



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 08:13 PM EDT

PDB ID : 3X0A / pdb_00003x0a
Title : Crystal structure of PIP4KIIBETA F205L 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 : 2.60 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

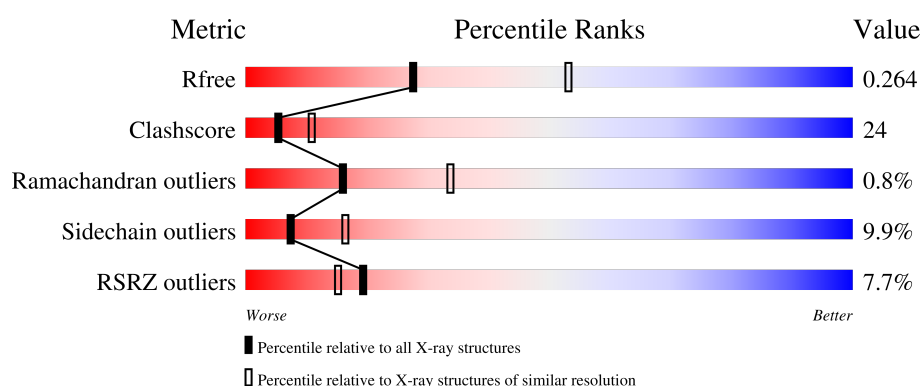
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	393	4% 50% 24% 6% 19%
1	B	393	9% 41% 30% 6% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5324 atoms, of which 58 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.

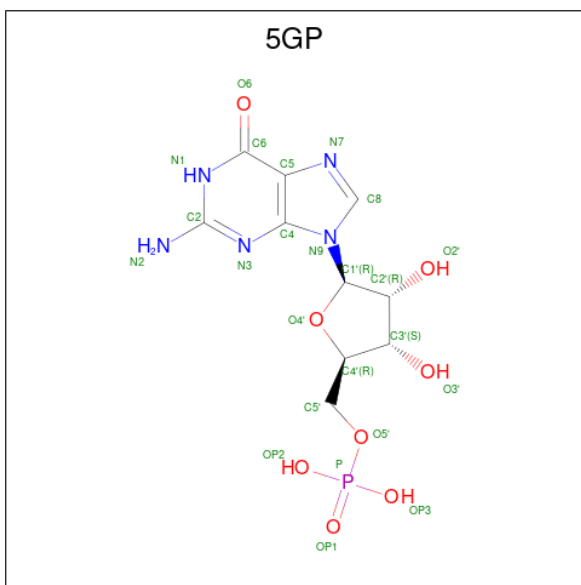
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2620	1667	447	492	14			
1	B	303	Total	C	N	O	S	0	0	0
			2491	1593	426	459	13			

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	205	LEU	PHE	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	205	LEU	PHE	engineered mutation	UNP P78356

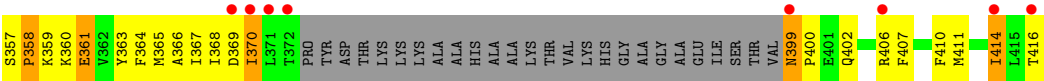
- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



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
			34	10	10	5	8	1		
2	A	1	Total	C	H	N	O		0	0
			31	10	12	5	4			
2	B	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	21	Total	O	0	0
			21	21		
3	B	19	Total	O	0	0
			19	19		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.93Å 183.01Å 106.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.60 48.18 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.18-2.60) 98.4 (48.18-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.228 , 0.272 0.216 , 0.264	Depositor DCC
R_{free} test set	1622 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.010 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)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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	0.60	3/2673 (0.1%)	0.92	12/3597 (0.3%)
1	B	0.68	5/2542 (0.2%)	0.94	8/3418 (0.2%)
All	All	0.64	8/5215 (0.2%)	0.93	20/7015 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	LYS	C-N	9.29	1.45	1.33
1	A	241	ASN	C-N	-7.54	1.24	1.33
1	B	40	GLU	C-O	-6.68	1.16	1.24
1	A	218	LYS	N-CA	-6.50	1.38	1.46
1	B	278	ASP	CA-C	6.10	1.59	1.52
1	B	207	HIS	CG-ND1	-5.74	1.31	1.38
1	B	259	ASN	CA-C	-5.36	1.45	1.52
1	A	207	HIS	CG-ND1	-5.06	1.32	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ARG	N-CA-C	9.07	124.33	112.72
1	B	40	GLU	O-C-N	-8.66	115.08	121.84
1	B	40	GLU	CB-CA-C	8.20	121.69	109.63
1	B	338	GLY	N-CA-C	7.44	120.93	112.00
1	B	40	GLU	CA-C-O	6.67	125.80	119.13
1	A	218	LYS	N-CA-C	6.21	120.67	112.72
1	A	217	LEU	O-C-N	-6.10	115.30	123.23
1	A	217	LEU	CA-C-N	6.00	133.25	122.46
1	A	217	LEU	C-N-CA	6.00	133.25	122.46
1	A	99	CYS	CB-CA-C	-5.98	106.95	111.20
1	A	276	ILE	N-CA-C	5.90	117.33	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ASN	CA-C-N	5.77	128.81	120.79
1	B	259	ASN	C-N-CA	5.77	128.81	120.79
1	B	208	ARG	N-CA-CB	-5.75	102.30	110.81
1	B	277	MET	N-CA-C	5.71	115.92	107.88
1	A	62	VAL	CA-C-N	5.31	125.21	119.85
1	A	62	VAL	C-N-CA	5.31	125.21	119.85
1	A	204	VAL	N-CA-C	-5.19	105.34	111.00
1	A	56	GLU	N-CA-C	-5.04	105.70	111.14
1	A	415	LEU	N-CA-C	5.01	117.47	109.81

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	2620	0	2598	96	0
1	B	2491	0	2476	158	0
2	A	67	34	34	5	0
2	B	48	24	24	1	0
3	A	21	0	0	1	0
3	B	19	0	0	0	0
All	All	5266	58	5132	249	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 24.

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLU:HG2	1:B:242:ASP:OD1	1.46	1.11
1:B:42:ILE:HD12	1:B:42:ILE:H	1.21	1.02
1:B:251:HIS:ND1	1:B:416:THR:HG21	1.75	1.01
1:A:370:ILE:HG13	1:A:370:ILE:O	1.59	1.01
1:B:249:LYS:HD2	1:B:249:LYS:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:CD1	1:A:414:ILE:HD11	1.99	0.92
1:B:217:LEU:HB2	1:B:411:MET:HE1	1.53	0.91
1:A:77:ILE:HD11	1:B:77:ILE:HG12	1.50	0.90
1:B:234:ASP:O	1:B:236:PRO:HD3	1.72	0.90
1:B:251:HIS:ND1	1:B:416:THR:CG2	2.35	0.89
1:A:77:ILE:HD11	1:B:77:ILE:CG1	2.01	0.89
1:B:357:SER:OG	1:B:358:PRO:HD2	1.73	0.89
1:A:79:VAL:HG22	1:B:77:ILE:CD1	2.01	0.89
1:B:219:GLY:O	1:B:406:ARG:HG2	1.73	0.88
1:B:243:PHE:CZ	1:B:414:ILE:CG2	2.58	0.87
1:A:399:ASN:HB3	1:A:400:PRO:CD	2.06	0.85
1:B:94:LYS:HB2	1:B:190:THR:HB	1.57	0.84
1:B:243:PHE:CE2	1:B:414:ILE:CG2	2.62	0.83
1:B:217:LEU:CB	1:B:411:MET:HE1	2.08	0.82
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.62	0.81
1:A:399:ASN:HB3	1:A:400:PRO:HD2	1.63	0.80
1:B:249:LYS:O	1:B:249:LYS:CD	2.30	0.79
1:B:260:PHE:CE1	1:B:365:MET:HE3	2.17	0.79
1:B:242:ASP:O	1:B:246:GLU:CG	2.30	0.78
1:B:251:HIS:CE1	1:B:416:THR:HG21	2.19	0.78
1:A:79:VAL:HG22	1:B:77:ILE:HD12	1.66	0.77
1:B:249:LYS:O	1:B:249:LYS:CG	2.32	0.77
1:B:42:ILE:H	1:B:42:ILE:CD1	1.97	0.77
1:A:260:PHE:HB2	1:A:351:MET:HE1	1.64	0.77
1:B:243:PHE:CZ	1:B:414:ILE:HG21	2.18	0.76
1:A:371:LEU:O	1:A:372:THR:HG22	1.87	0.75
1:B:242:ASP:O	1:B:246:GLU:HG3	1.85	0.74
1:B:243:PHE:CE2	1:B:414:ILE:HG21	2.23	0.73
1:A:415:LEU:HD23	1:A:415:LEU:H	1.52	0.73
1:B:254:GLU:OE2	1:B:257:LYS:HD3	1.89	0.72
1:A:69:ASP:HB3	1:B:83:LEU:HD13	1.69	0.71
1:B:243:PHE:HE1	1:B:249:LYS:CG	2.03	0.71
1:A:141:THR:HG22	1:A:142:THR:O	1.90	0.71
1:A:370:ILE:O	1:A:370:ILE:CG1	2.30	0.71
1:A:218:LYS:HD2	1:A:224:ARG:CZ	2.21	0.70
1:B:281:LEU:HD12	1:B:366:ALA:O	1.92	0.70
1:B:357:SER:OG	1:B:358:PRO:CD	2.38	0.69
1:B:243:PHE:HE1	1:B:249:LYS:HG2	1.57	0.69
1:B:271:LEU:HD21	1:B:370:ILE:HD12	1.75	0.69
1:B:243:PHE:HE2	1:B:414:ILE:HG23	1.57	0.69
1:B:243:PHE:CE1	1:B:249:LYS:HG2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:PHE:CE2	1:B:414:ILE:HG23	2.28	0.68
1:B:243:PHE:HZ	1:B:414:ILE:CG2	2.05	0.68
1:B:249:LYS:O	1:B:249:LYS:HG3	1.93	0.68
1:B:40:GLU:HG2	1:B:42:ILE:HD13	1.74	0.68
1:B:227:SER:O	1:B:231:LYS:HG3	1.94	0.67
1:B:399:ASN:N	1:B:400:PRO:CD	2.57	0.67
1:A:411:MET:O	1:A:414:ILE:HB	1.95	0.67
1:B:78:LYS:HD2	1:B:94:LYS:NZ	2.10	0.67
1:B:40:GLU:CG	1:B:42:ILE:HD13	2.25	0.66
1:B:252:VAL:CG2	1:B:252:VAL:O	2.44	0.66
1:B:243:PHE:CE1	1:B:249:LYS:CG	2.80	0.65
1:B:283:VAL:HG22	1:B:365:MET:HG2	1.79	0.65
1:B:367:ILE:O	1:B:368:ILE:CG2	2.45	0.65
1:B:367:ILE:O	1:B:368:ILE:HG22	1.97	0.65
1:B:227:SER:OG	1:B:230:GLU:HB2	1.96	0.65
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.27	0.64
1:B:224:ARG:CZ	1:B:239:LYS:HG2	2.27	0.64
1:B:141:THR:HG23	1:B:142:THR:O	1.97	0.64
1:A:220:SER:HB3	1:A:222:VAL:HG23	1.78	0.64
1:A:225:GLU:HG2	1:A:241:ASN:HB2	1.80	0.64
1:A:94:LYS:HB2	1:A:190:THR:HB	1.79	0.64
1:B:160:MET:HE1	1:B:183:PHE:CD2	2.33	0.64
1:A:241:ASN:O	1:A:245:ASN:HB2	1.98	0.63
1:B:224:ARG:HB3	1:B:239:LYS:HG2	1.79	0.63
1:A:415:LEU:HD23	1:A:415:LEU:N	2.13	0.63
1:B:220:SER:HA	1:B:406:ARG:NE	2.14	0.62
1:B:367:ILE:HG22	1:B:368:ILE:N	2.14	0.62
1:B:225:GLU:HG3	1:B:241:ASN:HB2	1.81	0.62
1:A:371:LEU:C	1:A:372:THR:CG2	2.72	0.62
1:A:160:MET:HE1	1:A:164:LEU:HD13	1.82	0.62
1:B:250:LEU:HD22	1:B:363:TYR:CD2	2.35	0.61
1:B:235:LEU:HD12	1:B:235:LEU:H	1.65	0.61
1:A:56:GLU:OE2	1:B:48:TRP:NE1	2.31	0.60
1:B:224:ARG:HB3	1:B:239:LYS:CG	2.30	0.60
1:B:277:MET:O	1:B:278:ASP:HB2	2.02	0.60
1:B:216:ASP:C	1:B:217:LEU:HD23	2.27	0.60
1:B:242:ASP:O	1:B:246:GLU:CD	2.45	0.60
2:A:502:5GP:H2'	2:A:503:5GP:N3	2.17	0.59
1:B:243:PHE:HE2	1:B:414:ILE:CG2	2.14	0.59
1:B:224:ARG:HB3	1:B:239:LYS:HD3	1.83	0.59
1:A:141:THR:HG23	1:A:145:ARG:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ALA:O	1:B:231:LYS:HE2	2.03	0.58
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.86	0.58
1:A:355:GLU:N	1:A:355:GLU:OE2	2.38	0.57
1:B:265:LYS:NZ	1:B:269:GLU:OE2	2.37	0.57
1:B:367:ILE:C	1:B:368:ILE:HG23	2.28	0.57
1:B:287:ASP:OD1	1:B:290:ARG:HB2	2.05	0.56
1:A:415:LEU:N	1:A:415:LEU:CD2	2.68	0.56
1:B:367:ILE:C	1:B:368:ILE:CG2	2.79	0.56
1:A:218:LYS:HD2	1:A:224:ARG:NE	2.20	0.56
1:A:217:LEU:CD1	1:A:414:ILE:CD1	2.81	0.55
1:B:252:VAL:O	1:B:253:GLY:O	2.24	0.55
1:A:269:GLU:O	1:A:273:GLN:HG3	2.07	0.55
1:A:354:HIS:C	1:A:356:SER:H	2.14	0.55
1:B:243:PHE:HZ	1:B:414:ILE:HG22	1.71	0.55
1:B:152:VAL:HB	1:B:156:ASP:OD2	2.08	0.54
1:B:252:VAL:HG23	1:B:256:SER:HB2	1.88	0.54
1:B:369:ASP:OD2	2:B:501:5GP:OP1	2.26	0.54
1:A:264:LEU:O	1:A:268:VAL:HG22	2.07	0.54
1:B:74:TYR:CD1	1:B:74:TYR:C	2.85	0.53
1:B:279:TYR:HB3	1:B:370:ILE:HG22	1.90	0.53
1:A:202:ARG:HG3	1:A:203:ASN:N	2.24	0.53
1:B:252:VAL:O	1:B:252:VAL:HG23	2.07	0.53
1:B:141:THR:CG2	1:B:142:THR:O	2.56	0.53
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.91	0.53
1:A:371:LEU:O	1:A:372:THR:CG2	2.57	0.53
1:A:407:PHE:CE1	1:A:411:MET:HE3	2.44	0.53
1:B:42:ILE:HD12	1:B:42:ILE:N	2.06	0.53
1:B:238:PHE:HD2	1:B:242:ASP:HB3	1.74	0.53
1:B:250:LEU:HB2	1:B:414:ILE:O	2.09	0.53
1:B:281:LEU:HD12	1:B:366:ALA:C	2.34	0.53
1:A:96:LYS:NZ	2:A:502:5GP:OP3	2.39	0.52
1:A:204:VAL:HA	1:A:349:TYR:CD2	2.44	0.52
1:A:399:ASN:CB	1:A:400:PRO:CD	2.80	0.52
1:A:225:GLU:CG	1:A:241:ASN:HB2	2.40	0.52
1:B:236:PRO:HB2	1:B:238:PHE:CE1	2.45	0.52
1:B:46:LEU:HD21	1:B:149:ILE:HD13	1.92	0.52
1:B:254:GLU:HA	1:B:257:LYS:HB3	1.92	0.52
1:B:205:LEU:HD13	1:B:211:VAL:HG21	1.92	0.51
1:B:271:LEU:CD2	1:B:370:ILE:HD12	2.40	0.51
1:B:139:PHE:C	1:B:139:PHE:CD2	2.87	0.51
1:A:66:LEU:HD12	1:A:168:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.93	0.51
1:B:57:LEU:O	1:B:104:ARG:NH2	2.44	0.51
1:B:240:ASP:OD1	1:B:240:ASP:N	2.44	0.51
1:A:261:LEU:HD21	1:A:412:SER:HA	1.91	0.51
1:B:86:LYS:HE3	1:B:91:SER:OG	2.11	0.51
1:A:141:THR:CG2	1:A:142:THR:O	2.58	0.50
1:A:248:GLN:O	1:A:249:LYS:HD2	2.11	0.50
1:A:354:HIS:C	1:A:356:SER:N	2.68	0.50
1:B:49:GLY:HA3	1:B:95:PHE:CE1	2.47	0.50
1:B:399:ASN:O	1:B:402:GLN:HB2	2.10	0.50
1:A:43:LEU:HD21	1:A:140:LEU:HD11	1.94	0.49
1:B:243:PHE:CZ	1:B:249:LYS:HB3	2.47	0.49
1:A:206:SER:HB2	1:A:364:PHE:CE2	2.47	0.49
1:B:235:LEU:HD12	1:B:235:LEU:N	2.28	0.49
1:A:349:TYR:CD1	1:A:366:ALA:HB2	2.48	0.49
1:B:224:ARG:HB3	1:B:239:LYS:CD	2.42	0.49
1:B:159:GLU:OE2	1:B:159:GLU:HA	2.13	0.49
1:B:43:LEU:HD21	1:B:140:LEU:CD1	2.42	0.48
1:B:204:VAL:HG13	1:B:366:ALA:HB3	1.94	0.48
1:B:250:LEU:CD2	1:B:363:TYR:CE2	2.96	0.48
1:B:252:VAL:O	1:B:253:GLY:C	2.56	0.48
1:A:189:LEU:N	1:A:189:LEU:HD12	2.28	0.48
1:B:219:GLY:HA2	1:B:410:PHE:CG	2.49	0.48
1:A:141:THR:CG2	1:A:145:ARG:HA	2.44	0.48
1:B:250:LEU:HD21	1:B:285:ILE:HD11	1.96	0.48
1:A:249:LYS:O	1:A:250:LEU:HD23	2.14	0.48
1:B:217:LEU:HB3	1:B:411:MET:HE1	1.92	0.48
1:A:43:LEU:HD21	1:A:140:LEU:CD1	2.44	0.48
1:A:354:HIS:ND1	1:A:356:SER:OG	2.45	0.48
1:B:157:VAL:HG13	1:B:186:MET:HE3	1.95	0.48
1:B:260:PHE:HB2	1:B:351:MET:HE1	1.96	0.47
1:B:250:LEU:HD21	1:B:285:ILE:CD1	2.44	0.47
1:B:285:ILE:HD13	1:B:363:TYR:HD2	1.79	0.47
1:B:78:LYS:HD2	1:B:94:LYS:HZ2	1.78	0.47
1:B:160:MET:HG2	1:B:186:MET:SD	2.54	0.47
1:B:370:ILE:HG13	1:B:370:ILE:O	2.14	0.47
1:A:207:HIS:CD2	1:A:208:ARG:HG2	2.49	0.47
1:B:206:SER:HB2	1:B:364:PHE:CE2	2.50	0.47
1:A:100:PRO:HD2	3:A:604:HOH:O	2.14	0.47
1:A:160:MET:CE	1:A:164:LEU:HD13	2.43	0.47
1:A:239:LYS:O	1:A:242:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLY:O	1:A:352:LYS:HE3	2.14	0.47
1:B:367:ILE:CG2	1:B:368:ILE:N	2.77	0.47
1:B:139:PHE:HD2	1:B:139:PHE:O	1.98	0.47
1:B:288:VAL:CG1	1:B:339:PRO:HB2	2.45	0.47
1:A:213:ARG:NH1	1:A:246:GLU:OE2	2.47	0.46
1:A:371:LEU:C	1:A:372:THR:HG23	2.41	0.46
1:B:233:LYS:CG	1:B:234:ASP:H	2.28	0.46
1:A:274:LEU:C	1:A:276:ILE:H	2.24	0.46
1:B:276:ILE:CG2	1:B:277:MET:N	2.79	0.46
1:B:288:VAL:HG23	1:B:360:LYS:O	2.16	0.46
1:A:110:PHE:CE1	1:A:182:GLN:HB3	2.49	0.46
1:A:288:VAL:HG21	1:A:360:LYS:HG2	1.98	0.46
1:B:353:SER:OG	1:B:361:GLU:O	2.21	0.46
1:B:139:PHE:CD2	1:B:139:PHE:O	2.69	0.46
1:B:160:MET:HE1	1:B:183:PHE:CG	2.50	0.46
1:B:224:ARG:NH2	1:B:239:LYS:HE3	2.31	0.45
1:A:254:GLU:H	1:A:254:GLU:HG2	1.45	0.45
1:B:141:THR:HG23	1:B:145:ARG:HA	1.98	0.45
1:A:160:MET:O	1:A:164:LEU:HB2	2.17	0.45
1:B:99:CYS:N	1:B:100:PRO:CD	2.80	0.45
1:B:250:LEU:HD22	1:B:363:TYR:CE2	2.52	0.45
1:A:98:TYR:O	1:A:99:CYS:C	2.59	0.45
1:B:226:ALA:HB3	1:B:231:LYS:NZ	2.32	0.45
1:B:399:ASN:N	1:B:400:PRO:HD3	2.30	0.45
1:B:104:ARG:HA	1:B:107:ARG:CZ	2.48	0.44
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.99	0.44
1:B:48:TRP:HB2	1:B:89:LEU:HD21	1.99	0.44
1:A:253:GLY:HA2	1:A:354:HIS:CD2	2.52	0.44
1:B:104:ARG:HA	1:B:107:ARG:NH1	2.33	0.44
1:A:154:SER:OG	2:A:502:5GP:H4'	2.18	0.44
1:A:224:ARG:NH1	1:A:240:ASP:OD1	2.51	0.44
1:A:69:ASP:C	1:A:71:PHE:N	2.75	0.44
1:A:414:ILE:HG22	1:A:415:LEU:HD22	2.00	0.43
1:A:168:HIS:O	1:A:172:VAL:HG23	2.18	0.43
1:A:354:HIS:O	1:A:356:SER:N	2.52	0.43
2:A:502:5GP:H2'	2:A:503:5GP:N2	2.34	0.43
1:B:337:PHE:CD1	1:B:337:PHE:C	2.96	0.43
1:B:354:HIS:ND1	1:B:355:GLU:N	2.67	0.43
1:A:354:HIS:CE1	1:A:356:SER:HG	2.35	0.43
1:B:49:GLY:HA3	1:B:95:PHE:CZ	2.54	0.43
1:B:264:LEU:O	1:B:268:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:O	1:A:273:GLN:HB2	2.19	0.43
1:A:150:LYS:O	1:A:198:MET:HA	2.19	0.42
1:A:250:LEU:HD12	1:A:414:ILE:CG2	2.49	0.42
1:B:180:LEU:HB3	1:B:181:PRO:HD2	2.00	0.42
1:B:233:LYS:HG2	1:B:234:ASP:H	1.84	0.42
1:B:243:PHE:HE1	1:B:249:LYS:HG3	1.83	0.42
1:A:295:GLU:O	1:A:298:VAL:HG12	2.19	0.42
1:B:235:LEU:HD13	1:B:235:LEU:O	2.19	0.42
1:B:254:GLU:O	1:B:257:LYS:N	2.52	0.42
1:A:48:TRP:HB2	1:A:89:LEU:HD21	2.02	0.42
1:A:97:GLU:HG3	1:A:187:TYR:CE2	2.55	0.42
2:A:502:5GP:O2'	2:A:503:5GP:H1'	2.19	0.42
1:B:119:ASN:O	1:B:123:ARG:HB2	2.20	0.42
1:B:215:TYR:HB3	1:B:217:LEU:HD21	2.02	0.42
1:A:94:LYS:HB2	1:A:190:THR:CB	2.46	0.42
1:B:225:GLU:HG3	1:B:241:ASN:CB	2.48	0.42
1:B:268:VAL:HG11	1:B:407:PHE:CD2	2.55	0.42
1:B:82:HIS:CE1	1:B:83:LEU:HG	2.54	0.41
1:A:77:ILE:HD11	1:B:77:ILE:HG13	1.93	0.41
1:A:282:LEU:O	1:A:365:MET:HA	2.21	0.41
1:B:191:VAL:O	1:B:192:ASP:HB2	2.21	0.41
1:B:260:PHE:CZ	1:B:365:MET:HE3	2.54	0.41
1:A:240:ASP:OD1	1:A:240:ASP:N	2.54	0.41
1:B:224:ARG:O	1:B:239:LYS:HB3	2.21	0.41
1:B:240:ASP:O	1:B:244:LEU:HB2	2.19	0.41
1:B:254:GLU:O	1:B:255:GLU:C	2.64	0.41
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.56	0.41
1:A:234:ASP:OD1	1:A:234:ASP:N	2.53	0.41
1:A:159:GLU:HG2	1:A:373:PRO:HD3	2.03	0.41
1:B:124:SER:HB3	1:B:143:TYR:CD2	2.56	0.41
1:B:358:PRO:HB2	1:B:359:LYS:H	1.70	0.41
1:B:276:ILE:HG22	1:B:277:MET:N	2.35	0.41
1:A:215:TYR:O	1:A:282:LEU:HD12	2.21	0.40
1:B:203:ASN:OD1	1:B:205:LEU:N	2.54	0.40
1:A:59:ASN:HB3	1:B:34:LYS:O	2.21	0.40
1:A:82:HIS:O	1:A:83:LEU:HB2	2.20	0.40
1:A:152:VAL:HB	1:A:156:ASP:OD2	2.21	0.40
1:A:160:MET:HG2	1:A:371:LEU:HD21	2.03	0.40
1:A:251:HIS:O	1:A:353:SER:HA	2.22	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	311/393 (79%)	292 (94%)	16 (5%)	3 (1%)	12	28
1	B	291/393 (74%)	276 (95%)	13 (4%)	2 (1%)	18	38
All	All	602/786 (77%)	568 (94%)	29 (5%)	5 (1%)	16	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	PRO
1	A	358	PRO
1	B	253	GLY
1	A	355	GLU
1	A	400	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	296/352 (84%)	269 (91%)	27 (9%)	9	19
1	B	281/352 (80%)	251 (89%)	30 (11%)	6	14
All	All	577/704 (82%)	520 (90%)	57 (10%)	7	16

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU

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Mol	Chain	Res	Type
1	A	91	SER
1	A	115	GLN
1	A	123	ARG
1	A	138	ARG
1	A	141	THR
1	A	150	LYS
1	A	160	MET
1	A	220	SER
1	A	222	VAL
1	A	249	LYS
1	A	254	GLU
1	A	256	SER
1	A	258	LYS
1	A	266	ARG
1	A	295	GLU
1	A	298	VAL
1	A	348	VAL
1	A	355	GLU
1	A	370	ILE
1	A	371	LEU
1	A	372	THR
1	A	398	VAL
1	A	401	GLU
1	A	409	GLU
1	A	414	ILE
1	A	415	LEU
1	B	42	ILE
1	B	76	LYS
1	B	80	ASP
1	B	86	LYS
1	B	87	GLU
1	B	104	ARG
1	B	115	GLN
1	B	120	SER
1	B	123	ARG
1	B	139	PHE
1	B	141	THR
1	B	155	GLU
1	B	189	LEU
1	B	208	ARG
1	B	230	GLU
1	B	235	LEU

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Mol	Chain	Res	Type
1	B	239	LYS
1	B	240	ASP
1	B	244	LEU
1	B	252	VAL
1	B	257	LYS
1	B	263	LYS
1	B	276	ILE
1	B	277	MET
1	B	280	SER
1	B	287	ASP
1	B	361	GLU
1	B	370	ILE
1	B	399	ASN
1	B	414	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	B	82	HIS
1	B	115	GLN
1	B	128	ASN

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	A	503	-	21,21,26	1.79	5 (23%)	30,32,40	1.92	7 (23%)
2	5GP	B	501	-	26,26,26	1.37	4 (15%)	39,40,40	1.96	9 (23%)
2	5GP	B	502	-	26,26,26	2.15	10 (38%)	39,40,40	1.94	9 (23%)
2	5GP	A	502	-	26,26,26	1.15	3 (11%)	39,40,40	1.97	8 (20%)
2	5GP	A	501	-	26,26,26	1.60	6 (23%)	39,40,40	2.06	10 (25%)

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	A	503	-	-	0/4/20/26	0/3/3/3
2	5GP	B	501	-	-	0/10/26/26	0/3/3/3
2	5GP	B	502	-	-	0/10/26/26	0/3/3/3
2	5GP	A	502	-	-	3/10/26/26	0/3/3/3
2	5GP	A	501	-	-	3/10/26/26	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	5GP	C6-N1	-4.57	1.30	1.38
2	A	501	5GP	C6-N1	-4.33	1.30	1.38
2	A	503	5GP	C6-N1	-4.23	1.30	1.38
2	B	502	5GP	C5-N7	-4.19	1.30	1.39
2	B	501	5GP	C6-N1	-3.85	1.31	1.38
2	A	501	5GP	C5-N7	-3.67	1.31	1.39
2	A	503	5GP	C4-N9	-3.56	1.29	1.38
2	A	503	5GP	C5-N7	-3.51	1.32	1.39
2	B	502	5GP	C4-N9	-3.38	1.29	1.38
2	B	502	5GP	P-OP3	-3.17	1.43	1.54
2	A	502	5GP	C5-C4	3.11	1.47	1.38
2	B	501	5GP	C5-N7	-3.04	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	5GP	C8-N9	-2.81	1.31	1.37
2	A	501	5GP	C4-N9	-2.81	1.30	1.38
2	B	502	5GP	P-OP2	-2.79	1.44	1.54
2	B	502	5GP	O4'-C4'	-2.58	1.39	1.45
2	B	502	5GP	C2-N1	-2.51	1.31	1.37
2	B	502	5GP	C2'-C3'	-2.46	1.46	1.53
2	B	501	5GP	C5-C4	2.43	1.45	1.38
2	B	501	5GP	C4-N9	-2.40	1.32	1.38
2	A	502	5GP	C6-N1	-2.35	1.34	1.38
2	A	501	5GP	C8-N9	-2.26	1.32	1.37
2	B	502	5GP	P-O5'	-2.26	1.53	1.60
2	A	503	5GP	C2-N1	-2.22	1.32	1.37
2	A	501	5GP	C2-N1	-2.13	1.32	1.37
2	A	501	5GP	C5-C4	2.07	1.44	1.38
2	A	502	5GP	C5-N7	-2.04	1.35	1.39
2	A	503	5GP	C8-N9	-2.02	1.33	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	5GP	C5-C4-N3	-6.53	118.00	128.39
2	A	502	5GP	C5-C4-N3	-6.23	118.47	128.39
2	B	502	5GP	C5-C4-N3	-6.08	118.72	128.39
2	B	501	5GP	C5-C4-N3	-5.82	119.13	128.39
2	A	502	5GP	C2-N3-C4	5.09	121.07	112.30
2	A	502	5GP	N9-C4-N3	4.63	135.22	125.95
2	B	502	5GP	C2-N3-C4	4.60	120.23	112.30
2	B	501	5GP	C2-N3-C4	4.53	120.10	112.30
2	A	503	5GP	C5-C4-N3	-4.51	121.21	128.39
2	A	501	5GP	C2-N3-C4	4.51	120.07	112.30
2	B	502	5GP	N9-C4-N3	4.36	134.66	125.95
2	A	501	5GP	N9-C4-N3	4.29	134.53	125.95
2	B	501	5GP	N9-C4-N3	3.99	133.93	125.95
2	A	503	5GP	C2-N3-C4	3.62	118.54	112.30
2	B	501	5GP	C6-C5-N7	3.27	136.25	130.29
2	A	502	5GP	C6-C5-N7	3.26	136.22	130.29
2	A	503	5GP	N9-C4-N3	3.25	132.45	125.95
2	A	503	5GP	C6-C5-N7	3.19	136.10	130.29
2	A	501	5GP	C6-C5-N7	3.08	135.89	130.29
2	A	501	5GP	C4-C5-N7	-2.96	105.99	110.67
2	B	502	5GP	C6-C5-N7	2.85	135.48	130.29
2	A	503	5GP	O6-C6-C5	-2.77	119.21	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	5GP	C2'-C1'-N9	-2.66	105.85	113.25
2	A	502	5GP	C4-C5-N7	-2.66	106.46	110.67
2	A	501	5GP	OP2-P-OP3	2.62	117.61	107.80
2	B	501	5GP	C4-C5-N7	-2.56	106.61	110.67
2	A	501	5GP	C2-N1-C6	-2.52	120.54	125.11
2	A	501	5GP	C3'-C2'-C1'	2.52	106.23	101.46
2	B	502	5GP	OP3-P-OP1	2.51	120.63	110.83
2	A	502	5GP	C3'-C2'-C1'	2.51	106.21	101.46
2	A	501	5GP	N2-C2-N3	-2.48	114.84	119.67
2	B	501	5GP	C3'-C2'-C1'	2.40	106.00	101.46
2	A	501	5GP	O6-C6-C5	-2.36	120.31	126.53
2	B	502	5GP	OP2-P-O5'	-2.34	100.56	106.67
2	B	502	5GP	C4-C5-N7	-2.33	106.97	110.67
2	B	501	5GP	N2-C2-N3	-2.28	115.21	119.67
2	B	501	5GP	O6-C6-C5	-2.28	120.52	126.53
2	A	502	5GP	O6-C6-C5	-2.12	120.92	126.53
2	A	503	5GP	C1'-N9-C4	-2.10	120.27	126.49
2	A	503	5GP	N2-C2-N3	-2.07	115.62	119.67
2	B	501	5GP	C2'-C3'-C4'	2.06	106.59	102.61
2	B	502	5GP	O4'-C1'-N9	2.06	113.02	108.36
2	A	502	5GP	C8-N7-C5	2.01	107.84	104.26

There are no chirality outliers.

All (6) torsion outliers are listed below:

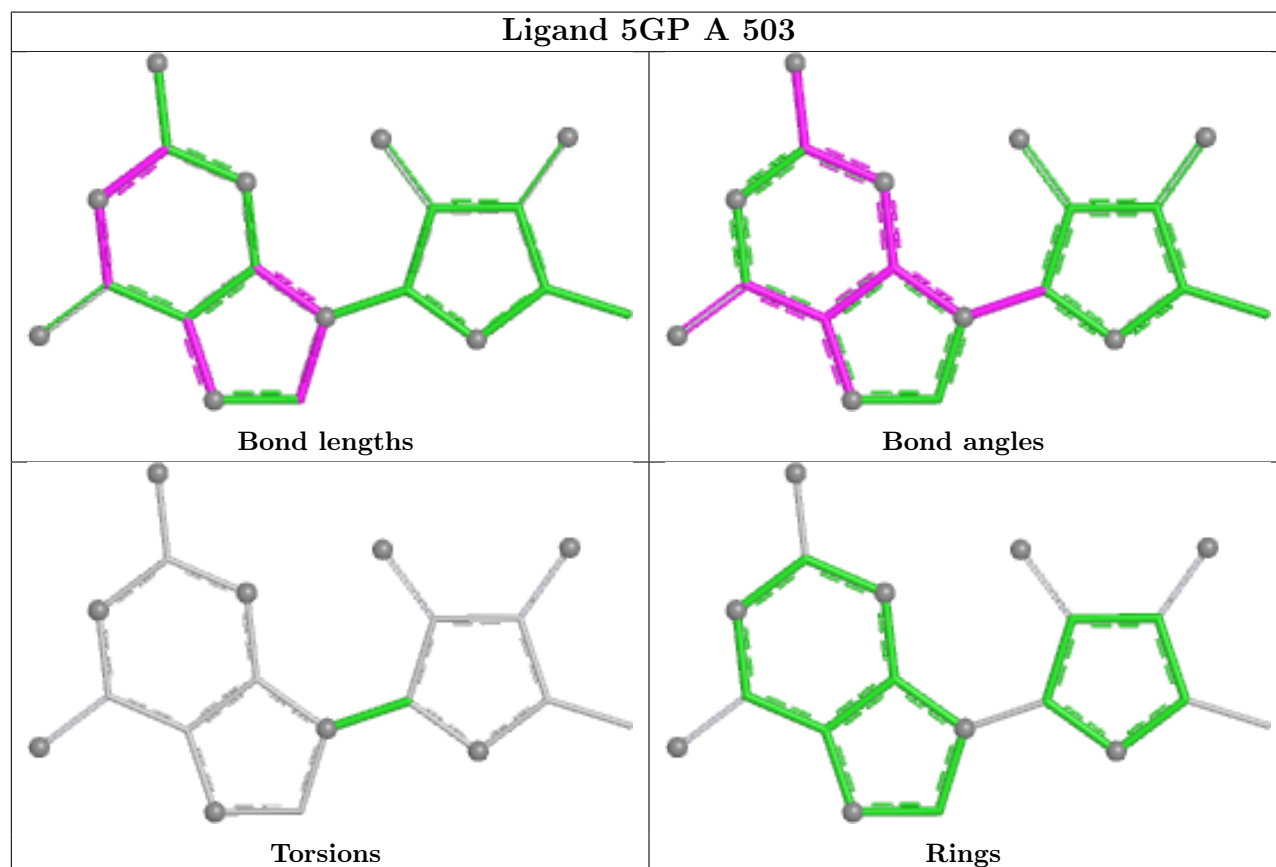
Mol	Chain	Res	Type	Atoms
2	A	501	5GP	C5'-O5'-P-OP3
2	A	501	5GP	C5'-O5'-P-OP2
2	A	502	5GP	C5'-O5'-P-OP3
2	A	502	5GP	C5'-O5'-P-OP2
2	A	501	5GP	C5'-O5'-P-OP1
2	A	502	5GP	C5'-O5'-P-OP1

There are no ring outliers.

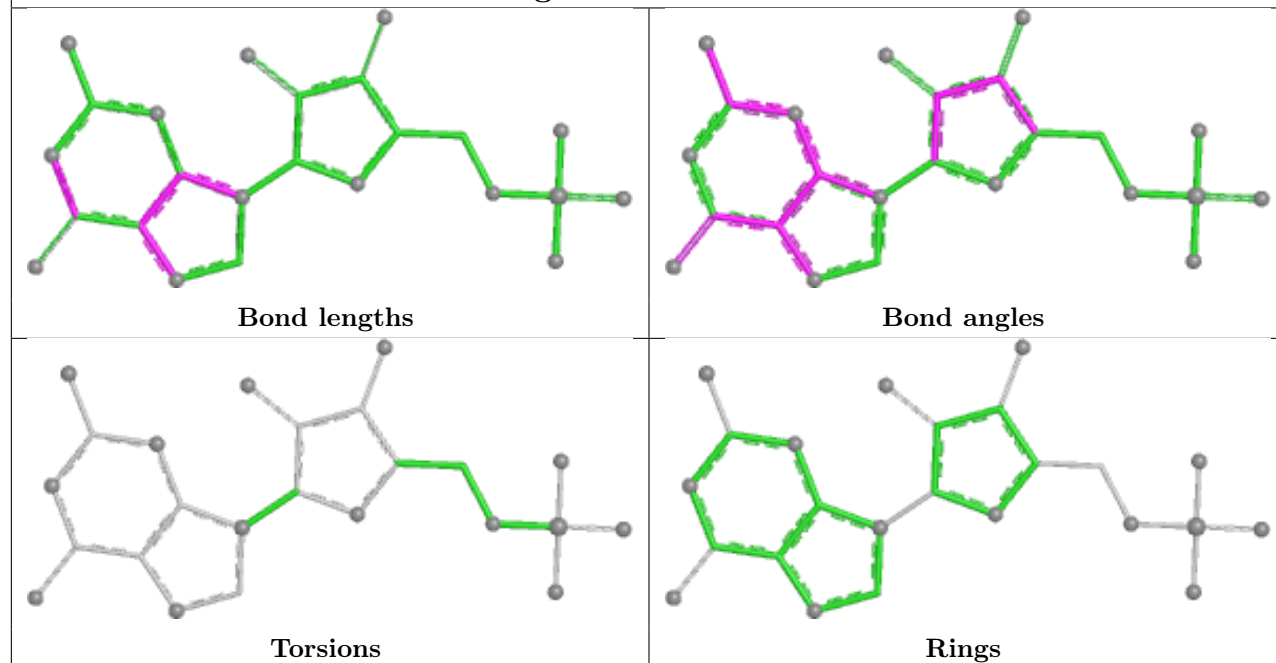
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	5GP	3	0
2	B	501	5GP	1	0
2	A	502	5GP	5	0

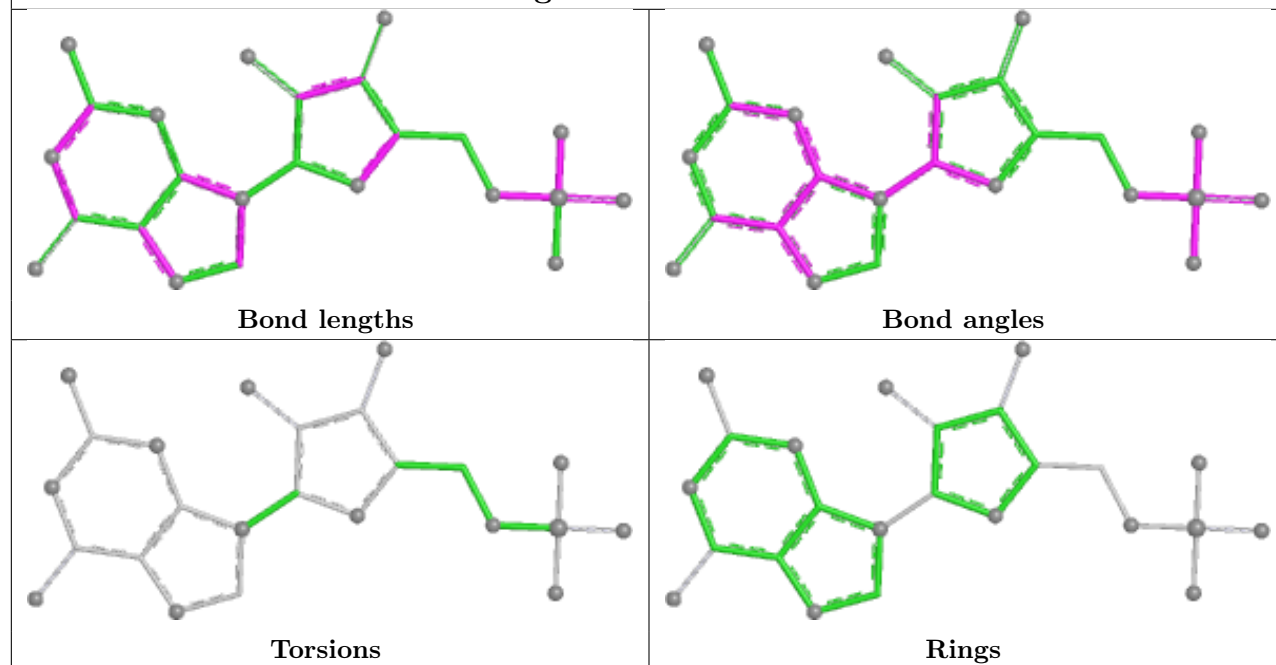
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

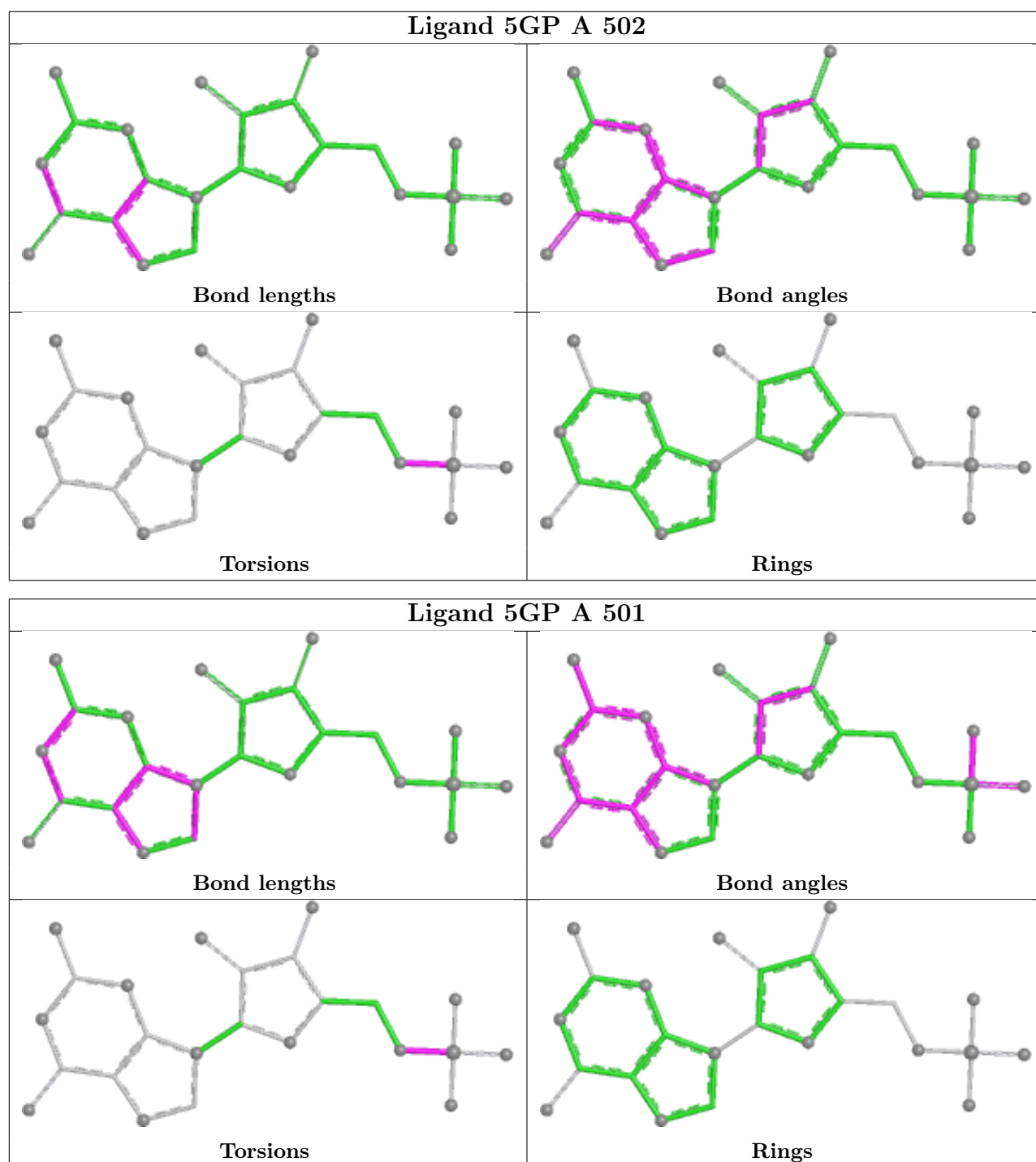


Ligand 5GP B 501



Ligand 5GP B 502





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	319/393 (81%)	0.32	14 (4%) 39 33	25, 76, 130, 155	0
1	B	303/393 (77%)	0.54	34 (11%) 10 8	25, 76, 149, 164	0
All	All	622/786 (79%)	0.43	48 (7%) 19 15	25, 76, 140, 164	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	THR	7.5
1	B	416	THR	7.2
1	B	220	SER	6.9
1	A	338	GLY	6.0
1	B	353	SER	5.8
1	B	337	PHE	5.8
1	B	250	LEU	5.7
1	B	249	LYS	5.2
1	A	398	VAL	5.0
1	B	247	GLY	4.5
1	B	211	VAL	4.4
1	B	356	SER	4.3
1	B	253	GLY	4.0
1	B	372	THR	3.8
1	B	254	GLU	3.7
1	B	354	HIS	3.6
1	B	252	VAL	3.6
1	B	338	GLY	3.4
1	A	339	PRO	3.3
1	B	236	PRO	3.3
1	A	302	ALA	3.2
1	A	371	LEU	3.1
1	B	223	ALA	3.1
1	B	243	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	242	ASP	3.0
1	B	258	LYS	2.9
1	A	304	ASP	2.9
1	B	251	HIS	2.9
1	A	373	PRO	2.9
1	B	235	LEU	2.9
1	B	245	ASN	2.8
1	B	208	ARG	2.8
1	B	406	ARG	2.4
1	B	246	GLU	2.3
1	B	244	LEU	2.3
1	A	246	GLU	2.3
1	B	369	ASP	2.3
1	B	371	LEU	2.2
1	B	414	ILE	2.2
1	B	339	PRO	2.2
1	A	277	MET	2.1
1	A	227	SER	2.1
1	B	241	ASN	2.1
1	A	223	ALA	2.0
1	A	293	GLN	2.0
1	A	402	GLN	2.0
1	B	370	ILE	2.0
1	B	399	ASN	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](#)

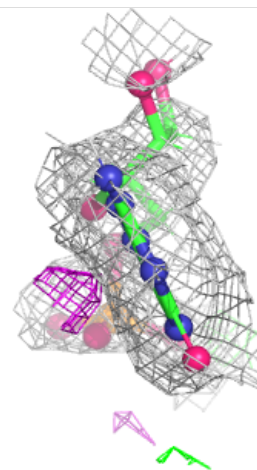
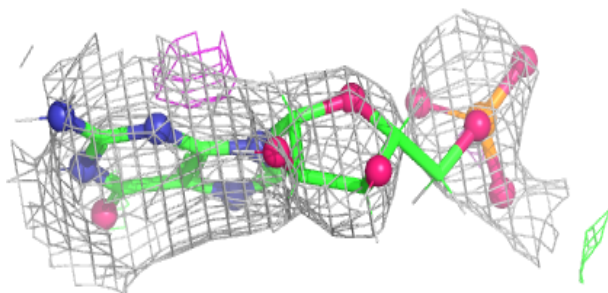
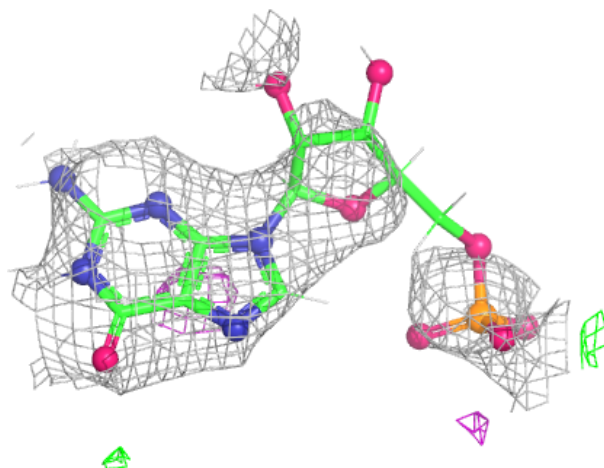
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	501	24/24	0.75	0.14	107,155,198,198	0
2	5GP	A	503	19/24	0.76	0.17	45,98,156,169	0
2	5GP	A	501	24/24	0.85	0.10	54,124,158,162	0
2	5GP	A	502	24/24	0.90	0.12	37,69,89,93	0
2	5GP	B	502	24/24	0.95	0.07	48,58,71,83	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.

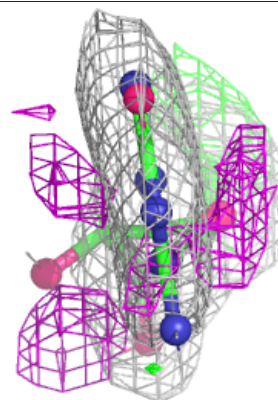
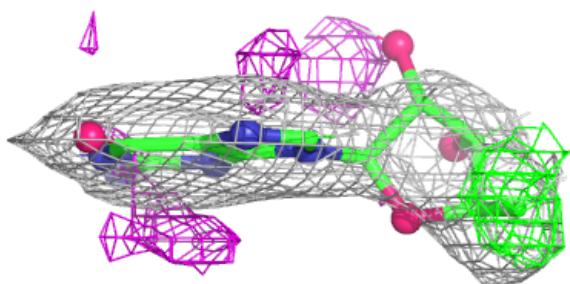
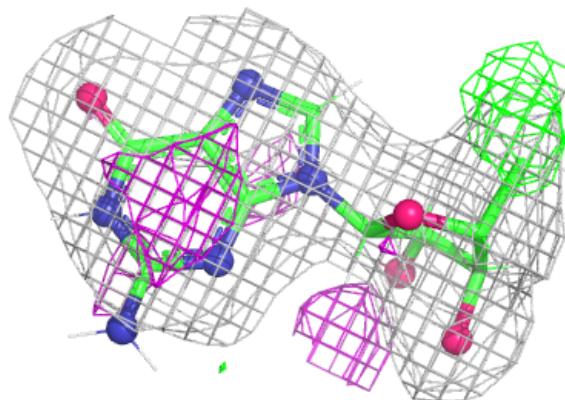
Electron density around 5GP B 501:

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



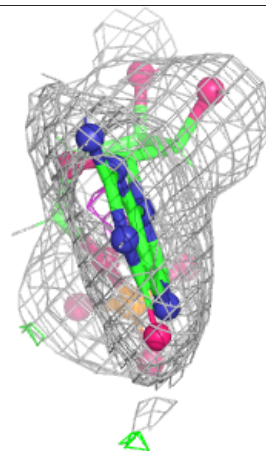
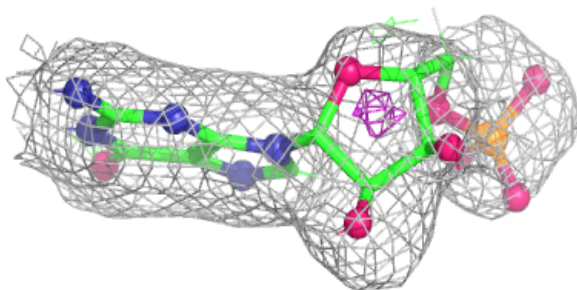
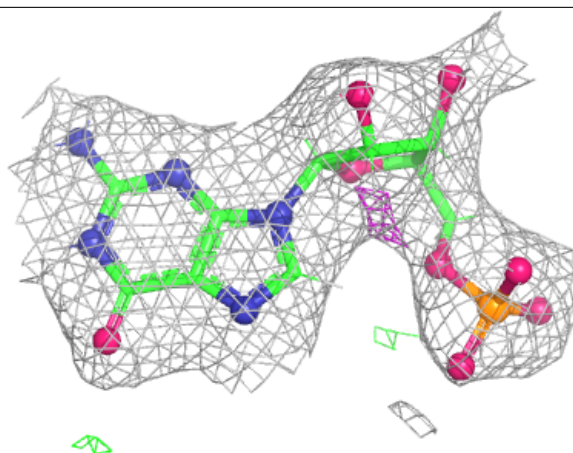
Electron density around 5GP A 503:

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



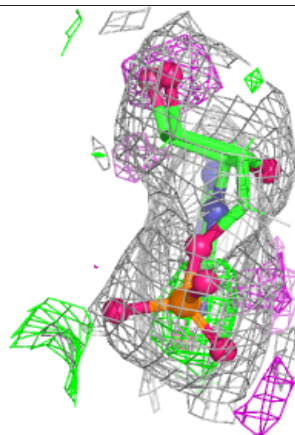
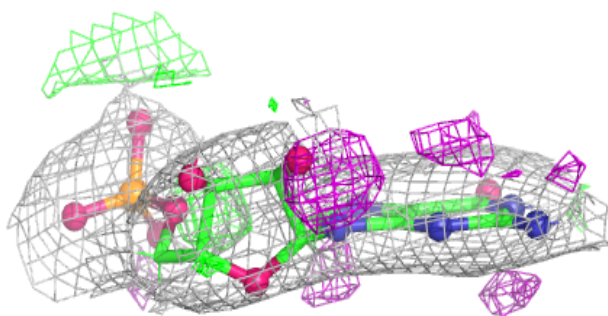
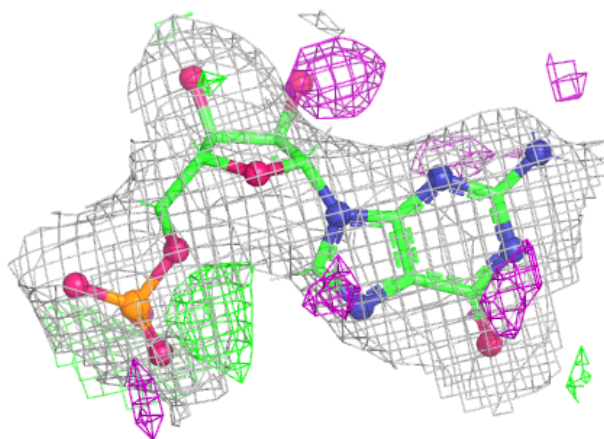
Electron density around 5GP A 501:

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

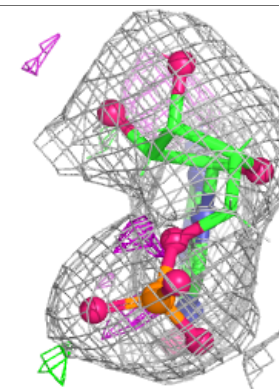
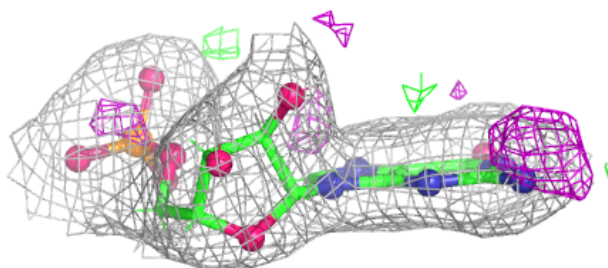
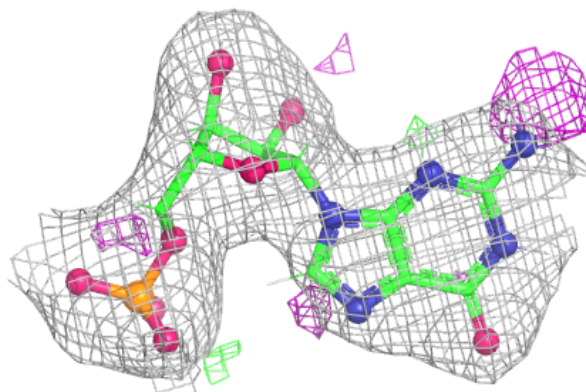


Electron density around 5GP A 502:

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

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

$2mF_o-DF_c$ (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.