Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 09:34 PM EST

PDB ID	:	4I02
Title	:	structure of the mutant Catabolite gene activator protein V140A
Authors	:	Pohl, E.; Townsend, P.D.; Rodgers, T.; Burnell, D.; McLeish, T.C.B.; Wilson, M.R.; Cann, M.J.
Deposited on	:	2012-11-16
Resolution	:	1.75 Å(reported)

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

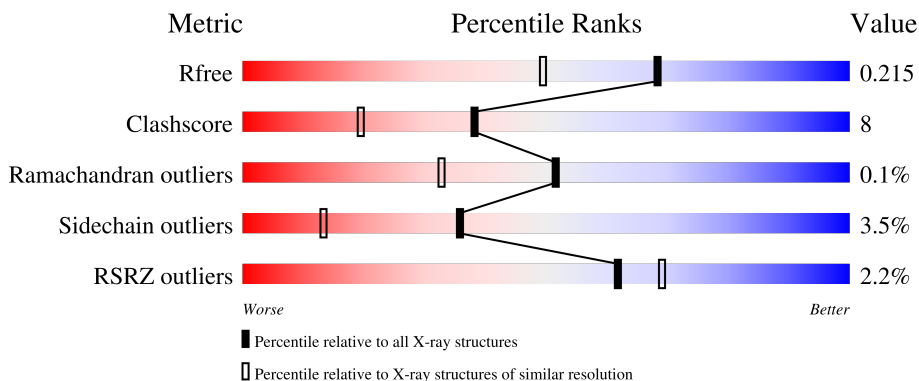|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.75 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		0.215
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		3.5%
RSRZ outliers		2.2%

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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	222	2% / 77% / 13% · 8%
1	B	222	% / 83% / 8% · 7%
1	C	222	% / 82% / 8% · 9%
1	D	222	3% / 82% / 11% · 7%
1	E	222	2% / 81% / 7% · 9%

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Mol	Chain	Length	Quality of chain
1	F	222	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10622 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 Catabolite gene activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	2	0
			1600	1015	279	297	9			
1	B	206	Total	C	N	O	S	0	1	0
			1611	1021	279	301	10			
1	C	201	Total	C	N	O	S	0	0	0
			1561	989	275	288	9			
1	D	207	Total	C	N	O	S	0	1	0
			1613	1021	279	303	10			
1	E	201	Total	C	N	O	S	0	1	0
			1558	987	273	289	9			
1	F	201	Total	C	N	O	S	0	0	0
			1554	985	273	287	9			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P0ACJ8
A	-10	ARG	-	expression tag	UNP P0ACJ8
A	-9	GLY	-	expression tag	UNP P0ACJ8
A	-8	SER	-	expression tag	UNP P0ACJ8
A	-7	HIS	-	expression tag	UNP P0ACJ8
A	-6	HIS	-	expression tag	UNP P0ACJ8
A	-5	HIS	-	expression tag	UNP P0ACJ8
A	-4	HIS	-	expression tag	UNP P0ACJ8
A	-3	HIS	-	expression tag	UNP P0ACJ8
A	-2	HIS	-	expression tag	UNP P0ACJ8
A	-1	GLY	-	expression tag	UNP P0ACJ8
A	0	SER	-	expression tag	UNP P0ACJ8
A	140	ALA	VAL	engineered mutation	UNP P0ACJ8
B	-11	MET	-	expression tag	UNP P0ACJ8
B	-10	ARG	-	expression tag	UNP P0ACJ8
B	-9	GLY	-	expression tag	UNP P0ACJ8
B	-8	SER	-	expression tag	UNP P0ACJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP P0ACJ8
B	-6	HIS	-	expression tag	UNP P0ACJ8
B	-5	HIS	-	expression tag	UNP P0ACJ8
B	-4	HIS	-	expression tag	UNP P0ACJ8
B	-3	HIS	-	expression tag	UNP P0ACJ8
B	-2	HIS	-	expression tag	UNP P0ACJ8
B	-1	GLY	-	expression tag	UNP P0ACJ8
B	0	SER	-	expression tag	UNP P0ACJ8
B	140	ALA	VAL	engineered mutation	UNP P0ACJ8
C	-11	MET	-	expression tag	UNP P0ACJ8
C	-10	ARG	-	expression tag	UNP P0ACJ8
C	-9	GLY	-	expression tag	UNP P0ACJ8
C	-8	SER	-	expression tag	UNP P0ACJ8
C	-7	HIS	-	expression tag	UNP P0ACJ8
C	-6	HIS	-	expression tag	UNP P0ACJ8
C	-5	HIS	-	expression tag	UNP P0ACJ8
C	-4	HIS	-	expression tag	UNP P0ACJ8
C	-3	HIS	-	expression tag	UNP P0ACJ8
C	-2	HIS	-	expression tag	UNP P0ACJ8
C	-1	GLY	-	expression tag	UNP P0ACJ8
C	0	SER	-	expression tag	UNP P0ACJ8
C	140	ALA	VAL	engineered mutation	UNP P0ACJ8
D	-11	MET	-	expression tag	UNP P0ACJ8
D	-10	ARG	-	expression tag	UNP P0ACJ8
D	-9	GLY	-	expression tag	UNP P0ACJ8
D	-8	SER	-	expression tag	UNP P0ACJ8
D	-7	HIS	-	expression tag	UNP P0ACJ8
D	-6	HIS	-	expression tag	UNP P0ACJ8
D	-5	HIS	-	expression tag	UNP P0ACJ8
D	-4	HIS	-	expression tag	UNP P0ACJ8
D	-3	HIS	-	expression tag	UNP P0ACJ8
D	-2	HIS	-	expression tag	UNP P0ACJ8
D	-1	GLY	-	expression tag	UNP P0ACJ8
D	0	SER	-	expression tag	UNP P0ACJ8
D	140	ALA	VAL	engineered mutation	UNP P0ACJ8
E	-11	MET	-	expression tag	UNP P0ACJ8
E	-10	ARG	-	expression tag	UNP P0ACJ8
E	-9	GLY	-	expression tag	UNP P0ACJ8
E	-8	SER	-	expression tag	UNP P0ACJ8
E	-7	HIS	-	expression tag	UNP P0ACJ8
E	-6	HIS	-	expression tag	UNP P0ACJ8
E	-5	HIS	-	expression tag	UNP P0ACJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP P0ACJ8
E	-3	HIS	-	expression tag	UNP P0ACJ8
E	-2	HIS	-	expression tag	UNP P0ACJ8
E	-1	GLY	-	expression tag	UNP P0ACJ8
E	0	SER	-	expression tag	UNP P0ACJ8
E	140	ALA	VAL	engineered mutation	UNP P0ACJ8
F	-11	MET	-	expression tag	UNP P0ACJ8
F	-10	ARG	-	expression tag	UNP P0ACJ8
F	-9	GLY	-	expression tag	UNP P0ACJ8
F	-8	SER	-	expression tag	UNP P0ACJ8
F	-7	HIS	-	expression tag	UNP P0ACJ8
F	-6	HIS	-	expression tag	UNP P0ACJ8
F	-5	HIS	-	expression tag	UNP P0ACJ8
F	-4	HIS	-	expression tag	UNP P0ACJ8
F	-3	HIS	-	expression tag	UNP P0ACJ8
F	-2	HIS	-	expression tag	UNP P0ACJ8
F	-1	GLY	-	expression tag	UNP P0ACJ8
F	0	SER	-	expression tag	UNP P0ACJ8
F	140	ALA	VAL	engineered mutation	UNP P0ACJ8

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).
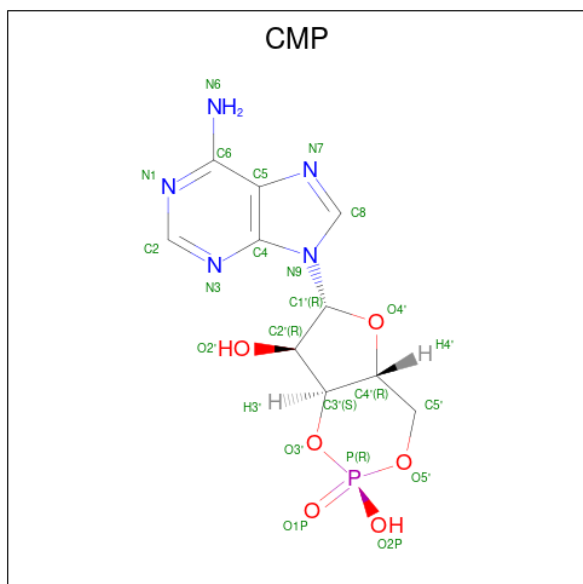
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	22	10	5	6	1	0	0

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total 22	C 10	N 5	O 6	P 1			0	0
2	B	1	Total 22	C 10	N 5	O 6	P 1			0	0
2	B	1	Total 22	C 10	N 5	O 6	P 1			0	0
2	C	1	Total 22	C 10	N 5	O 6	P 1			0	0
2	D	1	Total 22	C 10	N 5	O 6	P 1			0	0
2	D	1	Total 22	C 10	N 5	O 6	P 1			0	0
2	E	1	Total 22	C 10	N 5	O 6	P 1			0	0
2	F	1	Total 22	C 10	N 5	O 6	P 1			0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total 157	O 157	0	0
3	B	157	Total 157	O 157	0	0
3	C	149	Total 149	O 149	0	0
3	D	155	Total 155	O 155	0	0
3	E	152	Total 152	O 152	0	0
3	F	157	Total 157	O 157	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.
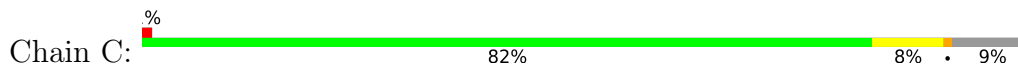
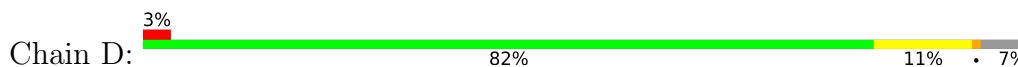• Molecule 1: Catabolite gene activator
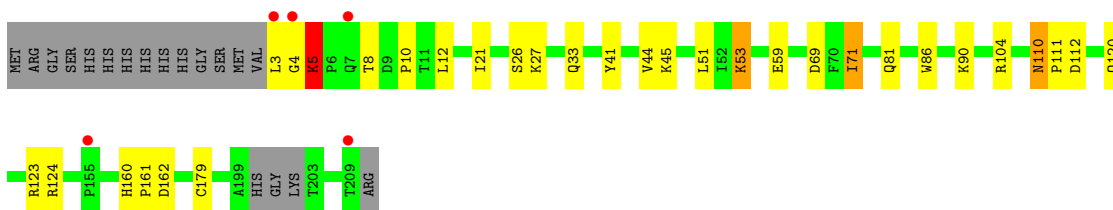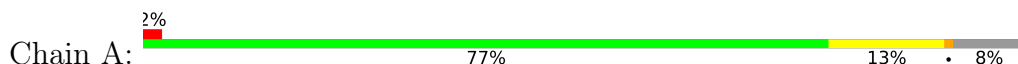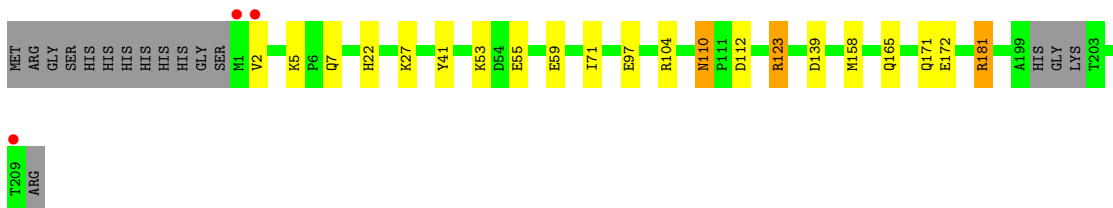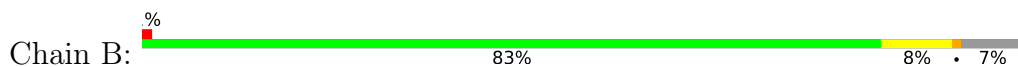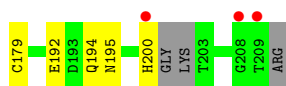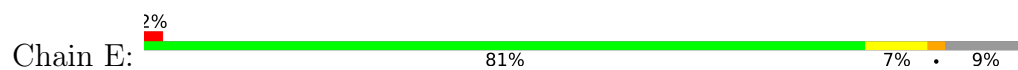
Chain A:

• Molecule 1: Catabolite gene activator

Chain B:

• Molecule 1: Catabolite gene activator

Chain C:

• Molecule 1: Catabolite gene activator

Chain D:

C179 E192 D193 Q194 N195 H200 GLY LYS T203 G208 T209 ARG

• Molecule 1: Catabolite gene activator

Chain E:

2%

81% 7% • 9%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET VAL LEU GLY LYS PRO GLN THR D9 P10 K27 L30 M60 N66 I71 V95 F103 R104 I107 Q108 V109 N110 P111 R123 Q126 Q154 M158 T159 H160 P161 D162 R170 R181

A199 H200 G201 T209 ARG

• Molecule 1: Catabolite gene activator

Chain F:

2%

80% 10% • 9%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET VAL LEU GLY LYS PRO GLN THR D9 P10 T11 L12 H20 Y24 N66 I71 W86 C93 K102 Q108 V109 N110 M121 A122 R123 K131 L149 Q154 P161 Q165 I166 K167 Q171

R181 K189 A199 T203 V206 T209 ARG
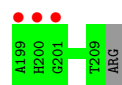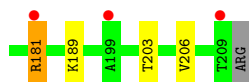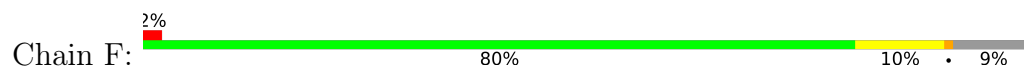
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.26Å 50.19Å 276.32Å 90.00° 94.48° 90.00°	Depositor
Resolution (Å)	48.32 – 1.75 48.32 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.32-1.75) 99.5 (48.32-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.185 , 0.216 0.185 , 0.215	Depositor DCC
R_{free} test set	7906 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10622	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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 54.44 % 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 3.6532e-05. 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: CMP

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	0.64	0/1630	0.73	1/2198 (0.0%)
1	B	0.63	0/1638	0.71	1/2210 (0.0%)
1	C	0.63	1/1586 (0.1%)	0.70	0/2141
1	D	0.60	1/1641 (0.1%)	0.70	1/2217 (0.0%)
1	E	0.62	0/1585	0.71	1/2141 (0.0%)
1	F	0.62	1/1578 (0.1%)	0.72	1/2130 (0.0%)
All	All	0.63	3/9658 (0.0%)	0.71	5/13037 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	86	TRP	CD2-CE2	5.28	1.47	1.41
1	D	14	TRP	CD2-CE2	5.03	1.47	1.41
1	C	14	TRP	CD2-CE2	5.02	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	F	121	MET	CG-SD-CE	-6.88	89.19	100.20
1	D	179	CYS	CA-CB-SG	-5.32	104.42	114.00
1	B	139	ASP	CB-CG-OD1	5.30	123.07	118.30

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	CYS	CA-CB-SG	-5.29	104.48	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	LEU	Peptide

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	1600	0	1629	35	0
1	B	1611	0	1640	29	0
1	C	1561	0	1580	21	0
1	D	1613	0	1623	22	0
1	E	1558	0	1572	18	0
1	F	1554	0	1570	17	0
2	A	44	0	22	3	0
2	B	44	0	22	5	0
2	C	22	0	11	1	0
2	D	44	0	22	7	0
2	E	22	0	11	1	0
2	F	22	0	11	1	0
3	A	157	0	0	6	0
3	B	157	0	0	6	0
3	C	149	0	0	6	0
3	D	155	0	0	5	1
3	E	152	0	0	4	0
3	F	157	0	0	8	1
All	All	10622	0	9713	147	1

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 8.

All (147) 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)
2:B:302:CMP:H2	2:B:302:CMP:C2	0.97	1.50
2:A:302:CMP:H2	2:A:302:CMP:C2	0.97	1.50
2:D:302:CMP:H2	2:D:302:CMP:C2	0.97	1.50
2:F:301:CMP:H2	2:F:301:CMP:C2	0.97	1.49
2:C:301:CMP:H2	2:C:301:CMP:C2	0.97	1.48
2:A:301:CMP:H2	2:A:301:CMP:C2	0.97	1.48
2:E:301:CMP:H2	2:E:301:CMP:C2	0.97	1.48
2:B:301:CMP:H2	2:B:301:CMP:C2	0.97	1.47
2:D:301:CMP:C2	2:D:301:CMP:H2	0.97	1.47
1:F:9:ASP:HA	3:F:466:HOH:O	1.40	1.17
1:C:105:GLN:HG2	3:C:510:HOH:O	1.60	0.98
1:E:160:HIS:HD2	1:E:162:ASP:H	1.00	0.97
1:C:160:HIS:HD2	1:C:162:ASP:H	1.08	0.96
1:E:160:HIS:CD2	1:E:162:ASP:H	1.85	0.93
1:B:123:ARG:CB	1:B:123:ARG:HH11	1.83	0.91
1:A:33[A]:GLN:OE1	3:A:557:HOH:O	1.89	0.90
1:D:41:TYR:CD1	1:D:97[A]:GLU:HG2	2.07	0.90
1:C:181:ARG:HB3	1:C:181:ARG:NH1	1.87	0.90
1:B:123:ARG:HH11	1:B:123:ARG:HB2	1.35	0.89
1:D:131:LYS:HE3	3:D:493:HOH:O	1.78	0.83
1:B:123:ARG:HH11	1:B:123:ARG:CG	1.92	0.82
1:A:69:ASP:OD1	1:A:123:ARG:NH2	2.14	0.81
1:C:160:HIS:CD2	1:C:162:ASP:H	1.98	0.81
1:A:123:ARG:NH1	3:A:547:HOH:O	2.17	0.78
1:D:160:HIS:HD2	1:D:162:ASP:H	1.30	0.77
1:A:21:ILE:HD11	1:A:44:VAL:HG21	1.65	0.77
1:A:123:ARG:HH22	1:A:124:ARG:HH21	1.33	0.76
1:F:20:HIS:HE1	3:F:545:HOH:O	1.66	0.76
1:A:160:HIS:HD2	1:A:162:ASP:H	1.32	0.75
1:E:160:HIS:HD2	1:E:162:ASP:N	1.82	0.74
1:C:181:ARG:CB	1:C:181:ARG:HH11	2.02	0.73
1:B:41:TYR:CE2	1:B:97[A]:GLU:HG2	2.23	0.72
1:A:4:GLY:O	1:A:5:LYS:CB	2.37	0.71
1:C:158:MET:HE2	3:C:544:HOH:O	1.89	0.71
1:B:22:HIS:CD2	1:B:97[A]:GLU:OE1	2.45	0.70
1:B:123:ARG:HB2	1:B:123:ARG:NH1	2.06	0.69
1:A:21:ILE:CD1	1:A:44:VAL:HG21	2.23	0.69
1:D:160:HIS:CD2	1:D:162:ASP:H	2.09	0.69
1:F:66:ASN:HD21	1:F:154:GLN:HE22	1.42	0.68
1:B:53:LYS:NZ	3:B:485:HOH:O	2.14	0.67
1:C:181:ARG:NH1	1:C:181:ARG:CB	2.58	0.66
1:C:66:ASN:HD21	1:C:154:GLN:HE22	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:TYR:HD1	1:D:97[A]:GLU:HG2	1.59	0.66
1:A:104:ARG:NH2	3:A:510:HOH:O	2.29	0.65
1:A:160:HIS:CD2	1:A:162:ASP:H	2.13	0.65
1:B:27:LYS:HE3	3:C:521:HOH:O	1.96	0.65
1:A:45:LYS:HE2	3:A:543:HOH:O	1.97	0.65
1:A:12:LEU:HD13	3:A:540:HOH:O	1.97	0.64
1:B:181:ARG:HB2	1:B:181:ARG:HH11	1.63	0.64
1:F:131:LYS:HE2	3:F:531:HOH:O	1.98	0.63
1:A:4:GLY:O	1:A:5:LYS:HB2	1.97	0.62
1:D:131:LYS:CE	3:D:493:HOH:O	2.41	0.62
1:E:66:ASN:HD21	1:E:154:GLN:HE22	1.45	0.62
1:F:131:LYS:CE	3:F:531:HOH:O	2.48	0.62
1:B:41:TYR:CD2	1:B:97[A]:GLU:HG2	2.35	0.61
1:B:158:MET:HG2	1:D:158:MET:SD	2.41	0.60
1:E:160:HIS:CD2	1:E:161:PRO:HD2	2.36	0.60
1:B:123:ARG:HH11	1:B:123:ARG:HG2	1.66	0.60
1:A:51[B]:LEU:HD13	1:A:86:TRP:HB2	1.84	0.60
1:A:5:LYS:HD2	1:A:5:LYS:C	2.22	0.59
1:F:131:LYS:HD3	3:F:469:HOH:O	2.02	0.58
1:B:104:ARG:NH2	3:B:491:HOH:O	2.35	0.58
1:A:123:ARG:NH2	1:A:124:ARG:HH21	2.00	0.58
1:F:108:GLN:NE2	3:F:501:HOH:O	2.23	0.57
1:B:123:ARG:NH1	1:B:123:ARG:HG2	2.18	0.57
1:E:160:HIS:CG	1:E:161:PRO:HD2	2.40	0.57
1:B:41:TYR:CD2	1:B:97[A]:GLU:CG	2.89	0.56
1:F:181:ARG:NH1	3:F:492:HOH:O	2.38	0.56
1:B:123:ARG:CG	1:B:123:ARG:NH1	2.59	0.56
1:F:171:GLN:HE21	1:F:181:ARG:NH1	2.03	0.55
1:B:110:ASN:HD22	1:B:110:ASN:C	2.10	0.55
1:A:120:GLN:HA	1:A:123:ARG:HG2	1.88	0.55
1:A:51[B]:LEU:HD13	1:A:51[B]:LEU:H	1.72	0.54
1:C:181:ARG:HG3	3:C:518:HOH:O	2.07	0.54
1:B:59:GLU:O	2:B:302:CMP:H8	2.09	0.52
1:E:170:ARG:HG2	3:E:532:HOH:O	2.10	0.52
1:F:167:LYS:HE2	1:F:203:THR:OG1	2.10	0.52
1:C:181:ARG:HB3	1:C:181:ARG:HH11	1.59	0.51
1:F:24:TYR:HB2	1:F:93:CYS:SG	2.51	0.51
1:C:208:GLY:HA2	3:C:526:HOH:O	2.11	0.51
1:E:108[A]:GLN:OE1	3:E:494:HOH:O	2.19	0.51
1:A:10:PRO:HD2	3:A:455:HOH:O	2.10	0.50
1:D:110:ASN:ND2	1:D:112:ASP:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:NH1	1:A:124:ARG:HE	2.11	0.49
1:B:110:ASN:ND2	1:B:112:ASP:H	2.11	0.49
1:C:171:GLN:NE2	1:C:181:ARG:HD2	2.28	0.48
1:D:192:GLU:OE2	1:D:200:HIS:NE2	2.47	0.48
1:A:111:PRO:HB3	1:E:111:PRO:HB3	1.95	0.48
1:D:88:ARG:HD3	3:D:458:HOH:O	2.13	0.48
1:C:160:HIS:HD2	1:C:162:ASP:N	1.93	0.47
1:C:181:ARG:HH11	1:C:181:ARG:HB2	1.78	0.47
1:D:171:GLN:HG3	2:D:302:CMP:O5'	2.15	0.47
1:A:53:LYS:HB3	1:A:53:LYS:HE2	1.61	0.47
1:C:110:ASN:C	1:C:110:ASN:HD22	2.17	0.47
1:C:181:ARG:HB3	1:C:181:ARG:CZ	2.44	0.47
1:D:194:GLN:NE2	3:D:514:HOH:O	2.47	0.47
1:F:66:ASN:HD21	1:F:154:GLN:NE2	2.10	0.47
1:B:165:GLN:NE2	3:B:504:HOH:O	2.49	0.46
1:A:110:ASN:ND2	1:A:112:ASP:H	2.13	0.46
1:B:172:GLU:OE2	3:B:546:HOH:O	2.20	0.46
1:F:10:PRO:HD2	3:F:467:HOH:O	2.15	0.46
1:E:110:ASN:C	1:E:110:ASN:HD22	2.19	0.45
1:D:58:LYS:HE3	2:D:302:CMP:C6	2.52	0.45
1:B:181:ARG:NH1	3:B:422:HOH:O	2.48	0.45
1:E:30:LEU:HD21	1:E:95:VAL:HG21	1.99	0.45
1:B:171:GLN:HG3	2:B:302:CMP:O5'	2.17	0.44
1:C:150:ASN:HA	1:C:153:LYS:HE3	1.98	0.44
1:E:104:ARG:NE	3:E:447:HOH:O	2.46	0.44
1:F:165:GLN:HE21	1:F:167:LYS:HE3	1.82	0.44
1:A:59:GLU:O	2:A:302:CMP:H1'	2.18	0.44
1:C:110:ASN:ND2	1:C:112:ASP:H	2.16	0.44
1:A:110:ASN:HD22	1:A:110:ASN:C	2.21	0.44
1:E:103:PHE:CE2	1:E:107:ILE:HD11	2.53	0.44
1:C:66:ASN:HD21	1:C:154:GLN:NE2	2.11	0.44
1:A:90:LYS:HB2	1:A:90:LYS:HE3	1.81	0.43
1:D:58:LYS:HD2	2:D:302:CMP:H2'	1.99	0.43
1:D:110:ASN:C	1:D:110:ASN:HD22	2.20	0.43
1:B:5:LYS:HD2	1:D:195:ASN:HB3	1.99	0.43
1:F:102:LYS:HE2	1:F:102:LYS:HB3	1.70	0.43
1:A:41:TYR:HB2	1:A:71:ILE:HG13	2.01	0.43
1:A:160:HIS:CD2	1:A:161:PRO:HD2	2.54	0.43
1:A:26:SER:O	1:A:27:LYS:HB2	2.19	0.43
1:B:59:GLU:O	2:B:302:CMP:H1'	2.19	0.42
1:E:27:LYS:NZ	3:E:548:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:CB	3:B:547:HOH:O	2.68	0.42
1:B:181:ARG:HH11	1:B:181:ARG:CB	2.32	0.42
1:D:90:LYS:HB3	1:D:90:LYS:HE3	1.67	0.42
1:E:9:ASP:HA	1:E:10:PRO:HD3	1.77	0.42
1:F:149:LEU:HD23	1:F:149:LEU:HA	1.87	0.42
1:B:181:ARG:HB2	1:B:181:ARG:NH1	2.32	0.42
1:D:117:LEU:C	1:D:117:LEU:HD23	2.40	0.42
1:A:81:GLN:HE22	1:E:123:ARG:HH22	1.68	0.42
1:C:105:GLN:NE2	3:C:510:HOH:O	2.46	0.42
1:E:160:HIS:CG	1:E:161:PRO:CD	3.03	0.42
1:D:64:TYR:CE1	1:D:90:LYS:HD2	2.55	0.42
1:A:160:HIS:CG	1:A:161:PRO:HD2	2.54	0.41
1:B:110:ASN:C	1:B:110:ASN:ND2	2.73	0.41
1:E:123:ARG:NH2	1:E:126:GLN:OE1	2.54	0.41
1:C:189:LYS:HE2	1:C:193:ASP:OD1	2.20	0.41
1:F:9:ASP:OD2	1:F:12:LEU:HD12	2.20	0.41
1:A:123:ARG:HH12	1:A:124:ARG:HE	1.68	0.41
1:D:58:LYS:HE3	2:D:302:CMP:C5	2.55	0.41
1:D:104:ARG:NH2	3:D:543:HOH:O	2.54	0.41
1:D:59:GLU:O	2:D:302:CMP:H1'	2.21	0.41
1:A:120:GLN:O	1:A:123:ARG:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:413:HOH:O	3:F:530:HOH:O[1_465]	2.16	0.04

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	202/222 (91%)	198 (98%)	3 (2%)	1 (0%)	29	12
1	B	203/222 (91%)	201 (99%)	2 (1%)	0	100	100
1	C	199/222 (90%)	199 (100%)	0	0	100	100
1	D	204/222 (92%)	201 (98%)	3 (2%)	0	100	100
1	E	200/222 (90%)	199 (100%)	1 (0%)	0	100	100
1	F	199/222 (90%)	197 (99%)	2 (1%)	0	100	100
All	All	1207/1332 (91%)	1195 (99%)	11 (1%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LYS

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	172/190 (90%)	167 (97%)	5 (3%)	42	19
1	B	174/190 (92%)	168 (97%)	6 (3%)	37	14
1	C	166/190 (87%)	161 (97%)	5 (3%)	41	18
1	D	173/190 (91%)	167 (96%)	6 (4%)	36	13
1	E	165/190 (87%)	158 (96%)	7 (4%)	30	9
1	F	164/190 (86%)	157 (96%)	7 (4%)	29	9
All	All	1014/1140 (89%)	978 (96%)	36 (4%)	36	13

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	THR
1	A	53	LYS
1	A	71	ILE

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Mol	Chain	Res	Type
1	A	110	ASN
1	B	2	VAL
1	B	7	GLN
1	B	71	ILE
1	B	110	ASN
1	B	123	ARG
1	B	181	ARG
1	C	9	ASP
1	C	58	LYS
1	C	71	ILE
1	C	110	ASN
1	C	158	MET
1	D	33	GLN
1	D	71	ILE
1	D	110	ASN
1	D	123	ARG
1	D	149	LEU
1	D	158	MET
1	E	9	ASP
1	E	60	MET
1	E	71	ILE
1	E	108[A]	GLN
1	E	108[B]	GLN
1	E	110	ASN
1	E	170	ARG
1	F	71	ILE
1	F	102	LYS
1	F	110	ASN
1	F	123	ARG
1	F	181	ARG
1	F	189	LYS
1	F	206	VAL

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	81	GLN
1	A	110	ASN
1	A	160	HIS
1	A	165	GLN
1	B	22	HIS
1	B	110	ASN

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Mol	Chain	Res	Type
1	B	154	GLN
1	B	165	GLN
1	B	194	GLN
1	C	110	ASN
1	C	154	GLN
1	C	160	HIS
1	C	171	GLN
1	C	200	HIS
1	D	33	GLN
1	D	110	ASN
1	D	160	HIS
1	E	20	HIS
1	E	110	ASN
1	E	154	GLN
1	E	160	HIS
1	E	194	GLN
1	F	110	ASN
1	F	154	GLN
1	F	165	GLN
1	F	171	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 ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	CMP	B	301	-	22,25,25	1.67	3 (13%)	24,39,39	1.92	9 (37%)
2	CMP	D	301	-	22,25,25	1.90	4 (18%)	24,39,39	2.04	8 (33%)
2	CMP	E	301	-	22,25,25	1.56	4 (18%)	24,39,39	2.10	8 (33%)
2	CMP	A	302	-	22,25,25	2.01	5 (22%)	24,39,39	1.72	6 (25%)
2	CMP	C	301	-	22,25,25	1.44	3 (13%)	24,39,39	2.13	7 (29%)
2	CMP	D	302	-	22,25,25	2.07	5 (22%)	24,39,39	1.71	6 (25%)
2	CMP	B	302	-	22,25,25	1.86	6 (27%)	24,39,39	1.66	6 (25%)
2	CMP	F	301	-	22,25,25	1.53	3 (13%)	24,39,39	1.76	5 (20%)
2	CMP	A	301	-	22,25,25	2.20	3 (13%)	24,39,39	2.34	7 (29%)

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	CMP	B	301	-	-	0/0/31/31	0/4/4/4
2	CMP	D	301	-	-	0/0/31/31	0/4/4/4
2	CMP	E	301	-	-	0/0/31/31	0/4/4/4
2	CMP	A	302	-	-	0/0/31/31	0/4/4/4
2	CMP	C	301	-	-	0/0/31/31	0/4/4/4
2	CMP	D	302	-	-	0/0/31/31	0/4/4/4
2	CMP	B	302	-	-	0/0/31/31	0/4/4/4
2	CMP	F	301	-	-	0/0/31/31	0/4/4/4
2	CMP	A	301	-	-	0/0/31/31	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CMP	P-O5'	7.98	1.66	1.57
2	D	301	CMP	P-O5'	6.44	1.65	1.57
2	A	302	CMP	P-O5'	6.16	1.64	1.57
2	D	302	CMP	P-O5'	6.07	1.64	1.57
2	B	301	CMP	P-O5'	5.75	1.64	1.57
2	B	302	CMP	P-O5'	5.27	1.63	1.57
2	F	301	CMP	P-O5'	4.33	1.62	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	CMP	P-O3'	4.32	1.64	1.57
2	E	301	CMP	P-O5'	4.07	1.62	1.57
2	B	302	CMP	P-O3'	3.95	1.64	1.57
2	C	301	CMP	P-O3'	3.82	1.64	1.57
2	A	302	CMP	P-O3'	3.59	1.63	1.57
2	A	301	CMP	P-O3'	3.40	1.63	1.57
2	E	301	CMP	O4'-C1'	3.19	1.45	1.41
2	D	301	CMP	O4'-C1'	3.10	1.45	1.41
2	A	302	CMP	C5-C4	3.07	1.49	1.40
2	E	301	CMP	P-O3'	3.06	1.62	1.57
2	B	301	CMP	P-O3'	2.93	1.62	1.57
2	A	301	CMP	O4'-C1'	2.91	1.45	1.41
2	D	301	CMP	P-O3'	2.87	1.62	1.57
2	B	302	CMP	C5-C4	2.87	1.48	1.40
2	D	302	CMP	C2-N3	2.80	1.36	1.32
2	D	302	CMP	C5-C4	2.70	1.48	1.40
2	D	302	CMP	O4'-C1'	2.51	1.44	1.41
2	B	301	CMP	O4'-C1'	2.50	1.44	1.41
2	C	301	CMP	C2-N3	2.49	1.36	1.32
2	F	301	CMP	C2-N3	2.44	1.36	1.32
2	E	301	CMP	C2-N3	2.37	1.35	1.32
2	A	302	CMP	O5'-C5'	-2.30	1.42	1.46
2	C	301	CMP	C5-C4	2.26	1.46	1.40
2	D	301	CMP	C2-N3	2.19	1.35	1.32
2	F	301	CMP	O4'-C1'	2.16	1.44	1.41
2	B	302	CMP	C2-N3	2.13	1.35	1.32
2	B	302	CMP	O4'-C1'	2.13	1.44	1.41
2	B	302	CMP	O5'-C5'	-2.12	1.43	1.46
2	A	302	CMP	O4'-C1'	2.11	1.44	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	CMP	N3-C2-N1	-5.76	119.67	128.68
2	E	301	CMP	N3-C2-N1	-5.69	119.79	128.68
2	A	301	CMP	N3-C2-N1	-5.43	120.19	128.68
2	F	301	CMP	N3-C2-N1	-4.99	120.88	128.68
2	A	301	CMP	O5'-P-O3'	-4.76	99.12	105.68
2	A	301	CMP	O3'-C3'-C2'	4.51	120.03	115.61
2	D	301	CMP	N3-C2-N1	-4.22	122.09	128.68
2	B	301	CMP	O2P-P-O1P	4.05	121.43	108.73
2	C	301	CMP	C2-N1-C6	4.02	125.62	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	302	CMP	O2P-P-O1P	3.95	121.10	108.73
2	A	301	CMP	C2-N1-C6	3.93	125.48	118.75
2	D	302	CMP	O3'-C3'-C2'	3.85	119.38	115.61
2	A	301	CMP	O2P-P-O1P	3.82	120.70	108.73
2	B	301	CMP	N3-C2-N1	-3.78	122.76	128.68
2	A	302	CMP	O3'-C3'-C2'	3.54	119.07	115.61
2	A	302	CMP	N3-C2-N1	-3.53	123.17	128.68
2	D	301	CMP	O2P-P-O1P	3.42	119.44	108.73
2	D	301	CMP	O3'-C3'-C2'	3.42	118.95	115.61
2	F	301	CMP	O2P-P-O1P	3.36	119.27	108.73
2	D	301	CMP	O5'-P-O3'	-3.35	101.06	105.68
2	E	301	CMP	C2-N1-C6	3.33	124.46	118.75
2	E	301	CMP	O2P-P-O1P	3.32	119.14	108.73
2	B	302	CMP	O3'-C3'-C2'	3.30	118.84	115.61
2	E	301	CMP	O3'-C3'-C4'	3.30	113.20	110.71
2	B	302	CMP	N3-C2-N1	-3.27	123.57	128.68
2	F	301	CMP	C1'-N9-C4	-3.08	121.23	126.64
2	D	302	CMP	O3'-C3'-C4'	-3.01	108.44	110.71
2	C	301	CMP	O2P-P-O1P	2.99	118.08	108.73
2	D	301	CMP	C2-N1-C6	2.98	123.86	118.75
2	D	302	CMP	N3-C2-N1	-2.96	124.05	128.68
2	D	302	CMP	O2P-P-O1P	2.95	117.96	108.73
2	D	301	CMP	O2P-P-O3'	2.94	113.89	107.04
2	E	301	CMP	O5'-P-O3'	-2.92	101.66	105.68
2	A	302	CMP	O2P-P-O1P	2.86	117.69	108.73
2	C	301	CMP	C1'-N9-C4	-2.84	121.66	126.64
2	D	301	CMP	C1'-N9-C4	-2.82	121.69	126.64
2	F	301	CMP	O3'-C3'-C2'	2.76	118.31	115.61
2	B	301	CMP	O5'-P-O3'	-2.65	102.02	105.68
2	A	302	CMP	C5'-C4'-C3'	2.60	117.77	112.49
2	B	301	CMP	N6-C6-N1	2.54	123.85	118.57
2	C	301	CMP	O3'-C3'-C4'	2.52	112.61	110.71
2	C	301	CMP	O5'-P-O3'	-2.49	102.25	105.68
2	B	301	CMP	O3'-C3'-C2'	2.44	117.99	115.61
2	C	301	CMP	N6-C6-N1	2.43	123.61	118.57
2	A	302	CMP	O3'-C3'-C4'	-2.42	108.88	110.71
2	E	301	CMP	C1'-N9-C4	-2.39	122.44	126.64
2	B	301	CMP	C2-N1-C6	2.30	122.70	118.75
2	B	302	CMP	O3'-C3'-C4'	-2.29	108.98	110.71
2	E	301	CMP	N6-C6-N1	2.27	123.29	118.57
2	B	301	CMP	C1'-N9-C4	-2.23	122.72	126.64
2	A	301	CMP	N6-C6-N1	2.21	123.17	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	CMP	O2P-P-O3'	2.21	112.19	107.04
2	B	301	CMP	O3'-P-O1P	-2.20	105.69	110.39
2	B	301	CMP	C5'-C4'-C3'	-2.19	108.06	112.49
2	D	302	CMP	O5'-P-O3'	-2.19	102.66	105.68
2	D	301	CMP	O5'-P-O1P	-2.18	105.41	110.44
2	B	302	CMP	O5'-P-O1P	-2.15	105.48	110.44
2	F	301	CMP	C2-N1-C6	2.07	122.29	118.75
2	A	302	CMP	C2-N1-C6	2.06	122.28	118.75
2	D	302	CMP	N6-C6-N1	2.03	122.79	118.57
2	A	301	CMP	C1'-N9-C4	-2.03	123.08	126.64
2	B	302	CMP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CMP	1	0
2	D	301	CMP	1	0
2	E	301	CMP	1	0
2	A	302	CMP	2	0
2	C	301	CMP	1	0
2	D	302	CMP	6	0
2	B	302	CMP	4	0
2	F	301	CMP	1	0
2	A	301	CMP	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 CMP B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP D 302

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand CMP A 301

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	204/222 (91%)	0.07	5 (2%)	57	63	9, 20, 44, 63	0
1	B	206/222 (92%)	0.03	3 (1%)	73	80	9, 19, 40, 57	0
1	C	201/222 (90%)	-0.01	3 (1%)	73	80	10, 21, 43, 56	0
1	D	207/222 (93%)	0.05	7 (3%)	45	51	10, 20, 41, 57	0
1	E	201/222 (90%)	0.04	5 (2%)	57	63	9, 22, 47, 59	0
1	F	201/222 (90%)	0.02	4 (1%)	65	72	11, 21, 44, 61	0
All	All	1220/1332 (91%)	0.03	27 (2%)	62	69	9, 21, 43, 63	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	VAL	5.0
1	D	2	VAL	4.4
1	B	209	THR	3.3
1	C	208	GLY	3.2
1	A	4	GLY	3.2
1	A	3	LEU	3.1
1	C	200	HIS	3.0
1	E	201	GLY	3.0
1	D	200	HIS	2.8
1	B	1	MET	2.7
1	C	209	THR	2.6
1	F	181	ARG	2.6
1	F	209	THR	2.6
1	F	161	PRO	2.5
1	D	8	THR	2.5
1	E	199	ALA	2.4
1	E	181	ARG	2.4
1	D	209	THR	2.4
1	E	158	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	199	ALA	2.3
1	A	155	PRO	2.2
1	A	7	GLN	2.2
1	D	1	MET	2.1
1	E	200	HIS	2.1
1	A	209	THR	2.0
1	D	208	GLY	2.0
1	D	4	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CMP	A	302	22/22	0.88	0.13	25,36,42,44	0
2	CMP	B	302	22/22	0.89	0.12	22,32,40,42	0
2	CMP	D	302	22/22	0.91	0.14	24,33,37,44	0
2	CMP	C	301	22/22	0.98	0.09	9,11,13,13	0
2	CMP	B	301	22/22	0.99	0.09	7,9,11,12	0
2	CMP	D	301	22/22	0.99	0.09	8,11,12,13	0
2	CMP	A	301	22/22	0.99	0.09	8,9,11,11	0
2	CMP	E	301	22/22	0.99	0.09	9,10,12,12	0
2	CMP	F	301	22/22	0.99	0.08	10,11,12,12	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.
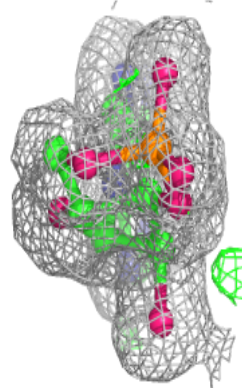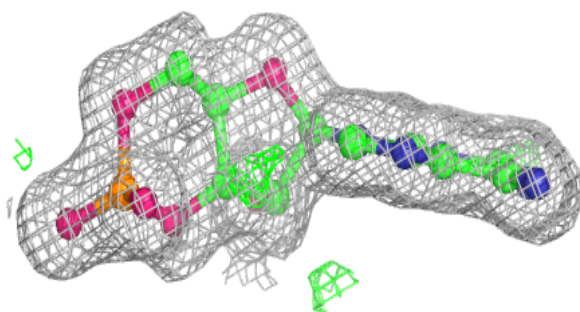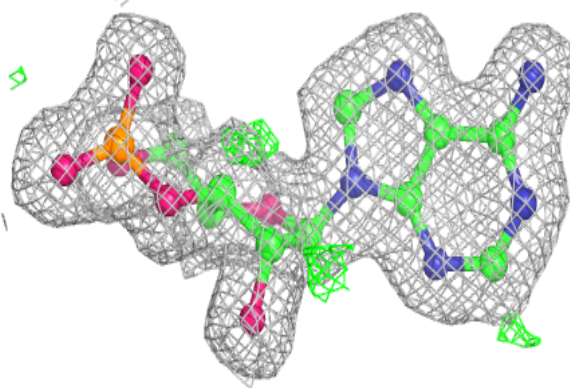
Electron density around CMP A 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
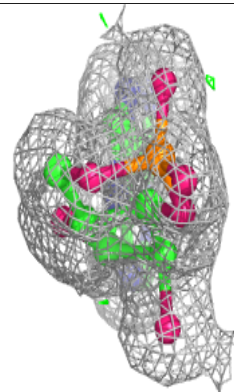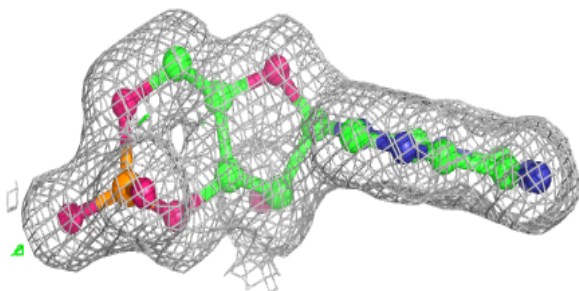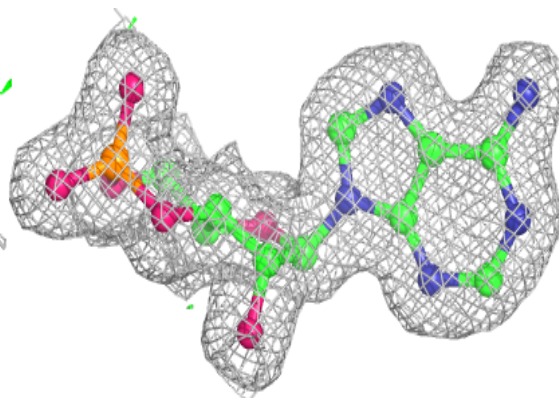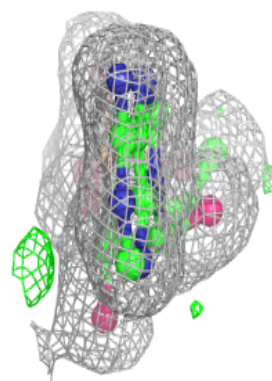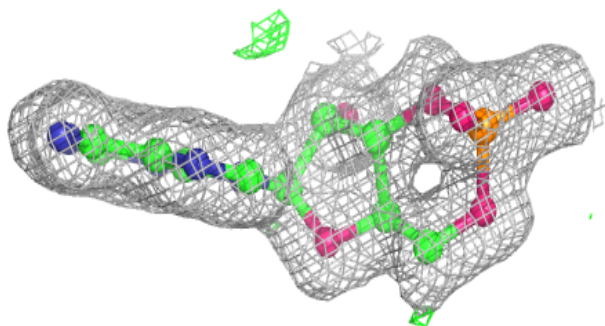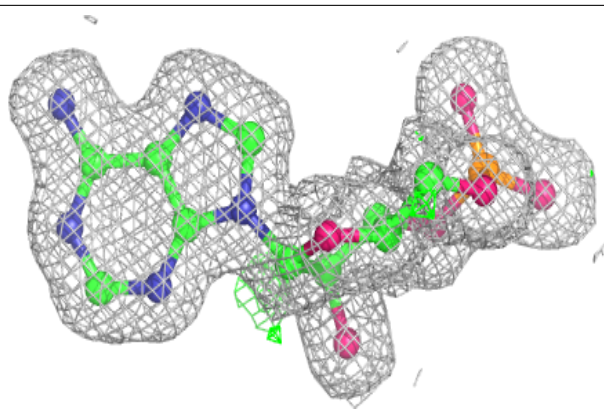and green (positive)
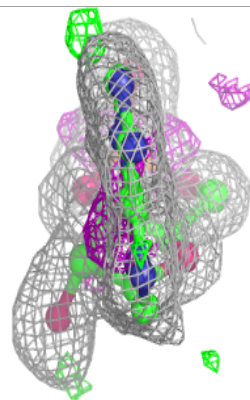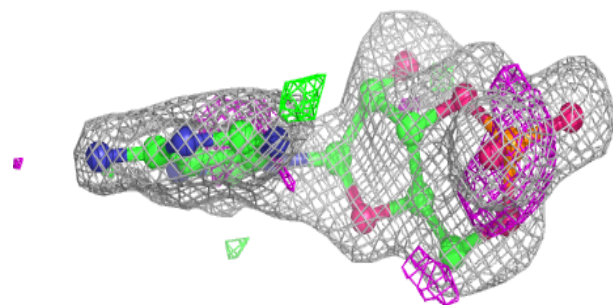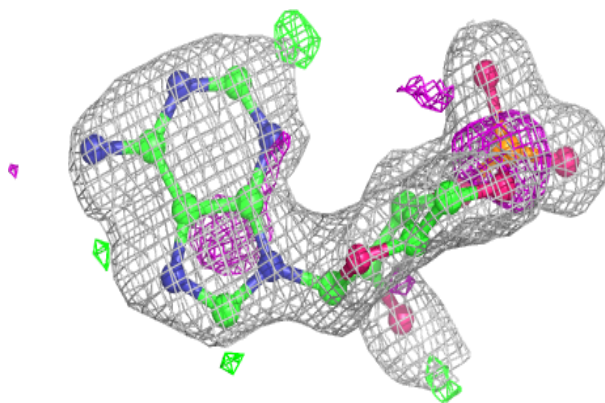
Electron density around CMP B 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
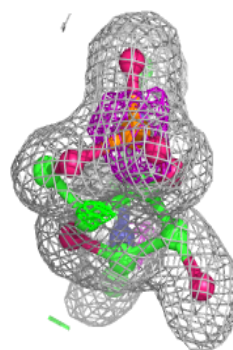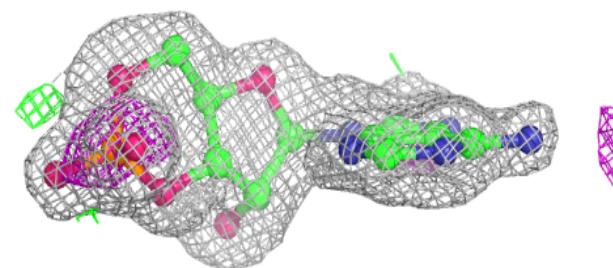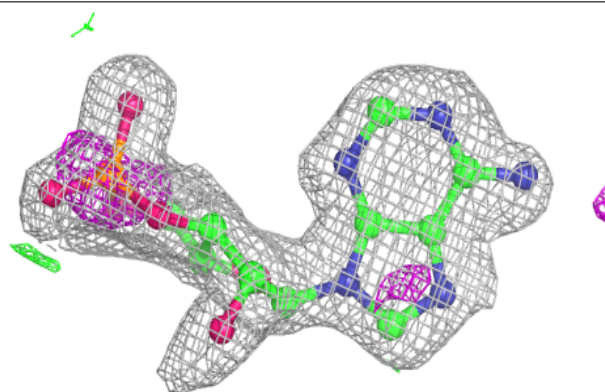
Electron density around CMP D 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
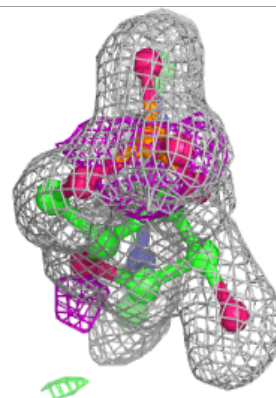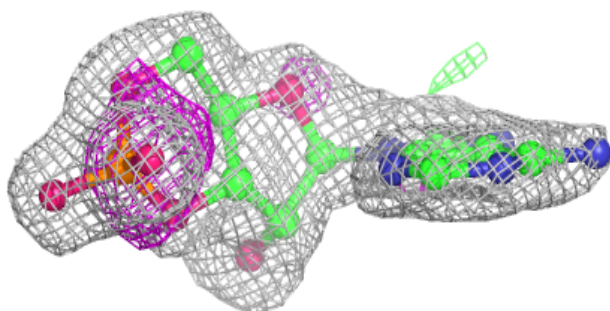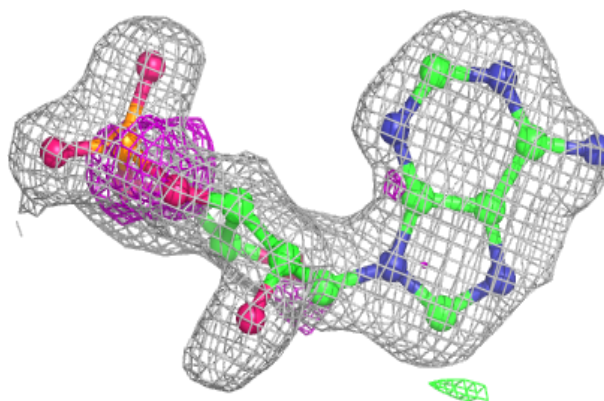
Electron density around CMP C 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
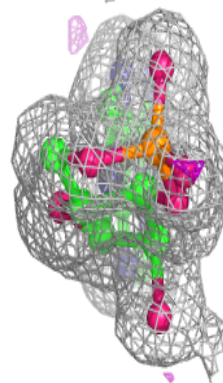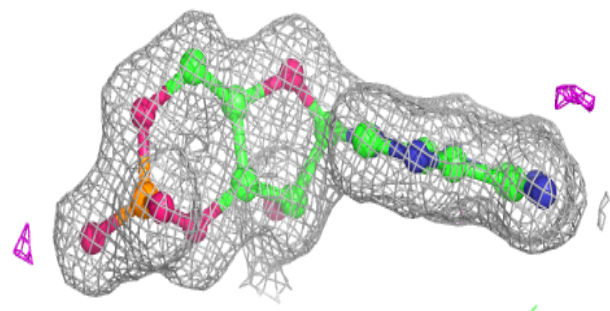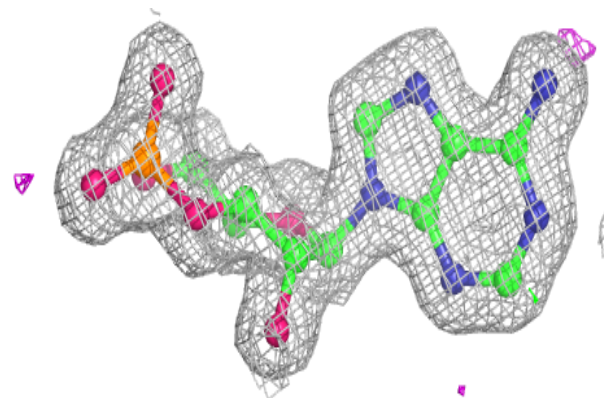
Electron density around CMP B 301:

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 CMP D 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
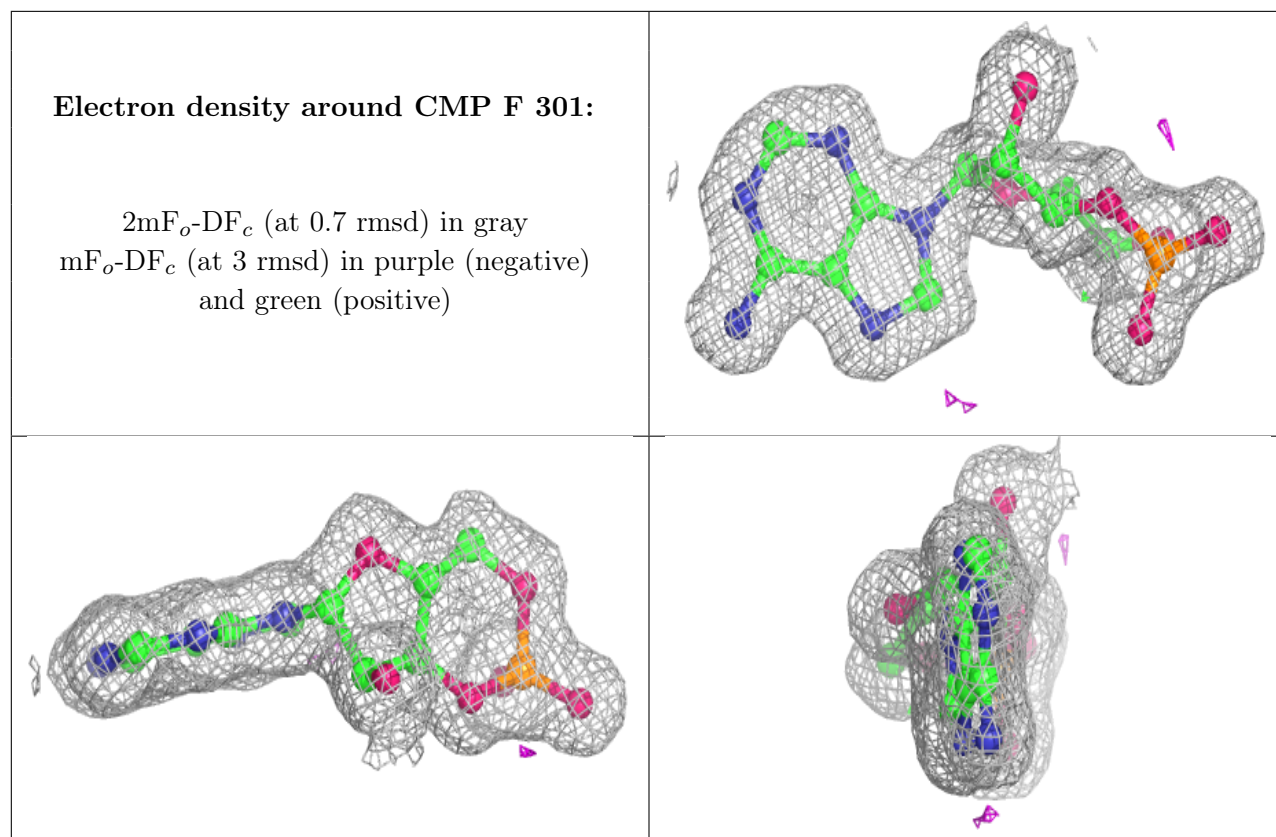and green (positive)

Electron density around CMP 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 CMP 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 CMP 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)
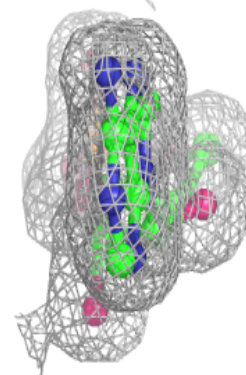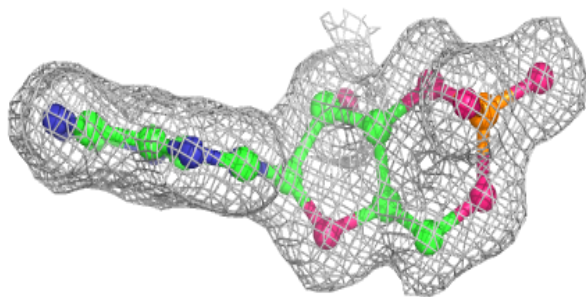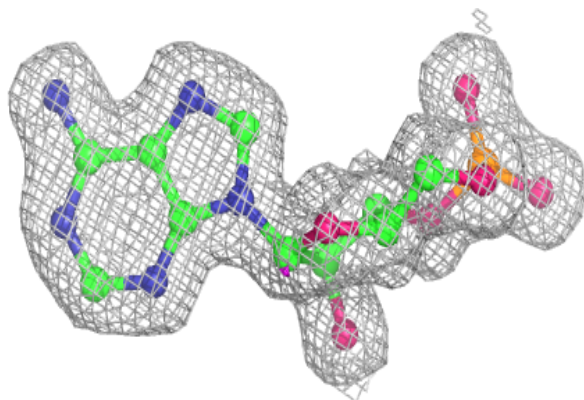
6.5 Other polymers (i)

There are no such residues in this entry.