



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:07 AM UTC

PDB ID : 8UH7 / pdb_00008uh7
Title : Structure of T4 Bacteriophage clamp loader bound to the T4 clamp, primer-template DNA, and ATP analog
Authors : Gee, C.L.; Marcus, K.; Kelch, B.A.; Makino, D.L.
Deposited on : 2023-10-07
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

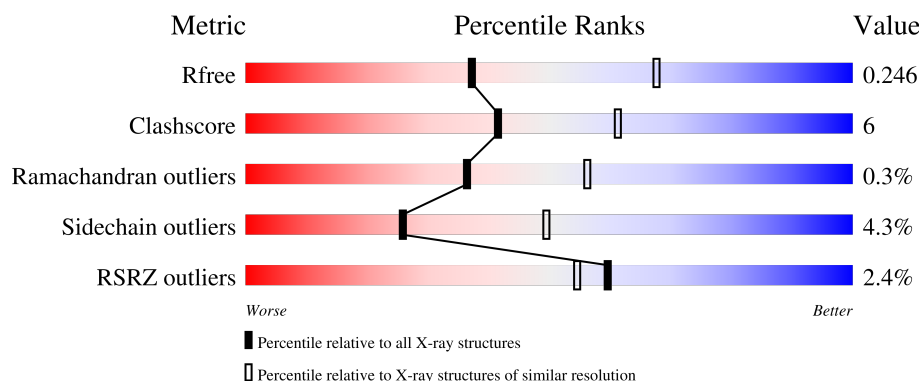
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	187	5% 76% 21% ..
2	B	324	% 85% 13% .
2	C	324	82% 16% .
2	D	324	% 84% 13% ..
2	E	324	% 81% 13% ..

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Mol	Chain	Length	Quality of chain
3	F	228	12% 75% 21%
3	G	228	77% 22%
3	H	228	% 82% 17%
4	I	30	7% 43% 37% 20%
5	J	20	5% 80% 20%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17800 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 Sliding-clamp-loader small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1495	963	247	279	6			

- Molecule 2 is a protein called Sliding-clamp-loader large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2509	1587	431	474	17			
2	C	320	Total	C	N	O	S	0	0	0
			2515	1590	432	476	17			
2	D	319	Total	C	N	O	S	0	0	0
			2509	1587	431	474	17			
2	E	314	Total	C	N	O	S	0	0	0
			2467	1564	422	465	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P04526
B	-3	PRO	-	expression tag	UNP P04526
B	-2	GLY	-	expression tag	UNP P04526
B	-1	GLY	-	expression tag	UNP P04526
B	0	SER	-	expression tag	UNP P04526
C	-4	GLY	-	expression tag	UNP P04526
C	-3	PRO	-	expression tag	UNP P04526
C	-2	GLY	-	expression tag	UNP P04526
C	-1	GLY	-	expression tag	UNP P04526
C	0	SER	-	expression tag	UNP P04526
D	-4	GLY	-	expression tag	UNP P04526
D	-3	PRO	-	expression tag	UNP P04526
D	-2	GLY	-	expression tag	UNP P04526
D	-1	GLY	-	expression tag	UNP P04526

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP P04526
E	-4	GLY	-	expression tag	UNP P04526
E	-3	PRO	-	expression tag	UNP P04526
E	-2	GLY	-	expression tag	UNP P04526
E	-1	GLY	-	expression tag	UNP P04526
E	0	SER	-	expression tag	UNP P04526

- Molecule 3 is a protein called Sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	G	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	H	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			

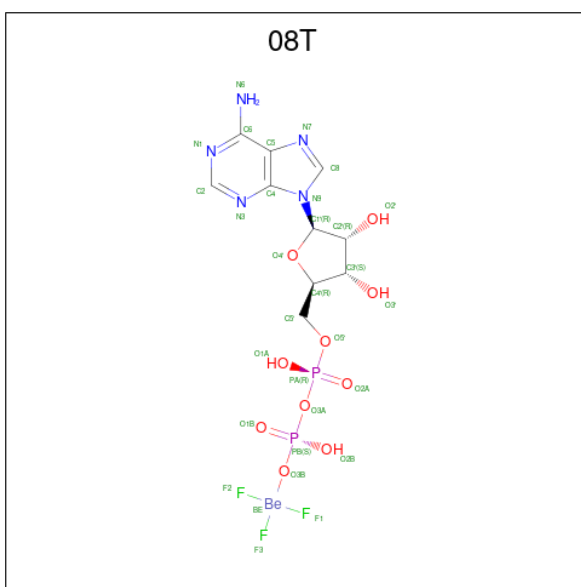
- Molecule 4 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			

- Molecule 5 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	20	Total	C	N	O	P	0	0	0
			408	195	81	113	19			

- Molecule 6 is [[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (CCD ID: 08T) (formula: C₁₀H₁₄BeF₃N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

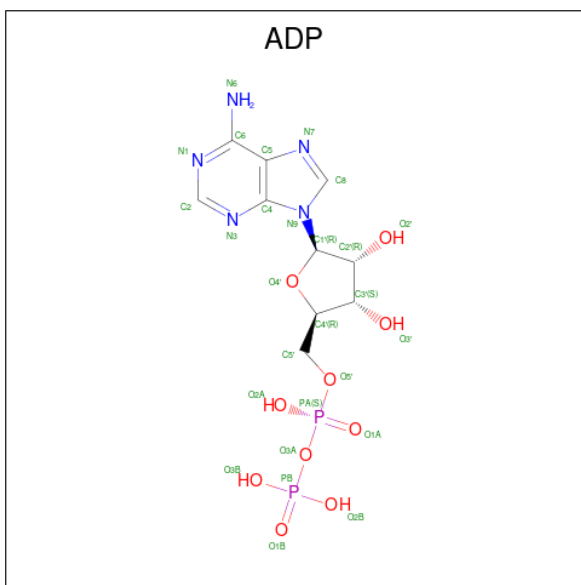


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	C	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	D	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

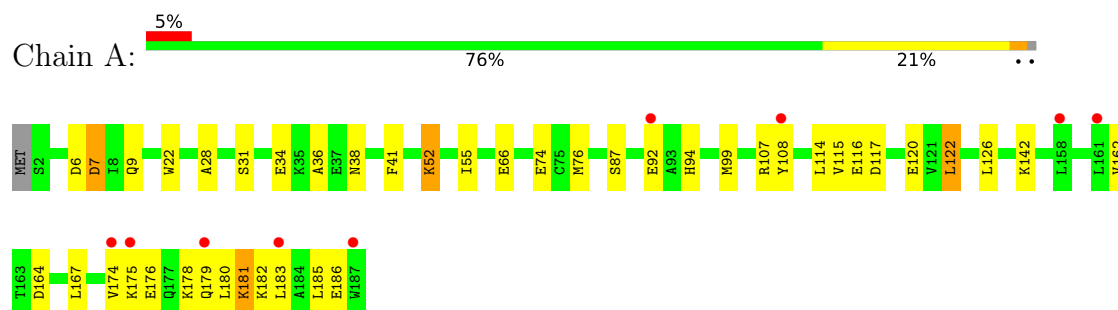
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O 1 1	0	0
9	B	7	Total O 7 7	0	0
9	C	6	Total O 6 6	0	0
9	D	9	Total O 9 9	0	0
9	E	7	Total O 7 7	0	0
9	F	1	Total O 1 1	0	0
9	G	2	Total O 2 2	0	0
9	J	1	Total O 1 1	0	0

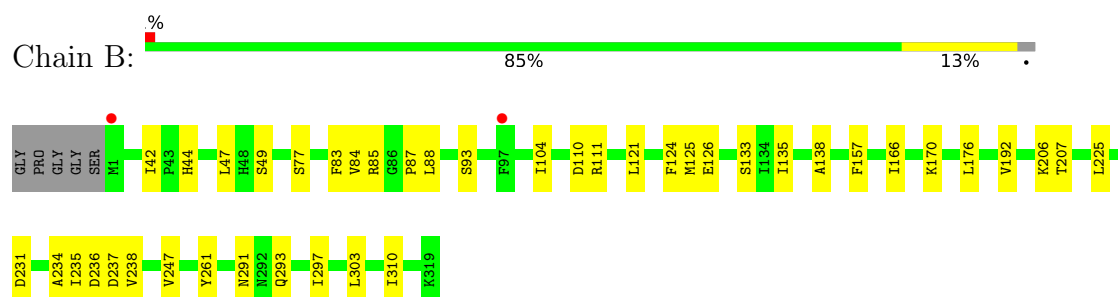
3 Residue-property plots [i](#)

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.

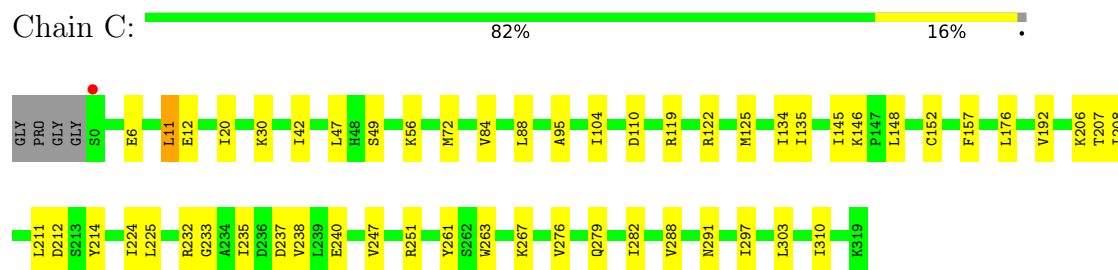
- Molecule 1: Sliding-clamp-loader small subunit



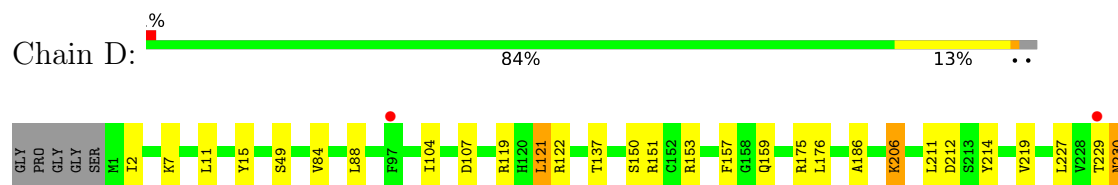
- Molecule 2: Sliding-clamp-loader large subunit



- Molecule 2: Sliding-clamp-loader large subunit

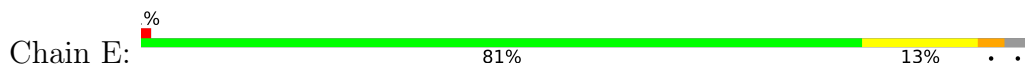


- Molecule 2: Sliding-clamp-loader large subunit

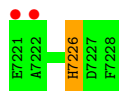
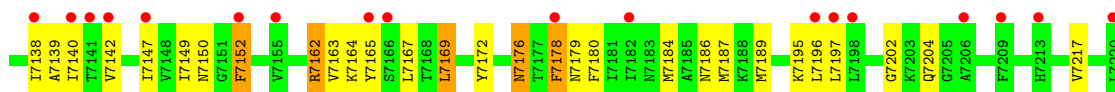
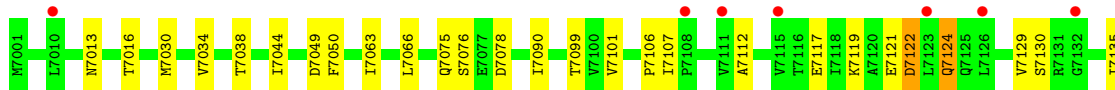
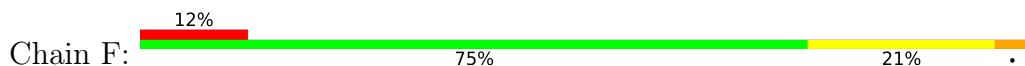




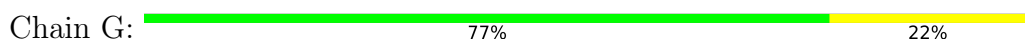
• Molecule 2: Sliding-clamp-loader large subunit



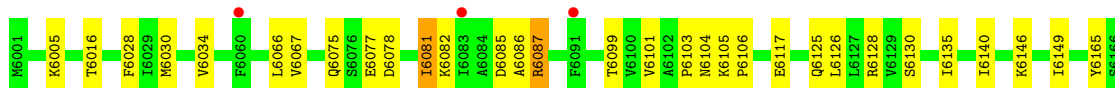
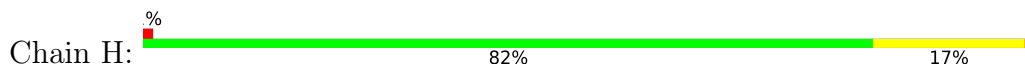
• Molecule 3: Sliding clamp



• Molecule 3: Sliding clamp

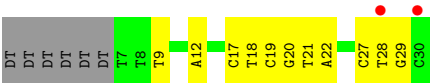


• Molecule 3: Sliding clamp

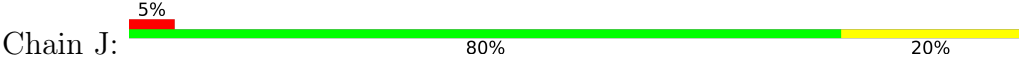




● Molecule 4: Template DNA strand



● Molecule 5: Primer DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.35Å 118.33Å 132.88Å 90.00° 102.05° 90.00°	Depositor
Resolution (Å)	49.65 – 2.63 49.65 – 2.63	Depositor EDS
% Data completeness (in resolution range)	65.9 (49.65-2.63) 65.9 (49.65-2.63)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.193 , 0.244 0.194 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17800	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 08T

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	0.12	0/1523	0.33	0/2051
2	B	0.12	0/2553	0.32	0/3441
2	C	0.13	0/2559	0.30	0/3449
2	D	0.13	0/2553	0.31	0/3441
2	E	0.14	0/2510	0.35	0/3382
3	F	0.11	0/1774	0.28	0/2395
3	G	0.11	0/1774	0.30	0/2395
3	H	0.11	0/1774	0.31	0/2395
4	I	0.22	0/544	0.47	0/838
5	J	0.20	0/459	0.34	0/706
All	All	0.13	0/18023	0.32	0/24493

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	1495	0	1521	26	0
2	B	2509	0	2537	26	0
2	C	2515	0	2542	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2509	0	2538	32	0
2	E	2467	0	2495	35	0
3	F	1750	0	1752	33	0
3	G	1750	0	1752	30	0
3	H	1750	0	1752	23	0
4	I	489	0	277	7	0
5	J	408	0	225	2	0
6	B	31	0	13	0	0
6	C	31	0	13	1	0
6	D	31	0	13	1	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	E	27	0	12	1	0
9	A	1	0	0	0	0
9	B	7	0	0	0	0
9	C	6	0	0	0	0
9	D	9	0	0	0	0
9	E	7	0	0	0	0
9	F	1	0	0	1	0
9	G	2	0	0	0	0
9	J	1	0	0	0	0
All	All	17800	0	17442	223	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 6.

All (223) 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:162:VAL:HG11	1:A:183:LEU:HD13	1.61	0.82
1:A:162:VAL:HG21	1:A:183:LEU:HD22	1.64	0.78
3:G:5146:LYS:HA	3:G:5171:ASP:HA	1.67	0.77
1:A:122:LEU:HD21	1:A:183:LEU:HD21	1.70	0.72
1:A:175:LYS:HG2	1:A:178:LYS:HG3	1.69	0.72
2:D:229:THR:O	2:D:230:ASN:ND2	2.22	0.72
2:B:88:LEU:HD22	2:B:104:ILE:HD13	1.74	0.69
2:E:116:GLU:OE1	2:E:119:ARG:NH1	2.26	0.68
3:F:7140:ILE:HG22	3:F:7149:ILE:HG12	1.75	0.67
1:A:55:ILE:HD11	1:A:92:GLU:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7149:ILE:HG13	3:F:7169:LEU:HD11	1.75	0.66
2:D:84:VAL:HG22	2:D:88:LEU:HD22	1.77	0.66
3:F:7030:MSE:HE1	3:F:7106:PRO:HA	1.78	0.64
2:D:88:LEU:HG	2:D:104:ILE:HD13	1.79	0.63
3:G:5063:ILE:HD13	3:G:5090:ILE:HG21	1.79	0.63
2:E:272:ILE:HG21	2:E:284:MET:HG3	1.80	0.62
3:F:7117:GLU:HG2	3:F:7195:LYS:HA	1.80	0.62
2:E:88:LEU:HD22	2:E:104:ILE:HD13	1.83	0.61
2:D:278:PRO:HA	2:D:281:ILE:HD13	1.84	0.60
3:H:6034:VAL:HG13	3:H:6101:VAL:HG21	1.84	0.59
4:I:21:DT:H2''	4:I:22:DA:C8	2.37	0.59
2:D:84:VAL:HA	2:D:88:LEU:HB2	1.84	0.59
3:H:6085:ASP:O	3:H:6087:ARG:N	2.36	0.59
2:C:235:ILE:HG22	2:C:238:VAL:HB	1.83	0.59
2:E:260:ASP:N	2:E:260:ASP:OD1	2.34	0.59
2:B:93:SER:HA	3:F:7099:THR:HG21	1.83	0.58
3:G:5140:ILE:HD13	3:G:5196:LEU:HD21	1.85	0.58
2:B:297:ILE:HD13	2:C:297:ILE:HD11	1.84	0.58
3:G:5129:VAL:HG13	3:G:5133:LEU:HD13	1.86	0.58
2:E:12:GLU:O	8:E:401:ADP:O3'	2.18	0.58
1:A:164:ASP:HA	1:A:167:LEU:HD12	1.85	0.57
2:B:303:LEU:HD21	2:C:288:VAL:HG12	1.85	0.57
2:C:88:LEU:HD22	2:C:104:ILE:HD13	1.87	0.56
1:A:120:GLU:HG3	1:A:142:LYS:HE3	1.86	0.56
1:A:179:GLN:HA	1:A:182:LYS:HB2	1.86	0.56
2:E:111:ARG:HH11	2:E:260:ASP:HB2	1.71	0.55
3:F:7038:THR:HB	3:F:7186:ASN:HB3	1.89	0.55
2:E:90:ASN:OD1	3:H:6186:ASN:ND2	2.37	0.55
2:E:235:ILE:HG22	2:E:238:VAL:HB	1.89	0.55
2:E:237:ASP:N	2:E:237:ASP:OD1	2.39	0.55
2:E:227:LEU:HD12	2:E:228:VAL:H	1.73	0.54
2:D:119:ARG:HA	2:D:122:ARG:HD3	1.91	0.53
2:D:283:ARG:NE	2:D:315:GLU:OE1	2.37	0.52
3:G:5078:ASP:OD1	3:G:5078:ASP:N	2.39	0.52
2:B:84:VAL:HG22	2:B:88:LEU:HD12	1.92	0.52
3:F:7112:ALA:HB2	3:F:7197:LEU:HD23	1.91	0.52
2:C:95:ALA:HB2	3:G:5222:ALA:HA	1.91	0.52
2:E:111:ARG:HH12	2:E:263:TRP:H	1.57	0.52
2:C:233:GLY:O	2:C:267:LYS:NZ	2.43	0.52
2:D:176:LEU:HD22	2:D:211:LEU:HD22	1.91	0.52
2:B:83:PHE:HA	2:B:87:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:SER:OG	2:B:111:ARG:NH1	2.43	0.51
2:E:186:ALA:HB3	2:E:219:VAL:HG13	1.91	0.51
4:I:28:DT:H2"	4:I:29:DG:N7	2.26	0.51
2:C:247:VAL:HG13	2:C:310:ILE:HD11	1.93	0.51
2:E:180:CYS:HA	2:E:185:ILE:HG13	1.94	0.51
3:G:5060:PHE:O	3:G:5063:ILE:HG13	2.11	0.50
3:G:5130:SER:HA	3:G:5135:ILE:HG13	1.92	0.50
2:D:11:LEU:HD12	2:D:212:ASP:HB2	1.93	0.50
5:J:9:DT:H2"	5:J:10:DA:C8	2.47	0.50
2:B:261:TYR:OH	2:B:291:ASN:OD1	2.22	0.50
1:A:41:PHE:O	1:A:108:TYR:OH	2.29	0.50
3:G:5122:ASP:HB3	3:G:5167:LEU:HD21	1.94	0.50
2:C:119:ARG:HA	2:C:122:ARG:HD3	1.94	0.50
2:B:110:ASP:HB3	2:B:138:ALA:HB1	1.94	0.50
3:F:7107:ILE:HD11	3:F:7217:VAL:HG21	1.93	0.50
2:C:237:ASP:OD1	2:C:238:VAL:N	2.44	0.49
3:H:6075:GLN:HA	3:H:6081:ILE:HA	1.92	0.49
2:C:20:ILE:O	2:C:30:LYS:NZ	2.45	0.49
2:B:110:ASP:OD1	2:C:122:ARG:NH2	2.34	0.49
2:C:247:VAL:O	2:C:251:ARG:HG3	2.12	0.49
3:F:7122:ASP:HB3	3:F:7167:LEU:HD21	1.95	0.49
3:F:7172:TYR:OH	3:F:7176:ASN:OD1	2.31	0.49
2:C:214:TYR:HB3	2:C:224:ILE:HG23	1.94	0.49
3:H:6140:ILE:HG12	3:H:6149:ILE:HG12	1.95	0.49
2:E:42:ILE:HD11	2:E:67:VAL:HG21	1.94	0.48
1:A:114:LEU:HD11	2:E:253:LEU:HD23	1.96	0.48
1:A:181:LYS:HD3	1:A:185:LEU:HD13	1.95	0.48
2:C:11:LEU:HD22	2:C:212:ASP:HB2	1.95	0.48
2:C:56:LYS:N	6:C:401:08T:O1B	2.37	0.48
2:E:272:ILE:HG23	2:E:276:VAL:HG21	1.94	0.48
3:G:5015:ALA:HB2	3:G:5057:LEU:HD23	1.95	0.48
3:F:7202:GLY:C	3:F:7204:GLN:H	2.22	0.47
3:G:5118:ILE:HD11	3:G:5196:LEU:HD22	1.96	0.47
2:C:110:ASP:OD1	2:D:122:ARG:NH2	2.36	0.47
2:D:49:SER:HB3	2:D:157:PHE:HB2	1.96	0.47
3:F:7152:PHE:HE2	3:F:7163:VAL:HG22	1.79	0.47
1:A:126:LEU:HD21	1:A:162:VAL:HG22	1.96	0.47
2:B:231:ASP:HB3	2:B:234:ALA:HB2	1.96	0.47
6:D:401:08T:F1	6:D:401:08T:O2B	2.23	0.47
2:E:26:PRO:HG2	2:E:158:GLY:HA2	1.97	0.47
3:H:6030:MSE:SE	3:H:6103:PRO:HG2	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:TYR:O	2:D:175:ARG:NH2	2.47	0.47
3:H:6028:PHE:CE2	3:H:6030:MSE:HE3	2.49	0.47
2:B:47:LEU:HD22	2:B:157:PHE:HE1	1.79	0.47
1:A:28:ALA:O	1:A:31:SER:HB3	2.15	0.47
2:D:107:ASP:OD1	2:D:137:THR:OG1	2.30	0.47
2:C:47:LEU:HD23	2:C:157:PHE:CZ	2.49	0.47
2:B:206:LYS:NZ	2:C:152:CYS:O	2.47	0.46
3:F:7162:ARG:HH12	3:F:7164:LYS:HD2	1.80	0.46
1:A:76:MET:HG3	2:E:310:ILE:HD12	1.97	0.46
2:C:261:TYR:OH	2:C:291:ASN:OD1	2.23	0.46
2:C:49:SER:HB3	2:C:157:PHE:HB2	1.97	0.46
3:G:5113:SER:HB3	3:G:5228:PHE:CE1	2.51	0.46
3:G:5134:GLN:O	3:G:5153:ASN:ND2	2.48	0.46
3:H:6067:VAL:HG22	3:H:6085:ASP:HB3	1.98	0.46
3:H:6212:GLU:HG3	3:H:6213:HIS:ND1	2.30	0.46
1:A:174:VAL:C	1:A:176:GLU:N	2.74	0.46
2:E:125:MET:HG2	2:E:134:ILE:HD12	1.96	0.46
3:G:5013:ASN:O	3:G:5016:THR:OG1	2.34	0.46
3:H:6030:MSE:HE1	3:H:6106:PRO:HA	1.96	0.46
2:D:237:ASP:OD1	2:D:237:ASP:N	2.47	0.46
3:H:6103:PRO:O	3:H:6105:LYS:N	2.44	0.46
3:H:6140:ILE:HD13	3:H:6196:LEU:HD21	1.98	0.46
2:E:272:ILE:O	2:E:276:VAL:HG23	2.16	0.46
3:G:5195:LYS:HE3	3:G:5197:LEU:HD11	1.97	0.46
4:I:27:DC:H2"	4:I:28:DT:C6	2.51	0.45
2:E:217:LYS:NZ	2:E:221:ASP:OD2	2.48	0.45
3:F:7034:VAL:HG22	3:F:7101:VAL:HG21	1.97	0.45
3:F:7063:ILE:HD11	3:G:5132:GLY:HA3	1.99	0.45
3:F:7180:PHE:HE2	3:F:7226:HIS:HA	1.80	0.45
3:G:5055:TYR:HB2	3:G:5095:ALA:HB2	1.99	0.45
3:G:5164:LYS:HA	3:G:5164:LYS:HD3	1.81	0.45
1:A:181:LYS:HE3	1:A:181:LYS:HB2	1.86	0.45
2:D:206:LYS:NZ	2:E:152:CYS:O	2.47	0.45
1:A:87:SER:OG	2:B:293:GLN:NE2	2.40	0.45
3:G:5129:VAL:HG11	3:G:5165:TYR:CD1	2.51	0.45
3:G:5066:LEU:HD21	3:H:6128:ARG:HB3	1.99	0.45
1:A:52:LYS:HD3	1:A:52:LYS:HA	1.40	0.44
2:B:49:SER:HB3	2:B:157:PHE:HB2	1.98	0.44
3:F:7076:SER:OG	3:F:7078:ASP:OD1	2.28	0.44
3:F:7129:VAL:HG21	3:F:7165:TYR:CZ	2.52	0.44
2:D:206:LYS:NZ	2:E:149:GLN:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:84:VAL:HG22	2:C:88:LEU:HD12	1.99	0.44
2:D:122:ARG:HB2	2:D:151:ARG:CZ	2.47	0.44
3:F:7013:ASN:O	3:F:7016:THR:OG1	2.29	0.44
2:D:297:ILE:HD12	2:E:297:ILE:HD11	1.99	0.44
2:B:192:VAL:HG22	2:B:225:LEU:HB2	2.00	0.44
2:D:299:ALA:HB2	2:E:295:HIS:ND1	2.33	0.44
3:F:7162:ARG:O	3:F:7162:ARG:HD3	2.18	0.44
4:I:17:DC:H2'	4:I:18:DT:H71	1.99	0.44
2:B:310:ILE:HD12	2:C:282:ILE:HD13	1.99	0.44
2:E:42:ILE:HG12	2:E:67:VAL:HG11	1.99	0.44
3:F:7187:MSE:HG3	3:F:7189:MSE:SE	2.68	0.44
2:C:303:LEU:HD21	2:D:288:VAL:HG12	2.00	0.43
3:G:5203:LYS:H	3:G:5203:LYS:HG2	1.58	0.43
5:J:11:DC:H2''	5:J:12:DG:C8	2.53	0.43
2:D:119:ARG:HB3	2:D:122:ARG:NH1	2.33	0.43
3:F:7049:ASP:OD1	3:F:7049:ASP:N	2.47	0.43
2:C:232:ARG:HB2	2:C:263:TRP:CE2	2.54	0.43
2:D:284:MET:HG3	2:D:285:TYR:N	2.33	0.43
3:H:6146:LYS:N	3:H:6146:LYS:HD2	2.34	0.43
1:A:74:GLU:OE1	1:A:107:ARG:NH1	2.52	0.43
2:D:294:TYR:HB3	2:E:293:GLN:HG3	2.00	0.43
2:B:166:ILE:O	2:B:170:LYS:HG2	2.18	0.43
2:C:192:VAL:HG22	2:C:225:LEU:HB2	2.00	0.43
2:B:121:LEU:O	2:B:124:PHE:HB3	2.19	0.43
2:E:36:ILE:HD11	2:E:153:ARG:HH21	1.84	0.43
3:H:6005:LYS:HD3	3:H:6005:LYS:HA	1.86	0.43
2:B:237:ASP:OD1	2:B:238:VAL:N	2.52	0.43
2:D:214:TYR:HE1	2:D:227:LEU:HG	1.82	0.43
3:G:5077:GLU:H	3:G:5077:GLU:CD	2.26	0.42
3:H:6196:LEU:HD13	3:H:6209:PHE:CE2	2.54	0.42
2:B:42:ILE:HG21	2:B:135:ILE:HD11	2.01	0.42
3:F:7063:ILE:HG21	3:F:7090:ILE:HG21	1.99	0.42
3:G:5088:SER:HB3	3:H:6167:LEU:HD13	2.01	0.42
1:A:38:ASN:ND2	4:I:9:DT:O2	2.52	0.42
2:C:176:LEU:HD11	2:C:207:THR:HG22	2.00	0.42
2:D:239:LEU:HD13	2:D:275:ARG:HD3	2.01	0.42
3:G:5028:PHE:CE1	3:G:5041:GLU:HB2	2.55	0.42
2:C:11:LEU:HB3	2:C:208:ILE:HG22	2.01	0.42
3:F:7044:ILE:HD12	3:F:7044:ILE:HA	1.87	0.42
2:C:42:ILE:HG21	2:C:135:ILE:HD11	2.02	0.42
4:I:19:DC:H2''	4:I:20:DG:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7121:GLU:O	3:F:7124:GLN:HG3	2.19	0.42
2:D:121:LEU:HD12	2:D:121:LEU:HA	1.86	0.42
3:F:7139:ALA:HA	3:F:7180:PHE:O	2.20	0.42
2:C:145:ILE:HD11	2:C:148:LEU:HD13	2.02	0.42
2:E:20:ILE:HD13	2:E:20:ILE:HA	1.88	0.42
2:D:186:ALA:HB3	2:D:219:VAL:HG13	2.01	0.41
3:F:7050:PHE:CD2	3:F:7075:GLN:HB2	2.55	0.41
1:A:22:TRP:CE3	2:B:85:ARG:HD3	2.54	0.41
2:C:125:MET:HG2	2:C:134:ILE:HD12	2.03	0.41
2:D:307:TYR:CE1	2:E:286:GLU:HA	2.55	0.41
2:E:91:PHE:CE2	2:E:102:LYS:HB3	2.56	0.41
2:B:247:VAL:HG13	2:B:310:ILE:HD11	2.03	0.41
2:B:121:LEU:O	2:B:125:MET:HG3	2.20	0.41
3:F:7176:ASN:OD1	3:F:7176:ASN:N	2.54	0.41
3:F:7130:SER:HA	3:F:7135:ILE:HB	2.03	0.41
3:G:5026:GLY:O	3:G:5048:ILE:N	2.47	0.41
2:C:176:LEU:HD22	2:C:211:LEU:HD22	2.03	0.41
3:G:5003:LEU:HD23	3:G:5003:LEU:HA	1.95	0.41
3:G:5181:ILE:HB	3:G:5221:GLU:HB2	2.02	0.41
3:H:6016:THR:HG22	3:H:6188:LYS:HD2	2.03	0.41
1:A:6:ASP:HB3	1:A:7:ASP:H	1.59	0.41
1:A:66:GLU:OE2	1:A:94:HIS:NE2	2.43	0.41
2:C:6:GLU:CD	2:C:6:GLU:H	2.28	0.41
2:D:229:THR:C	2:D:230:ASN:HD22	2.23	0.41
3:G:5140:ILE:HG21	3:G:5198:LEU:HD21	2.03	0.41
3:G:5180:PHE:CD1	3:G:5220:LEU:HD13	2.56	0.41
3:H:6087:ARG:HD2	3:H:6087:ARG:H	1.85	0.41
4:I:12:DA:H5'	4:I:12:DA:C8	2.56	0.41
2:B:44:HIS:CE1	2:B:133:SER:HA	2.56	0.41
2:C:206:LYS:HE2	2:D:150:SER:HA	2.03	0.41
2:E:305:LEU:HD12	2:E:305:LEU:HA	1.89	0.41
3:G:5196:LEU:HG	3:G:5198:LEU:HD11	2.03	0.41
1:A:174:VAL:C	1:A:176:GLU:H	2.28	0.40
2:E:119:ARG:HB3	2:E:122:ARG:HH21	1.86	0.40
3:H:6028:PHE:HE2	3:H:6030:MSE:HE3	1.85	0.40
3:H:6189:MSE:HE2	3:H:6189:MSE:HB3	2.03	0.40
1:A:181:LYS:HG3	1:A:182:LYS:N	2.36	0.40
2:B:176:LEU:HD11	2:B:207:THR:HG22	2.03	0.40
2:C:12:GLU:CD	2:D:153:ARG:HH12	2.29	0.40
2:D:247:VAL:HG13	2:D:310:ILE:HD11	2.03	0.40
2:E:44:HIS:CG	2:E:125:MET:HE3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7140:ILE:O	3:F:7179:ASN:HA	2.20	0.40
3:F:7178:PHE:N	3:F:7178:PHE:CD1	2.89	0.40
3:H:6130:SER:HA	3:H:6135:ILE:HB	2.04	0.40
1:A:183:LEU:HD23	1:A:186:GLU:OE1	2.21	0.40
3:F:7162:ARG:NH2	9:F:7301:HOH:O	2.55	0.40
3:F:7140:ILE:HD11	3:F:7180:PHE:CD1	2.56	0.40
2:E:243:LYS:HG2	2:E:318:TRP:CD2	2.56	0.40
3:H:6125:GLN:OE1	3:H:6165:TYR:OH	2.38	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	184/187 (98%)	177 (96%)	4 (2%)	3 (2%)	7	15
2	B	317/324 (98%)	303 (96%)	13 (4%)	1 (0%)	36	56
2	C	318/324 (98%)	304 (96%)	14 (4%)	0	100	100
2	D	317/324 (98%)	307 (97%)	10 (3%)	0	100	100
2	E	310/324 (96%)	295 (95%)	14 (4%)	1 (0%)	36	56
3	F	226/228 (99%)	206 (91%)	20 (9%)	0	100	100
3	G	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
3	H	226/228 (99%)	209 (92%)	16 (7%)	1 (0%)	30	49
All	All	2124/2167 (98%)	2017 (95%)	101 (5%)	6 (0%)	36	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	226	SER
3	H	6086	ALA

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Mol	Chain	Res	Type
1	A	36	ALA
1	A	7	ASP
1	A	9	GLN
2	B	236	ASP

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	162/163 (99%)	153 (94%)	9 (6%)	19	39
2	B	277/279 (99%)	275 (99%)	2 (1%)	76	89
2	C	278/279 (100%)	272 (98%)	6 (2%)	45	70
2	D	277/279 (99%)	269 (97%)	8 (3%)	37	63
2	E	272/279 (98%)	256 (94%)	16 (6%)	18	36
3	F	189/183 (103%)	173 (92%)	16 (8%)	10	21
3	G	189/183 (103%)	180 (95%)	9 (5%)	23	45
3	H	189/183 (103%)	177 (94%)	12 (6%)	16	34
All	All	1833/1828 (100%)	1755 (96%)	78 (4%)	26	49

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	52	LYS
1	A	99	MET
1	A	115	VAL
1	A	116	GLU
1	A	117	ASP
1	A	122	LEU
1	A	180	LEU
1	A	181	LYS
2	B	126	GLU
2	B	235	ILE

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Mol	Chain	Res	Type
2	C	11	LEU
2	C	72	MET
2	C	146	LYS
2	C	240	GLU
2	C	276	VAL
2	C	279	GLN
2	D	2	ILE
2	D	7	LYS
2	D	121	LEU
2	D	159	GLN
2	D	206	LYS
2	D	230	ASN
2	D	238	VAL
2	D	284	MET
2	E	90	ASN
2	E	109	PHE
2	E	111	ARG
2	E	170	LYS
2	E	185	ILE
2	E	214	TYR
2	E	219	VAL
2	E	221	ASP
2	E	228	VAL
2	E	237	ASP
2	E	248	LYS
2	E	260	ASP
2	E	276	VAL
2	E	297	ILE
2	E	310	ILE
2	E	314	CYS
3	F	7066	LEU
3	F	7119	LYS
3	F	7122	ASP
3	F	7124	GLN
3	F	7138	ILE
3	F	7142	VAL
3	F	7147	ILE
3	F	7150	ASN
3	F	7152	PHE
3	F	7162	ARG
3	F	7169	LEU
3	F	7176	ASN

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Mol	Chain	Res	Type
3	F	7178	PHE
3	F	7184	MSE
3	F	7196	LEU
3	F	7226	HIS
3	G	5001	MSE
3	G	5038	THR
3	G	5066	LEU
3	G	5078	ASP
3	G	5117	GLU
3	G	5119	LYS
3	G	5147	ILE
3	G	5161	THR
3	G	5189	MSE
3	H	6066	LEU
3	H	6077	GLU
3	H	6078	ASP
3	H	6081	ILE
3	H	6082	LYS
3	H	6087	ARG
3	H	6099	THR
3	H	6104	ASN
3	H	6117	GLU
3	H	6126	LEU
3	H	6184	MSE
3	H	6217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	136	ASN
2	B	65	HIS
2	B	101	GLN
2	B	139	ASN
2	B	295	HIS
2	C	200	ASN
2	C	279	GLN
2	E	65	HIS
2	E	140	ASN
2	E	311	GLN
3	F	7013	ASN
3	F	7075	GLN

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Mol	Chain	Res	Type
3	G	5176	ASN
3	G	5183	ASN
3	H	6183	ASN

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 8 ligands modelled in this entry, 4 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
6	08T	B	401	7	31,33,33	1.87	9 (29%)	41,52,52	2.09	10 (24%)
6	08T	C	401	7	31,33,33	1.84	9 (29%)	41,52,52	2.10	10 (24%)
6	08T	D	401	7	31,33,33	1.84	9 (29%)	41,52,52	2.11	10 (24%)
8	ADP	E	401	7	28,29,29	1.40	4 (14%)	43,45,45	1.89	8 (18%)

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
6	08T	B	401	7	-	2/16/38/38	0/3/3/3
6	08T	C	401	7	-	0/16/38/38	0/3/3/3
6	08T	D	401	7	-	2/16/38/38	0/3/3/3
8	ADP	E	401	7	-	2/16/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	401	ADP	C5-C4	4.71	1.47	1.39
6	B	401	08T	C2'-C3'	-4.23	1.41	1.53
6	D	401	08T	C2'-C3'	-4.15	1.42	1.53
6	C	401	08T	C2'-C3'	-4.14	1.42	1.53
6	D	401	08T	F2-BE	-3.76	1.45	1.54
6	B	401	08T	F2-BE	-3.70	1.45	1.54
6	C	401	08T	F2-BE	-3.69	1.45	1.54
6	B	401	08T	PB-O3A	-3.40	1.55	1.59
6	D	401	08T	PB-O3A	-3.29	1.55	1.59
6	C	401	08T	C6-N6	3.28	1.42	1.34
6	D	401	08T	C6-N6	3.28	1.42	1.34
6	B	401	08T	C5-N7	-3.26	1.33	1.39
6	B	401	08T	C6-N6	3.24	1.42	1.34
6	C	401	08T	C5-N7	-3.22	1.33	1.39
6	D	401	08T	C5-N7	-3.19	1.33	1.39
6	C	401	08T	PB-O3A	-3.08	1.56	1.59
6	B	401	08T	C8-N9	-2.76	1.32	1.37
6	D	401	08T	C8-N9	-2.74	1.32	1.37
6	C	401	08T	C8-N9	-2.72	1.32	1.37
6	C	401	08T	O4'-C4'	-2.71	1.39	1.45
8	E	401	ADP	C5-C6	2.68	1.48	1.41
6	B	401	08T	O4'-C4'	-2.65	1.39	1.45
6	D	401	08T	O4'-C4'	-2.55	1.39	1.45
8	E	401	ADP	C5-N7	-2.32	1.34	1.39
8	E	401	ADP	C8-N7	2.27	1.36	1.31
6	C	401	08T	C3'-C4'	-2.24	1.47	1.53
6	B	401	08T	C3'-C4'	-2.19	1.47	1.53
6	C	401	08T	C2'-C1'	-2.17	1.46	1.53
6	D	401	08T	C2'-C1'	-2.15	1.46	1.53
6	D	401	08T	C3'-C4'	-2.13	1.47	1.53
6	B	401	08T	C2'-C1'	-2.11	1.46	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	401	ADP	C5-C4-N3	-6.09	118.34	126.72
6	D	401	08T	C5-C4-N3	-5.92	118.56	126.72
6	C	401	08T	C5-C4-N3	-5.90	118.60	126.72
6	B	401	08T	C5-C4-N3	-5.89	118.60	126.72
6	C	401	08T	N3-C2-N1	-5.58	120.13	128.58
6	B	401	08T	N3-C2-N1	-5.47	120.30	128.58
6	D	401	08T	N3-C2-N1	-5.39	120.43	128.58
8	E	401	ADP	N3-C4-N9	4.84	135.39	127.17
6	C	401	08T	N3-C4-N9	4.21	134.33	127.17
6	B	401	08T	N3-C4-N9	4.18	134.27	127.17
6	D	401	08T	N3-C4-N9	4.17	134.26	127.17
6	C	401	08T	C2-N3-C4	4.02	121.65	111.83
6	B	401	08T	C2-N3-C4	3.98	121.56	111.83
6	D	401	08T	C2-N3-C4	3.96	121.51	111.83
8	E	401	ADP	C2-N3-C4	3.75	120.98	111.83
6	B	401	08T	C5-N7-C8	3.56	109.05	103.45
6	D	401	08T	C5-N7-C8	3.54	109.02	103.45
6	C	401	08T	C5-N7-C8	3.53	109.00	103.45
6	C	401	08T	N9-C8-N7	-3.52	108.94	113.94
6	B	401	08T	N9-C8-N7	-3.50	108.98	113.94
6	D	401	08T	N9-C8-N7	-3.49	108.98	113.94
8	E	401	ADP	C4-C5-N7	-3.47	106.61	110.58
6	D	401	08T	C4-C5-N7	-3.23	106.89	110.58
6	B	401	08T	C4-C5-N7	-3.17	106.95	110.58
8	E	401	ADP	N3-C2-N1	-3.14	123.82	128.58
6	C	401	08T	C4-C5-N7	-3.14	107.00	110.58
8	E	401	ADP	C3'-C2'-C1'	2.72	106.60	101.46
6	D	401	08T	C2'-C1'-N9	-2.68	106.64	113.30
8	E	401	ADP	C5-N7-C8	2.60	107.54	103.45
8	E	401	ADP	C4-N9-C8	2.52	108.38	105.74
6	C	401	08T	O5'-C5'-C4'	2.51	117.55	108.99
6	B	401	08T	O5'-C5'-C4'	2.44	117.30	108.99
6	D	401	08T	O5'-C5'-C4'	2.40	117.16	108.99
6	C	401	08T	C4-N9-C8	2.15	107.99	105.74
6	B	401	08T	C2'-C1'-N9	-2.10	108.09	113.30
6	C	401	08T	C2'-C1'-N9	-2.09	108.11	113.30
6	D	401	08T	C4-N9-C8	2.09	107.93	105.74
6	B	401	08T	C4-N9-C8	2.05	107.89	105.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	401	ADP	O4'-C4'-C5'-O5'
8	E	401	ADP	C3'-C4'-C5'-O5'
6	B	401	08T	PA-O3A-PB-O2B
6	D	401	08T	C3'-C4'-C5'-O5'
6	D	401	08T	O4'-C4'-C5'-O5'
6	B	401	08T	PA-O3A-PB-O1B

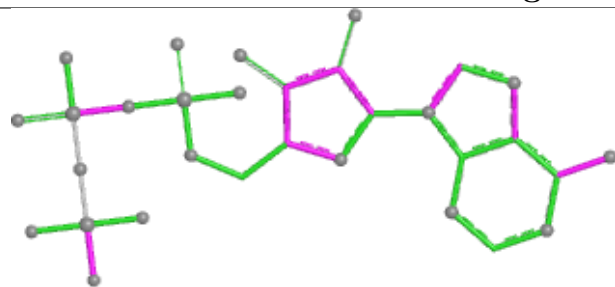
There are no ring outliers.

3 monomers are involved in 3 short contacts:

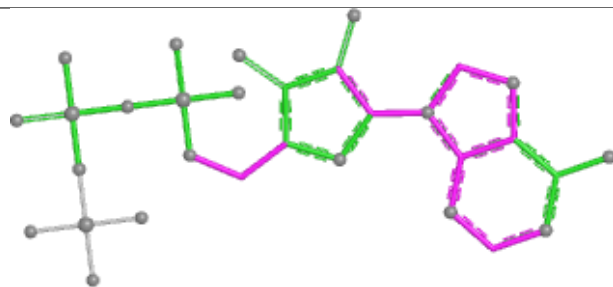
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	08T	1	0
6	D	401	08T	1	0
8	E	401	ADP	1	0

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.

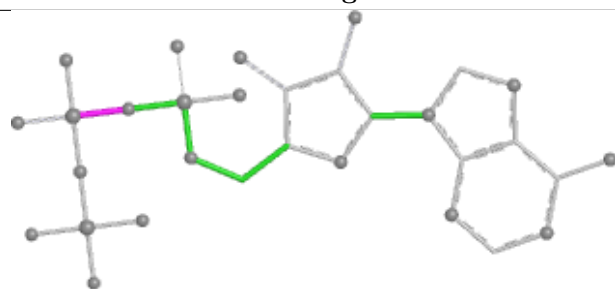
Ligand 08T B 401



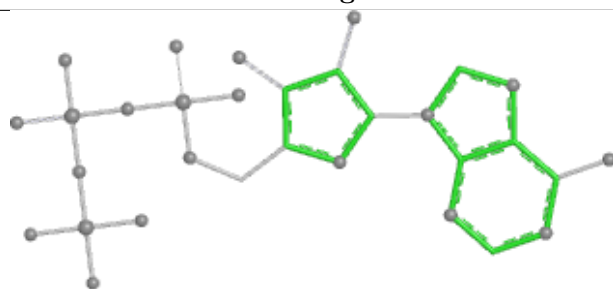
Bond lengths



Bond angles

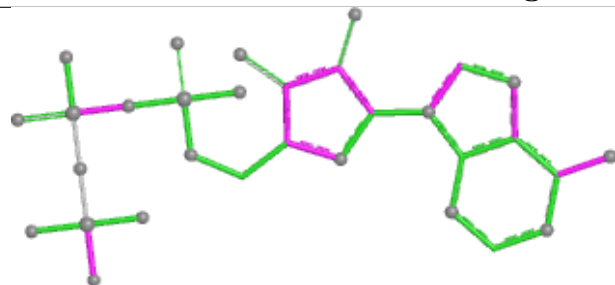


Torsions

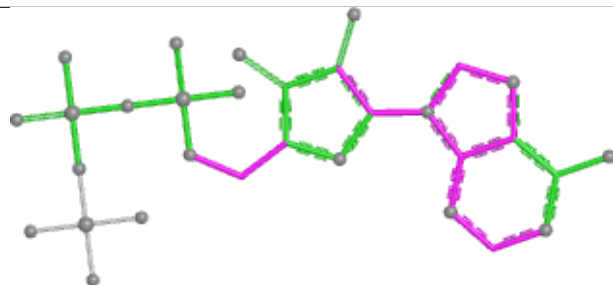


Rings

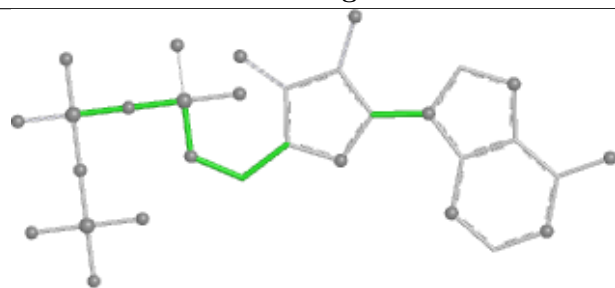
Ligand 08T C 401



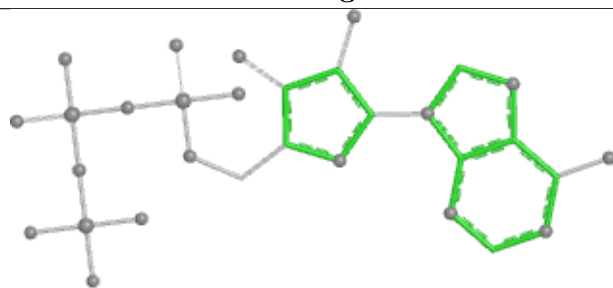
Bond lengths



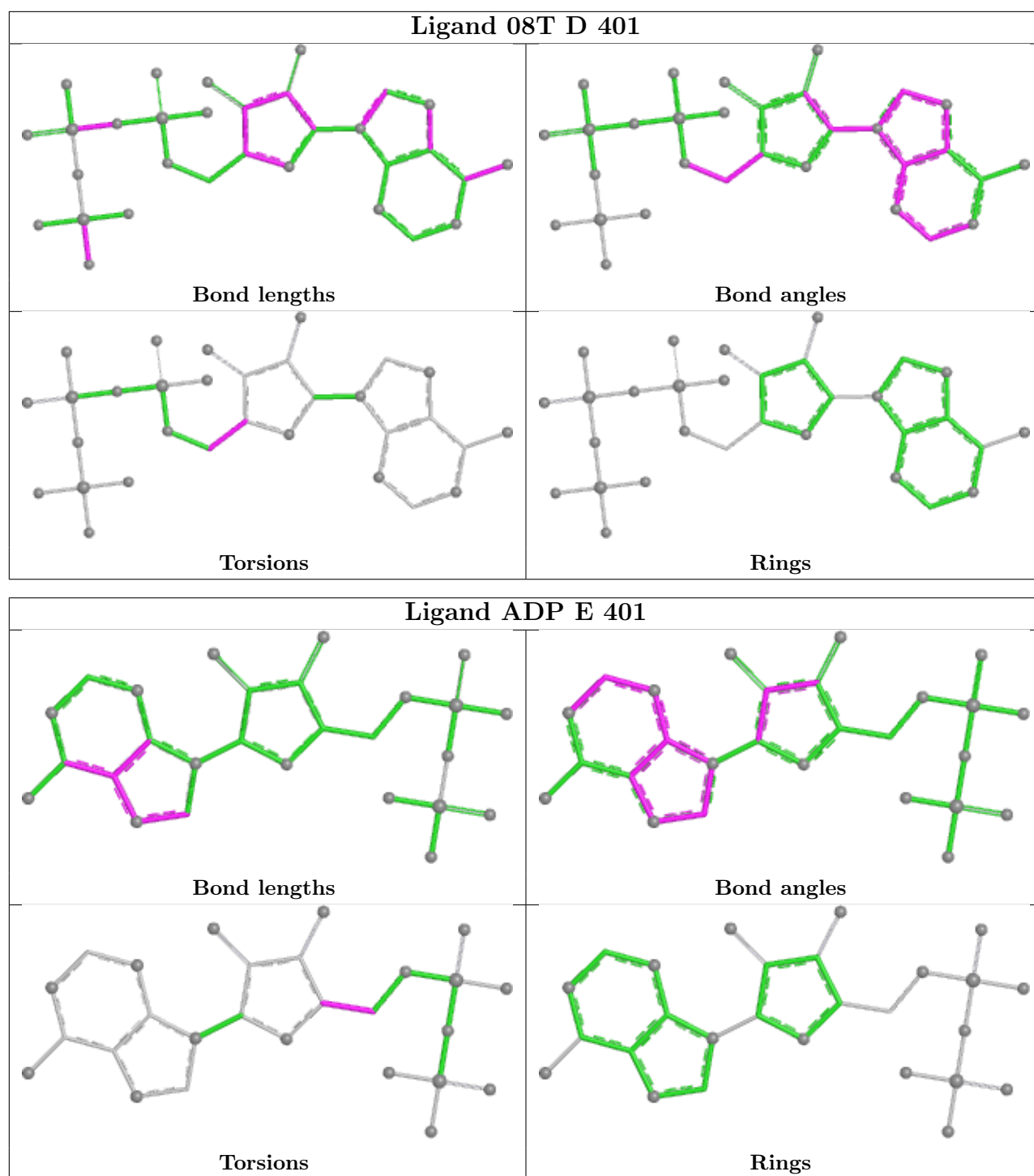
Bond angles



Torsions



Rings



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	186/187 (99%)	0.24	9 (4%) 35 30	18, 46, 87, 108	0
2	B	319/324 (98%)	-0.19	2 (0%) 85 83	16, 33, 55, 74	0
2	C	320/324 (98%)	-0.32	1 (0%) 90 88	12, 26, 50, 88	0
2	D	319/324 (98%)	-0.22	2 (0%) 85 83	9, 27, 74, 107	0
2	E	314/324 (96%)	-0.04	4 (1%) 75 71	14, 36, 68, 92	0
3	F	222/228 (97%)	1.03	27 (12%) 8 6	41, 87, 136, 147	0
3	G	222/228 (97%)	0.17	1 (0%) 87 85	26, 48, 73, 95	0
3	H	222/228 (97%)	0.38	3 (1%) 73 70	31, 60, 108, 128	0
4	I	24/30 (80%)	0.25	2 (8%) 17 13	20, 47, 165, 185	0
5	J	20/20 (100%)	0.45	1 (5%) 34 29	29, 67, 170, 177	0
All	All	2168/2217 (97%)	0.08	52 (2%) 59 54	9, 40, 104, 185	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	7.1
3	F	7178	PHE	5.2
1	A	187	TRP	4.1
3	F	7196	LEU	4.0
2	E	220	LEU	3.9
3	H	6083	ILE	3.7
3	F	7197	LEU	3.6
3	F	7209	PHE	3.5
2	C	0	SER	3.3
3	F	7115	VAL	3.2
3	F	7147	ILE	3.1
3	F	7206	ALA	3.0
2	D	229	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	97	PHE	2.9
3	F	7140	ILE	2.9
3	F	7123	LEU	2.8
2	B	97	PHE	2.7
3	F	7141	THR	2.7
2	E	114	LEU	2.6
3	F	7126	LEU	2.6
3	F	7182	ILE	2.6
3	F	7198	LEU	2.6
3	F	7111	VAL	2.5
3	F	7138	ILE	2.5
4	I	30	DC	2.5
2	E	228	VAL	2.5
3	H	6060	PHE	2.5
1	A	175	LYS	2.4
3	F	7108	PRO	2.4
1	A	161	LEU	2.4
3	H	6091	PHE	2.4
1	A	108	TYR	2.3
5	J	20	DA	2.3
3	F	7220	LEU	2.3
1	A	158	LEU	2.3
3	F	7165	TYR	2.3
3	F	7142	VAL	2.3
3	F	7221	GLU	2.3
1	A	179	GLN	2.3
3	F	7155	VAL	2.3
2	B	1	MET	2.2
3	F	7213	HIS	2.2
3	F	7222	ALA	2.1
3	F	7132	GLY	2.1
3	G	5135	ILE	2.1
2	E	227	LEU	2.1
3	F	7010	LEU	2.1
1	A	174	VAL	2.1
3	F	7152	PHE	2.1
4	I	28	DT	2.1
1	A	92	GLU	2.0
3	F	7166	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

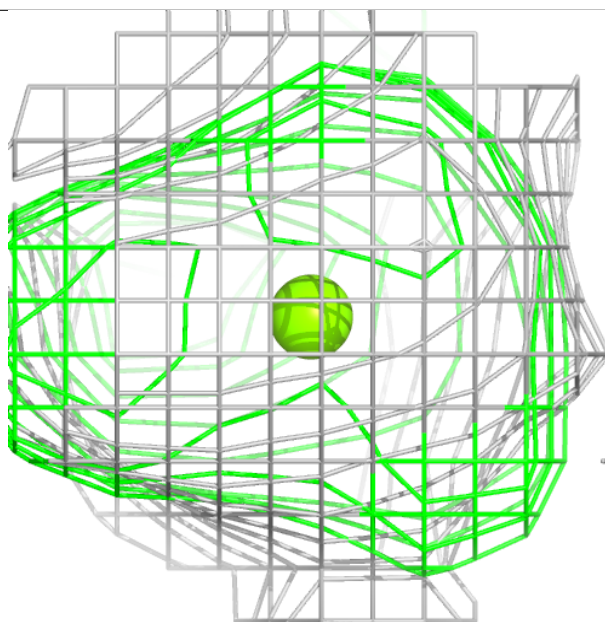
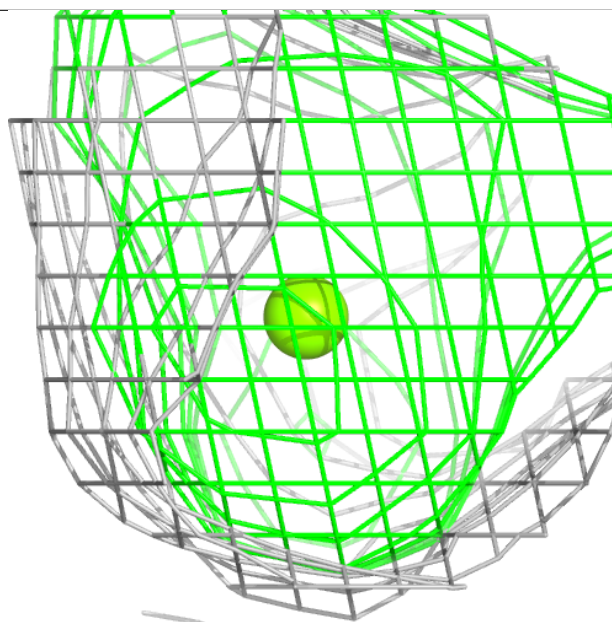
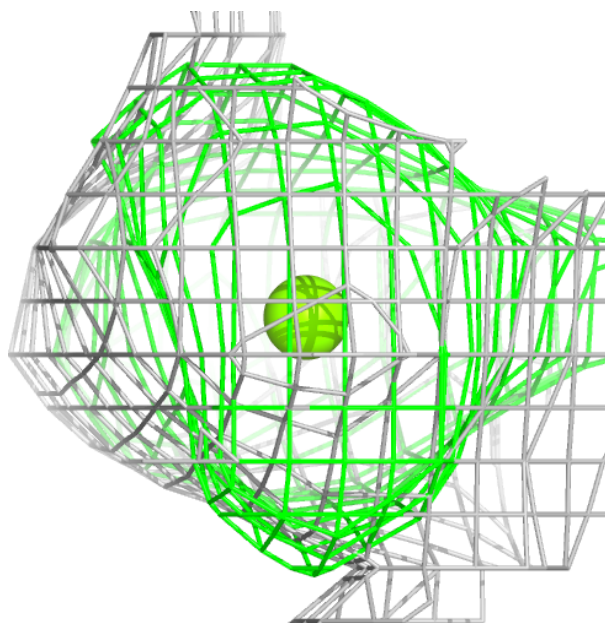
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	E	402	1/1	0.93	0.27	20,20,20,20	0
8	ADP	E	401	27/27	0.95	0.09	25,36,49,68	0
7	MG	D	402	1/1	0.96	0.15	11,11,11,11	0
7	MG	B	402	1/1	0.96	0.22	22,22,22,22	0
7	MG	C	402	1/1	0.96	0.18	12,12,12,12	0
6	08T	D	401	31/31	0.97	0.06	14,21,29,33	0
6	08T	B	401	31/31	0.97	0.06	14,26,37,49	0
6	08T	C	401	31/31	0.98	0.06	10,18,24,25	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.

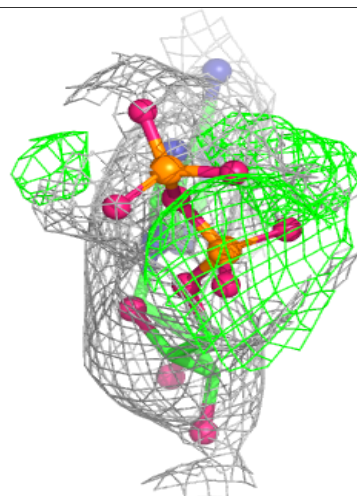
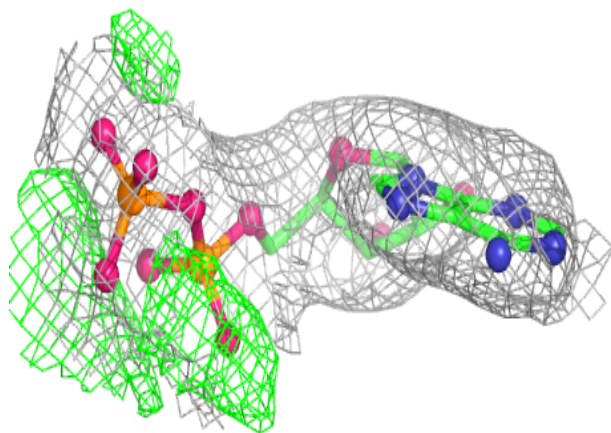
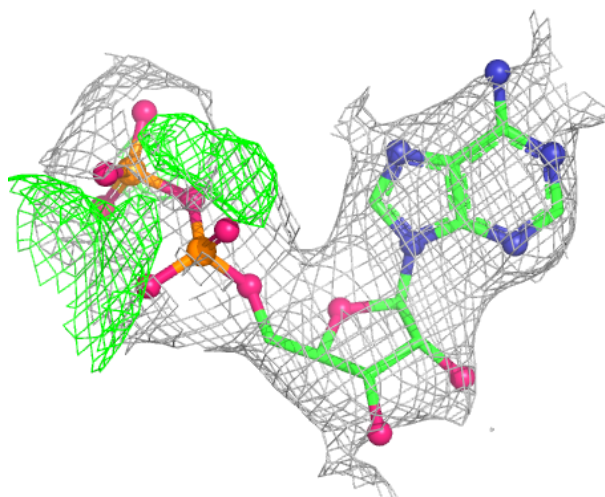
Electron density around MG E 402:

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



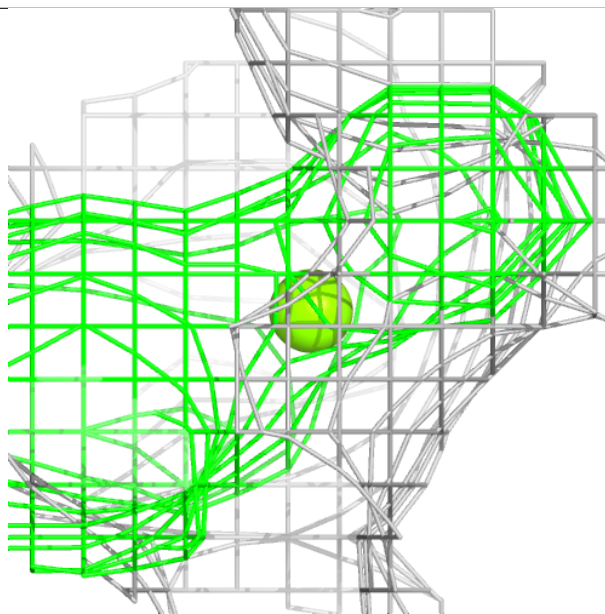
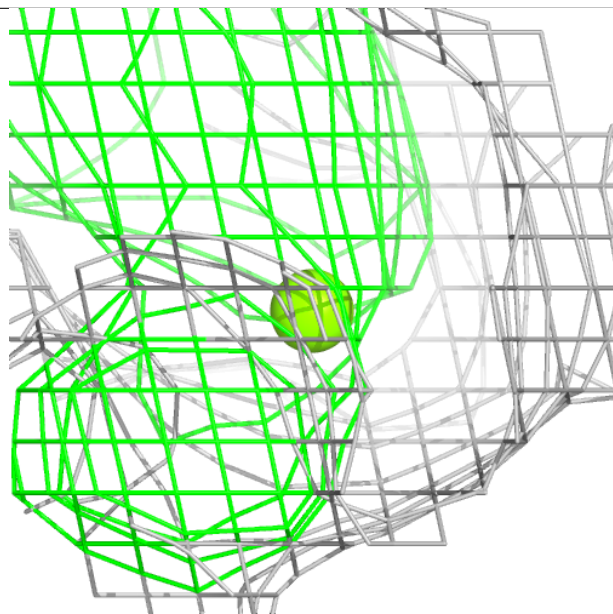
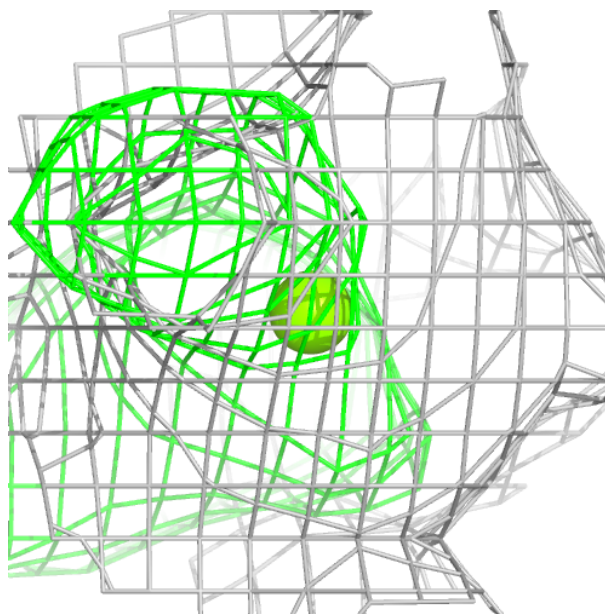
Electron density around ADP E 401:

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and green (positive)



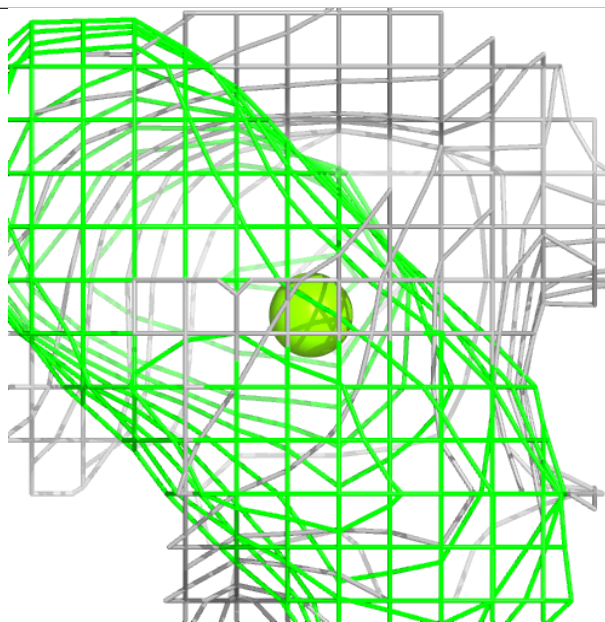
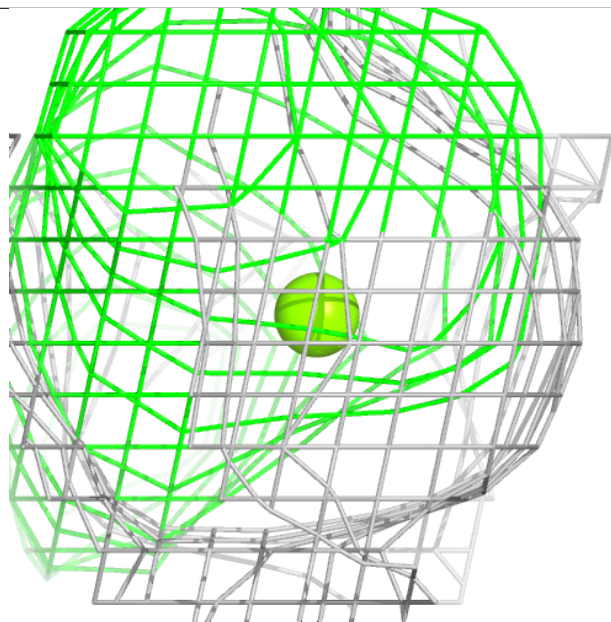
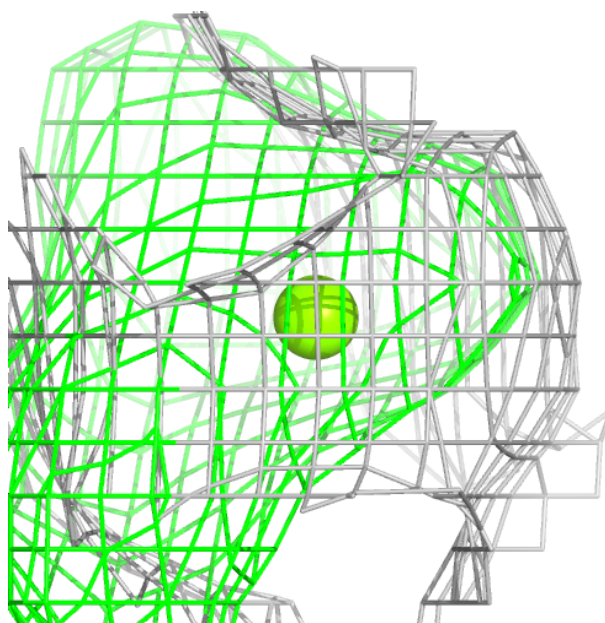
Electron density around MG D 402:

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



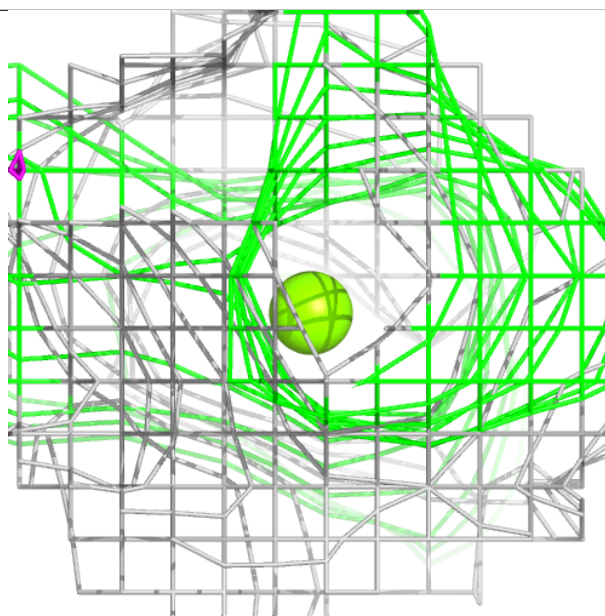
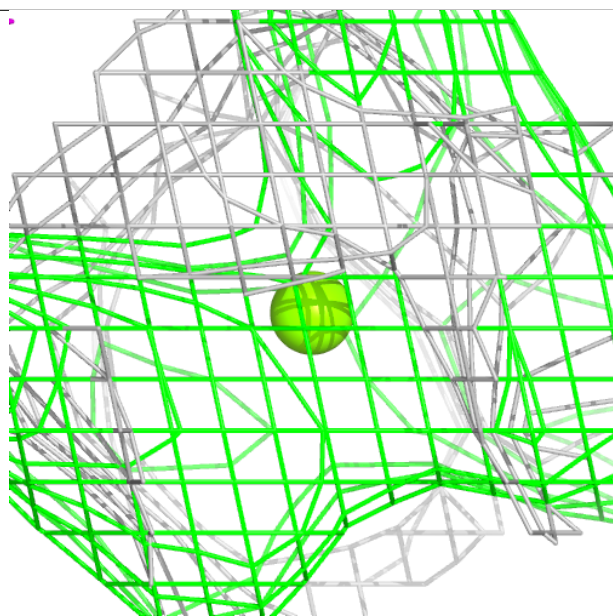
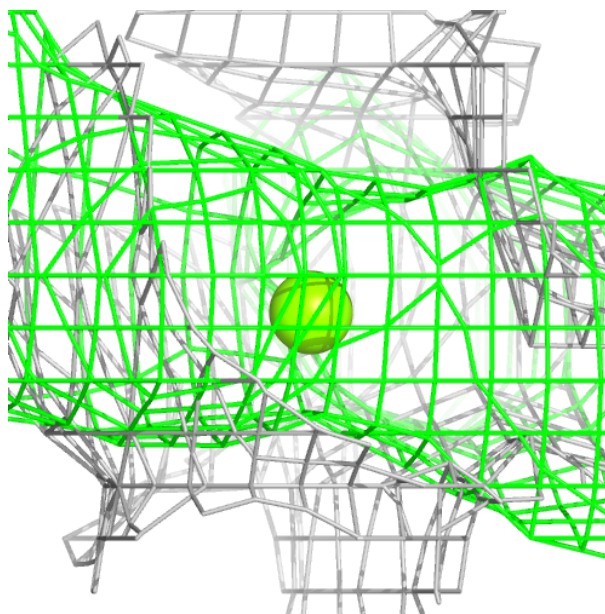
Electron density around MG B 402:

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



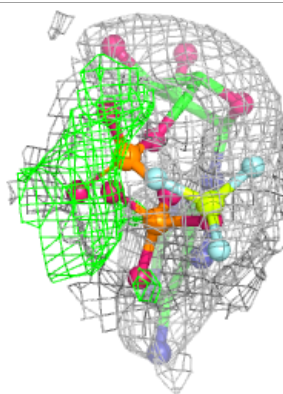
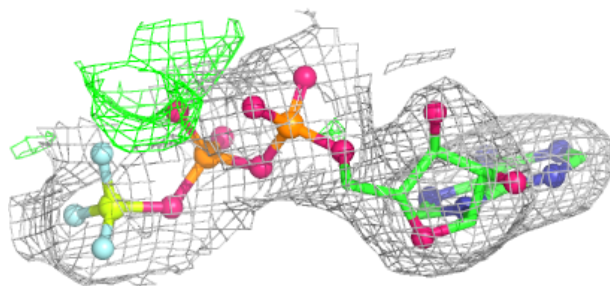
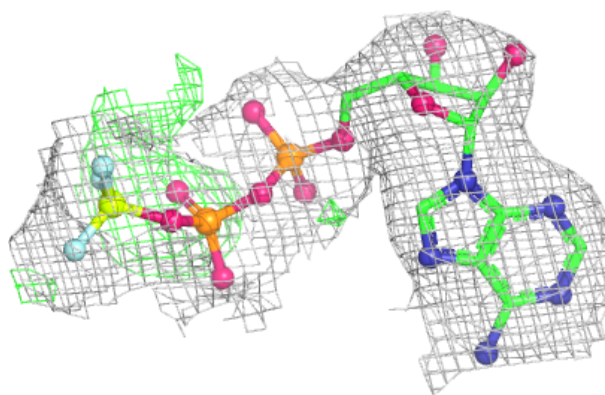
Electron density around MG C 402:

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

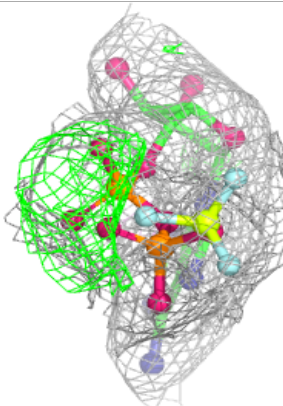
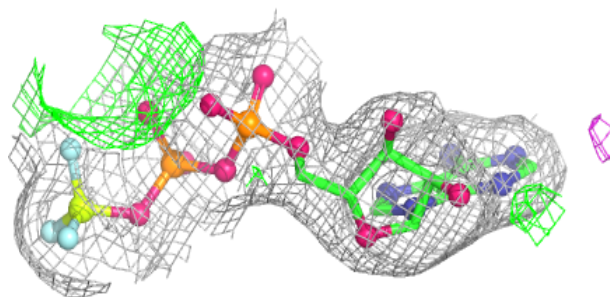
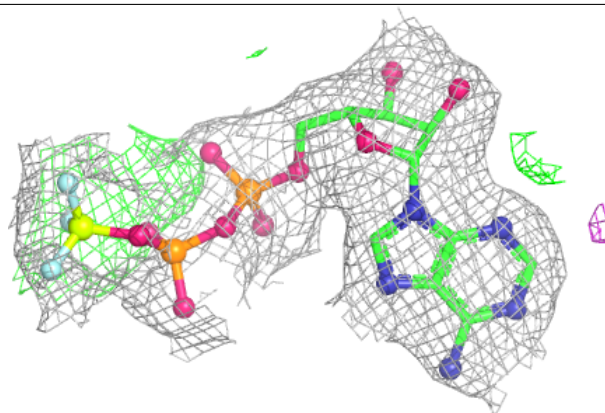


Electron density around 08T D 401:

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and green (positive)

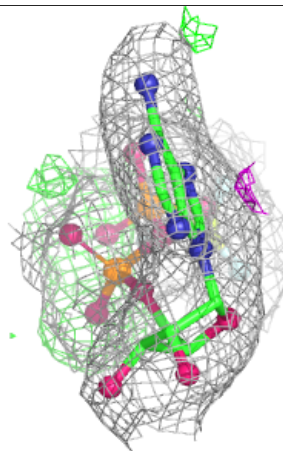
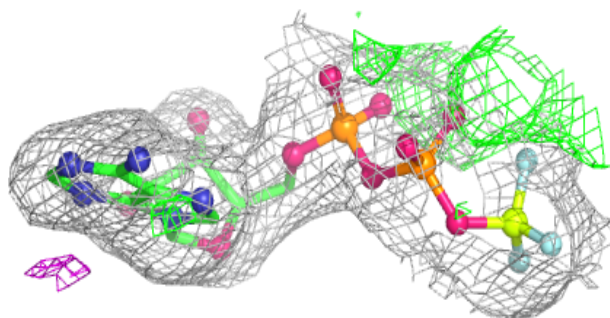
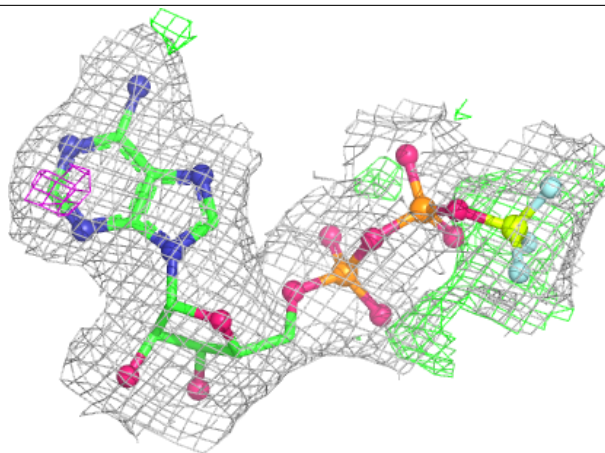
**Electron density around 08T B 401:**

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and green (positive)



Electron density around 08T C 401:

$2mF_o-DF_c$ (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.