



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 06:33 PM EDT

PDB ID : 3X06 / pdb_00003x06
Title : Crystal structure of PIP4KIIBETA T201M complex with GMP
Authors : Takeuchi, K.; Lo, Y.H.; Sumita, K.; Senda, M.; Terakawa, J.; Dimitoris, A.; Locasale, J.W.; Sasaki, M.; Yoshino, H.; Zhang, Y.; Kahoud, E.R.; Takano, T.; Yokota, T.; Emerling, B.; Asara, J.A.; Ishida, T.; Shimada, I.; Daikoku, T.; Cantley, L.C.; Senda, T.; Sasaki, A.T.
Deposited on : 2014-10-09
Resolution : 2.65 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](#) ①) 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

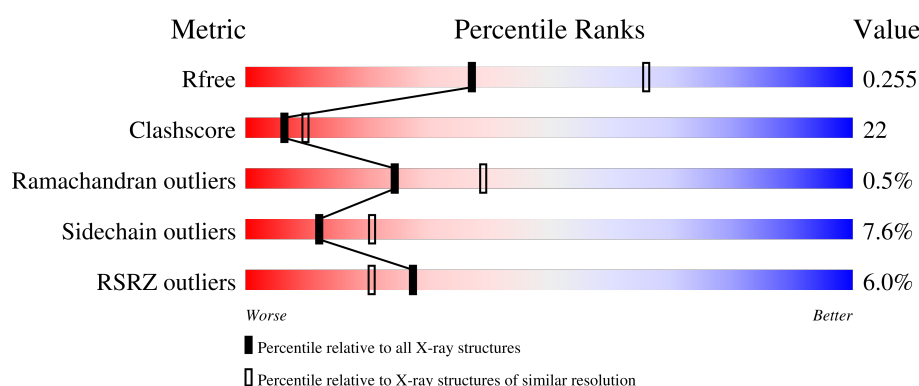
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	393	5% 51% 26% • 19%
1	B	393	5% 48% 26% • • 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5324 atoms, of which 60 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.

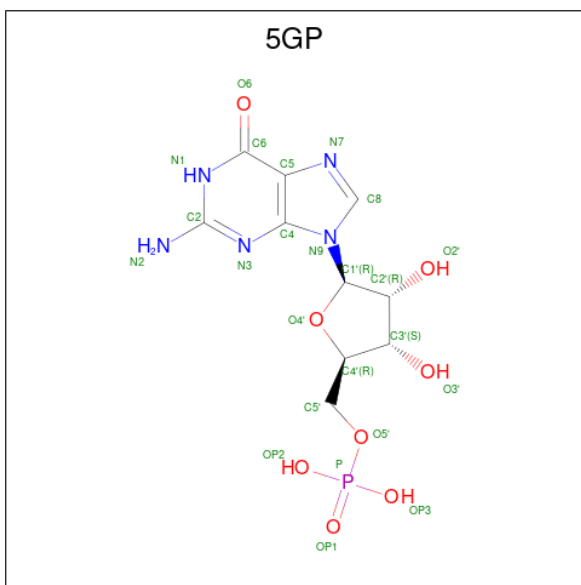
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2617	1666	446	490	15			
1	B	303	Total	C	N	O	S	0	0	0
			2496	1599	426	457	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP P78356
A	25	PRO	-	expression tag	UNP P78356
A	26	ASN	-	expression tag	UNP P78356
A	27	CYS	-	expression tag	UNP P78356
A	28	ALA	-	expression tag	UNP P78356
A	29	PRO	-	expression tag	UNP P78356
A	30	GLY	-	expression tag	UNP P78356
A	201	MET	THR	engineered mutation	UNP P78356
B	24	GLY	-	expression tag	UNP P78356
B	25	PRO	-	expression tag	UNP P78356
B	26	ASN	-	expression tag	UNP P78356
B	27	CYS	-	expression tag	UNP P78356
B	28	ALA	-	expression tag	UNP P78356
B	29	PRO	-	expression tag	UNP P78356
B	30	GLY	-	expression tag	UNP P78356
B	201	MET	THR	engineered mutation	UNP P78356

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		

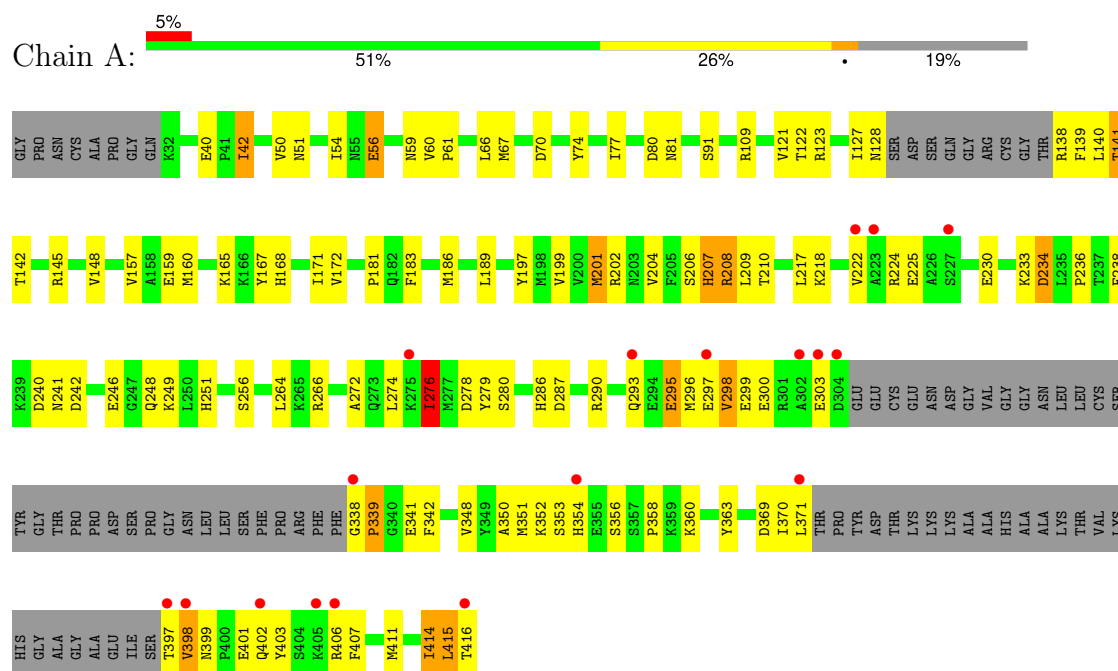
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	14	Total	O	0	0
			14	14		

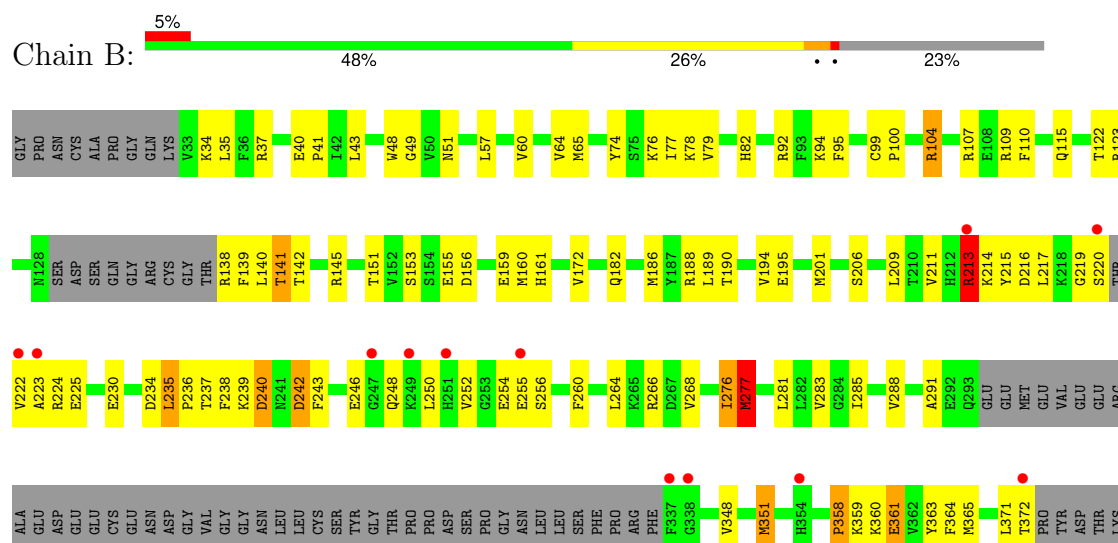
3 Residue-property plots [i](#)

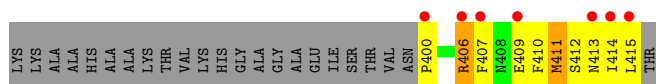
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta



- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.83Å 182.88Å 106.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.41 – 2.65 54.41 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (54.41-2.65) 99.0 (54.41-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.212 , 0.261 0.205 , 0.255	Depositor DCC
R_{free} test set	1549 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 81.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5324	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: 5GP

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	0.58	2/2670 (0.1%)	0.85	2/3590 (0.1%)
1	B	0.60	1/2549 (0.0%)	0.90	6/3426 (0.2%)
All	All	0.59	3/5219 (0.1%)	0.87	8/7016 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLU	C-N	-9.64	1.20	1.33
1	A	207	HIS	CG-ND1	-5.99	1.31	1.38
1	A	207	HIS	CD2-NE2	-5.17	1.32	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLU	O-C-N	8.17	130.91	122.09
1	B	213	ARG	CA-C-N	-6.13	114.34	122.99
1	B	213	ARG	C-N-CA	-6.13	114.34	122.99
1	B	277	MET	N-CA-C	5.75	115.83	108.24
1	A	276	ILE	N-CA-C	5.74	117.12	109.37
1	B	254	GLU	N-CA-C	-5.36	106.75	113.72
1	B	194	VAL	N-CA-C	5.18	115.43	108.17
1	A	56	GLU	N-CA-C	-5.02	105.70	111.07

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	2617	0	2591	109	0
1	B	2496	0	2482	128	0
2	A	96	48	48	2	0
2	B	24	12	12	0	0
3	A	17	0	0	0	0
3	B	14	0	0	1	0
All	All	5264	60	5133	228	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 22.

All (228) 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:399:ASN:OD1	1:A:402:GLN:HG2	1.35	1.23
1:B:235:LEU:HD12	1:B:235:LEU:H	1.12	1.13
1:B:243:PHE:HE2	1:B:414:ILE:CG2	1.63	1.10
1:B:243:PHE:CE2	1:B:414:ILE:CG2	2.45	0.99
1:A:141:THR:HG22	1:A:142:THR:O	1.65	0.95
1:B:222:VAL:HG12	1:B:223:ALA:H	1.29	0.94
1:B:236:PRO:HB2	1:B:238:PHE:CE1	2.03	0.94
1:B:243:PHE:CE2	1:B:414:ILE:HG21	2.03	0.93
1:B:277:MET:SD	1:B:400:PRO:N	2.42	0.92
1:B:213:ARG:CG	1:B:215:TYR:CE1	2.53	0.92
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.50	0.92
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.54	0.90
1:A:399:ASN:OD1	1:A:402:GLN:CG	2.20	0.88
1:B:243:PHE:HE2	1:B:414:ILE:HG22	1.40	0.86
1:B:141:THR:HG22	1:B:142:THR:O	1.76	0.84
1:B:235:LEU:HD12	1:B:235:LEU:N	1.93	0.82
1:B:213:ARG:HG3	1:B:215:TYR:CE1	2.15	0.81
1:A:398:VAL:HG12	1:A:402:GLN:HG3	1.63	0.80
1:B:213:ARG:CG	1:B:215:TYR:HE1	1.91	0.80
1:A:225:GLU:HG3	1:A:241:ASN:HB2	1.65	0.79
1:B:110:PHE:CE1	1:B:182:GLN:HG2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLY:HA2	1:B:410:PHE:CD2	2.19	0.78
1:A:338:GLY:N	1:A:339:PRO:HD3	2.00	0.77
1:A:183:PHE:CE1	1:A:201:MET:HE3	2.21	0.76
1:A:77:ILE:CD1	1:B:77:ILE:HD11	2.16	0.75
1:B:281:LEU:HD22	1:B:411:MET:CG	2.15	0.75
1:A:242:ASP:O	1:A:246:GLU:HG3	1.87	0.74
1:A:189:LEU:N	1:A:189:LEU:HD12	2.03	0.73
1:A:256:SER:HB3	1:A:351:MET:HE2	1.70	0.73
1:A:338:GLY:N	1:A:339:PRO:CD	2.53	0.72
1:A:77:ILE:HD12	1:B:79:VAL:HG22	1.72	0.72
1:B:213:ARG:HG2	1:B:215:TYR:CE1	2.23	0.71
1:B:242:ASP:O	1:B:246:GLU:HG3	1.91	0.71
1:B:216:ASP:C	1:B:217:LEU:HD23	2.16	0.71
1:B:235:LEU:H	1:B:235:LEU:CD1	1.95	0.71
1:A:77:ILE:HD11	1:B:77:ILE:CD1	2.21	0.70
1:B:78:LYS:HD2	1:B:94:LYS:HE2	1.73	0.70
1:A:128:ASN:HB3	1:A:140:LEU:HD23	1.74	0.70
1:B:141:THR:CG2	1:B:145:ARG:HA	2.21	0.70
1:A:217:LEU:HD13	1:A:414:ILE:CD1	2.23	0.68
1:A:141:THR:HG23	1:A:145:ARG:HA	1.76	0.68
1:A:224:ARG:NH1	1:A:240:ASP:OD1	2.24	0.68
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.76	0.68
1:B:141:THR:HG23	1:B:145:ARG:HA	1.75	0.68
1:A:218:LYS:HD2	1:A:224:ARG:NE	2.08	0.67
1:B:94:LYS:HB2	1:B:190:THR:HB	1.76	0.67
1:A:256:SER:HB3	1:A:351:MET:CE	2.24	0.67
1:A:42:ILE:H	1:A:42:ILE:HD13	1.60	0.66
1:A:42:ILE:HD13	1:A:42:ILE:N	2.10	0.66
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.25	0.66
1:B:243:PHE:CE2	1:B:414:ILE:HG22	2.22	0.66
1:A:141:THR:CG2	1:A:145:ARG:HA	2.26	0.66
1:B:281:LEU:HD22	1:B:411:MET:HG3	1.77	0.66
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.25	0.65
1:A:398:VAL:HA	1:A:402:GLN:OE1	1.96	0.65
1:B:406:ARG:HG2	1:B:407:PHE:N	2.10	0.64
1:B:250:LEU:HB2	1:B:415:LEU:HD23	1.79	0.64
1:B:216:ASP:O	1:B:217:LEU:HD23	1.97	0.64
1:A:217:LEU:CD1	1:A:414:ILE:CD1	2.75	0.64
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.81	0.63
1:B:242:ASP:OD1	1:B:242:ASP:N	2.29	0.63
1:B:213:ARG:HG2	1:B:215:TYR:HE1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LYS:HG3	1:B:237:THR:HA	1.81	0.63
1:A:138:ARG:HD3	1:A:140:LEU:HD11	1.80	0.62
1:A:138:ARG:HG2	1:A:139:PHE:N	2.15	0.62
1:B:159:GLU:OE2	1:B:159:GLU:HA	1.97	0.62
1:A:217:LEU:CD1	1:A:414:ILE:HD11	2.29	0.62
1:B:213:ARG:NH2	1:B:238:PHE:HE1	1.98	0.62
1:A:341:GLU:HG3	1:A:342:PHE:N	2.15	0.61
1:A:279:TYR:HB3	1:A:369:ASP:O	2.01	0.61
1:B:43:LEU:HD21	1:B:140:LEU:CD1	2.29	0.61
1:A:411:MET:HA	1:A:414:ILE:HD12	1.82	0.60
1:B:222:VAL:HG12	1:B:223:ALA:N	2.08	0.60
1:B:60:VAL:O	1:B:104:ARG:NH2	2.34	0.60
1:B:79:VAL:O	1:B:92:ARG:HA	2.01	0.60
1:B:161:HIS:HE1	3:B:606:HOH:O	1.83	0.60
1:A:341:GLU:OE2	1:A:352:LYS:HD2	2.01	0.60
1:A:339:PRO:O	1:A:360:LYS:NZ	2.35	0.59
1:A:341:GLU:HG3	1:A:342:PHE:H	1.68	0.59
1:B:213:ARG:HG2	1:B:215:TYR:OH	2.01	0.59
1:B:240:ASP:OD1	1:B:240:ASP:N	2.32	0.59
1:A:42:ILE:H	1:A:42:ILE:CD1	2.14	0.58
1:B:51:ASN:HB2	1:B:122:THR:HG21	1.84	0.58
1:B:189:LEU:HD12	1:B:189:LEU:N	2.19	0.58
1:A:399:ASN:H	1:A:402:GLN:CG	2.17	0.58
1:B:288:VAL:O	1:B:291:ALA:HB3	2.03	0.57
1:A:181:PRO:HB3	1:A:201:MET:CE	2.34	0.57
1:B:35:LEU:HD13	1:B:37:ARG:NH2	2.18	0.57
1:B:219:GLY:CA	1:B:410:PHE:CD2	2.87	0.57
1:A:109:ARG:CZ	1:A:172:VAL:HG22	2.34	0.57
1:B:213:ARG:NH2	1:B:238:PHE:CE1	2.72	0.56
1:B:264:LEU:HD11	1:B:407:PHE:HE1	1.70	0.56
1:A:66:LEU:HD12	1:A:168:HIS:CE1	2.40	0.56
1:A:139:PHE:CZ	1:A:148:VAL:HG11	2.40	0.56
1:B:78:LYS:HD2	1:B:94:LYS:CE	2.35	0.56
1:B:206:SER:HB2	1:B:364:PHE:CE2	2.41	0.56
1:B:214:LYS:HG3	1:B:236:PRO:O	2.06	0.56
1:A:183:PHE:HE1	1:A:201:MET:HE3	1.68	0.55
1:B:407:PHE:CD1	1:B:407:PHE:C	2.84	0.55
1:A:138:ARG:CG	1:A:139:PHE:N	2.69	0.55
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.88	0.55
1:B:225:GLU:HA	1:B:242:ASP:OD1	2.07	0.55
1:B:213:ARG:CB	1:B:215:TYR:HE1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:PHE:CE1	1:B:248:GLN:HG2	2.42	0.55
1:A:183:PHE:CE1	1:A:201:MET:CE	2.90	0.55
1:B:213:ARG:CG	1:B:215:TYR:CZ	2.89	0.55
1:A:40:GLU:OE1	1:A:138:ARG:NH2	2.41	0.54
1:B:153:SER:O	1:B:156:ASP:HB2	2.07	0.54
1:B:188:ARG:C	1:B:189:LEU:HD12	2.32	0.54
1:A:236:PRO:HB2	1:A:238:PHE:CE2	2.42	0.54
1:A:264:LEU:HD11	1:A:407:PHE:HE1	1.73	0.54
1:A:415:LEU:HD23	1:A:415:LEU:H	1.73	0.54
1:A:50:VAL:O	1:A:54:ILE:HG12	2.09	0.53
1:A:160:MET:HG2	1:A:186:MET:SD	2.48	0.53
1:B:49:GLY:HA3	1:B:95:PHE:CE1	2.44	0.53
1:B:141:THR:CG2	1:B:142:THR:O	2.54	0.52
1:B:214:LYS:CG	1:B:236:PRO:O	2.57	0.52
1:B:160:MET:HE2	1:B:371:LEU:HD11	1.90	0.52
1:B:48:TRP:HH2	1:B:77:ILE:HD13	1.75	0.52
1:B:206:SER:CB	1:B:209:LEU:HB2	2.40	0.52
1:B:213:ARG:HG2	1:B:215:TYR:CZ	2.44	0.52
1:A:139:PHE:CZ	1:A:148:VAL:CG1	2.93	0.51
1:A:217:LEU:CD1	1:A:414:ILE:HD13	2.38	0.51
1:B:260:PHE:HB2	1:B:351:MET:HE1	1.93	0.51
1:A:50:VAL:HG21	1:A:121:VAL:HG11	1.93	0.51
1:B:220:SER:CB	1:B:406:ARG:HD3	2.41	0.51
1:B:213:ARG:HG3	1:B:215:TYR:CZ	2.44	0.51
1:B:213:ARG:HB3	1:B:215:TYR:HE1	1.75	0.51
1:B:189:LEU:N	1:B:189:LEU:CD1	2.73	0.51
1:B:243:PHE:HE2	1:B:414:ILE:CB	2.23	0.50
1:B:243:PHE:HE1	1:B:248:GLN:HG2	1.74	0.50
1:A:181:PRO:HB3	1:A:201:MET:HE2	1.92	0.50
1:A:415:LEU:C	1:A:416:THR:HG23	2.36	0.50
1:A:217:LEU:HD12	1:A:414:ILE:HD13	1.94	0.50
1:B:206:SER:HB3	1:B:209:LEU:HB2	1.95	0.49
1:A:204:VAL:HG23	2:A:501:5GP:O6	2.12	0.49
1:A:138:ARG:HD3	1:A:140:LEU:CG	2.43	0.49
1:B:277:MET:SD	1:B:400:PRO:CD	3.00	0.49
1:A:234:ASP:OD1	1:A:234:ASP:N	2.45	0.49
1:A:189:LEU:N	1:A:189:LEU:CD1	2.73	0.49
1:A:206:SER:HB3	1:A:209:LEU:HB2	1.95	0.49
1:A:138:ARG:HD3	1:A:140:LEU:CD1	2.43	0.48
1:A:157:VAL:HG21	1:A:197:TYR:CD1	2.48	0.48
1:B:222:VAL:CG1	1:B:223:ALA:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:CG	1:B:215:TYR:OH	2.62	0.48
1:B:252:VAL:CG2	1:B:256:SER:HB2	2.43	0.48
1:A:67:MET:O	1:A:70:ASP:HB2	2.14	0.48
1:B:409:GLU:O	1:B:412:SER:N	2.47	0.47
1:B:201:MET:HB2	1:B:201:MET:HE3	1.73	0.47
1:A:230:GLU:OE1	1:A:233:LYS:HD2	2.13	0.47
1:B:288:VAL:HG23	1:B:360:LYS:O	2.14	0.47
1:A:230:GLU:CD	1:A:233:LYS:HD2	2.40	0.47
1:B:99:CYS:N	1:B:100:PRO:HD3	2.30	0.47
1:B:243:PHE:CE1	1:B:248:GLN:HB3	2.50	0.47
1:A:183:PHE:CD1	1:A:201:MET:HE3	2.50	0.47
1:A:141:THR:CG2	1:A:142:THR:O	2.52	0.46
1:A:59:ASN:HB3	1:B:34:LYS:O	2.15	0.46
1:B:104:ARG:HA	1:B:107:ARG:NH1	2.30	0.46
1:B:220:SER:HB2	1:B:406:ARG:HD3	1.97	0.46
1:B:110:PHE:CZ	1:B:182:GLN:HG2	2.49	0.46
1:B:252:VAL:HG23	1:B:256:SER:HB2	1.96	0.46
1:A:293:GLN:OE1	2:A:502:5GP:C6	2.64	0.46
1:A:415:LEU:H	1:A:415:LEU:CD2	2.27	0.46
1:A:251:HIS:O	1:A:353:SER:HA	2.16	0.46
1:A:248:GLN:HG3	1:A:249:LYS:N	2.30	0.46
1:B:358:PRO:HB2	1:B:359:LYS:H	1.60	0.45
1:A:74:TYR:CE2	1:B:82:HIS:CB	2.99	0.45
1:A:74:TYR:CZ	1:B:82:HIS:HB2	2.51	0.45
1:A:159:GLU:HA	1:A:159:GLU:OE2	2.16	0.45
1:A:181:PRO:HB3	1:A:201:MET:HE1	1.97	0.45
1:B:234:ASP:O	1:B:236:PRO:HD3	2.16	0.45
1:B:250:LEU:HD12	1:B:415:LEU:HD21	1.98	0.45
1:A:218:LYS:HD2	1:A:224:ARG:CZ	2.47	0.45
1:B:74:TYR:CD1	1:B:74:TYR:C	2.94	0.44
1:B:214:LYS:HB3	1:B:214:LYS:HE2	1.83	0.44
1:A:295:GLU:O	1:A:298:VAL:HG12	2.17	0.44
1:B:264:LEU:O	1:B:268:VAL:HG22	2.17	0.44
1:A:415:LEU:O	1:A:416:THR:CG2	2.66	0.44
1:B:237:THR:O	1:B:237:THR:HG22	2.17	0.44
1:A:81:ASN:O	1:A:91:SER:HB3	2.17	0.44
1:A:207:HIS:CE1	1:A:208:ARG:HG2	2.52	0.44
1:A:234:ASP:C	1:A:236:PRO:HD3	2.43	0.44
1:A:370:ILE:O	1:A:370:ILE:HG13	2.18	0.44
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.99	0.43
1:B:276:ILE:HG22	1:B:277:MET:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:O	1:A:416:THR:HG23	2.18	0.43
1:A:341:GLU:CG	1:A:342:PHE:H	2.30	0.43
1:A:74:TYR:CE2	1:B:82:HIS:HB3	2.53	0.43
1:A:80:ASP:OD1	1:A:80:ASP:C	2.61	0.43
1:B:220:SER:HB3	1:B:406:ARG:HD3	2.01	0.43
1:B:220:SER:C	1:B:222:VAL:HB	2.43	0.43
1:A:299:GLU:O	1:A:300:GLU:C	2.62	0.42
1:B:348:VAL:O	1:B:348:VAL:HG12	2.19	0.42
1:B:250:LEU:HD12	1:B:415:LEU:CD2	2.50	0.42
1:A:350:ALA:HA	1:A:363:TYR:O	2.19	0.42
1:B:43:LEU:CD2	1:B:140:LEU:CD1	2.97	0.42
1:A:354:HIS:C	1:A:356:SER:H	2.27	0.42
1:B:215:TYR:HB3	1:B:217:LEU:HD21	2.00	0.42
1:B:139:PHE:O	1:B:139:PHE:CD1	2.72	0.42
1:B:371:LEU:C	1:B:372:THR:HG23	2.44	0.42
1:B:409:GLU:O	1:B:410:PHE:C	2.62	0.42
1:A:186:MET:HG3	1:A:199:VAL:CG2	2.50	0.42
1:A:272:ALA:O	1:A:274:LEU:O	2.38	0.41
1:A:407:PHE:O	1:A:411:MET:HG2	2.20	0.41
1:B:40:GLU:HA	1:B:41:PRO:HD3	1.89	0.41
1:A:210:THR:O	1:A:286:HIS:ND1	2.45	0.41
1:B:240:ASP:HB3	1:B:410:PHE:CZ	2.55	0.41
1:A:341:GLU:CG	1:A:342:PHE:N	2.83	0.41
1:B:189:LEU:O	1:B:195:GLU:HA	2.21	0.41
1:A:202:ARG:CZ	1:A:348:VAL:HG21	2.51	0.41
1:B:283:VAL:HG22	1:B:365:MET:HG2	2.02	0.41
1:B:57:LEU:O	1:B:104:ARG:NH2	2.54	0.41
1:B:215:TYR:CD2	1:B:238:PHE:HB2	2.56	0.41
1:A:234:ASP:O	1:A:236:PRO:HD3	2.21	0.41
1:A:274:LEU:HB2	1:A:276:ILE:HG12	2.03	0.41
1:B:138:ARG:HG3	1:B:151:THR:OG1	2.21	0.41
1:B:160:MET:HG2	1:B:186:MET:SD	2.60	0.41
1:B:213:ARG:HB2	1:B:285:ILE:HB	2.02	0.41
1:B:240:ASP:HB3	1:B:410:PHE:CE2	2.56	0.41
1:A:293:GLN:O	1:A:297:GLU:HG3	2.21	0.41
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.86	0.40
1:A:278:ASP:HA	1:A:403:TYR:CZ	2.57	0.40
1:B:361:GLU:HG3	1:B:363:TYR:CZ	2.56	0.40
1:B:64:VAL:HG23	1:B:65:MET:HG2	2.02	0.40
1:B:141:THR:HG21	1:B:145:ARG:HA	1.98	0.40
1:A:167:TYR:O	1:A:171:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ASN:OD1	1:A:402:GLN:CD	2.65	0.40
1:B:224:ARG:HB3	1:B:239:LYS:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/393 (79%)	297 (96%)	11 (4%)	2 (1%)	21	34
1	B	293/393 (75%)	283 (97%)	9 (3%)	1 (0%)	36	52
All	All	603/786 (77%)	580 (96%)	20 (3%)	3 (0%)	24	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PRO
1	A	358	PRO
1	B	358	PRO

5.3.2 Protein sidechains [i](#)

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	295/352 (84%)	271 (92%)	24 (8%)	11	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	281/352 (80%)	261 (93%)	20 (7%)	13	23
All	All	576/704 (82%)	532 (92%)	44 (8%)	12	21

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	56	GLU
1	A	123	ARG
1	A	127	ILE
1	A	141	THR
1	A	165	LYS
1	A	201	MET
1	A	208	ARG
1	A	222	VAL
1	A	234	ASP
1	A	266	ARG
1	A	276	ILE
1	A	280	SER
1	A	295	GLU
1	A	296	MET
1	A	298	VAL
1	A	303	GLU
1	A	371	LEU
1	A	397	THR
1	A	398	VAL
1	A	401	GLU
1	A	406	ARG
1	A	414	ILE
1	A	415	LEU
1	B	76	LYS
1	B	104	ARG
1	B	115	GLN
1	B	123	ARG
1	B	141	THR
1	B	155	GLU
1	B	211	VAL
1	B	213	ARG
1	B	230	GLU
1	B	235	LEU
1	B	240	ASP
1	B	242	ASP

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Mol	Chain	Res	Type
1	B	266	ARG
1	B	276	ILE
1	B	277	MET
1	B	351	MET
1	B	361	GLU
1	B	406	ARG
1	B	411	MET
1	B	413	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	207	HIS
1	A	259	ASN
1	B	118	GLN
1	B	273	GLN
1	B	293	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	5GP	B	501	-	26,26,26	0.96	1 (3%)	39,40,40	1.72	8 (20%)
2	5GP	A	504	-	26,26,26	0.98	1 (3%)	39,40,40	1.89	10 (25%)
2	5GP	A	502	-	26,26,26	2.14	12 (46%)	39,40,40	2.08	10 (25%)
2	5GP	A	503	-	26,26,26	0.94	2 (7%)	39,40,40	1.91	10 (25%)
2	5GP	A	501	-	26,26,26	0.96	1 (3%)	39,40,40	1.77	8 (20%)

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	5GP	B	501	-	-	6/10/26/26	0/3/3/3
2	5GP	A	504	-	-	3/10/26/26	0/3/3/3
2	5GP	A	502	-	-	0/10/26/26	0/3/3/3
2	5GP	A	503	-	-	0/10/26/26	0/3/3/3
2	5GP	A	501	-	-	4/10/26/26	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	5GP	C6-N1	-4.85	1.29	1.38
2	A	502	5GP	C5-N7	-3.92	1.31	1.39
2	A	502	5GP	C4-N9	-3.25	1.29	1.38
2	A	502	5GP	C8-N9	-3.18	1.30	1.37
2	A	501	5GP	C6-N1	-2.99	1.33	1.38
2	B	501	5GP	C6-N1	-2.81	1.33	1.38
2	A	502	5GP	C2-N1	-2.79	1.30	1.37
2	A	502	5GP	P-OP2	-2.72	1.44	1.54
2	A	502	5GP	P-OP3	-2.60	1.45	1.54
2	A	504	5GP	C6-N1	-2.50	1.34	1.38
2	A	502	5GP	O4'-C4'	-2.39	1.39	1.45
2	A	503	5GP	C6-N1	-2.26	1.34	1.38
2	A	502	5GP	C2'-C3'	-2.20	1.47	1.53
2	A	502	5GP	P-O5'	-2.18	1.53	1.60
2	A	503	5GP	C5-N7	-2.17	1.34	1.39
2	A	502	5GP	P-OP1	-2.14	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	5GP	C3'-C4'	-2.08	1.47	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	5GP	C5-C4-N3	-6.38	118.24	128.39
2	A	503	5GP	C5-C4-N3	-6.30	118.36	128.39
2	A	504	5GP	C5-C4-N3	-5.99	118.86	128.39
2	A	501	5GP	C5-C4-N3	-5.81	119.15	128.39
2	B	501	5GP	C5-C4-N3	-5.71	119.30	128.39
2	A	503	5GP	C2-N3-C4	5.16	121.18	112.30
2	A	504	5GP	C2-N3-C4	5.08	121.05	112.30
2	A	502	5GP	C2-N3-C4	4.91	120.76	112.30
2	A	501	5GP	C2-N3-C4	4.51	120.06	112.30
2	B	501	5GP	C2-N3-C4	4.29	119.69	112.30
2	A	502	5GP	N9-C4-N3	4.24	134.43	125.95
2	A	502	5GP	C6-C5-N7	3.88	137.34	130.29
2	A	503	5GP	N9-C4-N3	3.72	133.39	125.95
2	A	504	5GP	N9-C4-N3	3.48	132.91	125.95
2	B	501	5GP	N9-C4-N3	3.43	132.81	125.95
2	A	501	5GP	N9-C4-N3	3.39	132.74	125.95
2	A	502	5GP	C4-C5-N7	-3.17	105.64	110.67
2	A	503	5GP	OP2-P-O5'	-2.93	99.03	106.67
2	A	501	5GP	OP2-P-O5'	-2.90	99.10	106.67
2	A	504	5GP	N9-C8-N7	-2.76	108.28	113.40
2	A	504	5GP	C2-N1-C6	-2.70	120.21	125.11
2	A	504	5GP	C5-C6-N1	2.66	120.02	113.25
2	A	503	5GP	C2-N1-C6	-2.65	120.31	125.11
2	A	503	5GP	C5-C6-N1	2.59	119.85	113.25
2	A	502	5GP	OP3-P-O5'	-2.53	100.06	106.67
2	A	503	5GP	O6-C6-C5	-2.47	120.02	126.53
2	B	501	5GP	N9-C8-N7	-2.46	108.84	113.40
2	A	504	5GP	OP2-P-O5'	-2.45	100.27	106.67
2	A	504	5GP	O6-C6-C5	-2.38	120.24	126.53
2	A	502	5GP	OP2-P-OP1	2.37	120.07	110.83
2	A	504	5GP	C4-C5-N7	-2.36	106.92	110.67
2	B	501	5GP	C4-C5-N7	-2.35	106.94	110.67
2	A	502	5GP	C2-N1-C6	-2.35	120.84	125.11
2	A	501	5GP	C4-C5-N7	-2.33	106.98	110.67
2	B	501	5GP	C5-C6-N1	2.33	119.18	113.25
2	A	501	5GP	C5-C6-N1	2.33	119.17	113.25
2	A	501	5GP	N9-C8-N7	-2.29	109.15	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	5GP	C5-C6-N1	2.24	118.94	113.25
2	A	503	5GP	N9-C8-N7	-2.21	109.29	113.40
2	A	503	5GP	C4-C5-N7	-2.19	107.20	110.67
2	A	504	5GP	C8-N7-C5	2.16	108.11	104.26
2	A	501	5GP	C2-N1-C6	-2.14	121.23	125.11
2	B	501	5GP	C2-N1-C6	-2.07	121.35	125.11
2	A	503	5GP	C8-N7-C5	2.05	107.91	104.26
2	A	502	5GP	C8-N7-C5	2.05	107.91	104.26
2	B	501	5GP	C8-N7-C5	2.04	107.89	104.26

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	5GP	C5'-O5'-P-OP1
2	A	501	5GP	C5'-O5'-P-OP3
2	A	501	5GP	C5'-O5'-P-OP2
2	A	501	5GP	C4'-C5'-O5'-P
2	A	504	5GP	C5'-O5'-P-OP1
2	A	504	5GP	C5'-O5'-P-OP3
2	A	504	5GP	C5'-O5'-P-OP2
2	B	501	5GP	C5'-O5'-P-OP3
2	B	501	5GP	C5'-O5'-P-OP2
2	B	501	5GP	C3'-C4'-C5'-O5'
2	B	501	5GP	O4'-C4'-C5'-O5'
2	B	501	5GP	C5'-O5'-P-OP1
2	B	501	5GP	C4'-C5'-O5'-P

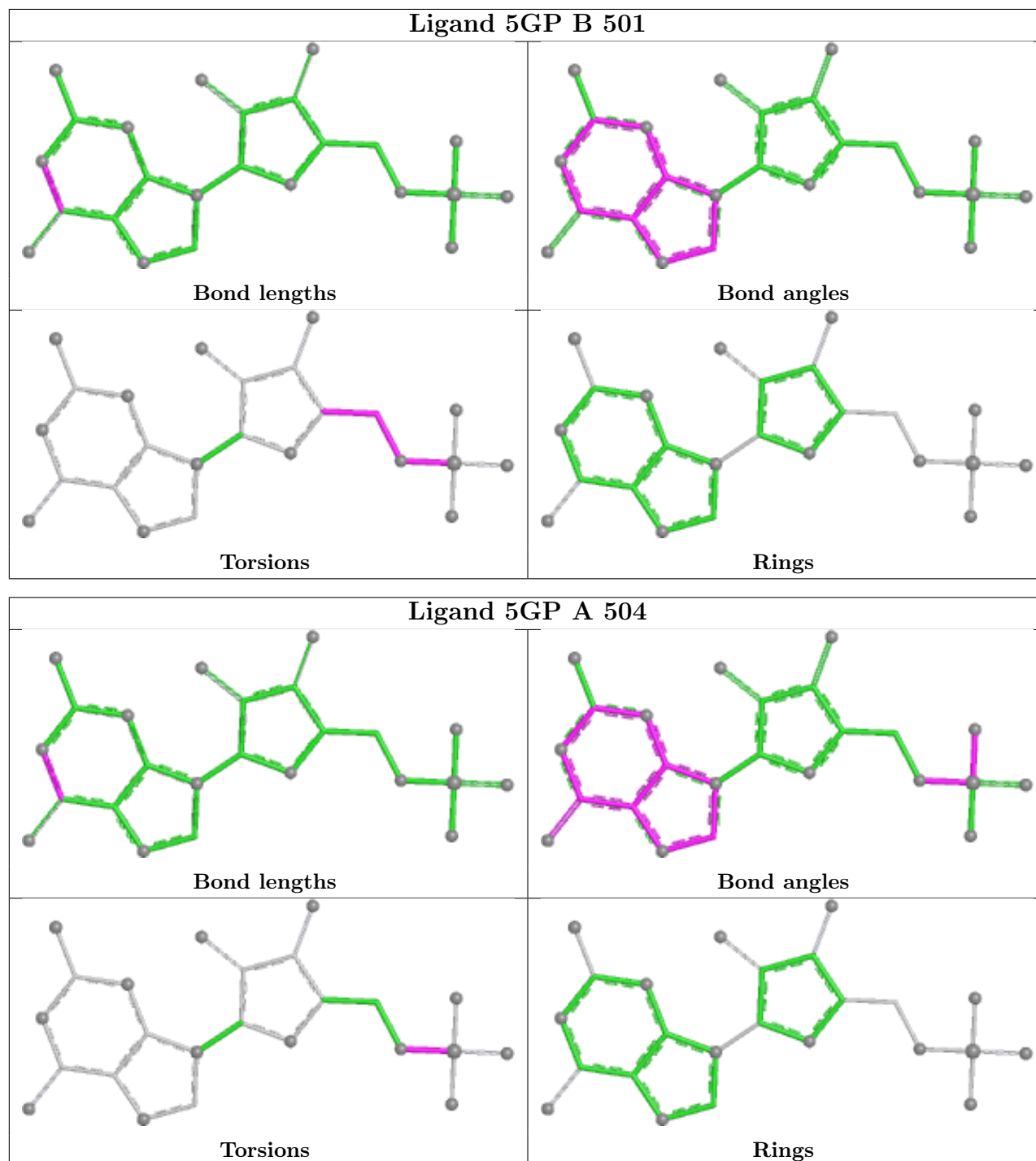
There are no ring outliers.

2 monomers are involved in 2 short contacts:

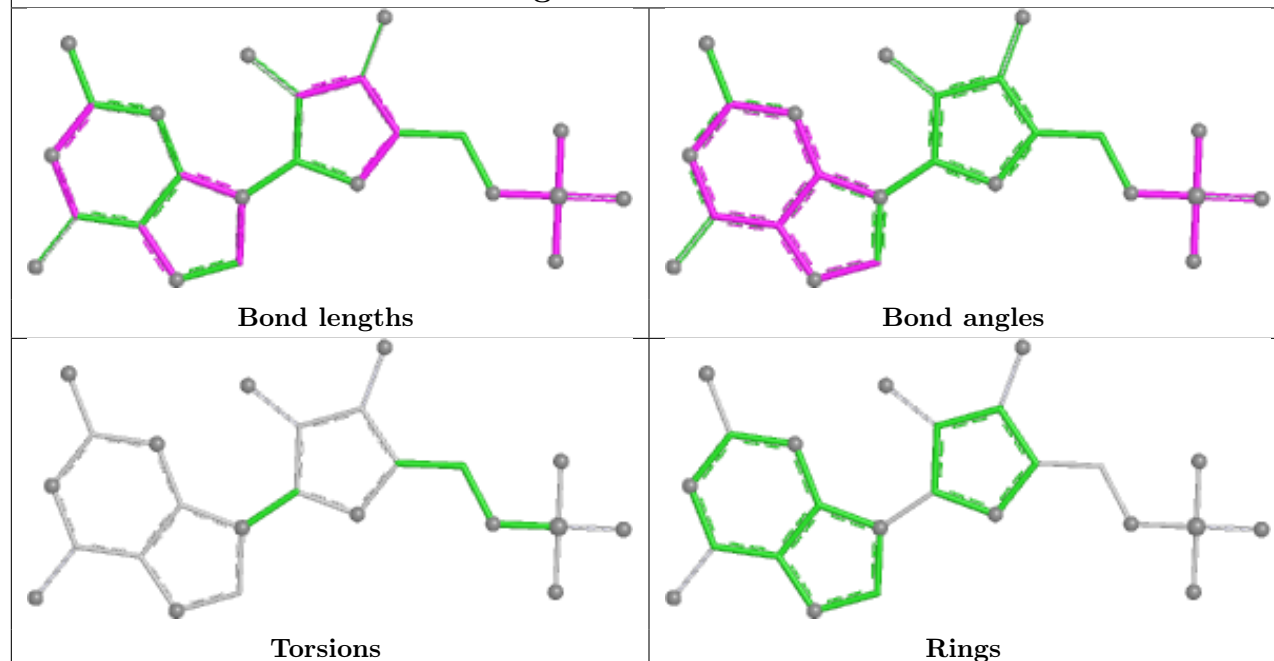
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	5GP	1	0
2	A	501	5GP	1	0

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

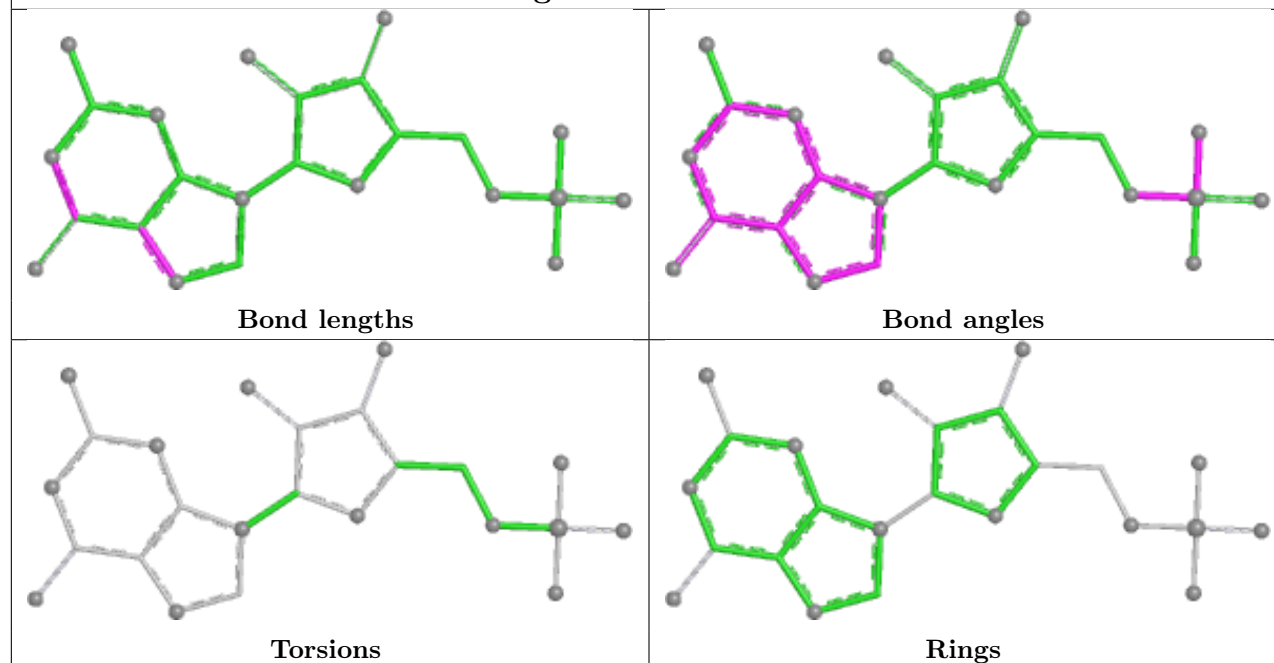
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

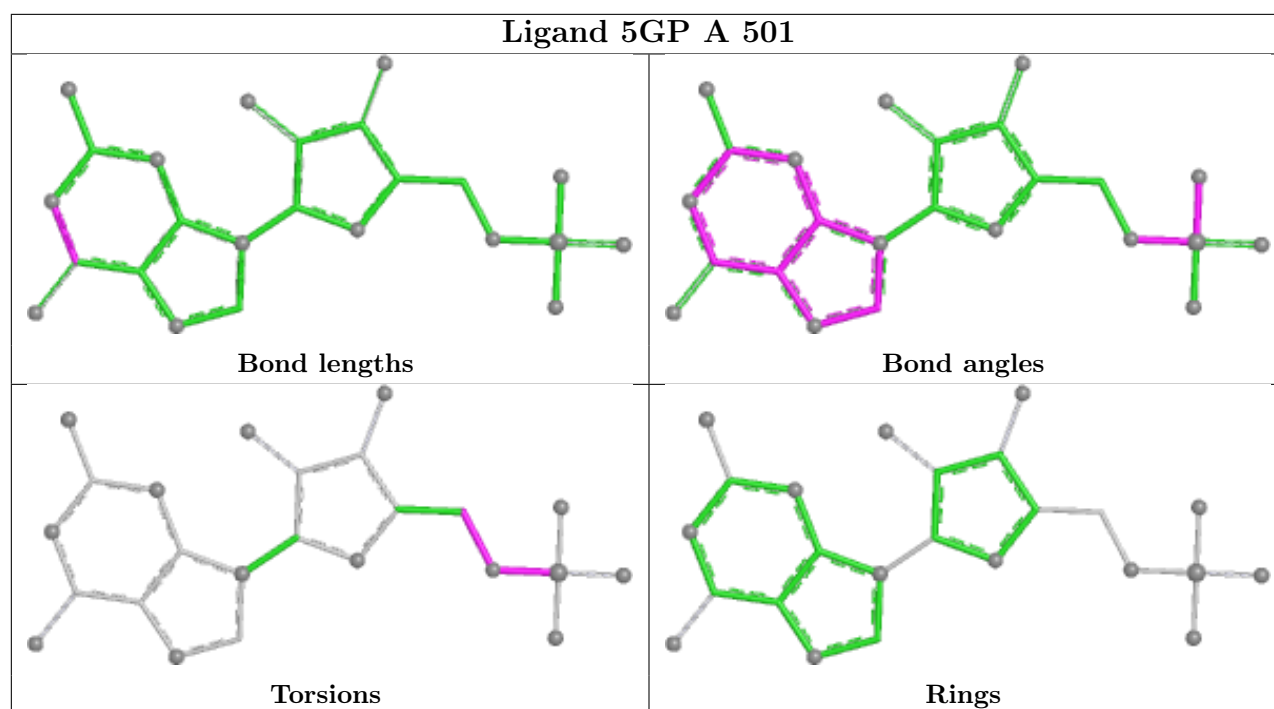


Ligand 5GP A 502



Ligand 5GP A 503





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	318/393 (80%)	0.27	18 (5%) 29 23	38, 70, 122, 158	0
1	B	303/393 (77%)	0.39	19 (6%) 26 19	38, 76, 143, 160	0
All	All	621/786 (79%)	0.33	37 (5%) 27 21	38, 73, 137, 160	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	SER	7.4
1	B	222	VAL	5.5
1	B	415	LEU	4.8
1	B	400	PRO	4.5
1	A	397	THR	4.4
1	B	337	PHE	3.8
1	B	414	ILE	3.7
1	A	223	ALA	3.6
1	B	372	THR	3.5
1	A	405	LYS	3.4
1	A	398	VAL	3.3
1	A	304	ASP	3.2
1	A	297	GLU	3.1
1	B	413	ASN	2.8
1	A	371	LEU	2.8
1	A	402	GLN	2.7
1	A	227	SER	2.7
1	B	251	HIS	2.7
1	A	338	GLY	2.6
1	B	247	GLY	2.6
1	B	338	GLY	2.5
1	B	407	PHE	2.4
1	A	416	THR	2.4
1	B	406	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	213	ARG	2.4
1	A	354	HIS	2.3
1	A	303	GLU	2.3
1	B	409	GLU	2.3
1	A	302	ALA	2.2
1	B	249	LYS	2.2
1	A	406	ARG	2.2
1	A	293	GLN	2.2
1	A	222	VAL	2.2
1	A	275	LYS	2.1
1	B	223	ALA	2.1
1	B	255	GLU	2.1
1	B	354	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

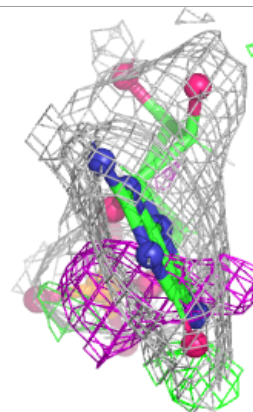
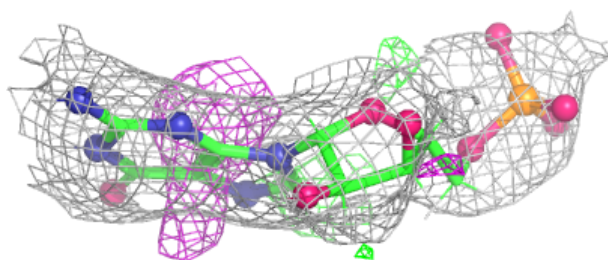
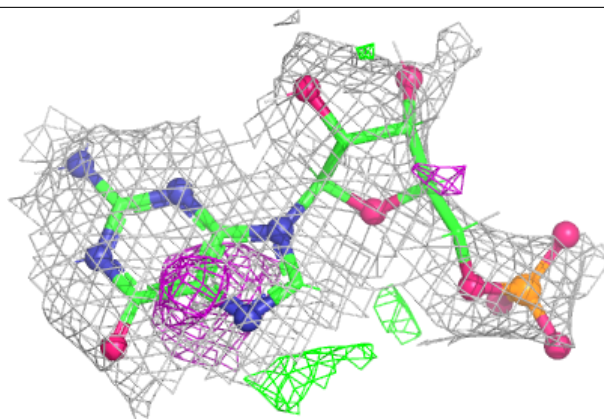
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5GP	A	501	24/24	0.79	0.15	72,149,195,202	0
2	5GP	A	503	24/24	0.81	0.12	70,111,175,180	0
2	5GP	B	501	24/24	0.85	0.10	97,157,195,203	0
2	5GP	A	502	24/24	0.91	0.12	65,83,102,118	0
2	5GP	A	504	24/24	0.95	0.09	54,77,95,100	0

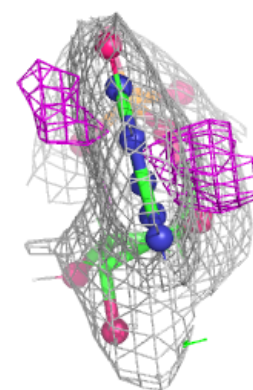
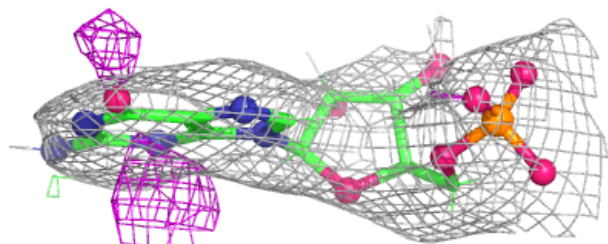
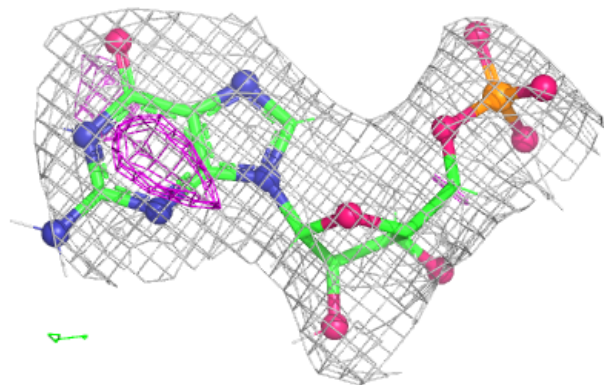
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5GP 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)

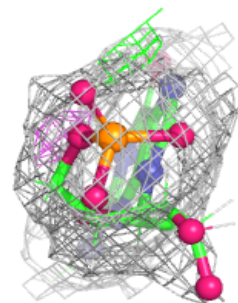
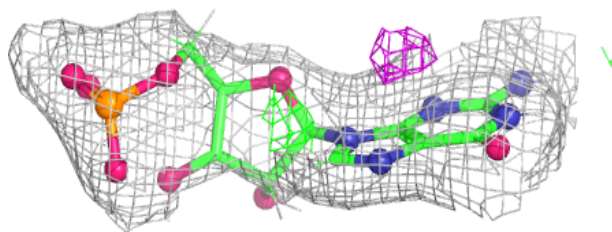
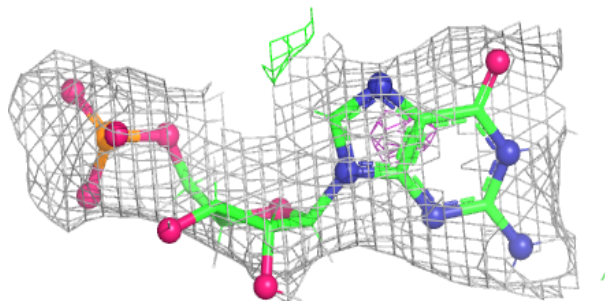
**Electron density around 5GP A 503:**

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

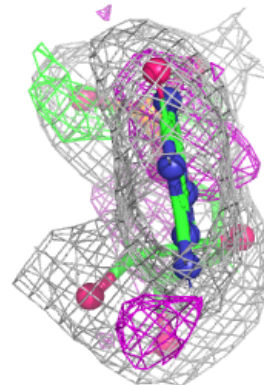
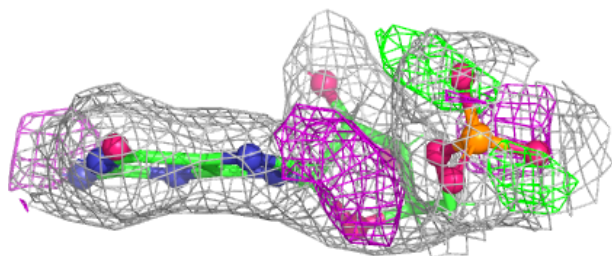
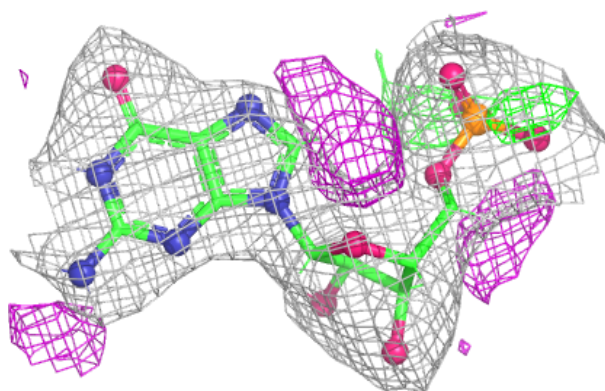


Electron density around 5GP B 501:

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

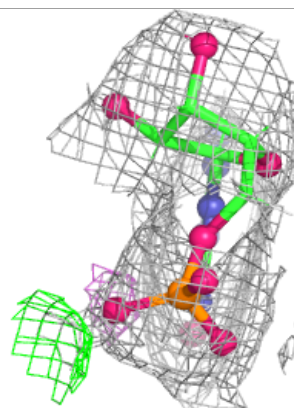
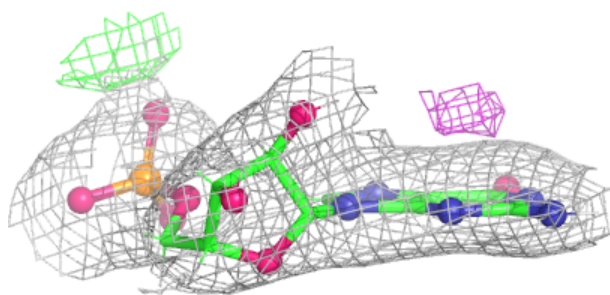
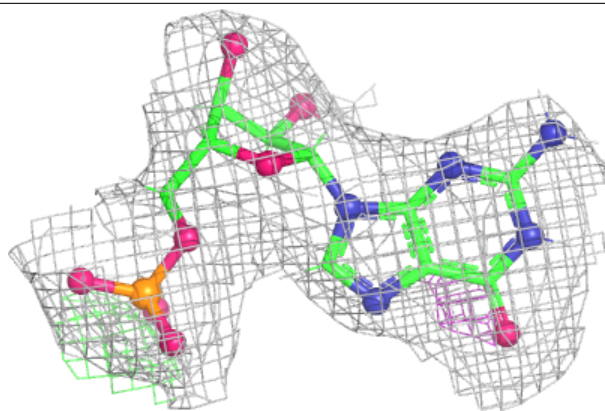
**Electron density around 5GP A 502:**

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



Electron density around 5GP A 504:

$2mF_o-DF_c$ (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.