



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:38 PM UTC

PDB ID : 6JWV / pdb_00006jwv
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS A437G with STZ-DHP
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

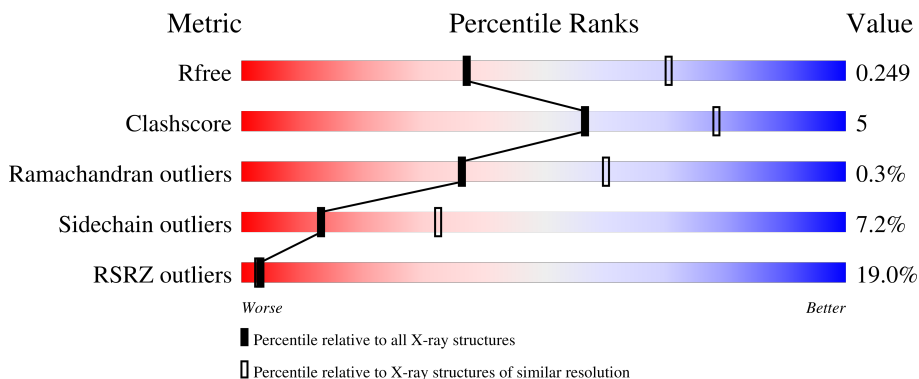
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	728	4% 61% 12% • 25%
1	B	728	24% 61% 11% • 26%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9403 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	543	Total	C	N	O	S	0	0	0
			4501	2897	741	841	22			
1	B	540	Total	C	N	O	S	0	0	0
			4454	2864	733	836	21			

There are 46 discrepancies between the modelled and reference sequences:

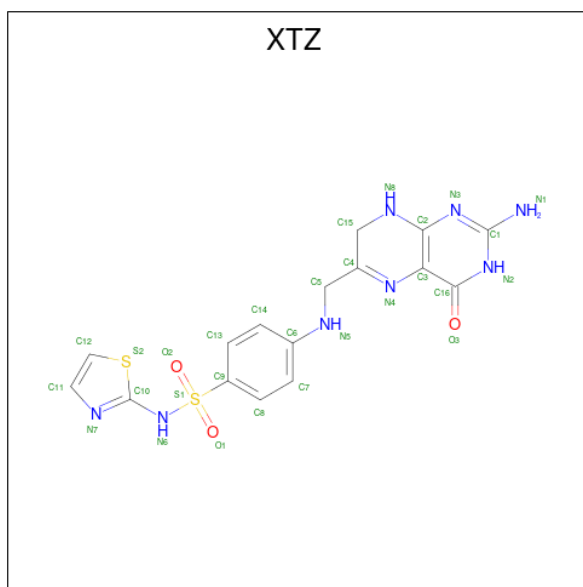
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression 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	437	GLY	ALA	engineered mutation	UNP Q25704

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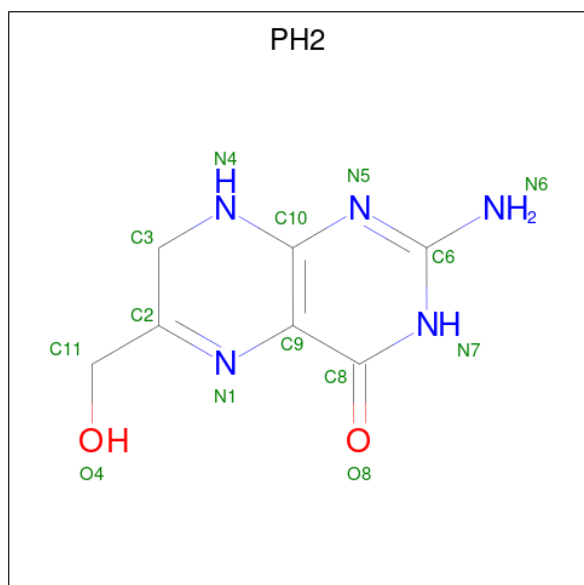
Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	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 (CCD ID: XTZ) (formula: C₁₆H₁₆N₈O₃S₂).



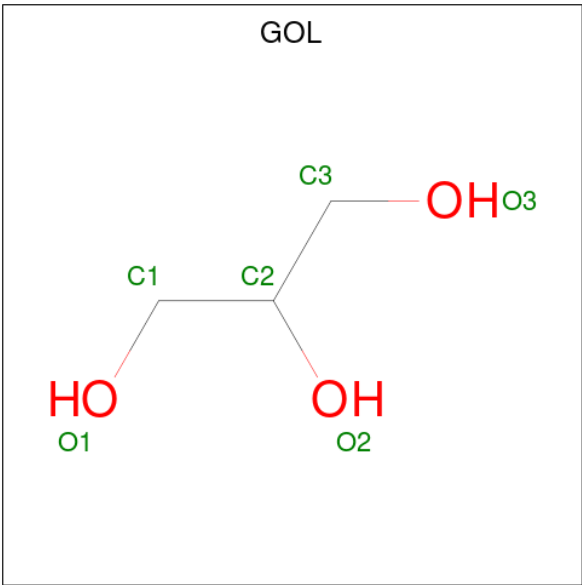
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	16	8	3	2		
2	B	1	Total	C	N	O	S	0	0
			29	16	8	3	2		

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



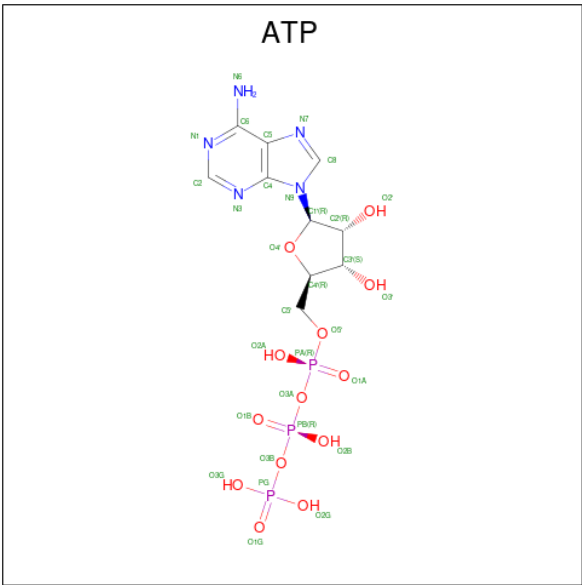
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	7	5	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

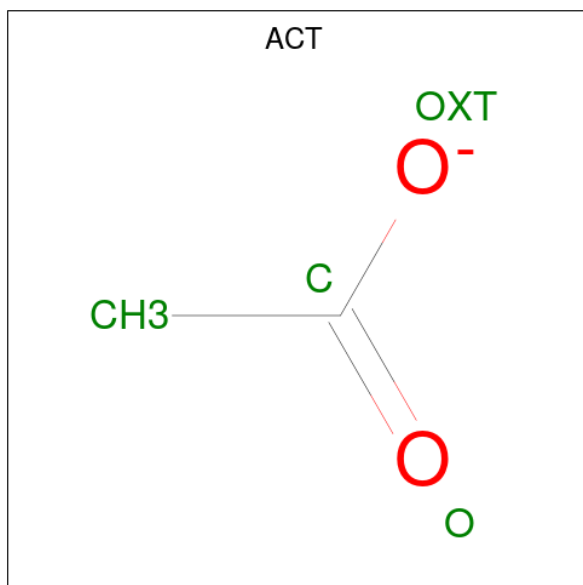
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0
6	B	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

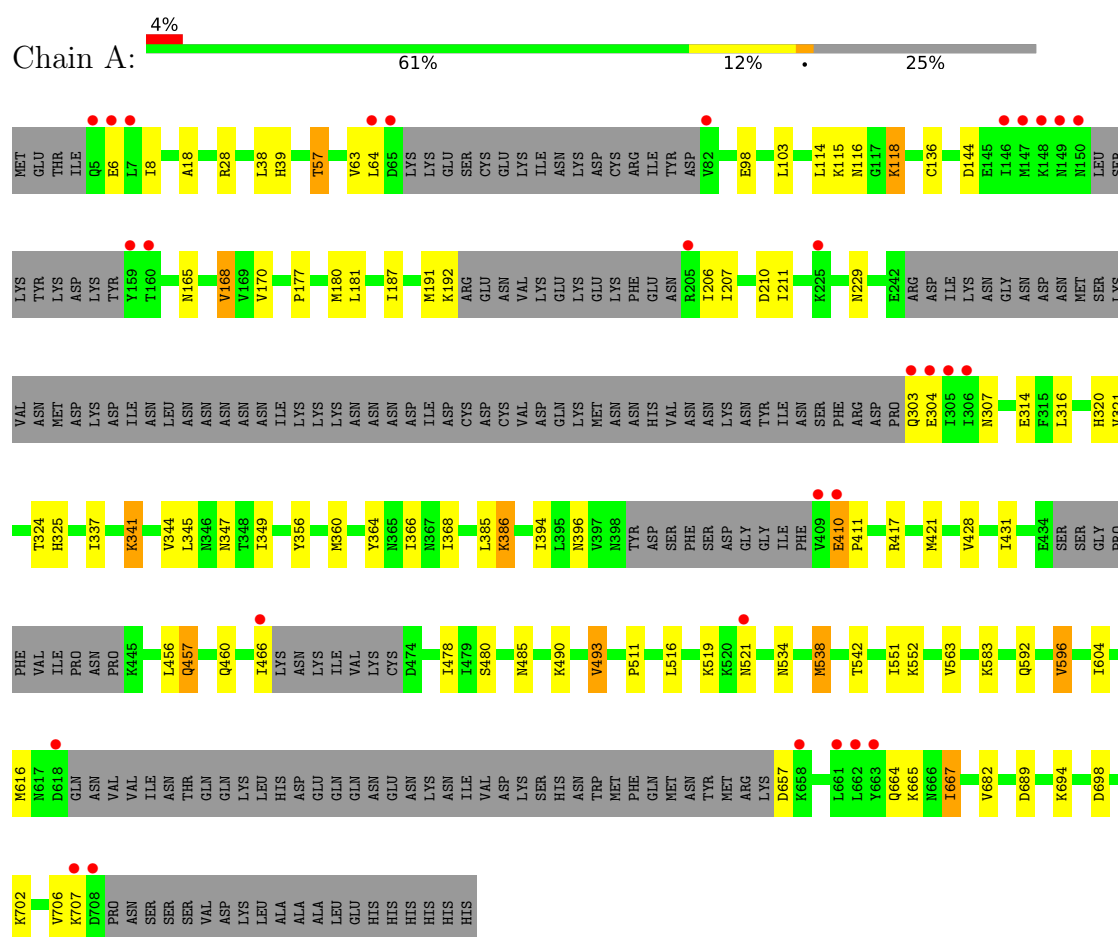
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	210	Total 210	O 210	0	0
9	B	102	Total 102	O 102	0	0

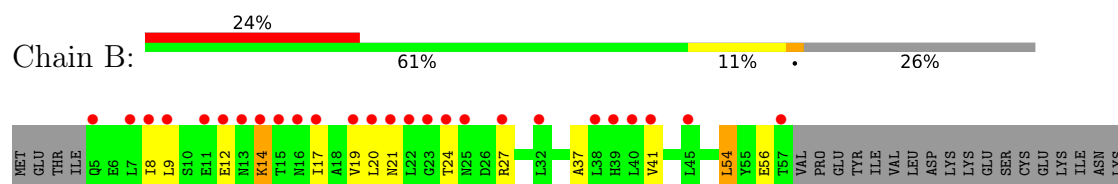
3 Residue-property plots

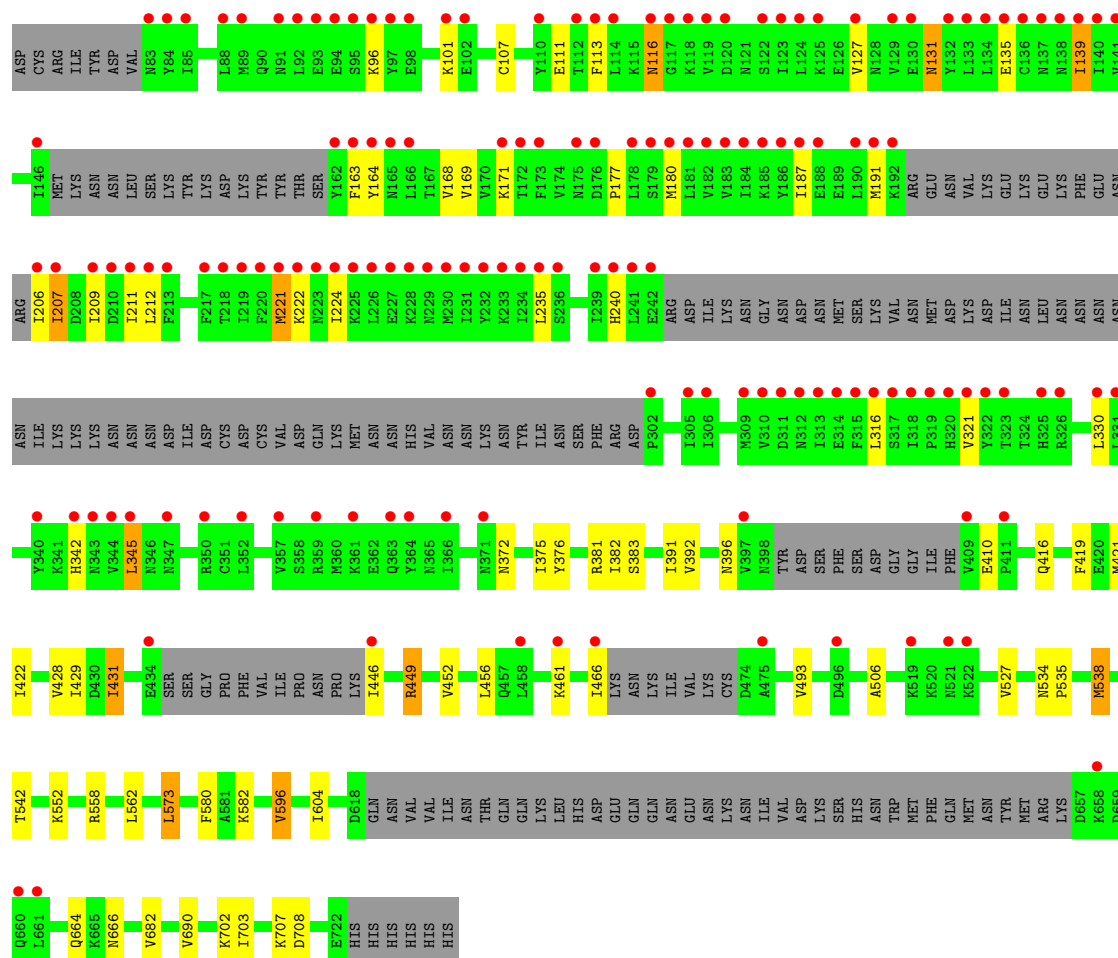
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase



- Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.89Å 136.72Å 138.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.70) 90.3 (30.00-2.71)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.14 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.206 , 0.257 0.202 , 0.249	Depositor DCC
R_{free} test set	4716 reflections (9.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9403	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PH2, GOL, ACT, MG, ATP, CA, XTZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	0/4568	0.99	1/6159 (0.0%)
1	B	0.63	0/4520	1.01	3/6095 (0.0%)
All	All	0.63	0/9088	1.00	4/12254 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	VAL	N-CA-C	6.13	116.86	111.90
1	B	708	ASP	CA-C-N	5.16	124.77	119.56
1	B	708	ASP	C-N-CA	5.16	124.77	119.56
1	A	538	MET	N-CA-C	5.08	116.50	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4501	0	4589	45	0
1	B	4454	0	4538	38	0
2	A	29	0	16	2	0
2	B	29	0	16	0	0
3	A	14	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	8	2	0
4	B	6	0	8	0	0
5	A	31	0	12	2	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	8	0	6	0	0
8	B	8	0	6	0	0
9	A	210	0	0	3	0
9	B	102	0	0	0	0
All	All	9403	0	9208	84	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 5.

All (84) 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:552:LYS:HD2	1:B:596:VAL:HG13	1.58	0.84
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.62	0.81
1:B:527:VAL:HG22	1:B:573:LEU:HD12	1.63	0.80
2:A:801:XTZ:H5	4:A:803:GOL:H11	1.65	0.79
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.66	0.77
1:A:57:THR:HG21	1:A:165:ASN:OD1	1.91	0.71
2:A:801:XTZ:N7	2:A:801:XTZ:H9	2.05	0.70
1:B:421:MET:HE3	1:B:429:ILE:HD12	1.74	0.70
1:B:375:ILE:HG21	1:B:382:ILE:HD13	1.75	0.69
1:A:394:ILE:O	1:A:421:MET:HE1	1.94	0.68
1:A:18:ALA:CB	1:A:180:MET:HE1	2.26	0.66
1:A:396:ASN:OD1	4:A:803:GOL:H2	1.97	0.64
1:B:56:GLU:O	1:B:372:ASN:HA	1.97	0.64
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.28	0.64
1:A:63:VAL:HG11	1:A:325:HIS:HB3	1.81	0.61
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.82	0.61
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.83	0.61
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.82	0.60
1:B:221:MET:HB3	1:B:224:ILE:HD11	1.82	0.60
1:A:6:GLU:HB3	1:A:8:ILE:HG22	1.83	0.60
1:B:419:PHE:HA	1:B:422:ILE:HD12	1.83	0.59
1:A:118:LYS:HD2	1:A:118:LYS:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:VAL:HG22	1:B:428:VAL:HB	1.85	0.58
1:A:485:ASN:HB2	9:A:1092:HOH:O	2.05	0.57
1:A:364:TYR:HB3	1:A:366:ILE:HG12	1.88	0.56
1:A:490:LYS:HD3	1:A:516:LEU:HD22	1.87	0.55
1:B:506:ALA:HB1	1:B:558:ARG:HG2	1.88	0.55
1:A:360:MET:HE2	1:A:368:ILE:HD13	1.89	0.55
1:B:187:ILE:HG22	1:B:191:MET:HE2	1.90	0.54
1:B:449:ARG:HH11	1:B:449:ARG:HG3	1.71	0.54
1:A:616:MET:HE3	1:A:665:LYS:HB3	1.89	0.53
1:B:376:TYR:O	1:B:383:SER:HB2	2.07	0.53
1:B:20:LEU:HB2	1:B:168:VAL:HG22	1.90	0.53
1:B:206:ILE:HG23	1:B:207:ILE:HG22	1.90	0.52
1:A:39:HIS:NE2	1:A:521:ASN:O	2.41	0.52
1:B:177:PRO:HB2	1:B:316:LEU:HD11	1.92	0.52
1:B:127:VAL:HB	1:B:131:ASN:HB3	1.92	0.51
1:A:534:ASN:O	1:A:538:MET:HB2	2.10	0.51
1:A:191:MET:HE3	1:A:207:ILE:HG21	1.94	0.50
1:A:181:LEU:HD21	5:A:804:ATP:H2'	1.92	0.50
1:A:187:ILE:HG22	1:A:191:MET:HE2	1.93	0.50
1:B:342:HIS:HB3	1:B:345:LEU:HG	1.93	0.50
1:B:431:ILE:HG21	1:B:456:LEU:HD21	1.93	0.49
1:B:375:ILE:HG12	1:B:382:ILE:HG23	1.95	0.49
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.44	0.48
1:A:592:GLN:HG2	1:B:703:ILE:O	2.14	0.47
1:A:385:LEU:HG	1:A:386:LYS:HD3	1.95	0.47
1:A:694:LYS:HE3	1:A:698:ASP:OD1	2.16	0.46
1:A:410:GLU:N	1:A:411:PRO:CD	2.78	0.46
1:A:667:ILE:HG13	1:A:689:ASP:OD2	2.16	0.46
1:A:493:VAL:HG13	1:A:519:LYS:HE3	1.97	0.46
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.98	0.46
1:B:107:CYS:SG	1:B:171:LYS:HD3	2.56	0.44
1:B:24:THR:HG23	1:B:164:TYR:HB2	1.99	0.44
1:B:391:ILE:HG21	1:B:690:VAL:HG13	1.99	0.44
1:A:428:VAL:HG22	1:A:478:ILE:HB	2.01	0.43
1:B:96:LYS:HG2	1:B:240:HIS:CD2	2.54	0.43
1:A:457:GLN:HG3	9:A:1029:HOH:O	2.19	0.43
1:A:114:LEU:HD21	1:A:337:ILE:HG22	2.01	0.42
1:A:604:ILE:HG12	1:A:682:VAL:HG11	2.01	0.42
1:A:39:HIS:NE2	1:A:521:ASN:C	2.77	0.42
1:B:180:MET:HE3	1:B:211:ILE:HG12	2.01	0.42
1:A:180:MET:HE3	1:A:211:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASP:HB3	1:A:320:HIS:CD2	2.54	0.42
1:A:38:LEU:HD21	1:A:168:VAL:HG11	2.01	0.42
1:A:118:LYS:H	1:A:118:LYS:CD	2.32	0.41
1:B:604:ILE:HG12	1:B:682:VAL:HG11	2.01	0.41
1:A:316:LEU:HA	5:A:804:ATP:C8	2.56	0.41
1:B:19:VAL:HG22	1:B:169:VAL:HG22	2.03	0.41
1:B:580:PHE:O	1:B:582:LYS:HD2	2.20	0.41
1:A:115:LYS:O	1:A:116:ASN:HB2	2.19	0.41
1:A:136:CYS:SG	9:A:961:HOH:O	2.62	0.41
1:B:17:ILE:HG13	1:B:113:PHE:HB2	2.03	0.41
1:A:324:THR:CG2	1:A:345:LEU:HD22	2.51	0.41
1:B:21:ASN:HB2	1:B:212:LEU:HD21	2.03	0.41
1:B:135:GLU:O	1:B:139:ILE:HG12	2.21	0.41
1:A:356:TYR:O	1:A:360:MET:HG2	2.21	0.41
1:A:341:LYS:HE2	1:A:345:LEU:O	2.21	0.40
1:A:385:LEU:O	1:A:386:LYS:HB2	2.21	0.40
1:A:38:LEU:CD2	1:A:168:VAL:HG11	2.52	0.40
1:B:12:GLU:O	1:B:14:LYS:HE3	2.21	0.40
1:B:37:ALA:O	1:B:41:VAL:HG23	2.22	0.40
1:B:116:ASN:HD22	1:B:116:ASN:HA	1.64	0.40
1:B:21:ASN:O	1:B:209:ILE:HA	2.21	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	525/728 (72%)	502 (96%)	22 (4%)	1 (0%)	43	68
1	B	522/728 (72%)	496 (95%)	24 (5%)	2 (0%)	30	54
All	All	1047/1456 (72%)	998 (95%)	46 (4%)	3 (0%)	36	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	LYS
1	B	538	MET
1	A	410	GLU

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	518/696 (74%)	480 (93%)	38 (7%)	13	32
1	B	512/696 (74%)	476 (93%)	36 (7%)	14	34
All	All	1030/1392 (74%)	956 (93%)	74 (7%)	13	32

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	57	THR
1	A	64	LEU
1	A	98	GLU
1	A	118	LYS
1	A	144	ASP
1	A	168	VAL
1	A	170	VAL
1	A	192	LYS
1	A	206	ILE
1	A	229	ASN
1	A	303	GLN
1	A	304	GLU
1	A	307	ASN
1	A	314	GLU
1	A	321	VAL
1	A	341	LYS
1	A	344	VAL
1	A	347	ASN
1	A	349	ILE

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Mol	Chain	Res	Type
1	A	386	LYS
1	A	417	ARG
1	A	457	GLN
1	A	460	GLN
1	A	466	ILE
1	A	480	SER
1	A	493	VAL
1	A	542	THR
1	A	551	ILE
1	A	563	VAL
1	A	583	LYS
1	A	596	VAL
1	A	657	ASP
1	A	664	GLN
1	A	667	ILE
1	A	702	LYS
1	A	706	VAL
1	A	707	LYS
1	B	8	ILE
1	B	9	LEU
1	B	14	LYS
1	B	27	ARG
1	B	54	LEU
1	B	101	LYS
1	B	111	GLU
1	B	116	ASN
1	B	131	ASN
1	B	139	ILE
1	B	163	PHE
1	B	207	ILE
1	B	221	MET
1	B	235	LEU
1	B	321	VAL
1	B	330	LEU
1	B	345	LEU
1	B	381	ARG
1	B	396	ASN
1	B	410	GLU
1	B	416	GLN
1	B	431	ILE
1	B	446	ILE
1	B	449	ARG

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Mol	Chain	Res	Type
1	B	461	LYS
1	B	466	ILE
1	B	493	VAL
1	B	538	MET
1	B	542	THR
1	B	562	LEU
1	B	573	LEU
1	B	596	VAL
1	B	664	GLN
1	B	666	ASN
1	B	702	LYS
1	B	707	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	21	ASN
1	A	131	ASN
1	A	138	ASN
1	A	143	ASN
1	A	149	ASN
1	A	307	ASN
1	A	347	ASN
1	A	363	GLN
1	A	460	GLN
1	A	485	ASN
1	A	614	HIS
1	B	25	ASN
1	B	116	ASN
1	B	165	ASN
1	B	240	HIS
1	B	303	GLN
1	B	307	ASN
1	B	334	ASN
1	B	367	ASN
1	B	416	GLN
1	B	495	ASN
1	B	710	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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$
8	ACT	A	807	-	3,3,3	0.91	0	3,3,3	0.24	0
2	XTZ	A	801	-	29,32,32	2.30	5 (17%)	35,46,46	2.67	10 (28%)
8	ACT	A	808	-	3,3,3	0.80	0	3,3,3	0.93	0
2	XTZ	B	801	-	29,32,32	2.29	4 (13%)	35,46,46	2.12	9 (25%)
4	GOL	A	803	-	5,5,5	0.57	0	5,5,5	0.87	0
3	PH2	A	802	6	12,15,15	1.54	3 (25%)	11,21,21	1.94	3 (27%)
5	ATP	A	804	6	32,33,33	1.43	4 (12%)	48,52,52	1.86	9 (18%)
8	ACT	B	804	-	3,3,3	0.81	0	3,3,3	0.81	0
8	ACT	B	805	-	3,3,3	0.86	0	3,3,3	0.79	0
4	GOL	B	802	-	5,5,5	0.41	0	5,5,5	0.45	0

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	XTZ	A	801	-	-	7/14/25/25	0/4/4/4
2	XTZ	B	801	-	-	7/14/25/25	0/4/4/4
4	GOL	A	803	-	-	2/4/4/4	-
3	PH2	A	802	6	-	0/0/11/11	0/2/2/2
5	ATP	A	804	6	-	4/22/38/38	0/3/3/3
4	GOL	B	802	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	XTZ	C9-S1	-9.66	1.61	1.76
2	A	801	XTZ	C9-S1	-9.65	1.61	1.76
5	A	804	ATP	C5-C4	4.59	1.47	1.39
2	A	801	XTZ	C3-C2	3.87	1.49	1.40
3	A	802	PH2	C9-C10	3.41	1.48	1.40
2	B	801	XTZ	C3-C2	3.14	1.47	1.40
2	B	801	XTZ	C10-N7	3.10	1.36	1.31
2	A	801	XTZ	C10-N7	3.09	1.36	1.31
5	A	804	ATP	C5-C6	2.82	1.48	1.41
2	B	801	XTZ	C11-C12	2.81	1.40	1.34
5	A	804	ATP	PB-O3B	2.70	1.62	1.59
2	A	801	XTZ	C11-C12	2.69	1.40	1.34
5	A	804	ATP	C5-N7	-2.44	1.34	1.39
2	A	801	XTZ	C16-N2	-2.31	1.34	1.38
3	A	802	PH2	C8-N7	-2.26	1.34	1.38
3	A	802	PH2	C3-C2	2.08	1.52	1.49

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	XTZ	O2-S1-O1	-11.10	106.04	119.52
2	B	801	XTZ	O2-S1-O1	-8.19	109.58	119.52
5	A	804	ATP	C5-C4-N3	-6.16	118.24	126.72
5	A	804	ATP	N3-C4-N9	5.09	135.82	127.17
3	A	802	PH2	C6-N5-C10	4.63	121.53	113.36
2	A	801	XTZ	O1-S1-C9	4.59	113.78	107.98
5	A	804	ATP	C2-N3-C4	4.20	122.09	111.83
2	B	801	XTZ	C1-N3-C2	4.19	120.76	113.36
2	A	801	XTZ	C1-N3-C2	4.08	120.56	113.36
5	A	804	ATP	N3-C2-N1	-4.01	122.50	128.58
2	B	801	XTZ	C9-S1-N6	3.91	112.30	106.06
2	A	801	XTZ	N6-C10-N7	3.64	125.32	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	XTZ	S2-C10-N6	-3.54	123.69	129.14
5	A	804	ATP	C4-C5-N7	-3.48	106.61	110.58
2	B	801	XTZ	C10-N6-S1	3.24	128.18	121.90
2	B	801	XTZ	C3-N4-C4	3.05	122.30	116.24
3	A	802	PH2	C9-N1-C2	2.90	121.99	116.24
2	A	801	XTZ	C10-N6-S1	2.78	127.28	121.90
5	A	804	ATP	C5-N7-C8	2.72	107.72	103.45
2	A	801	XTZ	C12-S2-C10	2.70	93.16	90.07
2	A	801	XTZ	C11-C12-S2	-2.67	106.86	110.27
2	A	801	XTZ	C8-C9-S1	2.61	122.63	119.76
2	B	801	XTZ	O3-C16-C3	-2.47	120.02	126.53
5	A	804	ATP	C4-N9-C8	2.46	108.32	105.74
5	A	804	ATP	C6-C5-N7	2.26	136.45	132.09
5	A	804	ATP	C2-N1-C6	2.24	122.40	118.73
2	B	801	XTZ	C3-C16-N2	2.18	118.79	113.25
2	A	801	XTZ	C14-C13-C9	2.16	121.54	119.44
2	B	801	XTZ	C11-C12-S2	-2.14	107.54	110.27
3	A	802	PH2	C9-C8-N7	2.10	118.61	113.25
2	B	801	XTZ	C12-S2-C10	2.09	92.47	90.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	XTZ	S2-C10-N6-S1
2	A	801	XTZ	N7-C10-N6-S1
2	B	801	XTZ	C10-N6-S1-O1
5	A	804	ATP	C5'-O5'-PA-O2A
4	A	803	GOL	C1-C2-C3-O3
2	B	801	XTZ	C7-C6-N5-C5
2	A	801	XTZ	C7-C6-N5-C5
2	B	801	XTZ	C14-C6-N5-C5
2	A	801	XTZ	C14-C6-N5-C5
4	A	803	GOL	O2-C2-C3-O3
2	B	801	XTZ	C10-N6-S1-C9
2	B	801	XTZ	C4-C5-N5-C6
5	A	804	ATP	C5'-O5'-PA-O1A
5	A	804	ATP	C5'-O5'-PA-O3A
2	A	801	XTZ	C13-C9-S1-O1
2	A	801	XTZ	C8-C9-S1-O1
5	A	804	ATP	O4'-C4'-C5'-O5'
2	B	801	XTZ	C8-C9-S1-O2

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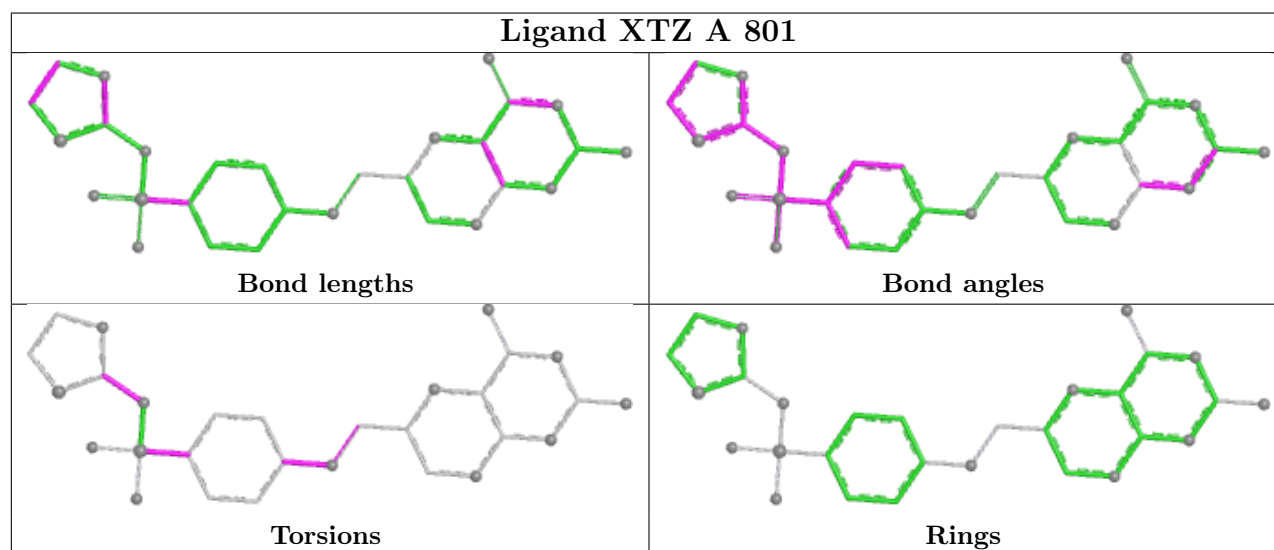
Mol	Chain	Res	Type	Atoms
2	A	801	XTZ	C4-C5-N5-C6
2	B	801	XTZ	C13-C9-S1-O2

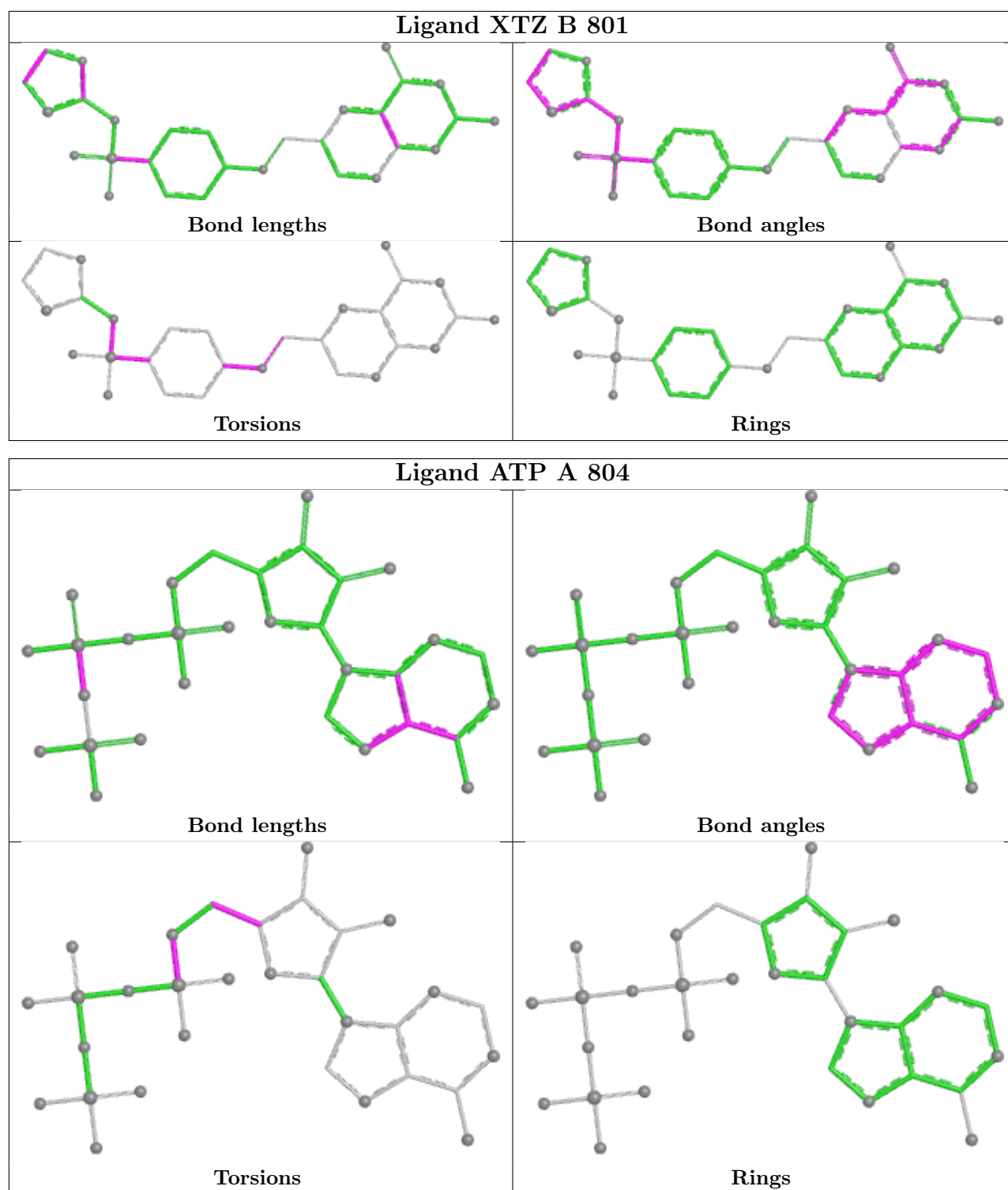
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	XTZ	2	0
4	A	803	GOL	2	0
5	A	804	ATP	2	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 ⓘ

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	543/728 (74%)	-0.01	30 (5%) 30 27	7, 25, 84, 120	0
1	B	540/728 (74%)	1.21	176 (32%) 1 1	8, 58, 120, 120	0
All	All	1083/1456 (74%)	0.60	206 (19%) 3 3	7, 34, 117, 120	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	ILE	6.6
1	B	187	ILE	6.4
1	B	315	PHE	6.2
1	A	82	VAL	6.2
1	B	220	PHE	6.1
1	B	302	PRO	5.8
1	B	219	ILE	5.8
1	B	146	ILE	5.5
1	B	226	LEU	5.5
1	B	9	LEU	5.4
1	A	466	ILE	5.3
1	B	231	ILE	5.3
1	B	316	LEU	5.2
1	B	7	LEU	5.2
1	B	134	LEU	5.2
1	B	221	MET	5.1
1	B	409	VAL	4.9
1	A	150	ASN	4.9
1	A	159	TYR	4.7
1	B	466	ILE	4.7
1	B	222	LYS	4.7
1	A	409	VAL	4.6
1	B	322	TYR	4.6
1	B	139	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	178	LEU	4.6
1	B	206	ILE	4.6
1	B	129	VAL	4.5
1	A	64	LEU	4.5
1	B	207	ILE	4.5
1	B	84	TYR	4.5
1	B	191	MET	4.4
1	B	123	ILE	4.4
1	B	313	ILE	4.3
1	B	446	ILE	4.3
1	A	160	THR	4.3
1	B	234	ILE	4.3
1	B	318	ILE	4.3
1	B	241	LEU	4.2
1	B	310	VAL	4.2
1	B	235	LEU	4.1
1	B	321	VAL	4.0
1	B	133	LEU	4.0
1	B	317	SER	4.0
1	B	132	TYR	4.0
1	B	305	ILE	3.9
1	B	25	ASN	3.8
1	B	97	TYR	3.8
1	B	183	VAL	3.8
1	B	21	ASN	3.8
1	B	140	ILE	3.8
1	B	85	ILE	3.7
1	B	163	PHE	3.7
1	B	182	VAL	3.7
1	B	124	LEU	3.6
1	B	211	ILE	3.6
1	B	136	CYS	3.6
1	B	45	LEU	3.5
1	A	147	MET	3.5
1	B	323	THR	3.5
1	B	357	VAL	3.5
1	B	176	ASP	3.4
1	B	344	VAL	3.4
1	B	224	ILE	3.4
1	B	229	ASN	3.4
1	B	122	SER	3.4
1	B	233	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	240	HIS	3.4
1	B	239	ILE	3.4
1	B	162	TYR	3.4
1	B	96	LYS	3.3
1	B	236	SER	3.3
1	B	40	LEU	3.3
1	B	319	PRO	3.3
1	B	306	ILE	3.3
1	B	230	MET	3.2
1	B	340	TYR	3.2
1	B	113	PHE	3.2
1	B	127	VAL	3.2
1	B	213	PHE	3.2
1	B	175	ASN	3.1
1	B	218	THR	3.1
1	B	141	VAL	3.1
1	A	148	LYS	3.1
1	B	658	LYS	3.1
1	B	24	THR	3.1
1	B	165	ASN	3.1
1	B	352	LEU	3.1
1	B	125	LYS	3.1
1	B	164	TYR	3.0
1	B	186	TYR	3.0
1	A	65	ASP	3.0
1	B	180	MET	3.0
1	B	326	ARG	3.0
1	B	190	LEU	3.0
1	B	363	GLN	3.0
1	A	7	LEU	3.0
1	B	519	LYS	3.0
1	B	364	TYR	3.0
1	B	179	SER	2.9
1	B	311	ASP	2.9
1	A	708	ASP	2.9
1	B	17	ILE	2.9
1	B	434	GLU	2.9
1	B	118	LYS	2.9
1	B	16	ASN	2.8
1	A	5	GLN	2.8
1	B	475	ALA	2.8
1	B	309	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	225	LYS	2.8
1	A	146	ILE	2.8
1	B	212	LEU	2.8
1	B	314	GLU	2.8
1	B	5	GLN	2.7
1	B	366	ILE	2.7
1	B	32	LEU	2.7
1	B	95	SER	2.7
1	B	325	HIS	2.7
1	A	205	ARG	2.7
1	B	192	LYS	2.7
1	B	185	LYS	2.7
1	B	181	LEU	2.7
1	B	320	HIS	2.7
1	B	137	ASN	2.7
1	B	210	ASP	2.6
1	B	88	LEU	2.6
1	A	6	GLU	2.6
1	B	13	ASN	2.6
1	A	303	GLN	2.6
1	B	92	LEU	2.6
1	B	112	THR	2.5
1	B	114	LEU	2.5
1	B	458	LEU	2.5
1	B	39	HIS	2.5
1	A	305	ILE	2.5
1	B	119	VAL	2.5
1	B	217	PHE	2.5
1	B	15	THR	2.5
1	B	22	LEU	2.5
1	B	93	GLU	2.5
1	B	138	ASN	2.5
1	B	228	LYS	2.5
1	B	166	LEU	2.5
1	B	102	GLU	2.5
1	B	135	GLU	2.5
1	B	57	THR	2.4
1	B	209	ILE	2.4
1	A	618	ASP	2.4
1	B	522	LYS	2.4
1	B	116	ASN	2.4
1	B	331	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	38	LEU	2.4
1	B	521	ASN	2.4
1	B	496	ASP	2.4
1	B	345	LEU	2.4
1	B	330	LEU	2.3
1	B	23	GLY	2.3
1	B	173	PHE	2.3
1	A	663	TYR	2.3
1	B	94	GLU	2.3
1	B	171	LYS	2.3
1	B	27	ARG	2.3
1	A	304	GLU	2.3
1	B	242	GLU	2.3
1	A	149	ASN	2.3
1	B	223	ASN	2.3
1	B	14	LYS	2.2
1	B	101	LYS	2.2
1	B	117	GLY	2.2
1	B	19	VAL	2.2
1	A	306	ILE	2.2
1	B	361	LYS	2.2
1	B	89	MET	2.2
1	B	232	TYR	2.2
1	B	83	ASN	2.2
1	B	397	VAL	2.2
1	B	359	ARG	2.2
1	B	110	TYR	2.2
1	B	660	GLN	2.2
1	A	661	LEU	2.2
1	A	707	LYS	2.2
1	B	184	ILE	2.2
1	B	98	GLU	2.2
1	B	91	ASN	2.2
1	A	662	LEU	2.2
1	A	410	GLU	2.1
1	A	658	LYS	2.1
1	A	521	ASN	2.1
1	B	343	ASN	2.1
1	B	371	ASN	2.1
1	B	120	ASP	2.1
1	B	188	GLU	2.1
1	B	20	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	312	ASN	2.1
1	B	347	ASN	2.1
1	B	342	HIS	2.1
1	A	225	LYS	2.1
1	B	11	GLU	2.0
1	B	12	GLU	2.0
1	B	130	GLU	2.0
1	B	227	GLU	2.0
1	B	350	ARG	2.0
1	B	411	PRO	2.0
1	B	461	LYS	2.0
1	B	172	THR	2.0
1	B	661	LEU	2.0
1	B	41	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 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(Å ²)	Q<0.9
8	ACT	A	808	4/4	0.79	0.18	60,60,60,61	0
4	GOL	B	802	6/6	0.82	0.20	32,39,43,45	0
4	GOL	A	803	6/6	0.84	0.18	28,30,35,36	0
8	ACT	B	805	4/4	0.84	0.16	37,37,38,38	0
5	ATP	A	804	31/31	0.86	0.11	31,52,86,88	0
2	XTZ	A	801	29/29	0.91	0.16	14,36,100,104	0
7	CA	B	803	1/1	0.91	0.09	83,83,83,83	0
6	MG	B	806	1/1	0.93	0.17	74,74,74,74	0
8	ACT	A	807	4/4	0.93	0.13	26,26,26,27	0

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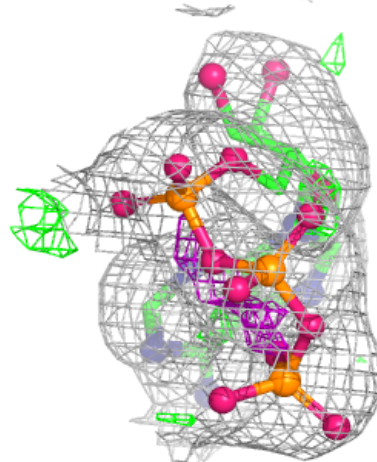
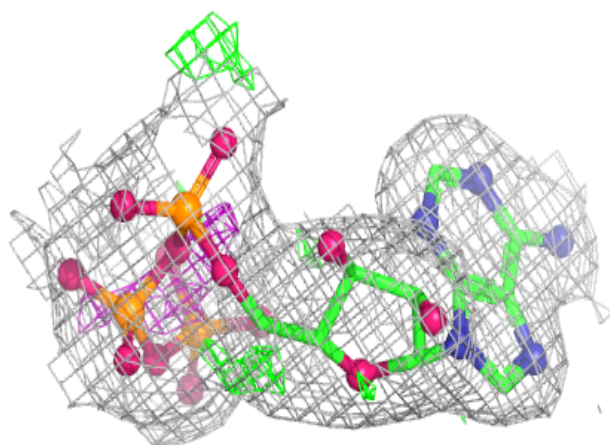
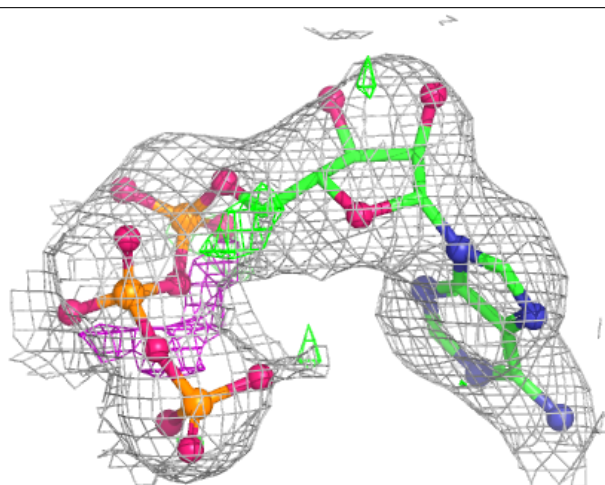
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	809	1/1	0.95	0.11	55,55,55,55	0
3	PH2	A	802	14/14	0.95	0.08	31,34,35,36	0
2	XTZ	B	801	29/29	0.95	0.10	13,25,48,50	0
6	MG	A	805	1/1	0.96	0.06	15,15,15,15	0
8	ACT	B	804	4/4	0.98	0.05	14,14,14,15	0
7	CA	A	806	1/1	0.99	0.02	19,19,19,19	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.

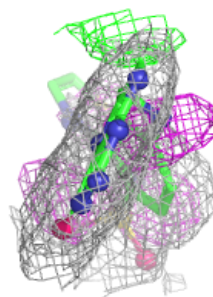
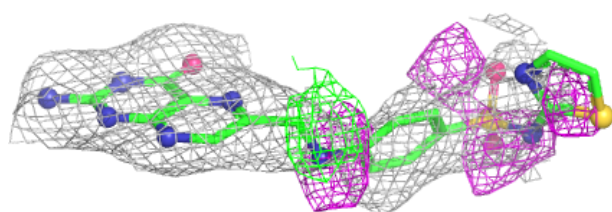
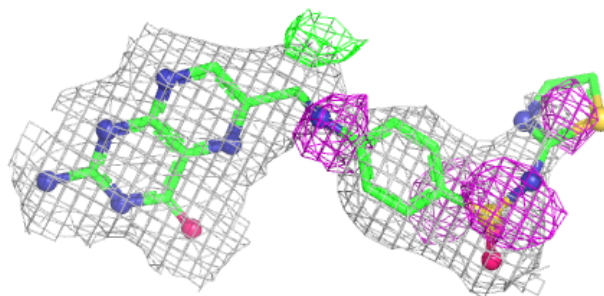
Electron density around ATP A 804:

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

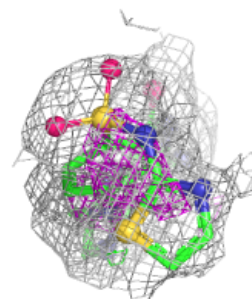
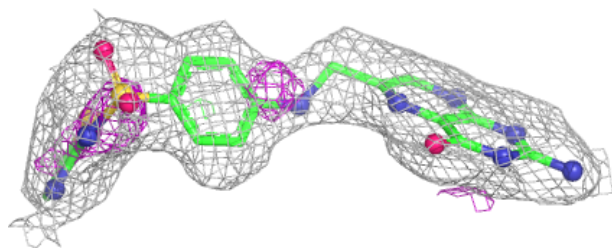
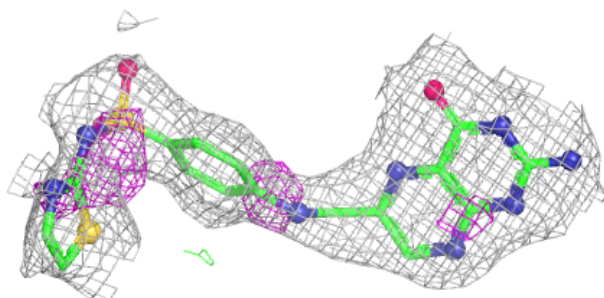


Electron density around XTZ A 801:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.