHE
1	A	256	GLU
1	B	51	LEU
1	B	54	GLU
1	B	73	GLN
1	B	82	LEU
1	B	102	TYR
1	B	106	ARG
1	B	116	LYS
1	B	122	ILE
1	B	130	THR
1	B	133	GLU
1	B	134	ARG
1	B	137	ASP
1	B	138	VAL
1	B	139	ASN

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Mol	Chain	Res	Type
1	B	141	ILE
1	B	146	GLU
1	B	157	ILE
1	B	164	TYR
1	B	192	GLN
1	B	196	SER
1	B	223	PHE
1	B	253	GLU
1	B	256	GLU
1	C	51	LEU
1	C	54	GLU
1	C	68	ARG
1	C	69	TYR
1	C	75	CYS
1	C	101	ILE
1	C	102	TYR
1	C	105	GLU
1	C	130	THR
1	C	141	ILE
1	C	149	LYS
1	C	185	ILE
1	C	223	PHE
1	D	23	ASP
1	D	51	LEU
1	D	58	SER
1	D	75	CYS
1	D	106	ARG
1	D	109	ARG
1	D	119	GLN
1	D	123	GLU
1	D	130	THR
1	D	134	ARG
1	D	139	ASN
1	D	185	ILE
1	D	204	LEU
1	D	223	PHE
1	D	253	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	C2I	D	501	3	40,50,50	5.71	20 (50%)	48,78,78	1.55	10 (20%)
2	C2I	A	501	3	40,50,50	5.57	20 (50%)	48,78,78	1.71	9 (18%)
2	C2I	B	501	3	40,50,50	5.66	19 (47%)	48,78,78	1.89	15 (31%)
2	C2I	C	501	3	40,50,50	5.69	20 (50%)	48,78,78	1.87	13 (27%)

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	C2I	D	501	3	-	10/22/62/62	0/6/7/7
2	C2I	A	501	3	-	13/22/62/62	0/6/7/7
2	C2I	B	501	3	-	11/22/62/62	0/6/7/7
2	C2I	C	501	3	-	10/22/62/62	0/6/7/7

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	C2I	C2'-C1'	-17.09	1.27	1.53
2	D	501	C2I	C2'-C1'	-16.56	1.28	1.53
2	B	501	C2I	C2'-C1'	-16.28	1.29	1.53
2	A	501	C2I	C2'-C1'	-15.69	1.29	1.53
2	D	501	C2I	C2A-C1A	-15.15	1.30	1.53
2	C	501	C2I	C2A-C1A	-14.59	1.31	1.53
2	B	501	C2I	C2A-C1A	-14.48	1.31	1.53
2	A	501	C2I	C2A-C1A	-13.76	1.32	1.53
2	B	501	C2I	O4'-C1'	11.37	1.57	1.41
2	A	501	C2I	O6-C6	11.34	1.43	1.23
2	D	501	C2I	C3A-C4A	-11.34	1.22	1.52
2	C	501	C2I	O6-C6	11.16	1.43	1.23
2	A	501	C2I	O4'-C1'	11.13	1.56	1.41
2	B	501	C2I	C3A-C4A	-11.07	1.23	1.52
2	C	501	C2I	C3A-C4A	-11.03	1.23	1.52
2	D	501	C2I	O6-C6	10.93	1.42	1.23
2	A	501	C2I	C3A-C4A	-10.89	1.23	1.52
2	B	501	C2I	O6-C6	10.81	1.42	1.23
2	C	501	C2I	O4'-C1'	10.73	1.56	1.41
2	D	501	C2I	O4'-C1'	10.70	1.56	1.41
2	D	501	C2I	C3'-C4'	-9.06	1.28	1.52
2	C	501	C2I	C3'-C4'	-9.06	1.28	1.52
2	B	501	C2I	C3'-C4'	-8.91	1.29	1.52
2	A	501	C2I	C3'-C4'	-8.64	1.29	1.52
2	B	501	C2I	O61-C61	8.40	1.38	1.23
2	C	501	C2I	O61-C61	7.84	1.37	1.23
2	D	501	C2I	O4A-C1A	7.76	1.51	1.41
2	D	501	C2I	O61-C61	7.67	1.37	1.23
2	A	501	C2I	O61-C61	7.62	1.36	1.23
2	A	501	C2I	O4A-C1A	7.50	1.51	1.41
2	C	501	C2I	O4A-C1A	7.30	1.51	1.41
2	C	501	C2I	C2A-C3A	7.11	1.68	1.52
2	B	501	C2I	C2A-C3A	7.11	1.68	1.52
2	A	501	C2I	C2A-C3A	6.99	1.68	1.52
2	A	501	C2I	O4A-C4A	6.99	1.60	1.45
2	A	501	C2I	C2'-C3'	6.97	1.68	1.52
2	B	501	C2I	O4A-C4A	6.95	1.60	1.45
2	B	501	C2I	O4A-C1A	6.94	1.50	1.41
2	C	501	C2I	O4A-C4A	6.76	1.60	1.45
2	D	501	C2I	C2A-C3A	6.70	1.67	1.52
2	D	501	C2I	C2'-C3'	6.64	1.67	1.52
2	D	501	C2I	O4A-C4A	6.63	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	C2I	C2'-C3'	6.16	1.66	1.52
2	B	501	C2I	C2'-C3'	5.93	1.66	1.52
2	B	501	C2I	O4'-C4'	5.09	1.56	1.45
2	A	501	C2I	O4'-C4'	4.89	1.55	1.45
2	D	501	C2I	O4'-C4'	4.72	1.55	1.45
2	C	501	C2I	O4'-C4'	4.70	1.55	1.45
2	C	501	C2I	C61-N11	-3.64	1.31	1.38
2	B	501	C2I	C61-N11	-3.42	1.31	1.38
2	A	501	C2I	C61-N11	-3.40	1.31	1.38
2	B	501	C2I	C5-C6	-3.40	1.40	1.47
2	D	501	C2I	C61-N11	-3.39	1.31	1.38
2	D	501	C2I	C51-C61	-3.24	1.41	1.47
2	C	501	C2I	C5-C6	-3.03	1.41	1.47
2	D	501	C2I	C5-C6	-2.94	1.41	1.47
2	A	501	C2I	C51-C61	-2.91	1.41	1.47
2	C	501	C2I	C51-C61	-2.88	1.41	1.47
2	A	501	C2I	C5-C6	-2.74	1.42	1.47
2	B	501	C2I	C51-C61	-2.62	1.42	1.47
2	C	501	C2I	C21-N11	2.61	1.35	1.30
2	B	501	C2I	C5'-C4'	2.60	1.59	1.51
2	A	501	C2I	O2'-C2'	2.52	1.48	1.43
2	A	501	C2I	C5'-C4'	2.43	1.59	1.51
2	A	501	C2I	C41-N31	-2.41	1.33	1.37
2	D	501	C2I	C5'-C4'	2.35	1.58	1.51
2	B	501	C2I	C21-N11	2.31	1.34	1.30
2	C	501	C2I	O2A-C2A	2.30	1.48	1.43
2	D	501	C2I	C41-N31	-2.29	1.33	1.37
2	D	501	C2I	O2A-C2A	2.29	1.48	1.43
2	B	501	C2I	O2A-C2A	2.26	1.48	1.43
2	B	501	C2I	C41-N31	-2.24	1.33	1.37
2	C	501	C2I	C5'-C4'	2.18	1.58	1.51
2	C	501	C2I	C41-N31	-2.09	1.34	1.37
2	A	501	C2I	C5A-C4A	2.08	1.58	1.51
2	A	501	C2I	O2A-C2A	2.04	1.47	1.43
2	D	501	C2I	P1-O2P	2.03	1.58	1.50
2	C	501	C2I	O2'-C2'	2.03	1.47	1.43
2	D	501	C2I	C6-N1	-2.01	1.34	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	C2I	P1-O3A-C3A	4.63	136.25	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	C2I	C3A-C2A-C1A	4.35	109.53	99.89
2	B	501	C2I	P1-O3A-C3A	4.23	134.79	119.41
2	A	501	C2I	C2'-C3'-C4'	4.20	110.67	103.22
2	C	501	C2I	O1P-P1-O3A	4.05	122.77	106.78
2	D	501	C2I	P1-O3A-C3A	3.94	133.76	119.41
2	B	501	C2I	C2'-C3'-C4'	3.80	109.95	103.22
2	C	501	C2I	O5A-C5A-C4A	-3.64	96.46	108.99
2	C	501	C2I	P1-O3A-C3A	3.63	132.61	119.41
2	B	501	C2I	O4A-C4A-C3A	-3.59	97.18	104.87
2	B	501	C2I	O5'-P1-O2P	-3.56	95.17	109.07
2	C	501	C2I	O3A-P1-O2P	-3.37	96.82	109.47
2	A	501	C2I	C8-N7-C5	3.30	109.28	102.99
2	A	501	C2I	O3A-C3A-C2A	3.16	123.15	111.68
2	D	501	C2I	C2'-C3'-C4'	3.14	108.80	103.22
2	B	501	C2I	N3-C2-N1	-3.07	118.45	125.84
2	D	501	C2I	O3A-C3A-C2A	3.03	122.66	111.68
2	A	501	C2I	C3A-C2A-C1A	3.02	106.59	99.89
2	B	501	C2I	C2-N1-C6	3.01	124.33	116.25
2	C	501	C2I	C8-N7-C5	3.01	108.72	102.99
2	C	501	C2I	C2-N1-C6	2.96	124.18	116.25
2	B	501	C2I	C8-N7-C5	2.94	108.60	102.99
2	C	501	C2I	O3A-C3A-C4A	-2.89	99.63	110.08
2	C	501	C2I	C2'-C3'-C4'	2.84	108.25	103.22
2	A	501	C2I	O2'-C2'-C1'	2.78	121.11	110.85
2	C	501	C2I	N3-C2-N1	-2.70	119.34	125.84
2	D	501	C2I	C2-N1-C6	2.67	123.43	116.25
2	C	501	C2I	O4A-C1A-C2A	-2.67	103.02	106.93
2	D	501	C2I	C8-N7-C5	2.63	107.99	102.99
2	D	501	C2I	O5A-C5A-C4A	-2.55	100.20	108.99
2	B	501	C2I	O3A-C3A-C2A	2.54	120.90	111.68
2	B	501	C2I	O1P-P1-O3A	2.52	116.71	106.78
2	D	501	C2I	N3-C2-N1	-2.51	119.81	125.84
2	D	501	C2I	C3A-C2A-C1A	2.49	105.41	99.89
2	B	501	C2I	C81-N71-C51	2.44	107.64	102.99
2	C	501	C2I	C4-C5-C6	-2.40	115.83	121.16
2	D	501	C2I	C4-C5-C6	-2.40	115.83	121.16
2	A	501	C2I	O11-P11-O5A	2.40	118.89	107.75
2	A	501	C2I	N3-C2-N1	-2.38	120.12	125.84
2	B	501	C2I	C3A-C2A-C1A	2.36	105.12	99.89
2	A	501	C2I	C2-N1-C6	2.33	122.50	116.25
2	B	501	C2I	O11-P11-O5A	2.28	118.33	107.75
2	B	501	C2I	C4-C5-C6	-2.20	116.29	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	C2I	O3'-P11-O21	-2.19	101.24	109.47
2	C	501	C2I	O3'-C3'-C2'	-2.16	103.85	111.68
2	B	501	C2I	O3A-P1-O2P	-2.08	101.67	109.47
2	B	501	C2I	O3'-C3'-C2'	-2.01	104.41	111.68

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	C2I	C2A-C3A-O3A-P1
2	A	501	C2I	C4'-C5'-O5'-P1
2	A	501	C2I	C5'-O5'-P1-O1P
2	A	501	C2I	C5'-O5'-P1-O2P
2	A	501	C2I	C5'-O5'-P1-O3A
2	B	501	C2I	C5'-O5'-P1-O2P
2	B	501	C2I	C5A-O5A-P11-O21
2	B	501	C2I	C5A-O5A-P11-O3'
2	C	501	C2I	C3A-O3A-P1-O1P
2	C	501	C2I	C5'-O5'-P1-O1P
2	C	501	C2I	C5'-O5'-P1-O2P
2	C	501	C2I	C5A-O5A-P11-O21
2	D	501	C2I	C2A-C3A-O3A-P1
2	D	501	C2I	C5A-O5A-P11-O3'
2	B	501	C2I	C2A-C3A-O3A-P1
2	A	501	C2I	C3A-O3A-P1-O5'
2	B	501	C2I	C4A-C3A-O3A-P1
2	B	501	C2I	C5'-O5'-P1-O3A
2	C	501	C2I	C5'-O5'-P1-O3A
2	D	501	C2I	C5'-O5'-P1-O3A
2	C	501	C2I	C3A-O3A-P1-O5'
2	D	501	C2I	C3A-O3A-P1-O5'
2	A	501	C2I	C5A-O5A-P11-O3'
2	C	501	C2I	C5A-O5A-P11-O3'
2	B	501	C2I	C4'-C5'-O5'-P1
2	C	501	C2I	C4'-C5'-O5'-P1
2	D	501	C2I	C4'-C5'-O5'-P1
2	C	501	C2I	C3A-O3A-P1-O2P
2	B	501	C2I	C4A-C5A-O5A-P11
2	D	501	C2I	C4A-C5A-O5A-P11
2	A	501	C2I	C5A-O5A-P11-O21
2	B	501	C2I	C5'-O5'-P1-O1P
2	B	501	C2I	C5A-O5A-P11-O11

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Mol	Chain	Res	Type	Atoms
2	D	501	C2I	C5'-O5'-P1-O1P
2	D	501	C2I	C5'-O5'-P1-O2P
2	D	501	C2I	C5A-O5A-P11-O11
2	D	501	C2I	C5A-O5A-P11-O21
2	A	501	C2I	C3'-C4'-C5'-O5'
2	A	501	C2I	O4'-C4'-C5'-O5'
2	A	501	C2I	C4A-C5A-O5A-P11
2	A	501	C2I	C3A-O3A-P1-O1P
2	C	501	C2I	C3A-C4A-C5A-O5A
2	B	501	C2I	C3A-O3A-P1-O5'
2	A	501	C2I	C3A-C4A-C5A-O5A

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	C2I	4	0
2	A	501	C2I	3	0
2	C	501	C2I	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 then 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 C2I D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand C2I A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand C2I B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand C2I C 501

Bond lengths

Bond angles

Torsions

Rings
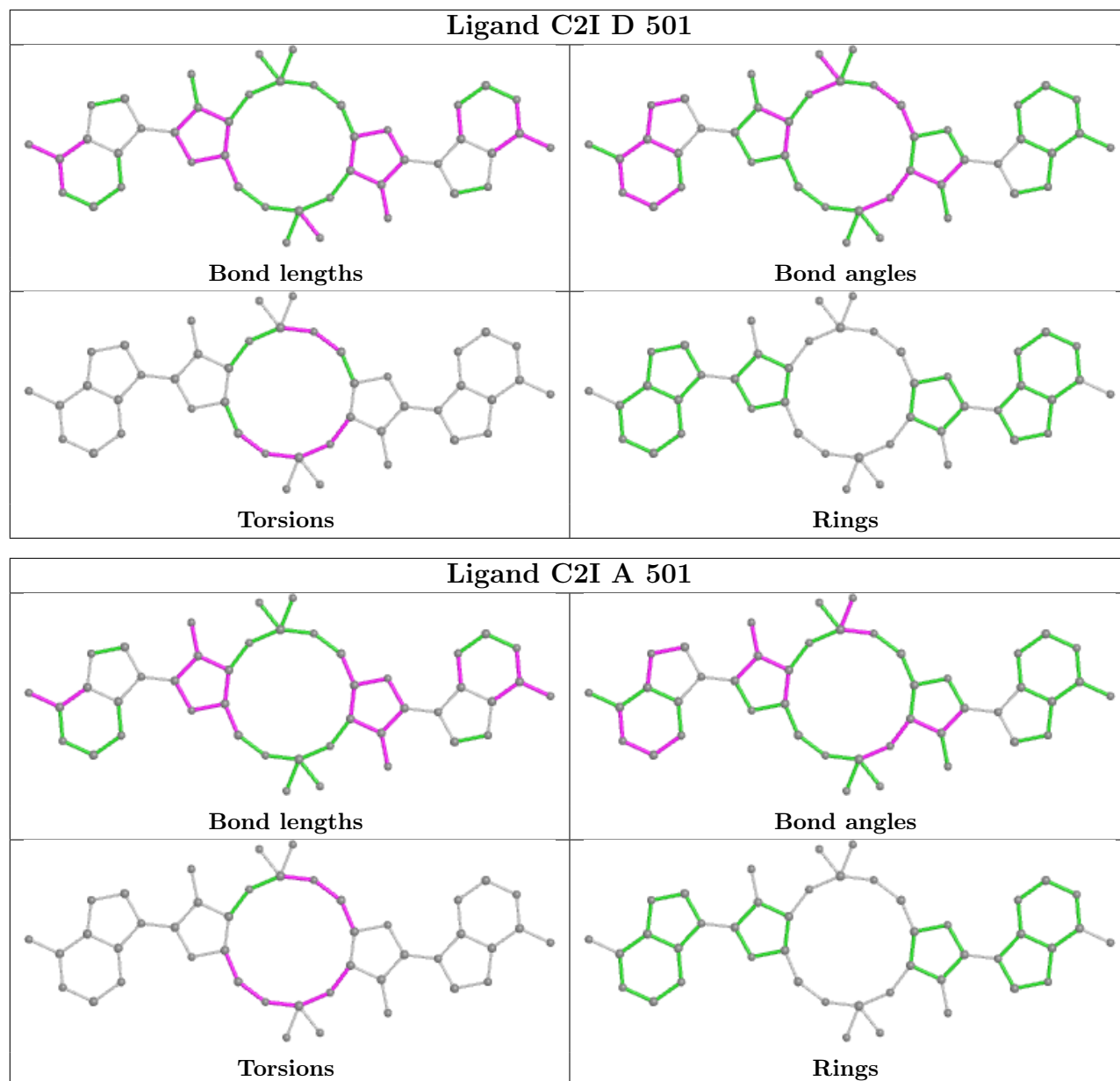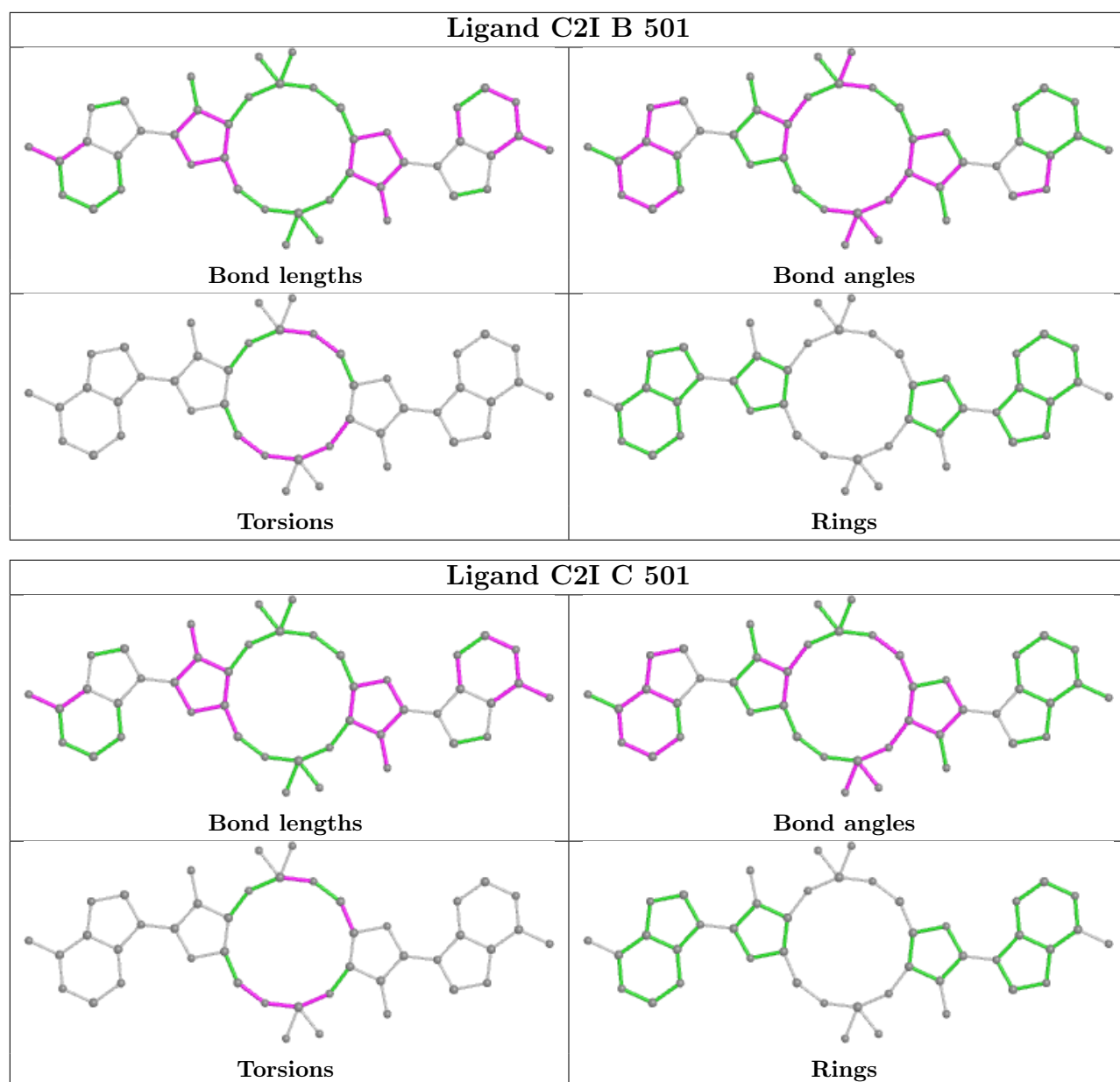
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	237/257 (92%)	0.66	29 (12%)	4	3	18, 32, 109, 142	0
1	B	237/257 (92%)	0.66	29 (12%)	4	3	21, 31, 110, 142	0
1	C	237/257 (92%)	0.42	20 (8%)	11	9	18, 32, 106, 153	0
1	D	237/257 (92%)	0.51	25 (10%)	6	5	20, 34, 108, 143	0
All	All	948/1028 (92%)	0.56	103 (10%)	5	5	18, 33, 109, 153	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	ILE	17.0
1	B	101	ILE	10.5
1	B	102	TYR	10.1
1	B	135	VAL	9.9
1	B	257	ALA	8.4
1	A	102	TYR	8.0
1	A	100	ALA	7.3
1	D	257	ALA	7.0
1	C	100	ALA	6.9
1	B	100	ALA	6.9
1	D	103	VAL	6.8
1	A	135	VAL	6.7
1	C	104	PRO	6.7
1	D	104	PRO	6.5
1	D	102	TYR	6.4
1	A	69	TYR	6.3
1	A	257	ALA	6.3
1	A	134	ARG	6.1
1	C	103	VAL	5.7
1	B	69	TYR	5.6
1	C	164	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	69	TYR	5.3
1	B	136	GLU	5.3
1	A	132	ALA	5.1
1	A	106	ARG	5.1
1	B	163	GLY	4.9
1	A	138	VAL	4.9
1	B	98	PRO	4.8
1	C	102	TYR	4.7
1	A	163	GLY	4.7
1	A	103	VAL	4.6
1	D	135	VAL	4.6
1	B	164	TYR	4.6
1	A	24	PHE	4.4
1	C	132	ALA	4.3
1	C	137	ASP	4.2
1	A	99	ASN	4.2
1	D	163	GLY	4.1
1	A	255	SER	4.1
1	B	134	ARG	4.0
1	A	140	HIS	3.9
1	B	103	VAL	3.9
1	A	133	GLU	3.8
1	D	101	ILE	3.8
1	C	134	ARG	3.8
1	B	104	PRO	3.8
1	C	163	GLY	3.7
1	C	135	VAL	3.7
1	A	22	LEU	3.6
1	B	99	ASN	3.6
1	B	254	PHE	3.4
1	A	68	ARG	3.2
1	C	136	GLU	3.1
1	C	24	PHE	3.1
1	B	50	GLY	3.1
1	D	255	SER	3.0
1	C	99	ASN	3.0
1	B	253	GLU	3.0
1	D	164	TYR	3.0
1	A	164	TYR	3.0
1	B	105	GLU	2.9
1	B	256	GLU	2.9
1	C	21	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	98	PRO	2.8
1	D	132	ALA	2.8
1	B	255	SER	2.8
1	D	66	ASP	2.8
1	A	131	GLU	2.7
1	D	131	GLU	2.7
1	D	136	GLU	2.7
1	B	106	ARG	2.7
1	C	107	CYS	2.6
1	A	51	LEU	2.6
1	D	134	ARG	2.6
1	C	106	ARG	2.6
1	B	132	ALA	2.6
1	D	137	ASP	2.6
1	A	21	SER	2.5
1	A	104	PRO	2.5
1	B	73	GLN	2.5
1	B	138	VAL	2.5
1	D	57	TYR	2.3
1	C	109	ARG	2.3
1	D	108	ILE	2.3
1	D	140	HIS	2.3
1	D	253	GLU	2.3
1	A	256	GLU	2.2
1	A	52	ASN	2.2
1	B	137	ASP	2.2
1	C	67	ASN	2.2
1	B	22	LEU	2.2
1	D	256	GLU	2.2
1	D	24	PHE	2.2
1	B	97	LEU	2.2
1	B	109	ARG	2.1
1	D	22	LEU	2.1
1	D	99	ASN	2.1
1	A	139	ASN	2.1
1	C	131	GLU	2.1
1	A	105	GLU	2.1
1	D	119	GLN	2.1
1	B	133	GLU	2.1
1	C	133	GLU	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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
3	CA	C	503	1/1	0.80	0.17	54,54,54,54	0
3	CA	B	503	1/1	0.81	0.23	94,94,94,94	0
3	CA	D	503	1/1	0.89	0.14	65,65,65,65	0
3	CA	A	502	1/1	0.94	0.06	24,24,24,24	0
2	C2I	B	501	44/44	0.94	0.14	25,31,38,40	0
2	C2I	C	501	44/44	0.95	0.13	23,30,40,50	0
2	C2I	D	501	44/44	0.95	0.15	28,35,46,54	0
2	C2I	A	501	44/44	0.96	0.13	24,31,38,40	0
3	CA	A	503	1/1	0.97	0.14	51,51,51,51	0
3	CA	D	502	1/1	0.98	0.05	27,27,27,27	0
3	CA	B	502	1/1	0.98	0.04	21,21,21,21	0
3	CA	C	502	1/1	0.99	0.08	26,26,26,26	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.
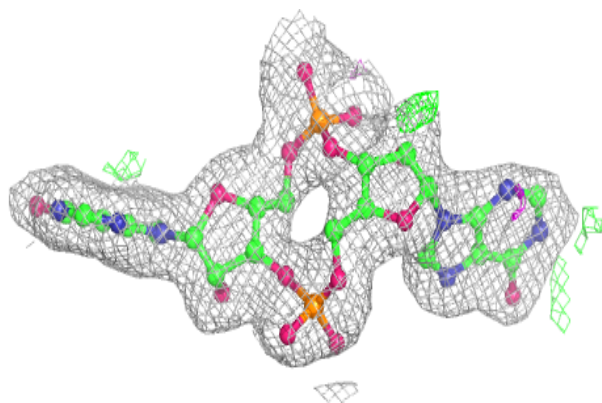
Electron density around CA C 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
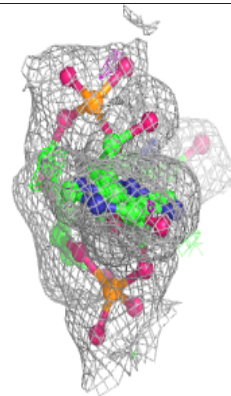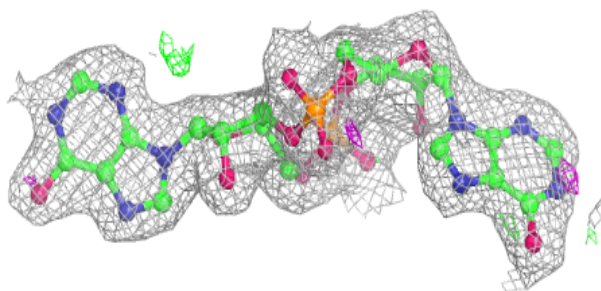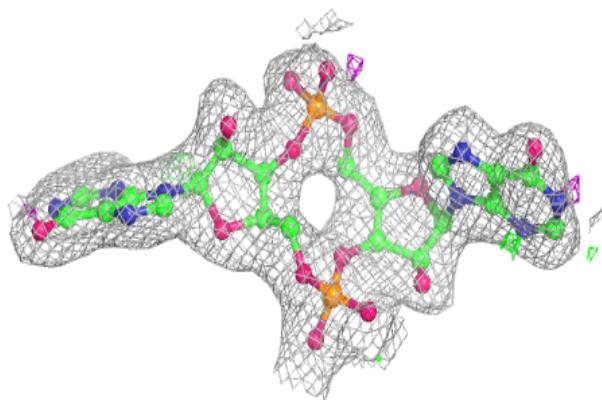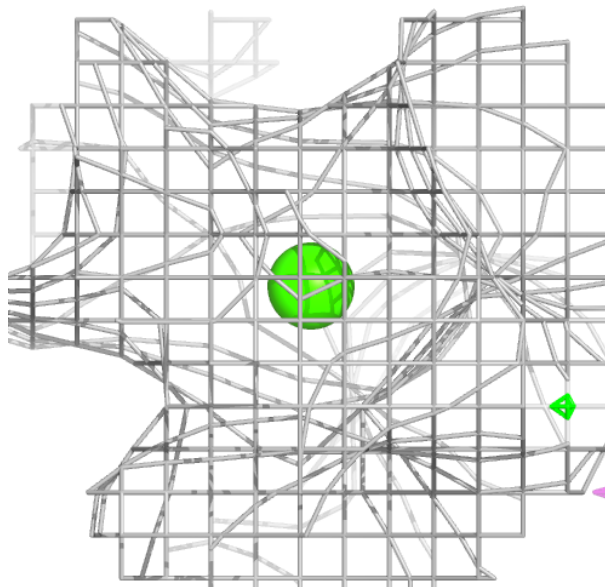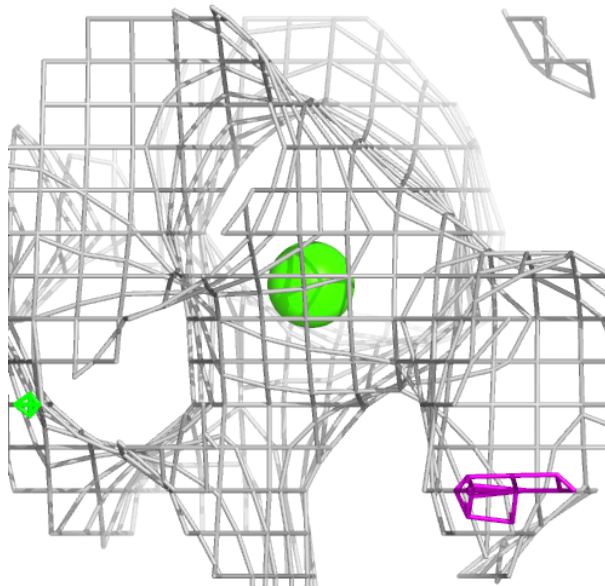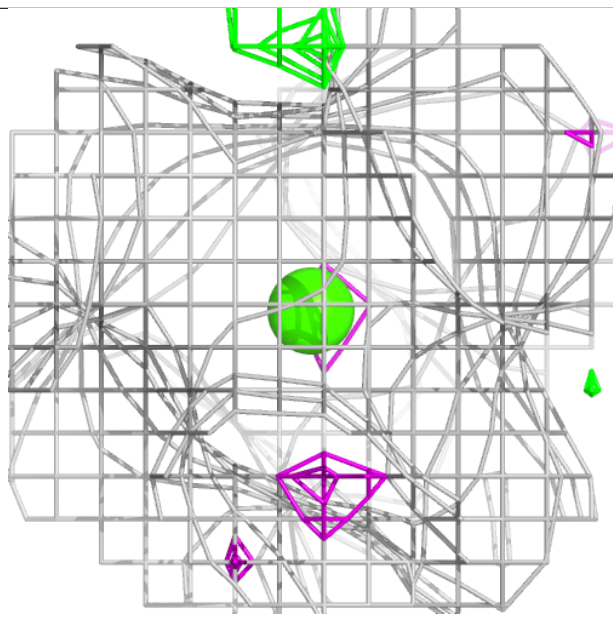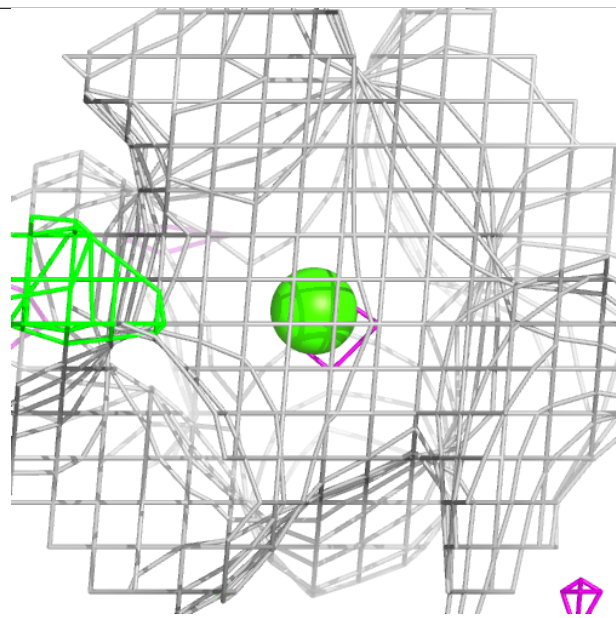mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
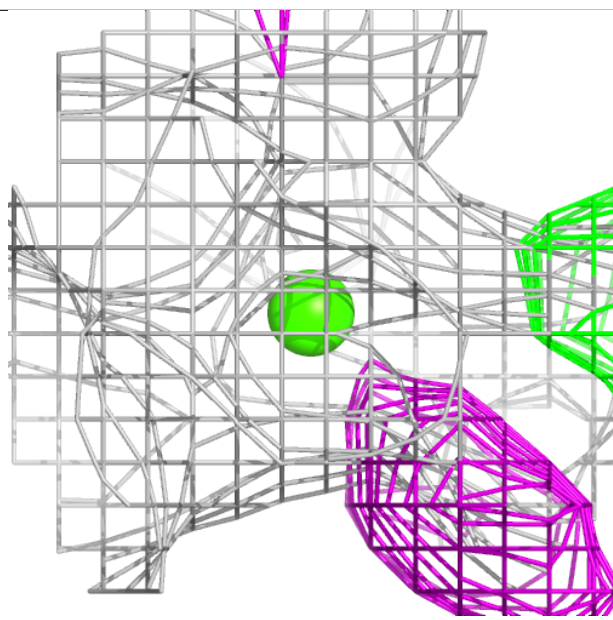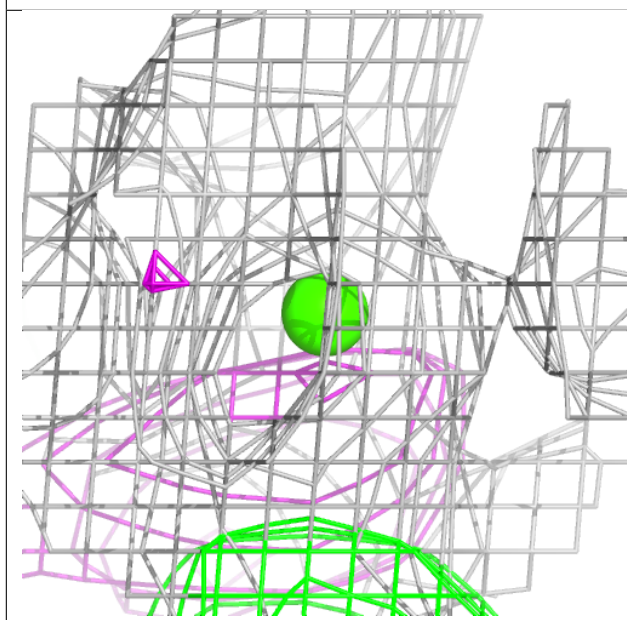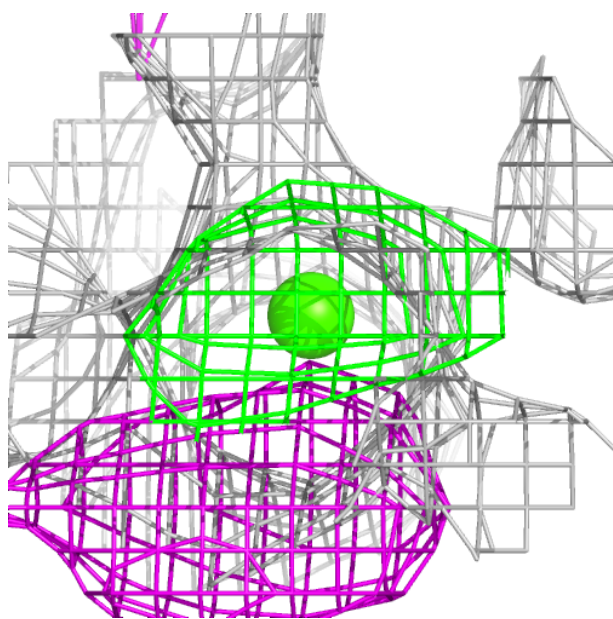
Electron density around CA B 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
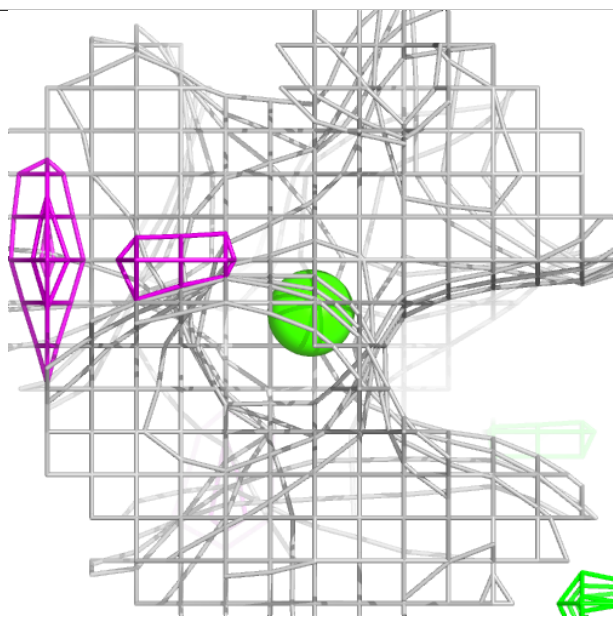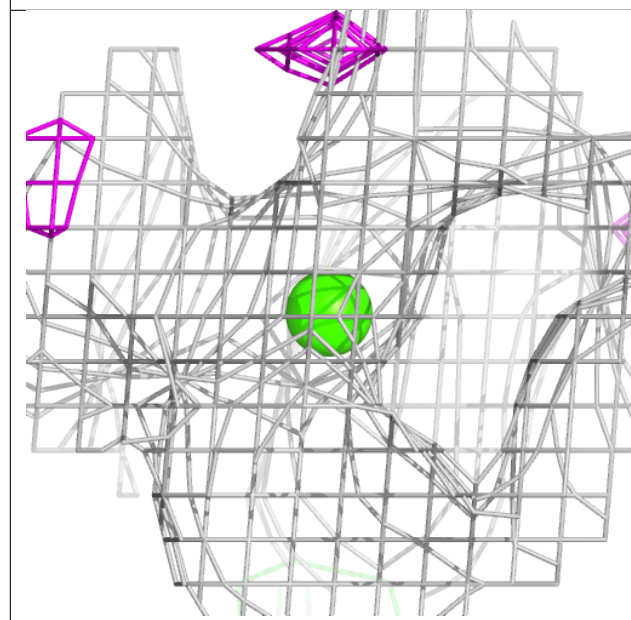
Electron density around CA D 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
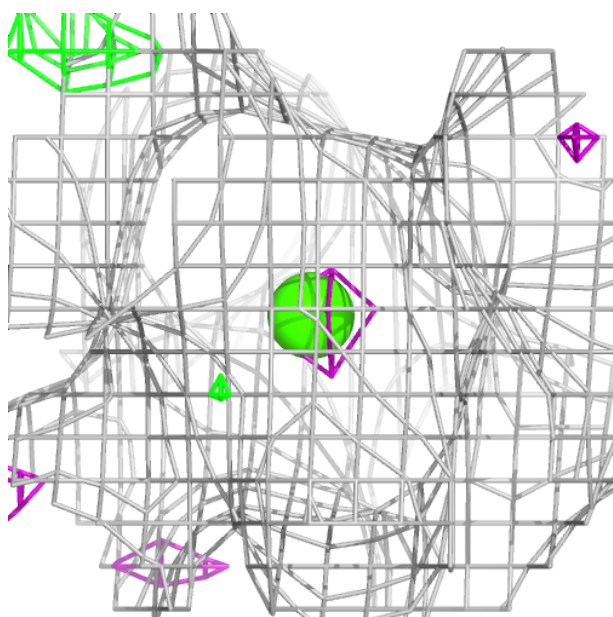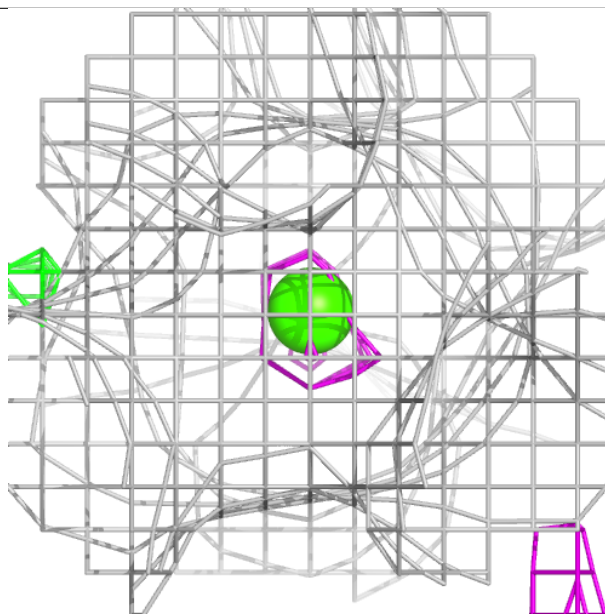and green (positive)
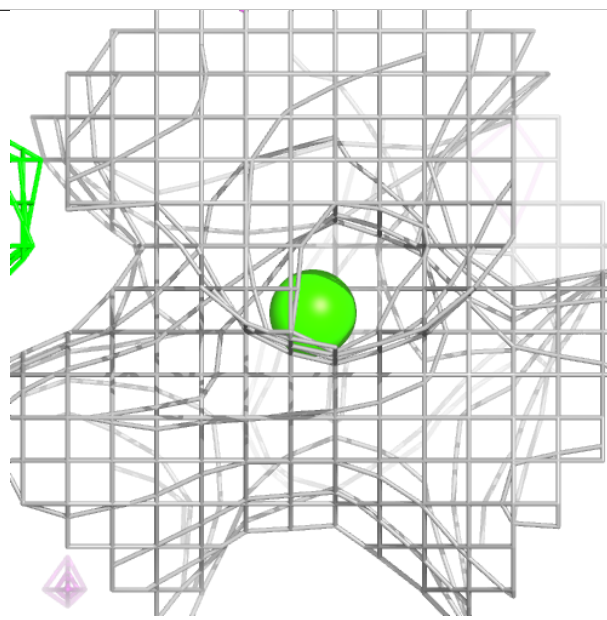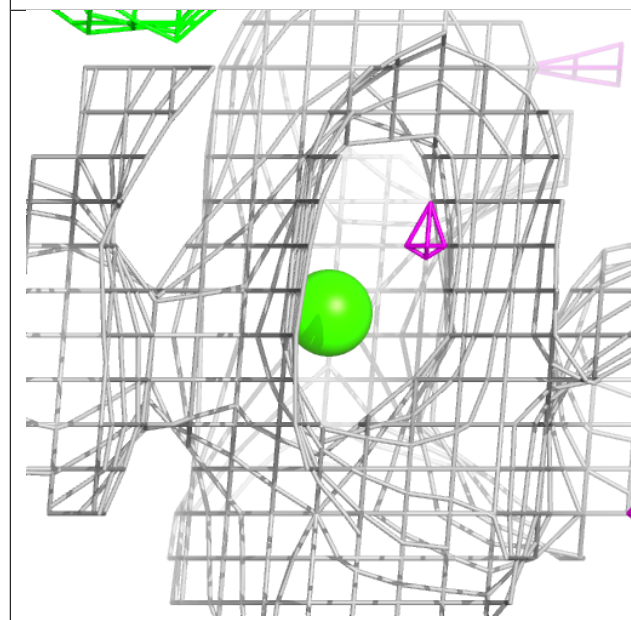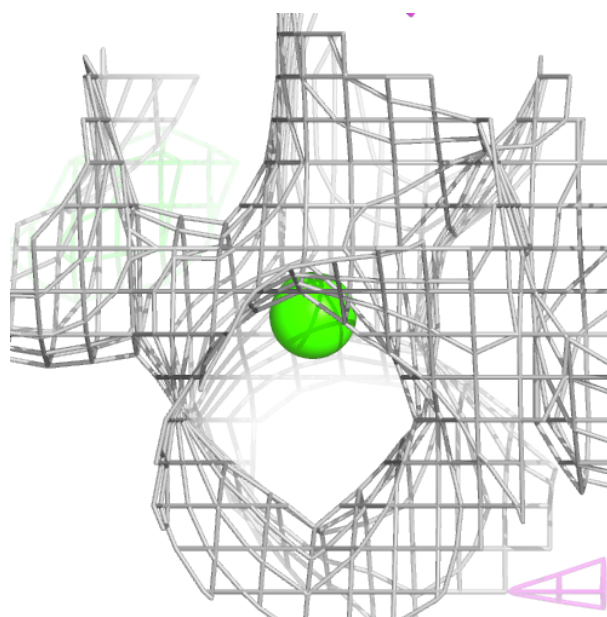
Electron density around CA A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
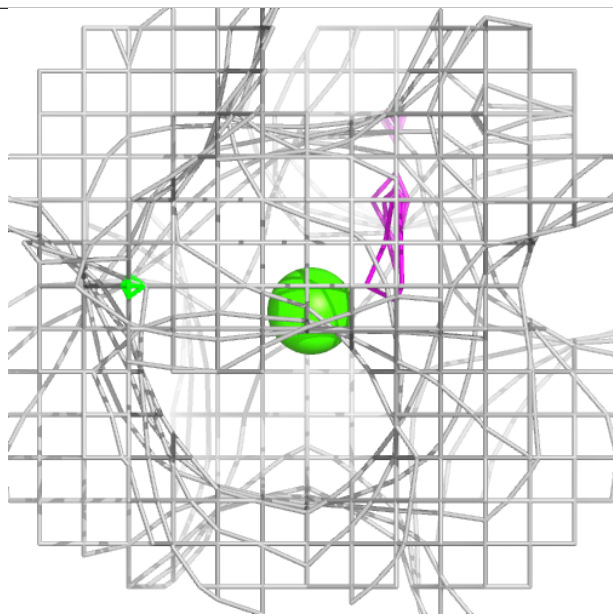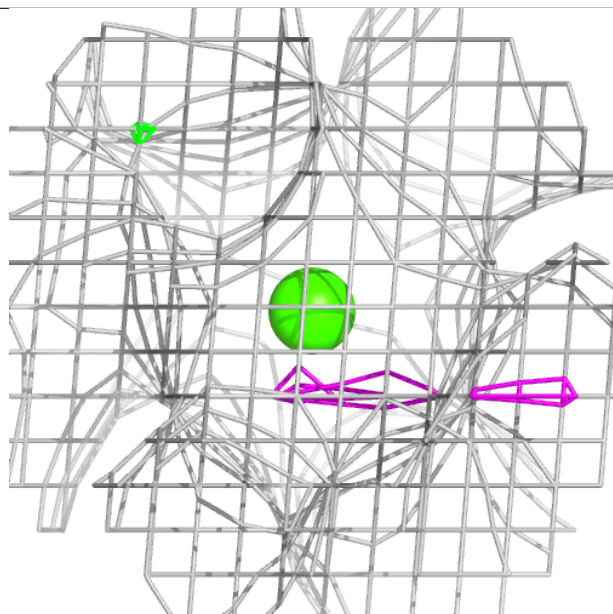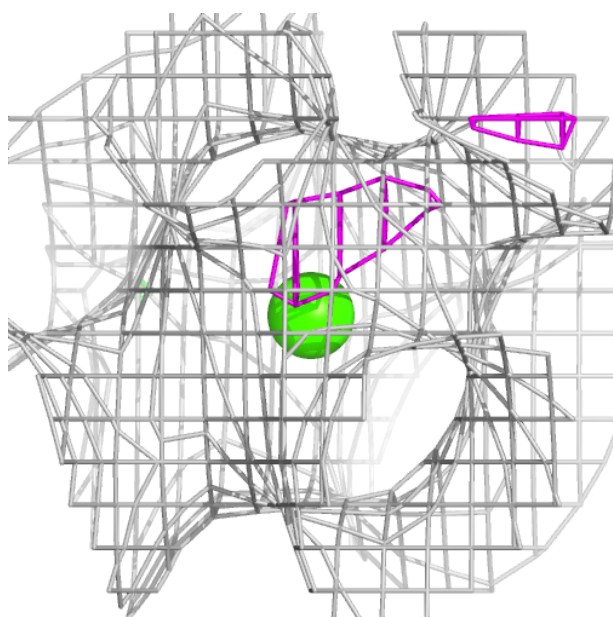
Electron density around C2I B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
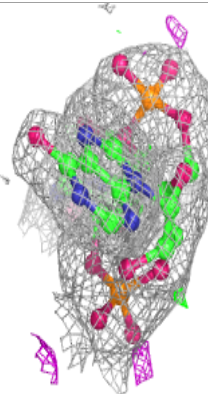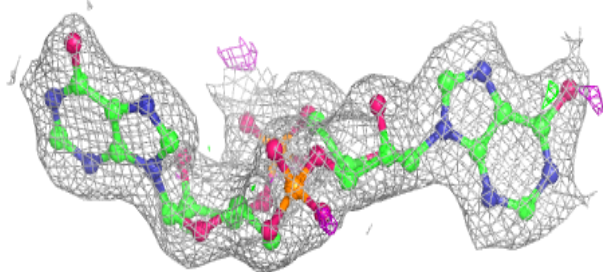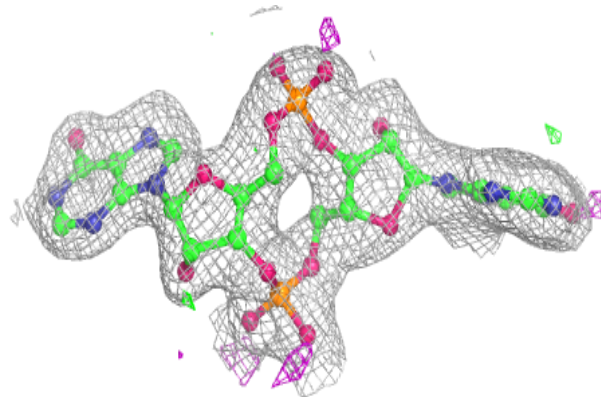
Electron density around C2I C 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
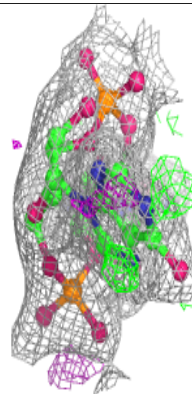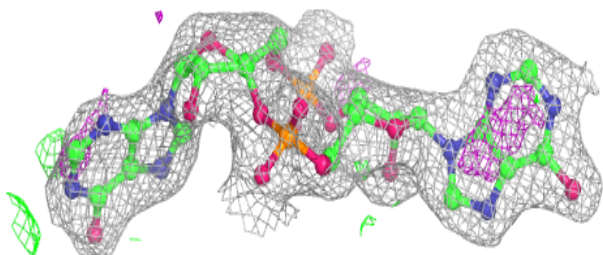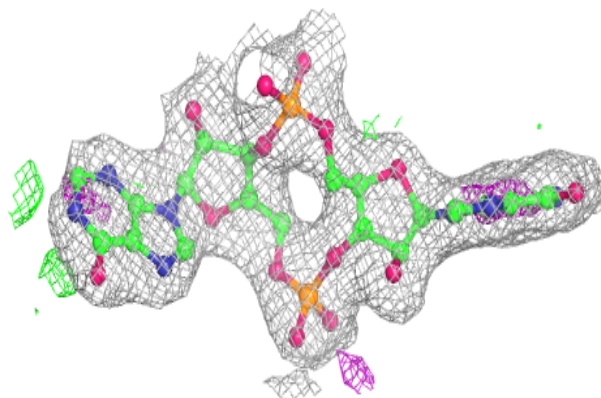
Electron density around C2I D 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
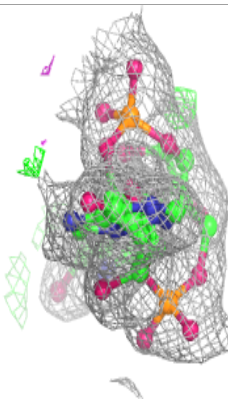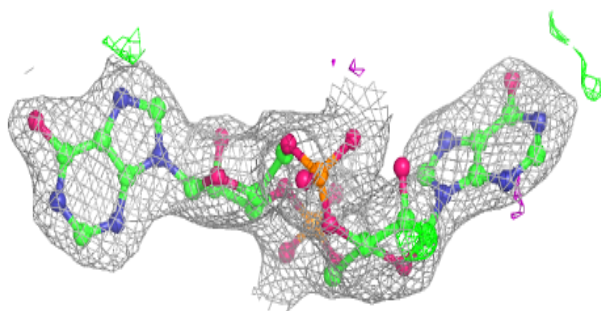
Electron density around C2I A 501:

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 CA A 503:

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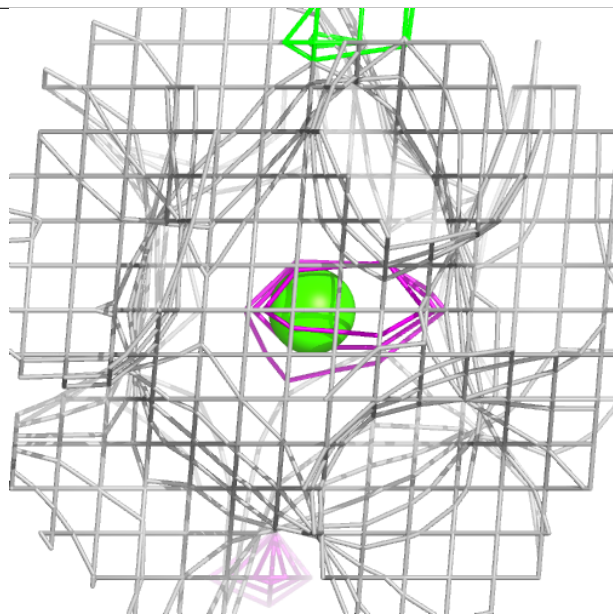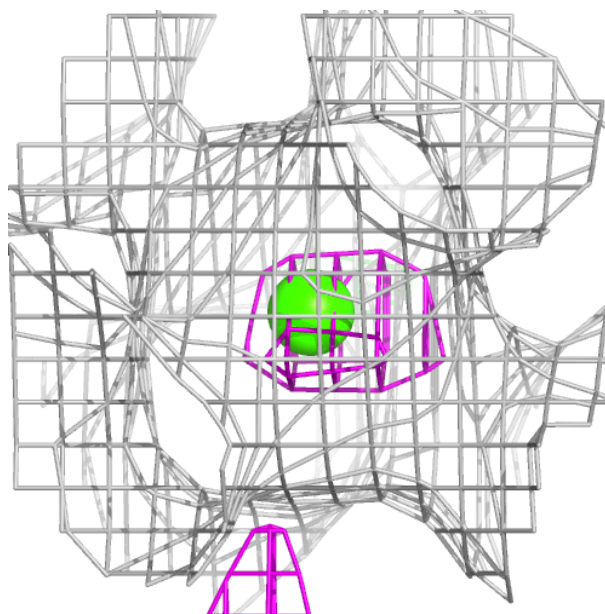mF_o-DF_c (at 3 rmsd) in purple (negative)
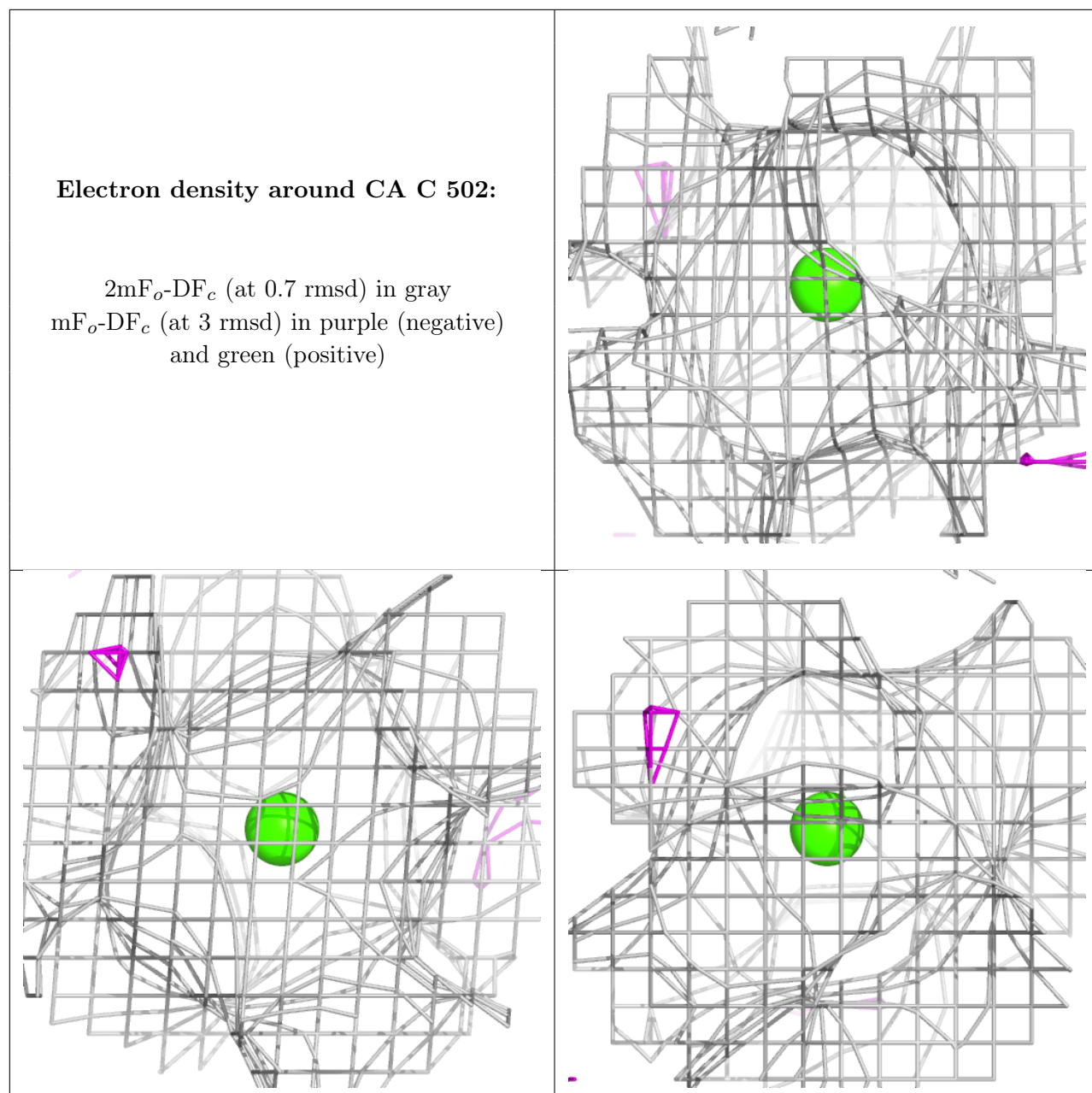and green (positive)

Electron density around CA D 502:

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

Electron density around CA B 502:

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

Electron density around CA C 502:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.