



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:36 AM BST

PDB ID : 6JWU
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS wild type with STZ-DHP
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

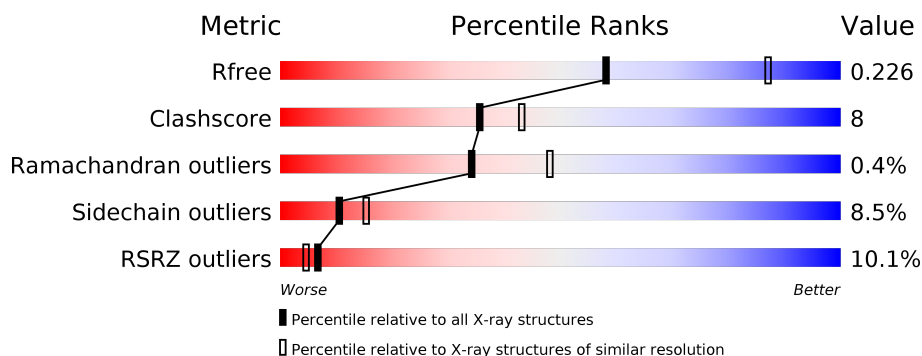
1 Overall quality at a glance

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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	728	<div> <div>7%</div> <div>59%</div> <div>16%</div> <div>•</div> <div>23%</div> </div>
1	B	728	<div> <div>8%</div> <div>56%</div> <div>15%</div> <div>•</div> <div>27%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	803	-	-	X	-
8	ACT	B	802	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9483 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 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4604	2968	754	859	23			
1	B	534	Total	C	N	O	S	0	0	0
			4396	2829	726	819	22			

There are 44 discrepancies between the modelled and reference sequences:

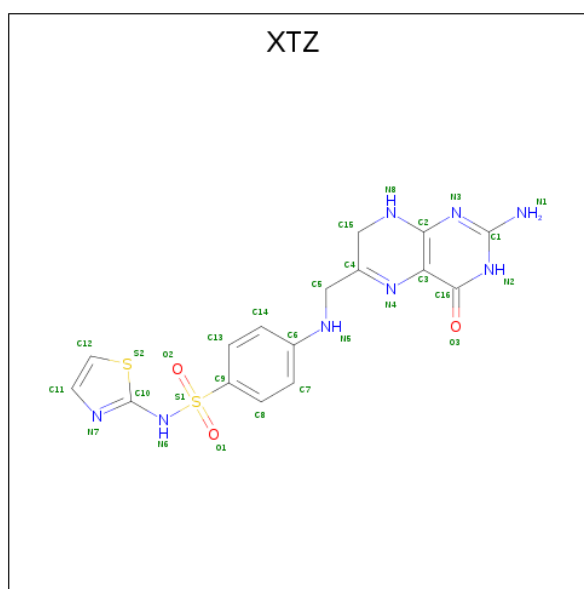
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag	UNP Q25704
A	714	VAL	-	expression tag	UNP Q25704
A	715	ASP	-	expression tag	UNP Q25704
A	716	LYS	-	expression tag	UNP Q25704
A	717	LEU	-	expression tag	UNP Q25704
A	718	ALA	-	expression tag	UNP Q25704
A	719	ALA	-	expression tag	UNP Q25704
A	720	ALA	-	expression tag	UNP Q25704
A	721	LEU	-	expression tag	UNP Q25704
A	722	GLU	-	expression tag	UNP Q25704
A	723	HIS	-	expression tag	UNP Q25704
A	724	HIS	-	expression tag	UNP Q25704
A	725	HIS	-	expression tag	UNP Q25704
A	726	HIS	-	expression tag	UNP Q25704
A	727	HIS	-	expression tag	UNP Q25704
A	728	HIS	-	expression tag	UNP Q25704
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704

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Chain	Residue	Modelled	Actual	Comment	Reference
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	UNP Q25704
B	714	VAL	-	expression tag	UNP Q25704
B	715	ASP	-	expression tag	UNP Q25704
B	716	LYS	-	expression tag	UNP Q25704
B	717	LEU	-	expression tag	UNP Q25704
B	718	ALA	-	expression tag	UNP Q25704
B	719	ALA	-	expression tag	UNP Q25704
B	720	ALA	-	expression tag	UNP Q25704
B	721	LEU	-	expression tag	UNP Q25704
B	722	GLU	-	expression tag	UNP Q25704
B	723	HIS	-	expression tag	UNP Q25704
B	724	HIS	-	expression tag	UNP Q25704
B	725	HIS	-	expression tag	UNP Q25704
B	726	HIS	-	expression tag	UNP Q25704
B	727	HIS	-	expression tag	UNP Q25704
B	728	HIS	-	expression tag	UNP Q25704

- Molecule 2 is 4-[[[(2-amino-4-oxo-3,4,7,8-tetrahydropteridin-6-yl)methyl]amino}-N-(1,3-thiazol-2-yl)benzenesulfonamide (three-letter code: XTZ) (formula: C₁₆H₁₆N₈O₃S₂).



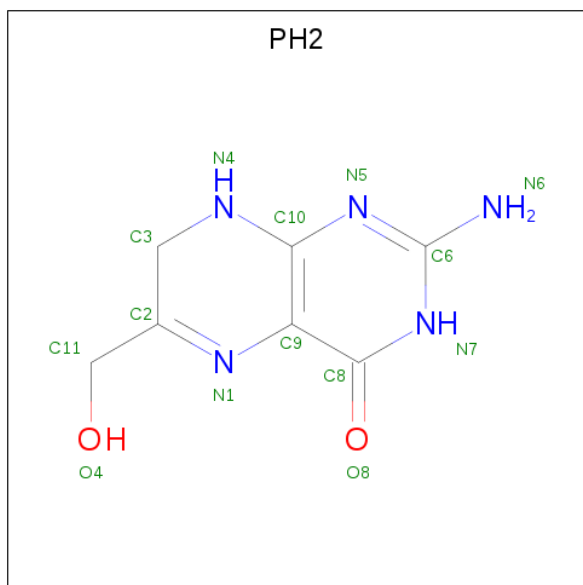
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	16	8	3	2		

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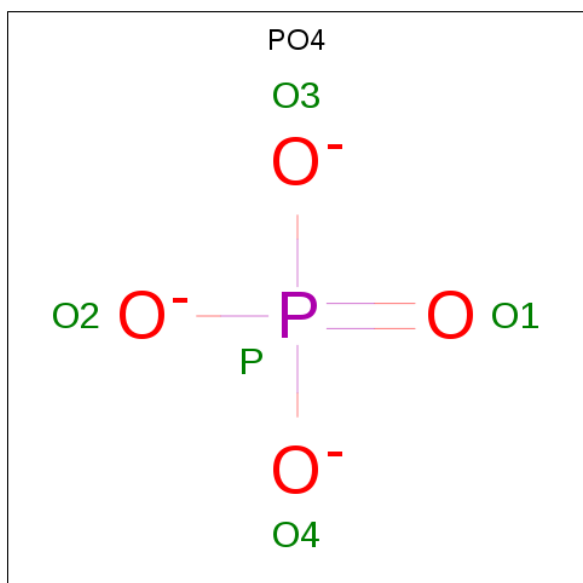
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			29	16	8	3	2		

- Molecule 3 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (three-letter code: PH2) (formula: C₇H₉N₅O₂).



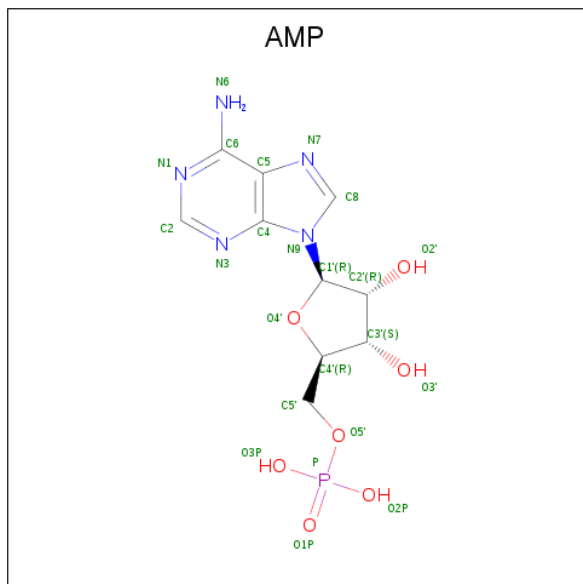
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	7	5	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 23 10 5 7 1	0	0
5	B	1	Total C N O P 23 10 5 7 1	0	0

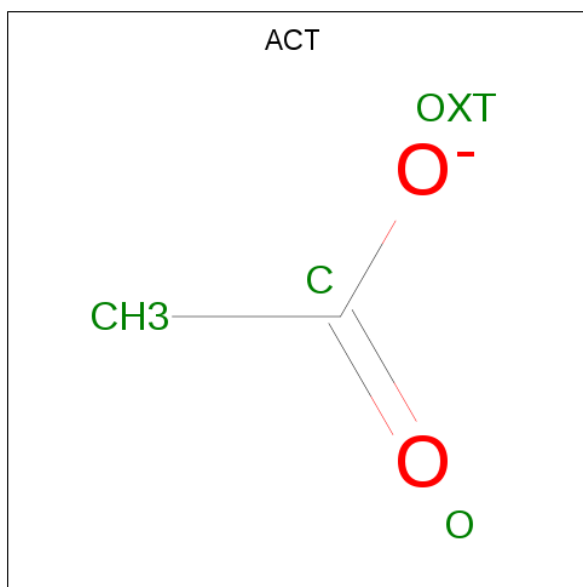
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	A	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	1	Total Ca 1 1	0	0

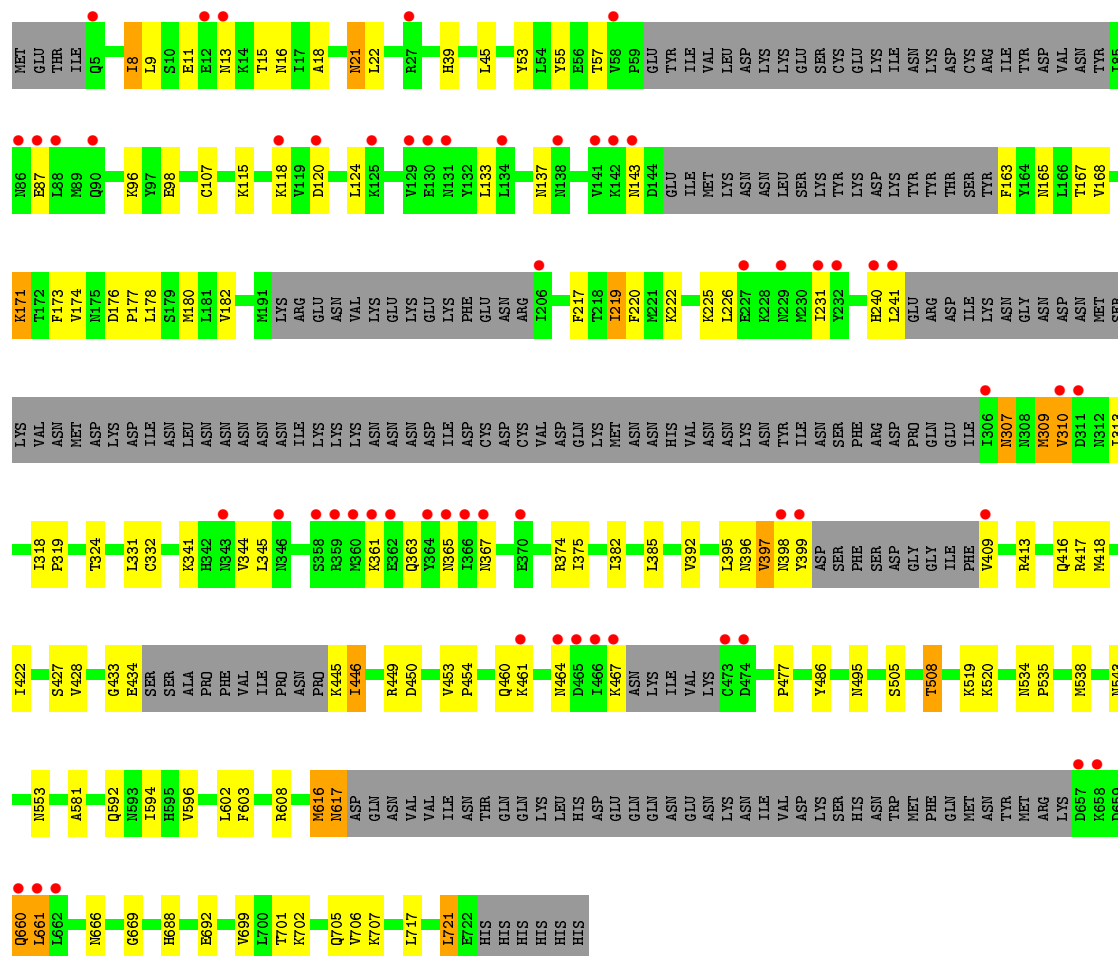
- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	204	Total O 204 204	0	0
9	B	122	Total O 122 122	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.15Å 136.96Å 137.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.66 – 2.65 32.64 – 2.65	Depositor EDS
% Data completeness (in resolution range)	85.8 (32.66-2.65) 85.8 (32.64-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.196 , 0.233 0.194 , 0.226	Depositor DCC
R_{free} test set	4839 reflections (10.28%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, PO4, XTZ, PH2, ACT, AMP, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/4677	0.81	0/6312
1	B	0.67	0/4461	0.79	0/6015
All	All	0.67	0/9138	0.80	0/12327

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	4604	0	4698	83	0
1	B	4396	0	4497	72	0
2	A	29	0	16	3	0
2	B	29	0	16	2	0
3	A	14	0	9	1	0
4	A	15	0	0	2	0
5	A	23	0	12	0	0
5	B	23	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	8	0	6	0	0
8	B	12	0	9	6	0
9	A	204	0	0	8	0
9	B	122	0	0	3	0
All	All	9483	0	9275	150	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 8.

All (150) 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:107:CYS:SG	1:A:171:LYS:HE3	1.87	1.14
1:B:107:CYS:SG	1:B:171:LYS:NZ	2.26	1.08
1:A:341:LYS:NZ	1:A:345:LEU:O	1.93	1.01
1:A:107:CYS:SG	1:A:171:LYS:CE	2.57	0.92
2:B:801:XTZ:H6	8:B:802:ACT:H1	1.66	0.77
1:A:51:THR:HG22	1:A:168:VAL:HG12	1.69	0.75
1:A:505:SER:O	1:A:508:THR:HB	1.87	0.75
1:B:505:SER:O	1:B:508:THR:HB	1.85	0.74
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.68	0.73
1:A:93:GLU:OE2	1:A:186:TYR:OH	2.06	0.73
2:A:801:XTZ:H5	4:A:803:PO4:O2	1.88	0.72
1:A:63:VAL:HG13	1:A:325:HIS:HB3	1.71	0.72
1:A:107:CYS:HG	1:A:171:LYS:HE3	1.55	0.72
1:A:691:LEU:HD11	1:B:661:LEU:HD11	1.71	0.71
1:A:2:GLU:HB3	1:A:5:GLN:HG3	1.71	0.71
1:B:519:LYS:NZ	9:B:902:HOH:O	2.23	0.71
1:A:398:ASN:HD21	1:A:409:VAL:HG23	1.54	0.70
1:B:55:TYR:OH	1:B:374:ARG:NH1	2.26	0.69
1:B:217:PHE:HB3	1:B:219:ILE:HD13	1.75	0.68
1:A:617:ASN:O	1:A:618:ASP:HB2	1.93	0.67
1:A:343:ASN:H	1:A:343:ASN:HD22	1.42	0.67
1:A:438:PRO:HG3	2:A:801:XTZ:S2	2.36	0.66
1:A:422:ILE:HD11	1:A:477:PRO:HG3	1.78	0.66
1:A:398:ASN:ND2	1:A:409:VAL:HG23	2.12	0.65
1:B:39:HIS:CD2	1:B:520:LYS:O	2.50	0.64
1:B:608:ARG:HA	1:B:666:ASN:OD1	1.98	0.64
1:B:341:LYS:NZ	1:B:345:LEU:O	2.31	0.63
1:B:422:ILE:HG12	1:B:477:PRO:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LYS:O	1:B:365:ASN:HA	1.98	0.63
1:A:128:ASN:OD1	1:A:131:ASN:ND2	2.32	0.62
1:A:191:MET:HE1	1:A:207:ILE:HG12	1.80	0.62
1:A:343:ASN:HD22	1:A:343:ASN:N	1.96	0.62
1:B:397:VAL:HG23	1:B:409:VAL:HG21	1.83	0.61
1:A:493:VAL:HG22	1:A:524:TYR:CZ	2.38	0.58
1:A:359:ARG:O	1:A:363:GLN:HB2	2.04	0.57
1:B:397:VAL:HG22	1:B:397:VAL:O	2.02	0.57
1:B:374:ARG:HD2	1:B:385:LEU:HD22	1.86	0.57
1:A:55:TYR:OH	1:A:374:ARG:NH1	2.36	0.57
1:A:131:ASN:ND2	9:A:910:HOH:O	2.37	0.56
1:B:692:GLU:N	1:B:692:GLU:OE1	2.30	0.56
1:B:96:LYS:HG2	1:B:240:HIS:CE1	2.40	0.56
1:B:660:GLN:HG3	1:B:660:GLN:O	2.06	0.56
1:B:398:ASN:O	1:B:399:TYR:HB2	2.06	0.55
1:B:396:ASN:ND2	8:B:802:ACT:O	2.39	0.55
1:B:701:THR:O	1:B:705:GLN:HG2	2.06	0.55
1:A:691:LEU:CD1	1:B:661:LEU:HD11	2.36	0.55
1:B:178:LEU:O	1:B:182:VAL:HG23	2.06	0.54
1:A:53:TYR:CG	1:A:374:ARG:HD2	2.42	0.54
1:A:4:ILE:CD1	9:A:999:HOH:O	2.56	0.53
1:A:119:VAL:HG21	1:A:215:ASN:HB3	1.90	0.53
1:A:434:GLU:HG3	9:A:1079:HOH:O	2.07	0.53
1:B:398:ASN:HB3	1:B:433:GLY:O	2.09	0.53
1:A:121:ASN:ND2	9:A:913:HOH:O	2.42	0.53
1:B:226:LEU:O	1:B:310:VAL:HG12	2.09	0.53
1:A:56:GLU:OE2	1:A:384:TYR:OH	2.26	0.52
1:A:55:TYR:OH	1:A:335:ASP:OD2	2.21	0.52
1:A:61:TYR:HB3	1:A:147:MET:HG2	1.91	0.52
1:B:538:MET:O	1:B:581:ALA:HA	2.10	0.52
1:A:368:ILE:O	1:A:368:ILE:HG13	2.10	0.51
1:A:38:LEU:CD2	1:A:168:VAL:HG11	2.41	0.51
1:B:167:THR:OG1	1:B:332:CYS:HB3	2.10	0.51
1:B:553:ASN:ND2	9:B:908:HOH:O	2.42	0.51
1:B:397:VAL:CG2	1:B:397:VAL:O	2.59	0.51
1:A:34:LEU:CD1	1:A:54:LEU:HD11	2.41	0.50
1:A:212:LEU:O	1:A:319:PRO:HA	2.11	0.50
1:A:304:GLU:O	1:A:308:ASN:ND2	2.45	0.50
1:B:53:TYR:CG	1:B:374:ARG:HD3	2.47	0.50
1:A:552:LYS:HE2	9:A:1054:HOH:O	2.12	0.49
1:B:45:LEU:HD22	1:B:180:MET:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ASN:OD1	1:B:307:ASN:N	2.45	0.49
1:A:4:ILE:HD13	9:A:999:HOH:O	2.11	0.48
2:B:801:XTZ:C5	8:B:802:ACT:H1	2.41	0.48
1:B:39:HIS:CG	1:B:520:LYS:O	2.66	0.48
1:B:495:ASN:HD22	1:B:495:ASN:N	2.10	0.48
1:B:688:HIS:CE1	8:B:802:ACT:H3	2.48	0.48
1:A:691:LEU:HD11	1:B:661:LEU:CD1	2.42	0.48
1:A:86:ASN:HB3	9:A:1083:HOH:O	2.12	0.48
1:B:450:ASP:O	1:B:454:PRO:HG2	2.14	0.48
1:B:397:VAL:CG2	1:B:409:VAL:HG21	2.43	0.48
1:A:703:ILE:O	1:B:592:GLN:HG2	2.14	0.48
1:A:573:LEU:HD23	1:A:601:PRO:HB2	1.96	0.48
1:B:688:HIS:HE1	8:B:802:ACT:H3	1.78	0.48
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.44	0.47
1:A:616:MET:CE	1:B:699:VAL:HG23	2.44	0.47
1:B:717:LEU:HG	1:B:721:LEU:HD22	1.95	0.47
1:A:538:MET:O	1:A:581:ALA:HA	2.15	0.47
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.45	0.47
1:B:8:ILE:HG22	1:B:9:LEU:HD23	1.96	0.47
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.88	0.47
1:A:617:ASN:N	1:A:617:ASN:HD22	2.14	0.46
1:B:124:LEU:HD11	1:B:176:ASP:OD2	2.16	0.46
1:A:324:THR:HB	9:A:914:HOH:O	2.16	0.46
1:A:89:MET:HB3	1:A:89:MET:HE2	1.66	0.46
1:B:594:ILE:CG1	1:B:602:LEU:HD21	2.45	0.46
1:A:180:MET:HE2	1:A:211:ILE:HD13	1.97	0.46
2:A:801:XTZ:C5	4:A:803:PO4:O2	2.62	0.46
1:B:434:GLU:H	1:B:434:GLU:CD	2.18	0.46
1:B:375:ILE:HG21	1:B:382:ILE:HG13	1.98	0.46
1:A:226:LEU:O	1:A:310:VAL:HG13	2.16	0.46
1:A:53:TYR:CD2	1:A:374:ARG:HD2	2.51	0.46
1:B:543:ASN:OD1	9:B:901:HOH:O	2.21	0.46
1:A:361:LYS:HD2	1:A:367:ASN:OD1	2.15	0.46
1:A:61:TYR:CE1	3:A:802:PH2:H31	2.52	0.45
1:B:18:ALA:HB2	1:B:180:MET:HE1	1.99	0.45
1:B:461:LYS:O	1:B:464:ASN:HB2	2.17	0.45
1:A:103:LEU:HD13	1:A:511:PRO:HB2	1.97	0.45
1:A:301:ASP:N	1:A:301:ASP:OD1	2.50	0.45
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.98	0.45
1:B:318:ILE:HA	1:B:319:PRO:C	2.36	0.45
1:A:2:GLU:N	1:A:2:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASN:ND2	1:B:174:VAL:O	2.51	0.44
1:A:395:LEU:HD23	1:A:431:ILE:HD12	1.99	0.44
1:A:343:ASN:ND2	1:A:343:ASN:N	2.65	0.44
1:A:63:VAL:HG21	1:A:322:TYR:CE1	2.52	0.44
1:A:5:GLN:HB2	1:A:9:LEU:HD12	2.00	0.44
1:B:413:ARG:O	1:B:416:GLN:HB2	2.18	0.43
1:B:453:VAL:N	1:B:454:PRO:CD	2.81	0.43
1:A:308:ASN:N	1:A:308:ASN:HD22	2.17	0.43
1:B:13:ASN:N	1:B:13:ASN:OD1	2.52	0.43
1:B:231:ILE:HD13	1:B:309:MET:HB3	2.01	0.43
1:A:699:VAL:HG23	1:B:616:MET:CE	2.48	0.43
1:B:486:TYR:CD1	8:B:807:ACT:H2	2.54	0.43
1:B:133:LEU:O	1:B:137:ASN:ND2	2.52	0.43
1:B:395:LEU:HD22	1:B:418:MET:CG	2.49	0.43
1:B:446:ILE:HA	1:B:446:ILE:HD12	1.83	0.42
1:A:584:HIS:O	1:A:588:ILE:HG12	2.19	0.42
1:A:20:LEU:HD21	1:A:180:MET:HE3	2.01	0.42
1:A:21:ASN:C	1:A:22:LEU:HD12	2.40	0.42
1:A:175:ASN:ND2	1:A:237:LYS:HE2	2.34	0.42
1:A:443:ASN:HB3	1:A:444:PRO:HD2	2.02	0.42
1:B:177:PRO:HB3	1:B:318:ILE:CD1	2.50	0.42
1:A:417:ARG:HD2	1:A:417:ARG:O	2.19	0.42
1:A:47:LYS:HE3	1:A:104:ILE:HD13	2.00	0.42
1:A:616:MET:CE	1:B:699:VAL:CG2	2.98	0.42
1:A:304:GLU:O	1:A:307:ASN:HB2	2.20	0.41
1:B:309:MET:O	1:B:313:ILE:HG13	2.20	0.41
1:A:14:LYS:HE2	1:A:120:ASP:HB3	2.01	0.41
1:A:398:ASN:ND2	1:A:407:ILE:HA	2.35	0.41
1:B:617:ASN:N	1:B:617:ASN:ND2	2.69	0.41
1:A:616:MET:HE2	1:B:699:VAL:HG23	2.02	0.41
1:B:177:PRO:CB	1:B:318:ILE:CD1	2.98	0.41
1:A:167:THR:OG1	1:A:332:CYS:HB3	2.20	0.41
1:A:306:ILE:O	1:A:310:VAL:HG23	2.19	0.41
1:B:55:TYR:CD2	1:B:331:LEU:HD21	2.56	0.41
1:B:706:VAL:HG23	1:B:706:VAL:O	2.21	0.41
1:A:463:TRP:O	1:A:466:ILE:HG12	2.21	0.41
1:A:493:VAL:CG2	1:A:524:TYR:CZ	3.03	0.41
1:A:699:VAL:HG21	1:B:669:GLY:CA	2.51	0.40
1:B:21:ASN:C	1:B:22:LEU:HD12	2.42	0.40
1:B:392:VAL:HG22	1:B:428:VAL:HB	2.04	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	542/728 (74%)	509 (94%)	30 (6%)	3 (1%)	25	37
1	B	516/728 (71%)	485 (94%)	30 (6%)	1 (0%)	47	64
All	All	1058/1456 (73%)	994 (94%)	60 (6%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	471	VAL
1	A	444	PRO
1	A	397	VAL
1	B	8	ILE

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	531/696 (76%)	488 (92%)	43 (8%)	11	17
1	B	506/696 (73%)	461 (91%)	45 (9%)	9	14
All	All	1037/1392 (74%)	949 (92%)	88 (8%)	10	15

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	6	GLU

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Mol	Chain	Res	Type
1	A	8	ILE
1	A	11	GLU
1	A	14	LYS
1	A	25	ASN
1	A	27	ARG
1	A	57	THR
1	A	93	GLU
1	A	116	ASN
1	A	165	ASN
1	A	192	LYS
1	A	206	ILE
1	A	220	PHE
1	A	301	ASP
1	A	303	GLN
1	A	308	ASN
1	A	324	THR
1	A	343	ASN
1	A	347	ASN
1	A	361	LYS
1	A	363	GLN
1	A	381	ARG
1	A	388	LYS
1	A	408	PHE
1	A	417	ARG
1	A	435	SER
1	A	449	ARG
1	A	493	VAL
1	A	508	THR
1	A	522	LYS
1	A	542	THR
1	A	562	LEU
1	A	576	ILE
1	A	616	MET
1	A	617	ASN
1	A	618	ASP
1	A	659	ASP
1	A	660	GLN
1	A	661	LEU
1	A	664	GLN
1	A	691	LEU
1	A	707	LYS
1	B	11	GLU

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Mol	Chain	Res	Type
1	B	15	THR
1	B	21	ASN
1	B	57	THR
1	B	87	GLU
1	B	98	GLU
1	B	115	LYS
1	B	118	LYS
1	B	120	ASP
1	B	143	ASN
1	B	163	PHE
1	B	165	ASN
1	B	168	VAL
1	B	171	LYS
1	B	173	PHE
1	B	219	ILE
1	B	220	PHE
1	B	222	LYS
1	B	225	LYS
1	B	241	LEU
1	B	307	ASN
1	B	309	MET
1	B	310	VAL
1	B	324	THR
1	B	344	VAL
1	B	363	GLN
1	B	367	ASN
1	B	397	VAL
1	B	417	ARG
1	B	427	SER
1	B	445	LYS
1	B	446	ILE
1	B	449	ARG
1	B	460	GLN
1	B	467	LYS
1	B	508	THR
1	B	596	VAL
1	B	603	PHE
1	B	616	MET
1	B	617	ASN
1	B	660	GLN
1	B	661	LEU
1	B	702	LYS

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Mol	Chain	Res	Type
1	B	707	LYS
1	B	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	121	ASN
1	A	131	ASN
1	A	138	ASN
1	A	308	ASN
1	A	343	ASN
1	A	398	ASN
1	A	521	ASN
1	A	553	ASN
1	A	557	GLN
1	A	617	ASN
1	B	21	ASN
1	B	91	ASN
1	B	100	ASN
1	B	131	ASN
1	B	138	ASN
1	B	143	ASN
1	B	240	HIS
1	B	367	ASN
1	B	457	GLN
1	B	495	ASN
1	B	553	ASN
1	B	617	ASN
1	B	664	GLN
1	B	710	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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
4	PO4	A	809	-	4,4,4	0.67	0	6,6,6	0.44	0
5	AMP	A	804	6	22,25,25	0.64	0	25,38,38	0.86	1 (4%)
8	ACT	B	807	-	1,3,3	3.22	1 (100%)	0,3,3	0.00	-
8	ACT	B	806	-	1,3,3	3.96	1 (100%)	0,3,3	0.00	-
4	PO4	A	810	-	4,4,4	0.43	0	6,6,6	0.44	0
8	ACT	A	808	-	1,3,3	3.09	1 (100%)	0,3,3	0.00	-
3	PH2	A	802	-	10,15,15	1.33	1 (10%)	10,21,21	3.27	5 (50%)
2	XTZ	A	801	-	25,32,32	2.25	2 (8%)	27,46,46	3.05	7 (25%)
8	ACT	A	807	-	1,3,3	4.22	1 (100%)	0,3,3	0.00	-
2	XTZ	B	801	-	25,32,32	2.38	2 (8%)	27,46,46	2.20	10 (37%)
4	PO4	A	803	-	4,4,4	0.95	0	6,6,6	0.51	0
5	AMP	B	803	6	22,25,25	0.64	0	25,38,38	0.98	2 (8%)
8	ACT	B	802	-	1,3,3	3.06	1 (100%)	0,3,3	0.00	-

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
5	AMP	A	804	6	-	3/6/26/26	0/3/3/3
3	PH2	A	802	-	-	0/0/11/11	0/2/2/2
2	XTZ	A	801	-	-	7/12/25/25	0/4/4/4
5	AMP	B	803	6	-	5/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XTZ	B	801	-	-	3/12/25/25	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	XTZ	C9-S1	-10.97	1.59	1.76
2	A	801	XTZ	C9-S1	-10.15	1.60	1.76
8	A	807	ACT	CH3-C	4.22	1.54	1.48
8	B	806	ACT	CH3-C	3.96	1.53	1.48
3	A	802	PH2	C8-N7	3.23	1.38	1.33
8	B	807	ACT	CH3-C	3.22	1.52	1.48
8	A	808	ACT	CH3-C	3.09	1.52	1.48
8	B	802	ACT	CH3-C	3.06	1.52	1.48
2	A	801	XTZ	C3-C2	2.58	1.48	1.41
2	B	801	XTZ	C3-C2	2.31	1.47	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	XTZ	O2-S1-O1	-10.17	107.05	119.55
2	A	801	XTZ	C9-S1-N6	8.10	117.02	106.83
3	A	802	PH2	C8-C9-C10	7.55	119.47	114.53
2	B	801	XTZ	O2-S1-O1	-5.14	113.23	119.55
3	A	802	PH2	C9-C8-N7	-4.71	116.99	123.43
2	A	801	XTZ	C16-N2-C1	4.68	123.37	115.93
2	B	801	XTZ	C16-N2-C1	4.07	122.40	115.93
2	A	801	XTZ	C3-C16-N2	-3.87	118.13	123.43
2	B	801	XTZ	C3-C16-N2	-3.82	118.21	123.43
3	A	802	PH2	C8-N7-C6	3.77	121.92	115.93
2	A	801	XTZ	C8-C9-S1	3.56	123.64	119.77
2	A	801	XTZ	C13-C9-S1	-3.51	115.95	119.77
2	B	801	XTZ	C9-S1-N6	3.50	111.24	106.83
2	B	801	XTZ	C16-C3-C2	3.23	116.64	114.53
2	B	801	XTZ	O2-S1-N6	2.98	114.19	106.73
2	B	801	XTZ	C1-N3-C2	2.98	121.21	114.54
2	B	801	XTZ	C10-N6-S1	2.97	129.56	124.16
2	B	801	XTZ	O1-S1-C9	-2.80	104.52	107.97
5	B	803	AMP	C3'-C2'-C1'	2.52	104.78	100.98
2	B	801	XTZ	N1-C1-N3	2.46	121.08	117.25
5	A	804	AMP	C5-C6-N6	2.42	124.03	120.35
5	B	803	AMP	C5-C6-N6	2.23	123.74	120.35
3	A	802	PH2	N7-C6-N5	-2.18	121.99	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	PH2	N6-C6-N5	2.12	120.55	117.25
2	A	801	XTZ	N1-C1-N3	2.05	120.44	117.25

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	803	AMP	C5'-O5'-P-O2P
5	B	803	AMP	C5'-O5'-P-O3P
5	A	804	AMP	C3'-C4'-C5'-O5'
5	B	803	AMP	O4'-C4'-C5'-O5'
5	B	803	AMP	C3'-C4'-C5'-O5'
2	A	801	XTZ	C10-N6-S1-O2
5	A	804	AMP	C5'-O5'-P-O1P
5	B	803	AMP	C5'-O5'-P-O1P
2	A	801	XTZ	C10-N6-S1-C9
2	A	801	XTZ	C10-N6-S1-O1
5	A	804	AMP	O4'-C4'-C5'-O5'
2	B	801	XTZ	C10-N6-S1-O2
2	A	801	XTZ	C13-C9-S1-O1
2	A	801	XTZ	C8-C9-S1-O1
2	B	801	XTZ	C8-C9-S1-O1
2	A	801	XTZ	C7-C6-N5-C5
2	B	801	XTZ	C13-C9-S1-O1
2	A	801	XTZ	C4-C5-N5-C6

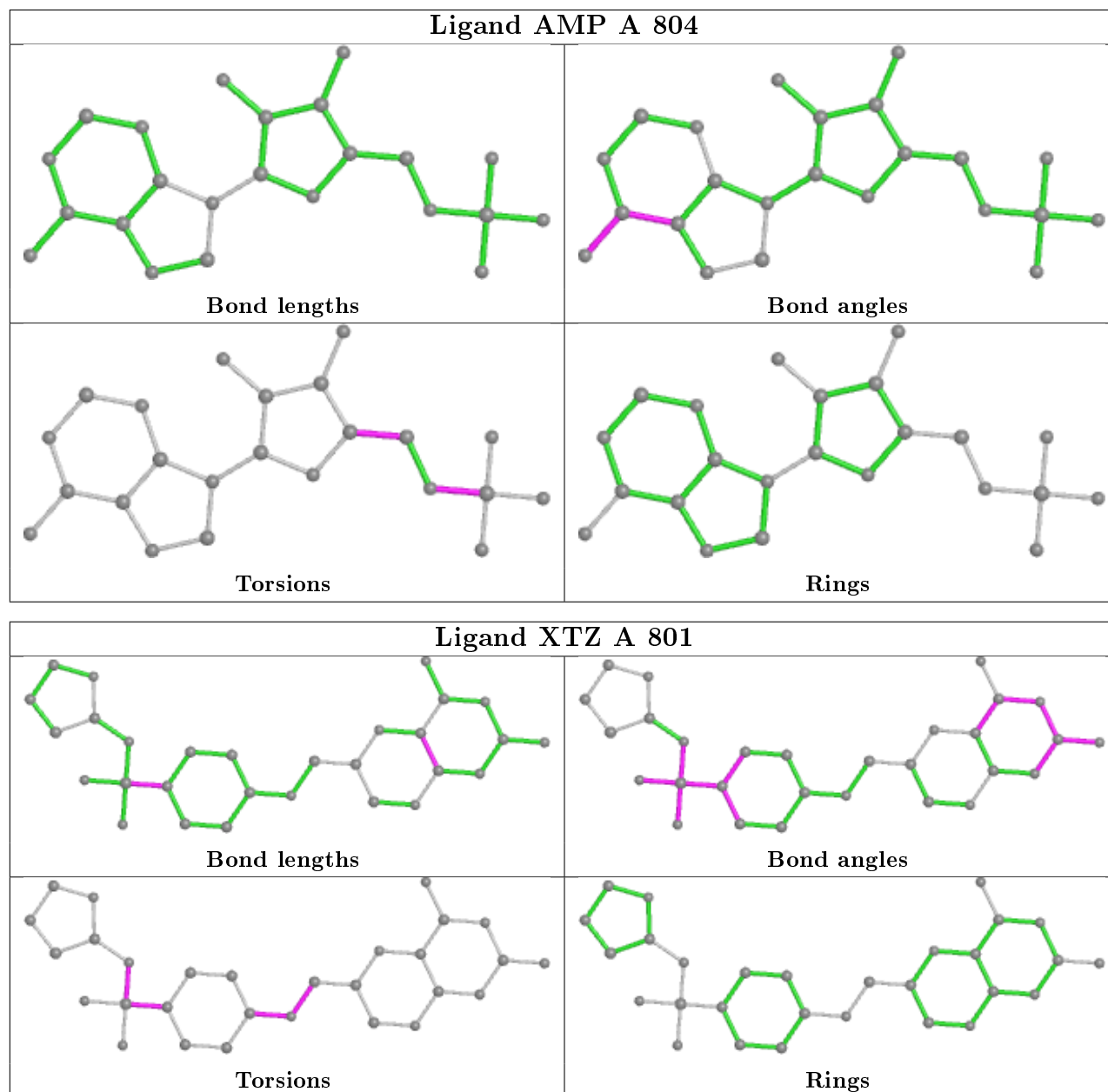
There are no ring outliers.

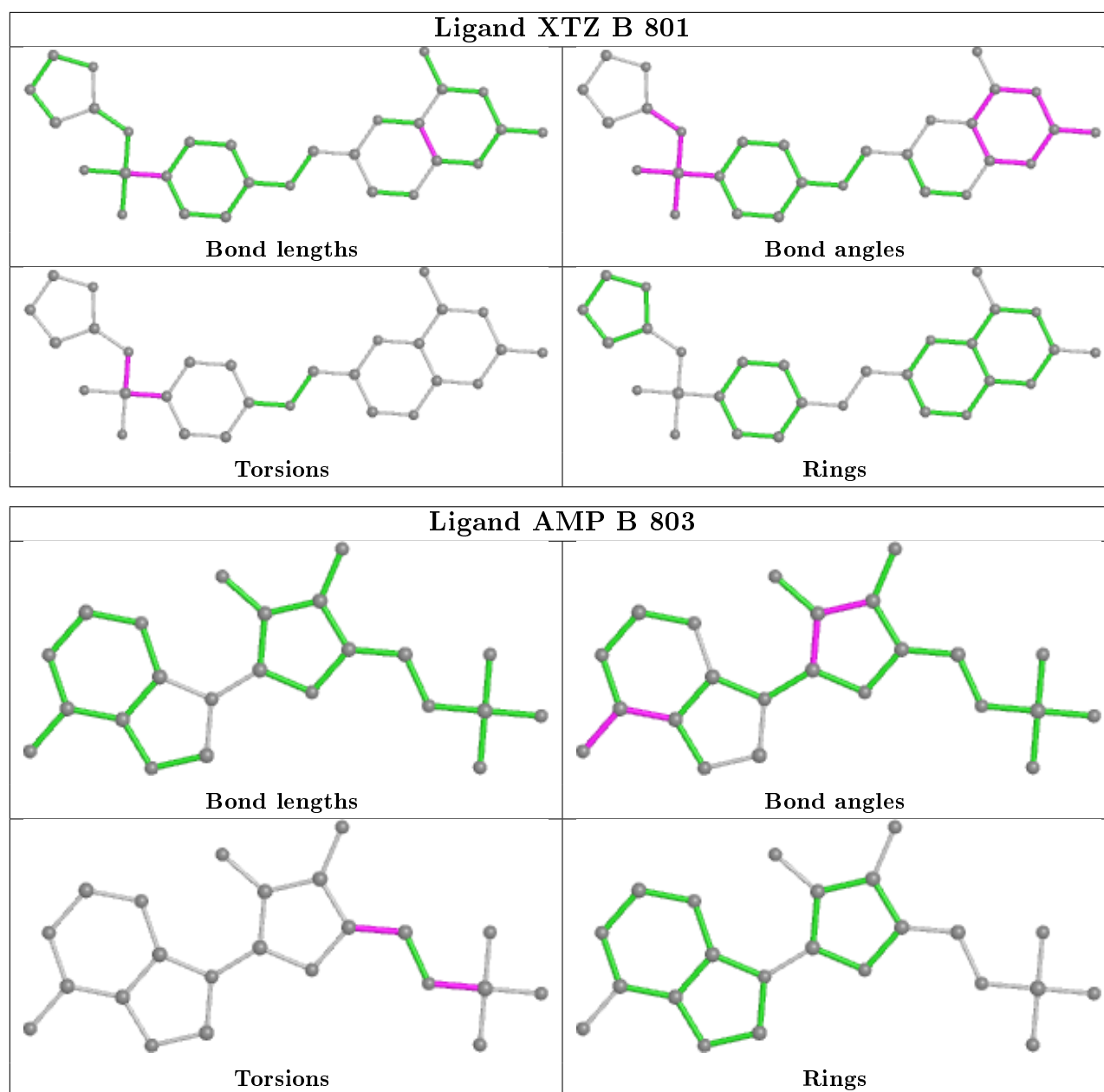
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	807	ACT	1	0
3	A	802	PH2	1	0
2	A	801	XTZ	3	0
2	B	801	XTZ	2	0
4	A	803	PO4	2	0
8	B	802	ACT	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.





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	558/728 (76%)	0.11	53 (9%) 8 6	6, 26, 100, 120	0
1	B	534/728 (73%)	0.24	57 (10%) 6 4	9, 48, 108, 120	0
All	All	1092/1456 (75%)	0.17	110 (10%) 7 4	6, 32, 105, 120	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	ILE	11.6
1	A	439	PHE	7.1
1	A	657	ASP	6.6
1	A	444	PRO	6.5
1	A	442	PRO	6.4
1	A	658	LYS	5.8
1	A	473	CYS	5.6
1	A	407	ILE	5.2
1	A	303	GLN	5.1
1	B	364	TYR	5.0
1	B	27	ARG	5.0
1	A	708	ASP	5.0
1	A	408	PHE	4.9
1	B	310	VAL	4.7
1	B	58	VAL	4.7
1	A	659	ASP	4.6
1	B	13	ASN	4.5
1	B	366	ILE	4.4
1	B	90	GLN	4.4
1	A	301	ASP	4.3
1	A	466	ILE	4.3
1	B	5	GLN	4.1
1	B	367	ASN	4.0
1	B	229	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	143	ASN	3.8
1	B	138	ASN	3.8
1	A	617	ASN	3.8
1	A	362	GLU	3.7
1	A	471	VAL	3.7
1	B	118	LYS	3.6
1	B	131	ASN	3.6
1	A	6	GLU	3.6
1	A	618	ASP	3.6
1	B	134	LEU	3.6
1	A	145	GLU	3.6
1	A	302	PRO	3.5
1	B	362	GLU	3.4
1	B	365	ASN	3.4
1	A	440	VAL	3.4
1	A	2	GLU	3.4
1	B	142	LYS	3.3
1	A	443	ASN	3.3
1	A	147	MET	3.3
1	A	118	LYS	3.2
1	B	466	ILE	3.2
1	A	148	LYS	3.2
1	B	125	LYS	3.2
1	B	358	SER	3.2
1	A	146	ILE	3.1
1	A	62	ILE	3.1
1	A	142	LYS	3.1
1	B	240	HIS	3.1
1	B	87	GLU	3.0
1	B	474	ASP	3.0
1	A	445	LYS	2.9
1	B	12	GLU	2.9
1	B	120	ASP	2.9
1	A	438	PRO	2.9
1	B	359	ARG	2.9
1	A	365	ASN	2.9
1	A	660	GLN	2.9
1	B	232	TYR	2.9
1	B	467	LYS	2.8
1	B	657	ASP	2.7
1	A	472	LYS	2.7
1	A	474	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	86	ASN	2.7
1	A	366	ILE	2.7
1	A	11	GLU	2.7
1	B	361	LYS	2.7
1	B	662	LEU	2.7
1	B	473	CYS	2.6
1	B	129	VAL	2.6
1	A	661	LEU	2.6
1	B	661	LEU	2.6
1	A	470	ILE	2.6
1	B	241	LEU	2.6
1	B	398	ASN	2.5
1	A	437	ALA	2.5
1	B	130	GLU	2.5
1	B	311	ASP	2.5
1	B	464	ASN	2.5
1	A	446	ILE	2.5
1	B	370	GLU	2.4
1	B	658	LYS	2.4
1	B	360	MET	2.4
1	A	242	GLU	2.4
1	B	227	GLU	2.4
1	A	61	TYR	2.4
1	B	343	ASN	2.4
1	B	461	LYS	2.3
1	B	465	ASP	2.3
1	B	231	ILE	2.3
1	B	206	ILE	2.3
1	A	367	ASN	2.2
1	B	660	GLN	2.2
1	A	149	ASN	2.2
1	A	305	ILE	2.2
1	A	358	SER	2.2
1	A	304	GLU	2.2
1	B	399	TYR	2.2
1	A	28	ARG	2.2
1	B	306	ILE	2.1
1	B	409	VAL	2.1
1	A	119	VAL	2.1
1	A	211	ILE	2.0
1	A	707	LYS	2.0
1	B	346	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	2.0
1	B	141	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

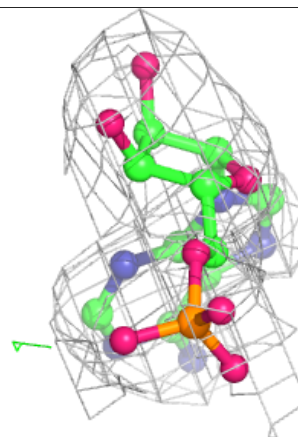
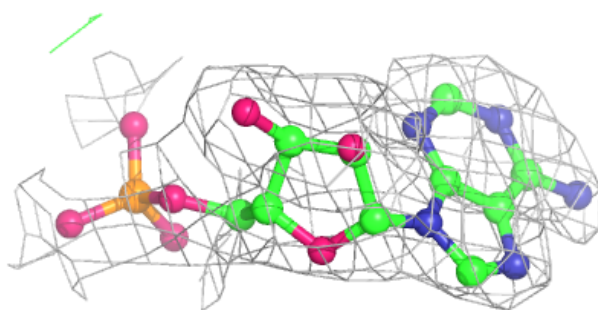
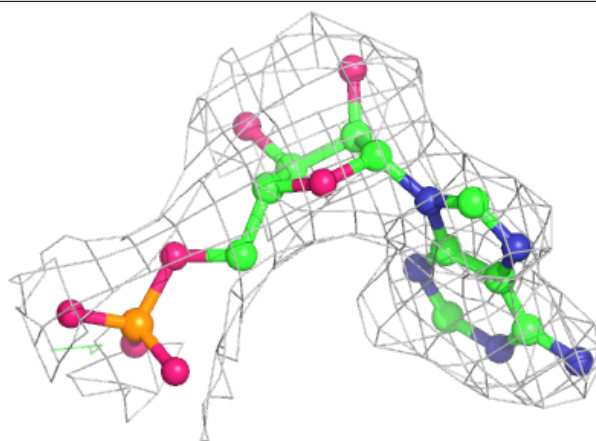
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	B	804	1/1	0.58	0.17	58,58,58,58	0
5	AMP	B	803	23/23	0.86	0.16	64,72,91,94	0
8	ACT	A	808	4/4	0.86	0.23	51,51,55,59	0
2	XTZ	A	801	29/29	0.89	0.23	14,31,90,94	0
8	ACT	B	802	4/4	0.89	0.22	37,43,44,46	0
2	XTZ	B	801	29/29	0.90	0.19	13,31,65,67	0
3	PH2	A	802	14/14	0.91	0.17	42,49,59,61	0
4	PO4	A	803	5/5	0.92	0.17	56,56,63,69	0
8	ACT	A	807	4/4	0.95	0.11	16,16,16,16	0
6	MG	A	805	1/1	0.95	0.15	15,15,15,15	0
8	ACT	B	806	4/4	0.95	0.16	17,17,18,18	0
5	AMP	A	804	23/23	0.96	0.19	24,31,49,53	0
4	PO4	A	810	5/5	0.97	0.21	63,65,69,75	0
4	PO4	A	809	5/5	0.97	0.22	55,56,57,61	0
8	ACT	B	807	4/4	0.98	0.17	28,28,28,29	0
7	CA	B	805	1/1	0.99	0.03	85,85,85,85	0
7	CA	A	806	1/1	0.99	0.09	18,18,18,18	0

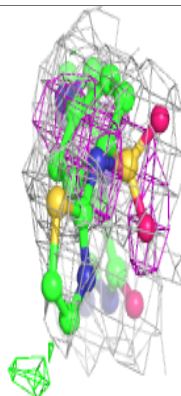
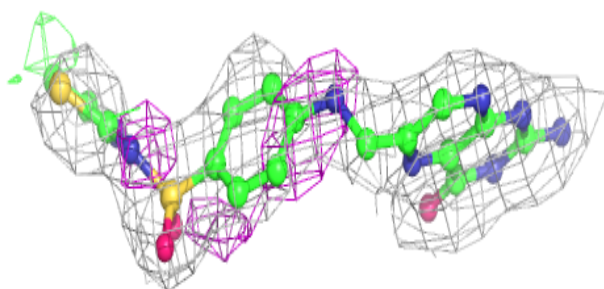
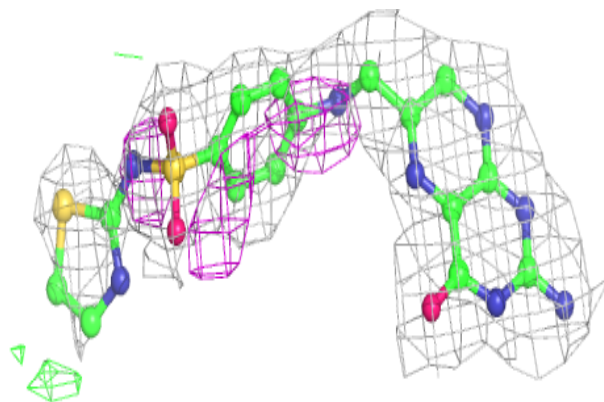
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP B 803:

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

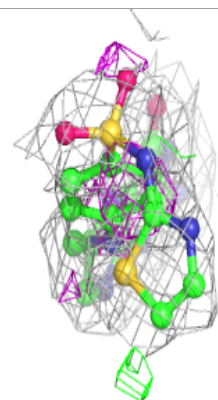
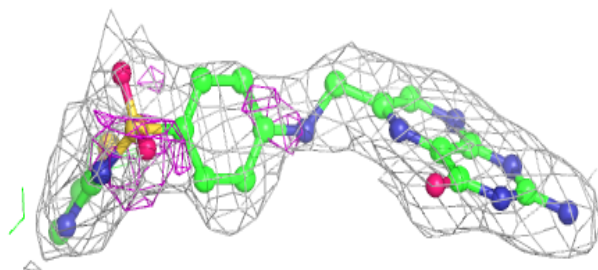
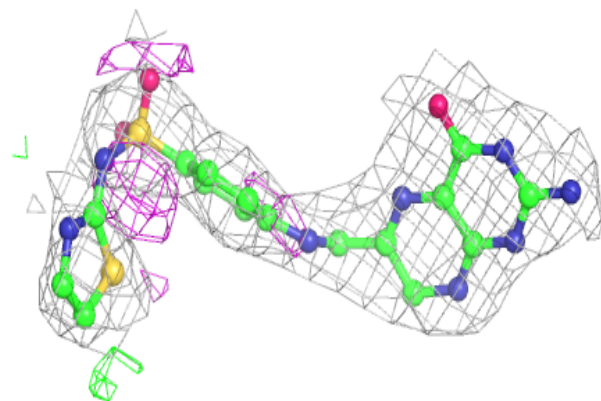
**Electron density around XTZ A 801:**

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

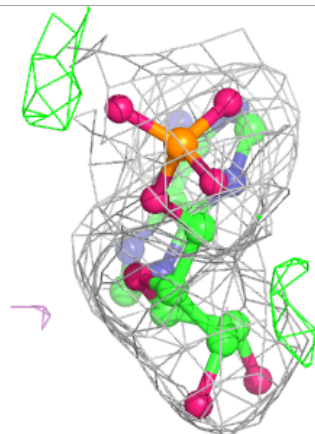
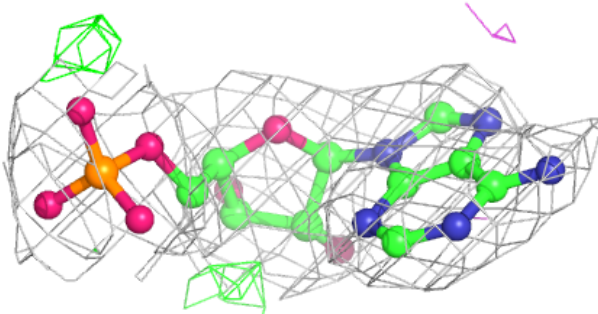
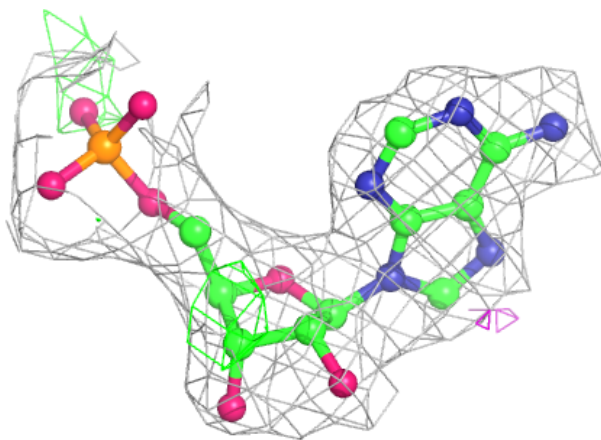


Electron density around XTZ B 801:

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

**Electron density around AMP A 804:**

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



6.5 Other polymers

There are no such residues in this entry.