Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 10:22 pm BST

PDB ID	:	4WOE
Title	:	The duplicated taurocyamine kinase from Schistosoma mansoni with bound transition state analog (TSA) components
Authors	:	Merceron, R.; Awama, A.; Montserret, R.; Marcillat, O.; Gouet, P.
Deposited on	:	2014-10-15
Resolution	:	2.30 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 (i) symbol.

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

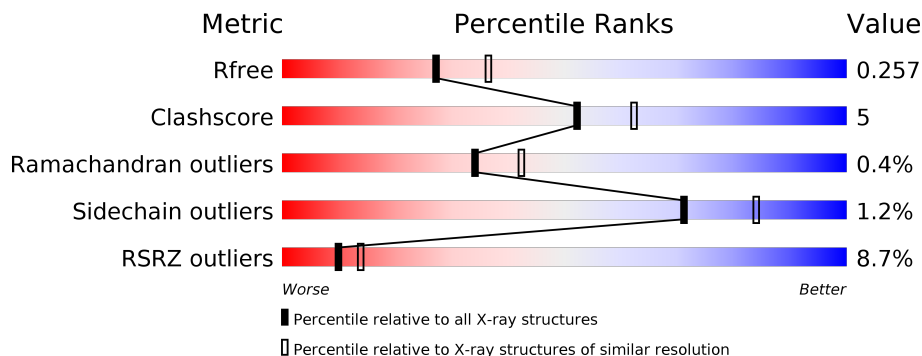|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		1.2%
RSRZ outliers		8.7%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	716	10% / 85% / 13% / •
1	B	716	7% / 89% / 8% / •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12052 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 Taurocyamine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	716	Total	C	N	O	S	0	0	0
			5648	3570	985	1064	29			
1	B	698	Total	C	N	O	S	0	0	0
			5506	3485	961	1031	29			

There are 8 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	ALA	engineered mutation	UNP P16641
A	235	GLY	ASP	engineered mutation	UNP P16641
A	237	THR	ILE	engineered mutation	UNP P16641
A	493	GLY	ASP	engineered mutation	UNP P16641
B	11	VAL	ALA	engineered mutation	UNP P16641
B	235	GLY	ASP	engineered mutation	UNP P16641
B	237	THR	ILE	engineered mutation	UNP P16641
B	493	GLY	ASP	engineered mutation	UNP P16641

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP

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

- Molecule 3 is Taurocyamine (three-letter code: 3S5) (formula: $C_3H_9N_3O_3S$).

3S5

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			10	3	3	3	1		
3	A	1	Total	C	N	O	S	0	0
			10	3	3	3	1		
3	B	1	Total	C	N	O	S	0	0
			10	3	3	3	1		
3	B	1	Total	C	N	O	S	0	0
			10	3	3	3	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO_3).
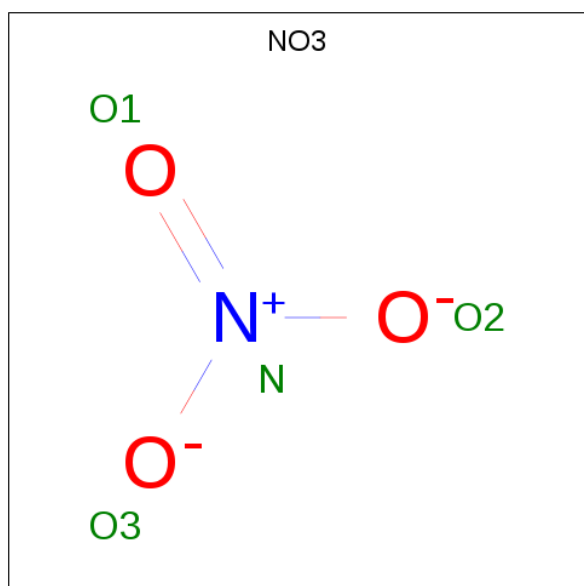
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	348	Total 348	O 348	0	0
6	B	391	Total 391	O 391	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Taurocyamine kinase
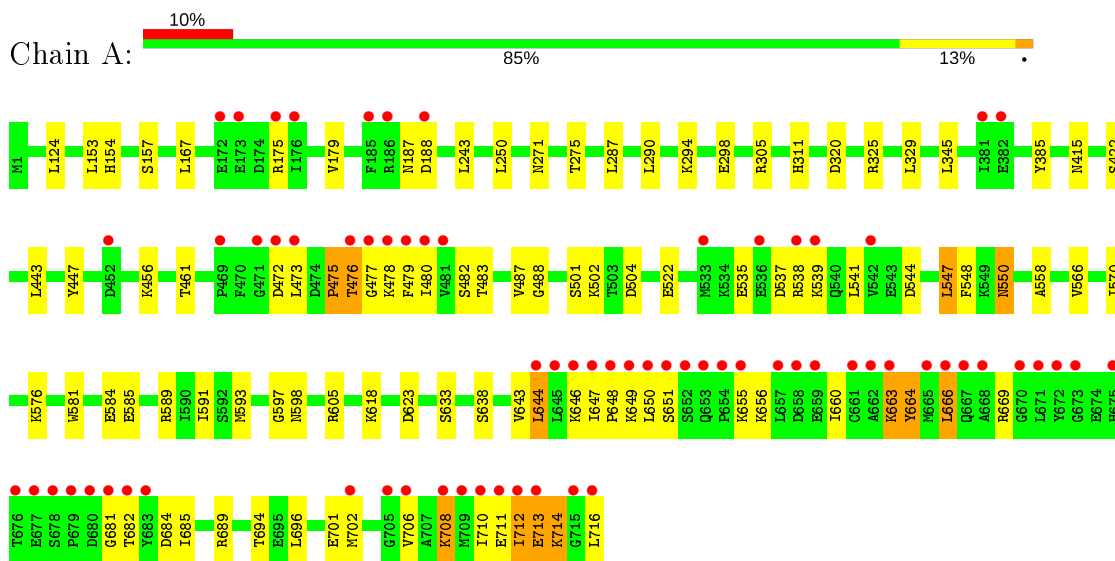
- Molecule 1: Taurocyamine kinase
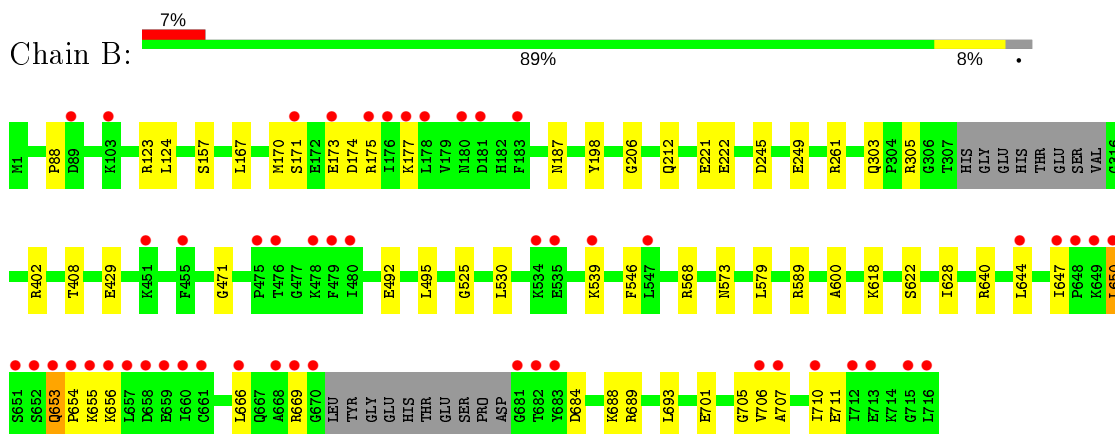
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.69Å 122.22Å 63.06Å 90.00° 108.06° 90.00°	Depositor
Resolution (Å)	46.74 – 2.30 46.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.74-2.30) 98.6 (46.74-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.185 , 0.256 0.188 , 0.257	Depositor DCC
R_{free} test set	3396 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12052	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1742e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 3S5, MG, ADP, NO3

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	0.45	1/5764 (0.0%)	0.61	5/7777 (0.1%)
1	B	0.43	0/5615	0.56	0/7570
All	All	0.44	1/11379 (0.0%)	0.59	5/15347 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	TYR	CD1-CE1	-6.94	1.28	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	LEU	CA-CB-CG	6.58	130.43	115.30
1	A	663	LYS	CD-CE-NZ	-6.14	97.58	111.70
1	A	547	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	666	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	664	TYR	CZ-CE2-CD2	-5.12	115.19	119.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	475	PRO	Peptide
1	A	714	LYS	Peptide

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	5648	0	5638	86	0
1	B	5506	0	5521	37	0
2	A	54	0	24	2	0
2	B	54	0	24	3	0
3	A	20	0	16	1	0
3	B	20	0	16	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	8	0	0	0	0
6	A	348	0	0	5	0
6	B	391	0	0	3	0
All	All	12052	0	11239	123	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 (123) 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:713:GLU:HG2	1:A:714:LYS:H	1.18	1.04
1:A:713:GLU:HG2	1:A:714:LYS:N	1.85	0.90
1:A:666:LEU:HD13	1:A:685:ILE:HD11	1.58	0.86
1:A:664:TYR:OH	1:A:708:LYS:NZ	2.13	0.81
1:A:547:LEU:HD13	1:A:570:ILE:HD11	1.63	0.80
1:A:689:ARG:NH1	1:A:701:GLU:OE2	2.24	0.71
1:B:653:GLN:HB3	1:B:656:LYS:HE3	1.73	0.69
1:A:646:LYS:HG2	1:A:682:THR:HG22	1.76	0.68
1:B:303:GLN:OE1	1:B:305:ARG:NH2	2.26	0.67
1:B:654:PRO:C	1:B:655:LYS:HD2	2.15	0.67
1:A:473:LEU:HD22	1:A:475:PRO:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ILE:O	1:A:649:LYS:HA	1.96	0.65
1:B:650:LEU:HG	1:B:653:GLN:HE22	1.61	0.64
1:B:123:ARG:HD3	2:B:801:ADP:O3B	1.99	0.63
1:A:710:ILE:O	1:A:713:GLU:HB3	1.98	0.62
1:A:650:LEU:HD11	1:A:656:LYS:HB3	1.80	0.62
1:A:660:ILE:HA	1:A:663:LYS:HD3	1.82	0.61
1:A:502:LYS:HE3	1:A:566:VAL:HG21	1.81	0.61
1:A:649:LYS:HE3	1:A:681:GLY:HA3	1.82	0.61
1:B:589:ARG:NH2	6:B:1213:HOH:O	2.34	0.61
1:A:656:LYS:O	1:A:660:ILE:HG12	2.01	0.60
1:B:669:ARG:HG2	1:B:684:ASP:HB3	1.83	0.60
1:A:650:LEU:HD22	1:A:712:ILE:HD11	1.83	0.59
1:A:305:ARG:HB2	1:A:320:ASP:HB3	1.85	0.59
1:A:480:ILE:HG23	1:A:643:VAL:HB	1.84	0.59
1:A:656:LYS:NZ	1:A:660:ILE:HD11	2.19	0.58
1:A:538:ARG:HG3	1:A:547:LEU:HD21	1.85	0.57
1:A:649:LYS:HG2	1:A:651:SER:OG	2.05	0.57
1:A:537:ASP:O	1:A:541:LEU:HD13	2.07	0.55
1:A:663:LYS:HE2	1:A:664:TYR:CE1	2.41	0.55
1:A:479:PHE:CZ	1:A:713:GLU:HB2	2.42	0.55
1:B:640:ARG:NH2	1:B:684:ASP:OD1	2.40	0.55
1:A:124:LEU:HG	1:A:243:LEU:HD21	1.88	0.54
1:A:548:PHE:CD2	1:A:584:GLU:HG3	2.42	0.54
1:A:548:PHE:CG	1:A:584:GLU:HG3	2.42	0.54
1:A:154:HIS:HE1	6:A:1151:HOH:O	1.90	0.53
1:B:402:ARG:HG2	1:B:408:THR:HG22	1.90	0.53
1:A:456:LYS:NZ	6:A:903:HOH:O	2.41	0.53
1:B:689:ARG:NH1	1:B:701:GLU:OE2	2.41	0.53
1:A:663:LYS:HG3	1:A:664:TYR:CD1	2.43	0.53
1:B:123:ARG:NH1	2:B:801:ADP:O1B	2.42	0.53
1:B:171:SER:HB3	1:B:173:GLU:HG3	1.91	0.52
1:B:170:MET:HB3	1:B:175:ARG:NH2	2.24	0.52
1:B:471:GLY:HA2	1:B:600:ALA:HB2	1.91	0.52
1:A:663:LYS:HG3	1:A:664:TYR:CE1	2.44	0.52
1:A:713:GLU:C	1:A:714:LYS:HD2	2.31	0.51
1:A:488:GLY:HA2	1:A:589:ARG:HD3	1.92	0.51
1:A:581:TRP:HH2	2:A:802:ADP:H5'2	1.74	0.51
1:A:472:ASP:HA	1:A:598:ASN:HA	1.92	0.51
1:B:647:ILE:HD12	1:B:650:LEU:HD23	1.90	0.51
1:B:666:LEU:HD11	1:B:705:GLY:HA3	1.92	0.51
1:B:710:ILE:HG13	1:B:711:GLU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:VAL:HA	1:A:638:SER:O	2.11	0.50
1:A:547:LEU:HD13	1:A:570:ILE:CD1	2.38	0.50
1:A:447:TYR:CZ	1:A:633:SER:HB2	2.46	0.50
1:A:480:ILE:HD13	1:A:643:VAL:HG11	1.94	0.49
1:A:456:LYS:HG2	1:A:623:ASP:HB3	1.94	0.49
1:B:245:ASP:O	1:B:249:GLU:HG3	2.12	0.49
1:A:655:LYS:NZ	6:A:1239:HOH:O	2.32	0.49
1:B:212:GLN:OE1	1:B:212:GLN:N	2.42	0.49
1:A:476:THR:HG23	1:A:478:LYS:H	1.77	0.48
1:B:707:ALA:HA	1:B:710:ILE:HG12	1.96	0.48
1:A:669:ARG:HB2	1:A:684:ASP:HB3	1.96	0.48
1:A:476:THR:OG1	1:A:477:GLY:N	2.35	0.48
1:A:522:GLU:OE2	1:A:605:ARG:HD3	2.14	0.48
1:A:656:LYS:HZ3	1:A:660:ILE:HD11	1.78	0.48
1:A:480:ILE:HG12	1:A:643:VAL:HG21	1.95	0.48
1:A:544:ASP:OD2	6:A:1244:HOH:O	2.20	0.47
1:A:538:ARG:HD2	1:A:550:ASN:HD21	1.79	0.47
1:B:187:ASN:HA	1:B:198:TYR:CZ	2.49	0.47
1:A:188:ASP:N	1:A:188:ASP:OD1	2.47	0.47
1:B:167:LEU:HD13	1:B:206:GLY:HA2	1.97	0.47
1:A:385:TYR:HB3	1:A:443:LEU:HG	1.96	0.46
1:A:666:LEU:HD13	1:A:685:ILE:CD1	2.39	0.46
1:A:294:LYS:HE3	1:A:294:LYS:HB3	1.77	0.46
1:A:660:ILE:HA	1:A:663:LYS:CD	2.45	0.46
1:A:664:TYR:HB2	1:A:666:LEU:HG	1.97	0.46
1:A:618:LYS:HD3	1:A:618:LYS:HA	1.58	0.46
1:B:622:SER:HB3	1:B:628:ILE:HD11	1.98	0.46
1:B:525:GLY:HA3	1:B:573:ASN:HA	1.99	0.45
1:A:153:LEU:HD23	1:A:250:LEU:HD21	1.98	0.45
1:A:708:LYS:HB2	1:A:708:LYS:HE3	1.61	0.45
1:A:591:ILE:HG21	1:A:593:MET:HE2	1.99	0.45
1:B:706:VAL:O	1:B:710:ILE:HG23	2.17	0.45
1:A:461:THR:HB	1:A:694:THR:HB	1.98	0.45
1:A:663:LYS:HE2	1:A:664:TYR:HE1	1.82	0.45
1:A:175:ARG:O	1:A:179:VAL:HG23	2.18	0.44
1:B:303:GLN:NE2	6:B:1125:HOH:O	2.48	0.44
1:A:576:LYS:HE2	1:A:576:LYS:HB2	1.79	0.44
1:B:653:GLN:CB	1:B:656:LYS:HB2	2.48	0.44
1:B:174:ASP:OD1	1:B:177:LYS:HE3	2.17	0.43
1:A:547:LEU:HD12	1:A:548:PHE:N	2.34	0.43
1:A:649:LYS:HE3	1:A:681:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:GLU:OE1	3:A:804:3S5:N03	2.51	0.43
1:A:664:TYR:OH	1:A:708:LYS:CE	2.67	0.43
1:A:702:MET:O	1:A:706:VAL:HG22	2.19	0.43
1:A:287:LEU:HD21	1:A:345:LEU:HD22	2.01	0.42
1:A:415:ASN:HB3	1:A:558:ALA:HB2	2.01	0.42
1:A:713:GLU:CG	1:A:714:LYS:N	2.67	0.42
1:A:482:SER:OG	2:A:802:ADP:N1	2.50	0.42
1:B:655:LYS:N	1:B:655:LYS:HD2	2.35	0.42
1:A:271:ASN:O	1:A:275:THR:HG22	2.20	0.42
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.74	0.42
1:A:483:THR:OG1	1:A:597:GLY:HA2	2.19	0.42
1:B:221:GLU:OE1	1:B:222:GLU:HB2	2.19	0.41
1:B:429:GLU:HB3	1:B:495:LEU:HD23	2.01	0.41
1:A:287:LEU:HD12	1:A:290:LEU:HD12	2.03	0.41
1:A:714:LYS:HE3	1:A:714:LYS:HA	2.03	0.41
1:A:325:ARG:NH1	1:A:329:LEU:HD23	2.36	0.41
1:B:123:ARG:HG2	1:B:124:LEU:N	2.34	0.41
1:A:548:PHE:HD1	1:A:581:TRP:CG	2.39	0.41
1:B:123:ARG:HH11	2:B:801:ADP:PB	2.44	0.41
1:A:644:LEU:HA	1:A:644:LEU:HD12	1.84	0.41
1:A:711:GLU:HA	1:A:713:GLU:OE1	2.20	0.41
1:A:648:PRO:HA	1:A:649:LYS:CB	2.49	0.41
1:A:501:SER:O	1:A:504:ASP:HB2	2.21	0.41
1:B:546:PHE:CZ	1:B:579:LEU:HD21	2.55	0.41
1:A:175:ARG:CZ	1:A:187:ASN:OD1	2.69	0.40
1:B:261:ARG:HD2	6:B:971:HOH:O	2.20	0.40
1:B:530:LEU:HD22	1:B:568:ARG:HB3	2.03	0.40
1:A:664:TYR:HD2	6:A:1131:HOH:O	2.03	0.40
1:B:492:GLU:OE1	1:B:618:LYS:HE2	2.21	0.40
1:A:535:GLU:O	1:A:539:LYS:HG3	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	714/716 (100%)	684 (96%)	27 (4%)	3 (0%)	34	42
1	B	692/716 (97%)	670 (97%)	20 (3%)	2 (0%)	41	50
All	All	1406/1432 (98%)	1354 (96%)	47 (3%)	5 (0%)	34	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	THR
1	B	88	PRO
1	A	157	SER
1	B	157	SER
1	A	712	ILE

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	613/613 (100%)	605 (99%)	8 (1%)	69	82
1	B	597/613 (97%)	591 (99%)	6 (1%)	76	87
All	All	1210/1226 (99%)	1196 (99%)	14 (1%)	71	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	311	HIS
1	A	422	SER
1	A	550	ASN
1	A	644	LEU
1	A	696	LEU
1	A	708	LYS
1	A	713	GLU

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Mol	Chain	Res	Type
1	B	539	LYS
1	B	644	LEU
1	B	650	LEU
1	B	653	GLN
1	B	688	LYS
1	B	693	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 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	$\#|Z| > 2$
5	NO3	A	807	4	1,3,3	0.89	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	3S5	B	803	-	9,9,9	1.57	3 (33%)	10,12,12	1.50	2 (20%)
2	ADP	A	802	4	24,29,29	0.96	1 (4%)	29,45,45	1.35	3 (10%)
3	3S5	B	804	-	9,9,9	1.51	3 (33%)	10,12,12	1.93	3 (30%)
2	ADP	B	802	-	24,29,29	1.03	2 (8%)	29,45,45	1.39	5 (17%)
3	3S5	A	803	-	9,9,9	1.51	2 (22%)	10,12,12	1.80	2 (20%)
3	3S5	A	804	-	9,9,9	1.46	3 (33%)	10,12,12	1.82	2 (20%)
2	ADP	A	801	4	24,29,29	1.05	2 (8%)	29,45,45	1.26	2 (6%)
2	ADP	B	801	4	24,29,29	1.03	2 (8%)	29,45,45	1.39	4 (13%)
5	NO3	A	808	-	1,3,3	0.82	0	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
3	3S5	B	803	-	-	3/7/7/7	-
2	ADP	A	802	4	-	9/12/32/32	0/3/3/3
3	3S5	B	804	-	-	0/7/7/7	-
2	ADP	B	802	-	-	6/12/32/32	0/3/3/3
3	3S5	A	803	-	-	3/7/7/7	-
3	3S5	A	804	-	-	0/7/7/7	-
2	ADP	A	801	4	-	5/12/32/32	0/3/3/3
2	ADP	B	801	4	-	4/12/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	3S5	O09-S07	2.80	1.53	1.45
3	B	803	3S5	O09-S07	2.76	1.53	1.45
2	B	802	ADP	C5-C4	2.74	1.48	1.40
2	B	801	ADP	C5-C4	2.56	1.47	1.40
2	A	801	ADP	C5-C4	2.52	1.47	1.40
3	B	804	3S5	C02-N04	2.49	1.38	1.33
3	B	803	3S5	C02-N04	2.45	1.38	1.33
2	A	802	ADP	C5-C4	2.42	1.47	1.40
3	B	804	3S5	O10-S07	2.35	1.52	1.45
2	A	801	ADP	O4'-C1'	2.34	1.44	1.41
3	A	804	3S5	O10-S07	2.32	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	3S5	O09-S07	2.30	1.51	1.45
3	B	803	3S5	O10-S07	2.25	1.51	1.45
2	B	802	ADP	C2-N3	2.23	1.35	1.32
3	B	804	3S5	O09-S07	2.19	1.51	1.45
2	B	801	ADP	O4'-C1'	2.10	1.44	1.41
3	A	803	3S5	O10-S07	2.09	1.51	1.45
3	A	804	3S5	C02-N04	2.08	1.37	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	804	3S5	O08-S07-C06	4.13	112.45	105.77
3	A	803	3S5	O09-S07-C06	4.02	111.75	106.92
3	A	804	3S5	O10-S07-C06	3.81	111.51	106.92
2	B	802	ADP	C3'-C2'-C1'	3.40	106.10	100.98
3	B	803	3S5	O09-S07-C06	3.38	110.98	106.92
3	A	803	3S5	O08-S07-C06	3.29	111.09	105.77
2	A	802	ADP	N3-C2-N1	-3.27	123.56	128.68
3	A	804	3S5	O09-S07-C06	3.24	110.81	106.92
2	A	802	ADP	C4-C5-N7	-3.20	106.06	109.40
2	B	801	ADP	N3-C2-N1	-3.11	123.82	128.68
2	A	801	ADP	N3-C2-N1	-3.08	123.86	128.68
2	B	802	ADP	N3-C2-N1	-3.02	123.95	128.68
2	B	801	ADP	C4-C5-N7	-2.79	106.49	109.40
2	B	802	ADP	PA-O3A-PB	-2.66	123.69	132.83
3	B	804	3S5	O10-S07-C06	2.65	110.10	106.92
2	B	802	ADP	C4-C5-N7	-2.61	106.68	109.40
2	B	801	ADP	PA-O3A-PB	-2.57	124.02	132.83
2	A	801	ADP	C4-C5-N7	-2.32	106.98	109.40
3	B	803	3S5	O08-S07-C06	2.27	109.43	105.77
2	A	802	ADP	PA-O3A-PB	-2.21	125.24	132.83
3	B	804	3S5	O09-S07-C06	2.10	109.44	106.92
2	B	801	ADP	O2A-PA-O1A	2.02	122.23	112.24
2	B	802	ADP	O2A-PA-O1A	2.01	122.17	112.24

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	ADP	PA-O3A-PB-O2B
2	A	802	ADP	C5'-O5'-PA-O3A
2	B	802	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	802	ADP	C5'-O5'-PA-O2A
2	B	802	ADP	C5'-O5'-PA-O3A
2	B	802	ADP	O4'-C4'-C5'-O5'
2	A	801	ADP	C5'-O5'-PA-O1A
2	B	801	ADP	C5'-O5'-PA-O1A
2	A	802	ADP	O4'-C4'-C5'-O5'
2	A	802	ADP	C3'-C4'-C5'-O5'
2	B	802	ADP	C3'-C4'-C5'-O5'
3	B	803	3S5	C05-C06-S07-O08
3	A	803	3S5	C05-C06-S07-O08
2	A	802	ADP	PB-O3A-PA-O1A
2	A	801	ADP	C5'-O5'-PA-O3A
2	B	801	ADP	C5'-O5'-PA-O3A
2	A	801	ADP	PB-O3A-PA-O1A
2	A	802	ADP	C5'-O5'-PA-O1A
2	A	802	ADP	C5'-O5'-PA-O2A
2	A	801	ADP	C5'-O5'-PA-O2A
2	B	801	ADP	C5'-O5'-PA-O2A
3	B	803	3S5	C05-C06-S07-O10
3	A	803	3S5	C05-C06-S07-O09
2	A	802	ADP	PB-O3A-PA-O2A
2	B	802	ADP	PB-O3A-PA-O2A
2	B	801	ADP	PB-O3A-PA-O1A
2	A	802	ADP	PA-O3A-PB-O3B
2	A	801	ADP	PB-O3A-PA-O2A
3	B	803	3S5	C05-C06-S07-O09
3	A	803	3S5	C05-C06-S07-O10

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	ADP	2	0
3	A	804	3S5	1	0
2	B	801	ADP	3	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 then 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 ADP A 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 801

Bond lengths

Bond angles

Torsions

Rings
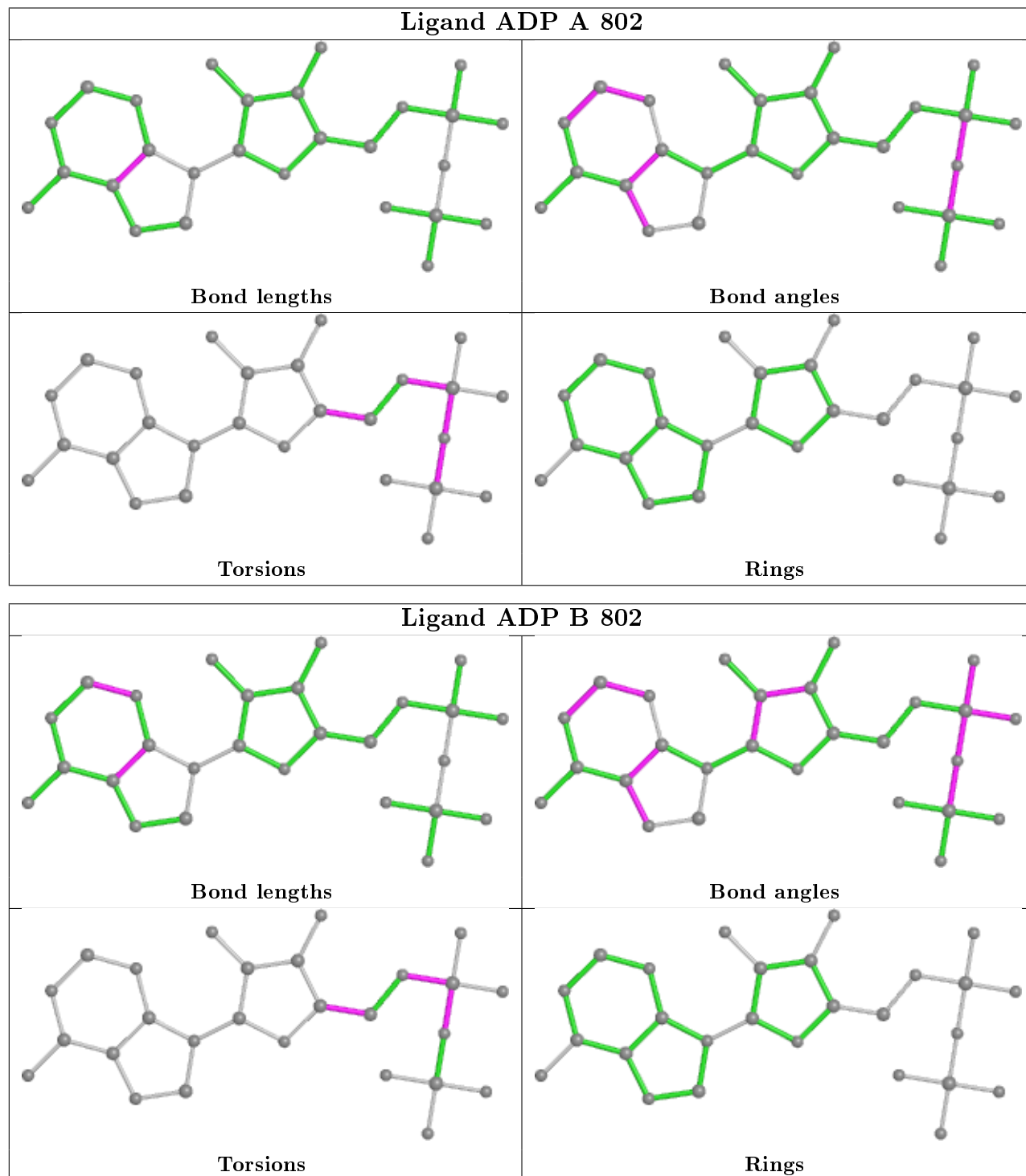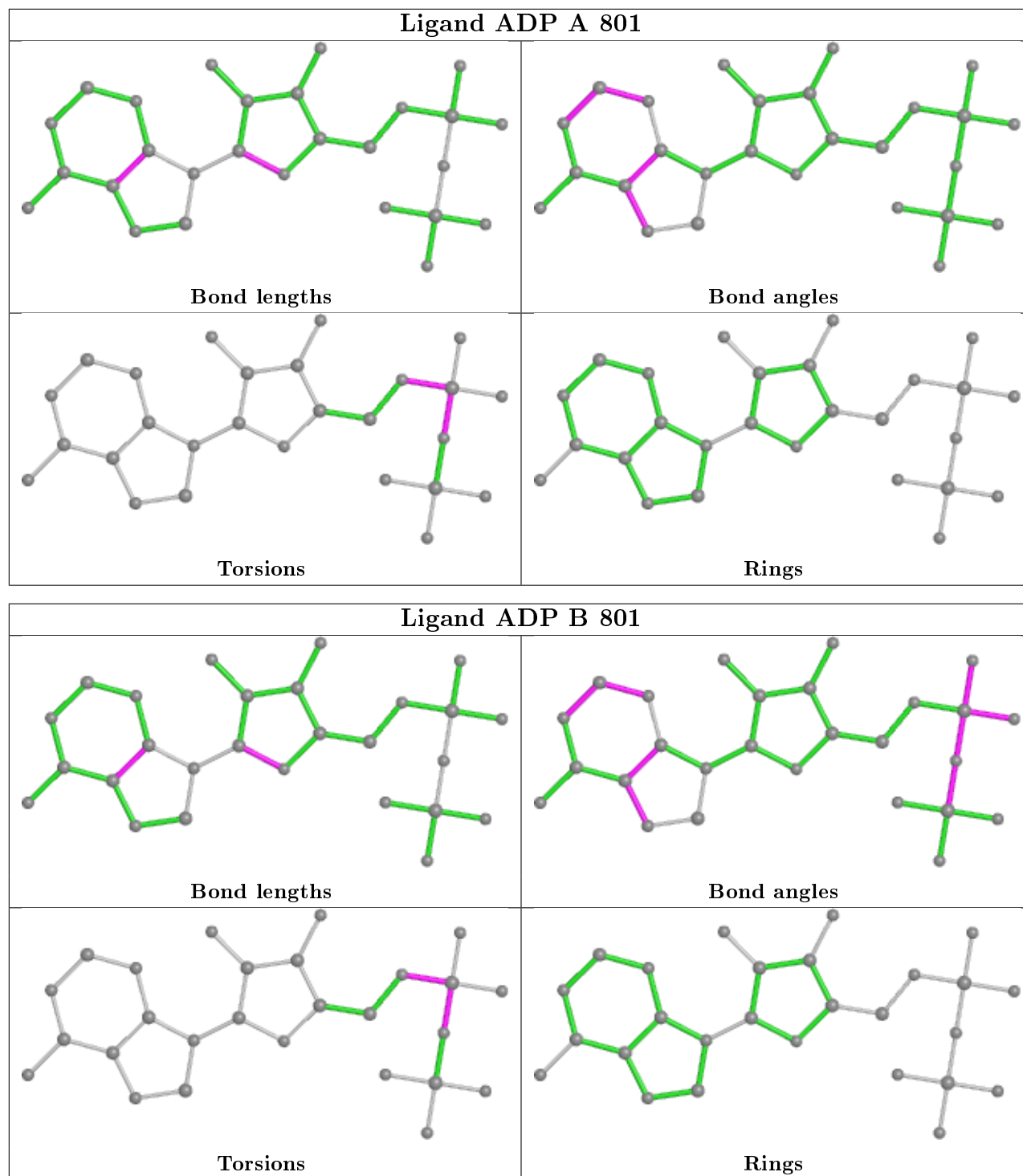
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	716/716 (100%)	0.37	71 (9%)	7	10	13, 22, 62, 94	0
1	B	698/716 (97%)	0.24	52 (7%)	14	19	11, 20, 55, 93	0
All	All	1414/1432 (98%)	0.31	123 (8%)	10	14	11, 21, 57, 94	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	GLY	10.0
1	B	657	LEU	9.8
1	A	652	SER	8.7
1	A	648	PRO	8.4
1	A	709	MET	7.6
1	A	679	PRO	7.5
1	A	654	PRO	7.4
1	B	652	SER	7.4
1	A	716	LEU	7.4
1	A	680	ASP	7.2
1	B	716	LEU	7.1
1	B	654	PRO	6.8
1	A	682	THR	6.7
1	A	712	ILE	6.3
1	B	653	GLN	6.2
1	B	648	PRO	6.1
1	B	710	ILE	6.1
1	A	480	ILE	5.7
1	A	681	GLY	5.7
1	A	671	LEU	5.5
1	A	662	ALA	5.5
1	A	479	PHE	5.5
1	B	176	ILE	5.5
1	A	661	CYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	665	MET	5.3
1	A	706	VAL	5.3
1	A	702	MET	5.1
1	A	710	ILE	5.0
1	A	650	LEU	5.0
1	B	681	GLY	4.9
1	B	476	THR	4.9
1	B	655	LYS	4.8
1	A	672	TYR	4.6
1	A	651	SER	4.6
1	A	659	GLU	4.6
1	B	647	ILE	4.5
1	B	475	PRO	4.5
1	B	650	LEU	4.5
1	B	668	ALA	4.5
1	B	651	SER	4.4
1	A	713	GLU	4.3
1	A	657	LEU	4.2
1	A	708	LYS	4.2
1	B	666	LEU	4.1
1	B	715	GLY	4.0
1	A	472	ASP	4.0
1	A	655	LYS	3.9
1	A	666	LEU	3.9
1	A	677	GLU	3.8
1	B	661	CYS	3.7
1	A	676	THR	3.7
1	A	478	LYS	3.6
1	A	649	LYS	3.6
1	B	682	THR	3.6
1	A	538	ARG	3.5
1	B	480	ILE	3.5
1	B	669	ARG	3.5
1	B	656	LYS	3.4
1	B	649	LYS	3.4
1	A	645	LEU	3.4
1	B	659	GLU	3.3
1	B	173	GLU	3.3
1	B	479	PHE	3.3
1	B	178	LEU	3.2
1	A	477	GLY	3.2
1	B	670	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	539	LYS	3.2
1	A	658	ASP	3.1
1	A	536	GLU	3.1
1	B	713	GLU	3.1
1	A	469	PRO	3.0
1	A	673	GLY	3.0
1	B	660	ILE	3.0
1	A	653	GLN	3.0
1	A	678	SER	2.9
1	B	103	LYS	2.9
1	A	711	GLU	2.9
1	A	670	GLY	2.9
1	A	668	ALA	2.9
1	B	478	LYS	2.8
1	A	382	GLU	2.8
1	B	535	GLU	2.8
1	B	171	SER	2.8
1	A	481	VAL	2.8
1	A	644	LEU	2.7
1	B	683	TYR	2.7
1	A	476	THR	2.7
1	A	647	ILE	2.6
1	A	542	VAL	2.6
1	B	180	ASN	2.6
1	B	183	PHE	2.6
1	A	173	GLU	2.6
1	B	451	LYS	2.6
1	A	683	TYR	2.5
1	B	177	LYS	2.5
1	A	705	GLY	2.5
1	A	176	ILE	2.5
1	B	658	ASP	2.5
1	A	675	HIS	2.4
1	A	452	ASP	2.4
1	A	471	GLY	2.4
1	B	706	VAL	2.3
1	B	712	ILE	2.3
1	A	539	LYS	2.3
1	A	667	GLN	2.3
1	B	181	ASP	2.3
1	A	533	MET	2.3
1	A	663	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	185	PHE	2.2
1	A	186	ARG	2.2
1	A	646	LYS	2.2
1	A	188	ASP	2.1
1	B	547	LEU	2.1
1	B	455	PHE	2.1
1	A	381	ILE	2.1
1	A	473	LEU	2.1
1	B	89	ASP	2.1
1	A	172	GLU	2.1
1	B	534	LYS	2.1
1	B	707	ALA	2.1
1	A	175	ARG	2.0
1	B	644	LEU	2.0
1	B	175	ARG	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 carbohydrates 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
4	MG	A	806	1/1	0.72	0.17	38,38,38,38	0
2	ADP	B	802	27/27	0.79	0.30	38,52,60,74	0
4	MG	A	805	1/1	0.86	0.14	43,43,43,43	0
4	MG	B	805	1/1	0.92	0.13	42,42,42,42	0
5	NO3	A	807	4/4	0.93	0.14	34,36,45,46	0
3	3S5	B	803	10/10	0.94	0.18	24,33,48,51	0
2	ADP	A	802	27/27	0.94	0.20	30,33,36,39	0
5	NO3	A	808	4/4	0.94	0.22	27,30,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	3S5	A	803	10/10	0.95	0.23	24,35,46,48	0
2	ADP	B	801	27/27	0.95	0.17	21,35,42,48	0
3	3S5	B	804	10/10	0.96	0.16	21,25,30,32	0
3	3S5	A	804	10/10	0.97	0.12	22,25,30,31	0
2	ADP	A	801	27/27	0.97	0.12	19,23,27,31	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.
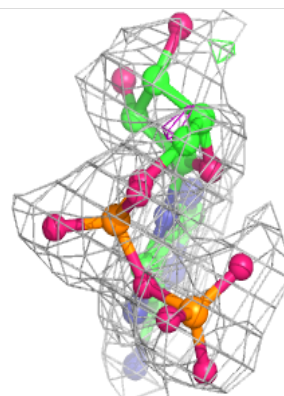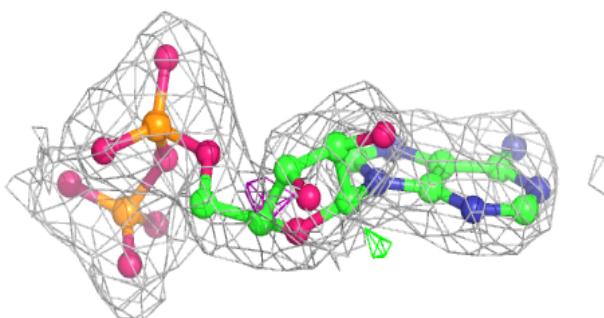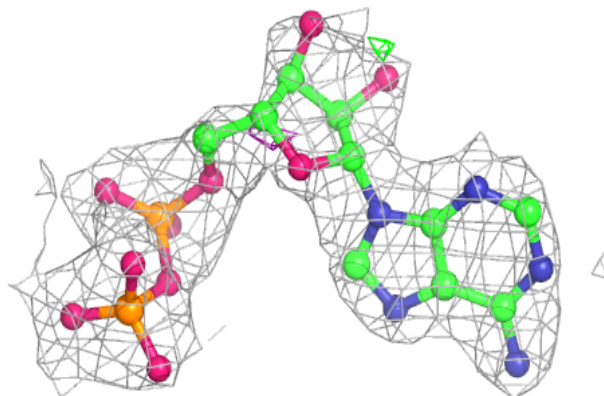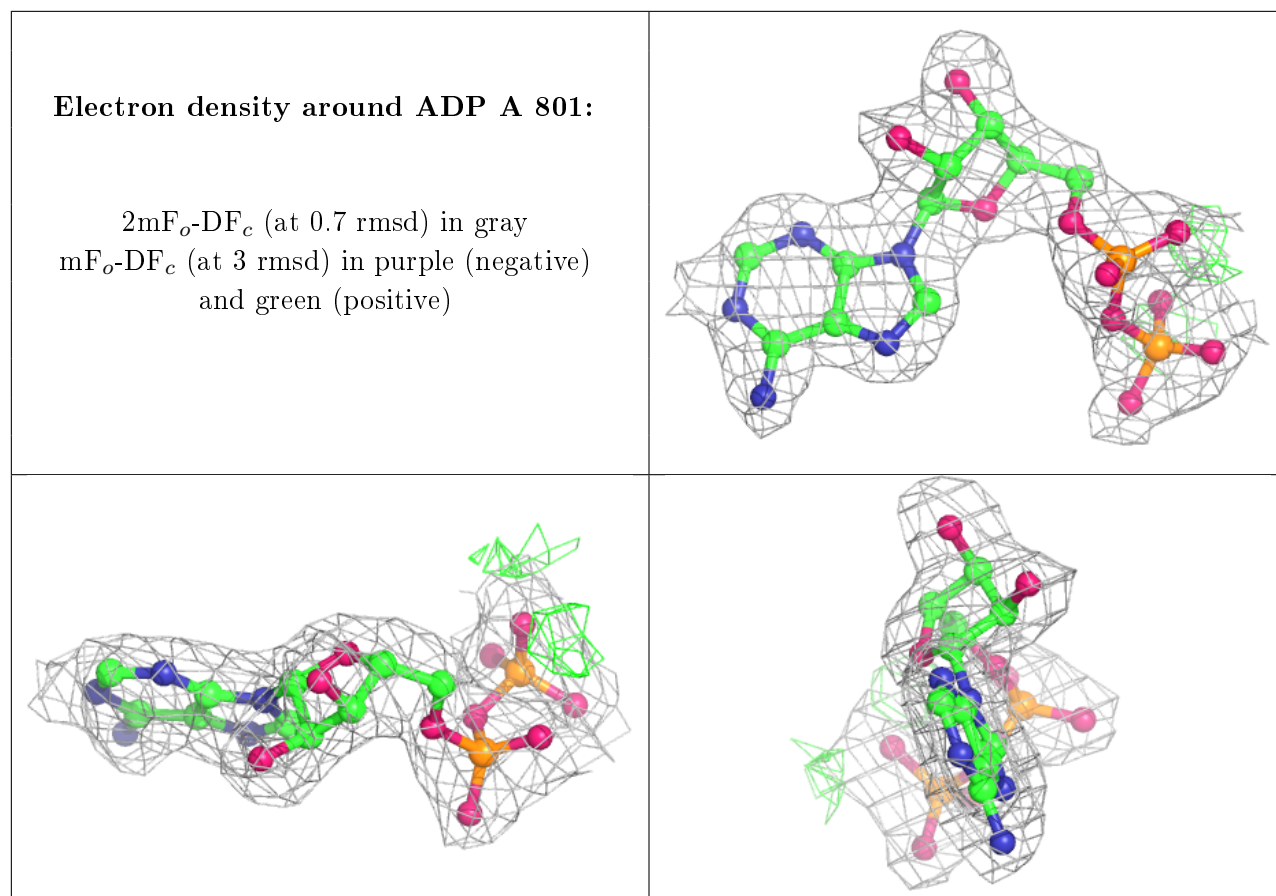
Electron density around ADP B 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
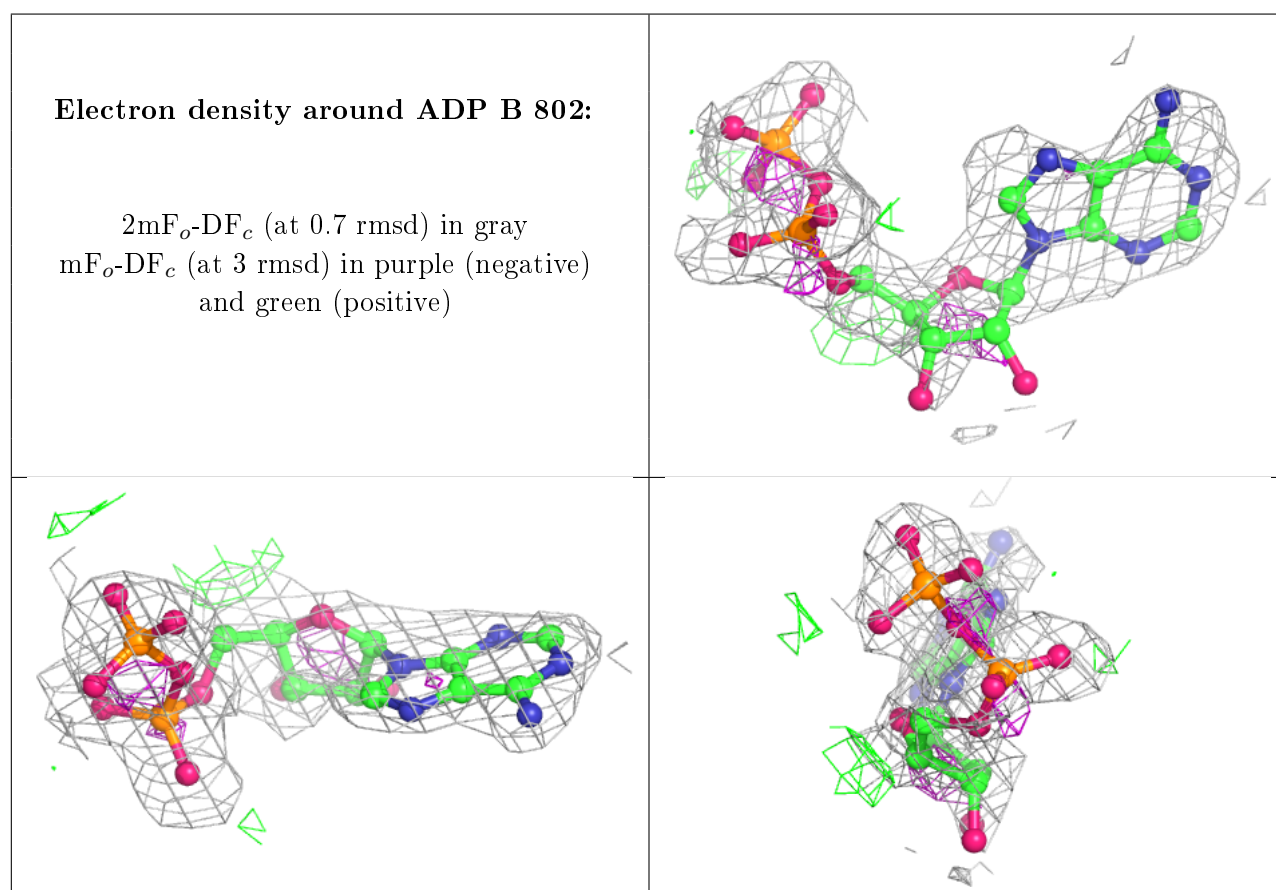
Electron density around ADP A 802:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
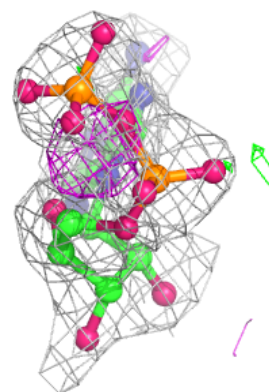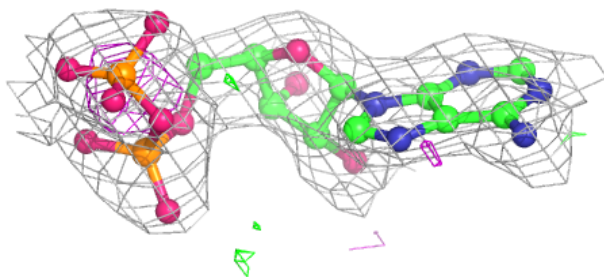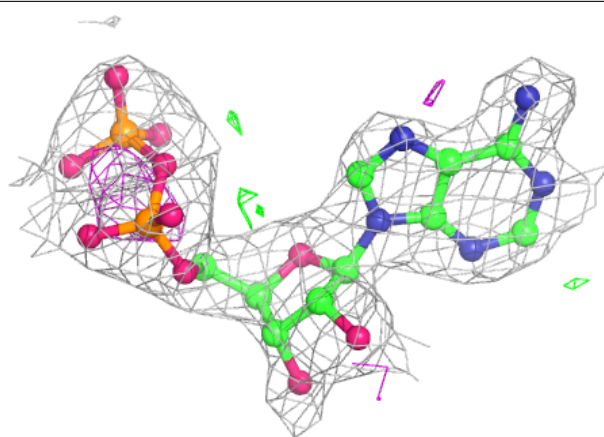
Electron density around ADP B 801:

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

Electron density around ADP A 801:

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

6.5 Other polymers (i)

There are no such residues in this entry.