



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:32 am BST

PDB ID : 4E7S
Title : Myosin VI D23R I24R R569E (MD) pre-powerstroke state
Authors : Isabet, T.; Sweeney, H.L.; Houdusse, A.
Deposited on : 2012-03-19
Resolution : 2.25 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 : 2.11
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

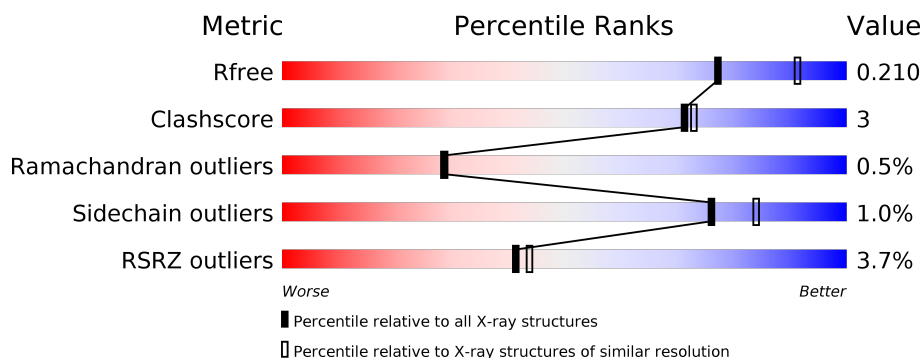
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	798	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7% • 5%</div> </div> </div>
1	B	798	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>9% 6%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12540 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 Myosin-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	2	0
			6034	3843	1040	1122	29			
1	B	752	Total	C	N	O	S	0	1	0
			5930	3781	1023	1098	28			

There are 26 discrepancies between the modelled and reference sequences:

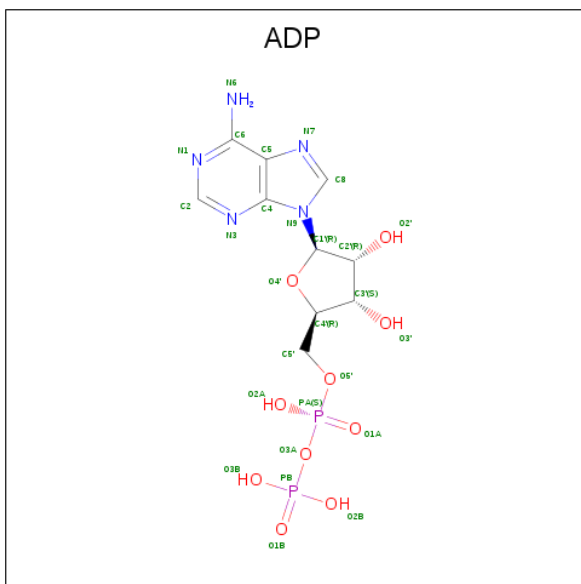
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP F1RQI7
A	-7	ASP	-	expression tag	UNP F1RQI7
A	-6	TYR	-	expression tag	UNP F1RQI7
A	-5	LYS	-	expression tag	UNP F1RQI7
A	-4	ASP	-	expression tag	UNP F1RQI7
A	-3	ASP	-	expression tag	UNP F1RQI7
A	-2	ASP	-	expression tag	UNP F1RQI7
A	-1	ASP	-	expression tag	UNP F1RQI7
A	0	LYS	-	expression tag	UNP F1RQI7
A	1	GLY	-	expression tag	UNP F1RQI7
A	23	ARG	ASP	engineered mutation	UNP F1RQI7
A	24	ARG	ILE	engineered mutation	UNP F1RQI7
A	569	GLU	ARG	engineered mutation	UNP F1RQI7
B	-8	MET	-	expression tag	UNP F1RQI7
B	-7	ASP	-	expression tag	UNP F1RQI7
B	-6	TYR	-	expression tag	UNP F1RQI7
B	-5	LYS	-	expression tag	UNP F1RQI7
B	-4	ASP	-	expression tag	UNP F1RQI7
B	-3	ASP	-	expression tag	UNP F1RQI7
B	-2	ASP	-	expression tag	UNP F1RQI7
B	-1	ASP	-	expression tag	UNP F1RQI7
B	0	LYS	-	expression tag	UNP F1RQI7
B	1	GLY	-	expression tag	UNP F1RQI7
B	23	ARG	ASP	engineered mutation	UNP F1RQI7
B	24	ARG	ILE	engineered mutation	UNP F1RQI7

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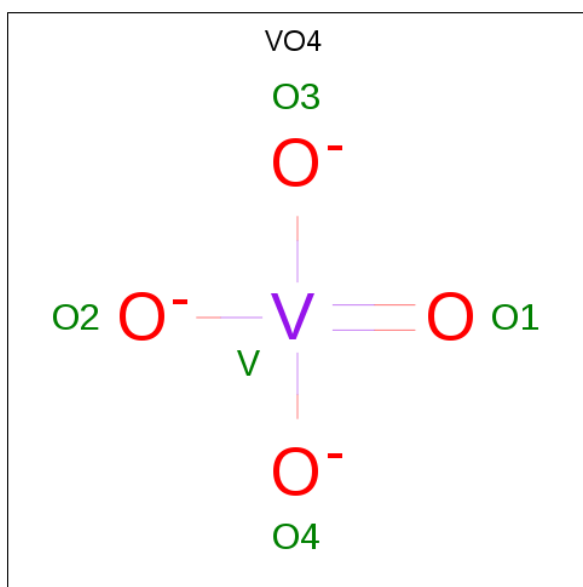
Chain	Residue	Modelled	Actual	Comment	Reference
B	569	GLU	ARG	engineered mutation	UNP F1RQI7

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			5	4	1		
3	B	1	Total	O	V	0	0
			5	4	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	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

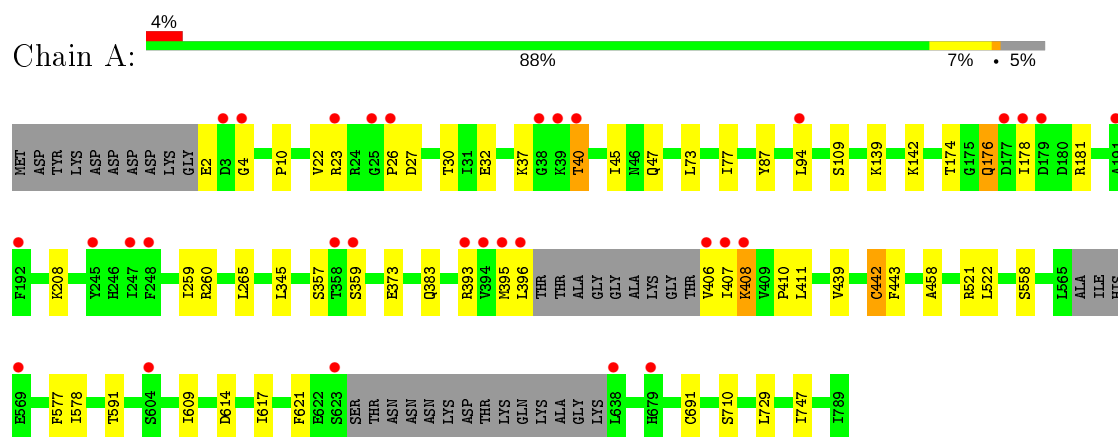
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		
7	B	210	Total	O	0	0
			210	210		

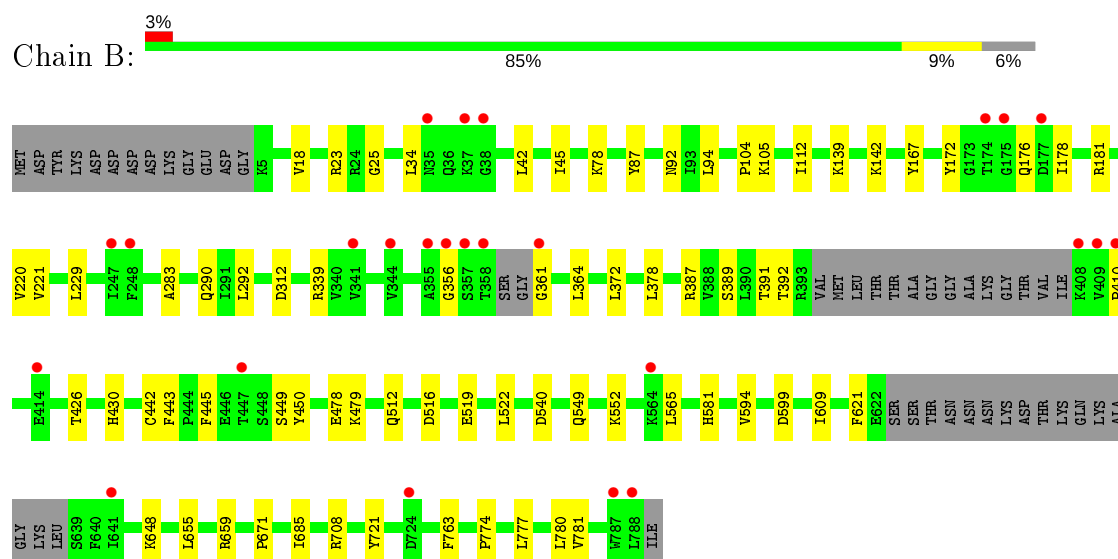
3 Residue-property plots [i](#)

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: Myosin-VI



• Molecule 1: Myosin-VI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.95Å 135.14Å 196.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.25 29.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.77-2.25) 98.9 (29.77-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.179 , 0.216 0.173 , 0.210	Depositor DCC
R_{free} test set	5150 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12540	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: VO4, GOL, MG, PO4, ADP

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	0.51	0/6158	0.59	0/8315
1	B	0.45	0/6055	0.55	0/8184
All	All	0.48	0/12213	0.57	0/16499

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	6034	0	5865	37	0
1	B	5930	0	5727	44	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	32	3	0
5	B	12	0	16	2	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	259	0	0	6	0
7	B	210	0	0	3	0
All	All	12540	0	11664	82	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 3.

All (82) 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:2:GLU:O	1:A:4:GLY:HA2	1.77	0.84
1:A:609:ILE:HG21	1:A:621:PHE:CE1	2.15	0.80
5:A:807:GOL:H31	7:A:1145:HOH:O	1.83	0.78
1:B:292:LEU:HG	5:B:806:GOL:H31	1.66	0.75
1:A:174:THR:HG23	1:A:176:GLN:H	1.56	0.71
1:A:22:VAL:HG23	1:A:23:ARG:H	1.56	0.70
1:B:139:LYS:O	1:B:142:LYS:HE3	1.99	0.62
1:A:10:PRO:HD3	1:A:47:GLN:O	2.02	0.60
1:A:393:ARG:HB2	1:A:411:LEU:HD21	1.85	0.59
1:A:396:LEU:HD12	1:A:406:VAL:N	2.22	0.55
1:B:777:LEU:O	1:B:781:VAL:HG23	2.05	0.55
1:A:609:ILE:HG21	1:A:621:PHE:CD1	2.41	0.55
1:B:387:ARG:O	1:B:391:THR:HG22	2.08	0.54
1:A:591:THR:HG23	7:A:1123:HOH:O	2.06	0.54
1:A:32:GLU:OE1	1:A:40:THR:HG22	2.08	0.54
1:B:18:VAL:HG11	1:B:34:LEU:HD22	1.91	0.53
1:A:208:LYS:HE2	7:A:1060:HOH:O	2.08	0.52
1:A:407:ILE:HG12	1:A:408:LYS:N	2.24	0.52
1:A:521:ARG:O	1:A:522:LEU:HB2	2.10	0.52
1:A:458:ALA:O	7:A:1015:HOH:O	2.19	0.52
1:B:478:GLU:OE1	1:B:581:HIS:HB3	2.10	0.51
1:B:361:GLY:HA2	1:B:410:PRO:HB2	1.94	0.50
1:B:540:ASP:OD1	1:B:594:VAL:HG23	2.11	0.50
1:A:691[B]:CYS:SG	5:A:807:GOL:H11	2.51	0.50
1:B:391:THR:HG23	1:B:392:THR:HG23	1.94	0.50
1:A:729:LEU:HD11	1:B:42:LEU:HB3	1.93	0.49
1:B:479:LYS:HE3	1:B:655:LEU:HD11	1.93	0.49
1:B:142:LYS:HD3	1:B:450:TYR:OH	2.13	0.48
1:B:78:LYS:HD3	7:B:1107:HOH:O	2.12	0.48
1:B:721:TYR:OH	1:B:774:PRO:HB3	2.13	0.48
1:A:396:LEU:O	1:A:396:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ASP:HB3	1:A:617:ILE:HG12	1.96	0.48
1:B:221:VAL:CG1	1:B:445:PHE:HB2	2.44	0.48
1:A:27:ASP:C	1:A:45:ILE:HD12	2.34	0.48
1:A:22:VAL:HG23	1:A:23:ARG:N	2.28	0.47
1:B:512:GLN:NE2	1:B:516:ASP:OD1	2.47	0.47
1:A:395:MET:O	1:A:407:ILE:HG22	2.15	0.47
1:B:25:GLY:O	1:B:45:ILE:HD11	2.14	0.47
1:A:259:ILE:HD12	7:A:990:HOH:O	2.15	0.47
1:B:356:GLY:HA2	1:B:361:GLY:N	2.31	0.46
1:B:339:ARG:HG3	1:B:378:LEU:HD22	1.97	0.46
1:B:565:LEU:HD23	1:B:565:LEU:N	2.31	0.46
1:B:23:ARG:HD3	7:B:1088:HOH:O	2.16	0.46
1:B:478:GLU:OE1	1:B:581:HIS:CB	2.64	0.45
1:A:139:LYS:O	1:A:142:LYS:HD2	2.16	0.45
1:B:522:LEU:HA	1:B:522:LEU:HD23	1.82	0.45
1:B:283:ALA:HA	1:B:312:ASP:OD1	2.17	0.45
1:B:426:THR:HG22	1:B:430:HIS:ND1	2.32	0.45
1:B:655:LEU:HB3	1:B:659:ARG:NH2	2.31	0.45
1:A:27:ASP:O	1:A:45:ILE:HD12	2.17	0.44
1:B:87:TYR:HB3	1:B:94:LEU:HD11	1.99	0.44
5:A:807:GOL:H2	7:A:906:HOH:O	2.16	0.44
1:B:290:GLN:O	5:B:806:GOL:H32	2.18	0.44
1:A:359:SER:O	1:A:410:PRO:HG2	2.18	0.44
1:B:112:ILE:HG23	1:B:167:TYR:CD1	2.53	0.43
1:B:34:LEU:HA	1:B:34:LEU:HD12	1.92	0.43
1:B:609:ILE:HG21	1:B:621:PHE:CZ	2.54	0.43
1:A:10:PRO:CG	1:A:47:GLN:HB3	2.49	0.42
1:A:87:TYR:HB3	1:A:94:LEU:HD11	2.01	0.42
1:B:378:LEU:HA	1:B:378:LEU:HD23	1.89	0.42
1:B:549:GLN:HE22	1:B:552:LYS:HZ1	1.65	0.42
1:A:373:GLU:HG3	1:A:383:GLN:NE2	2.35	0.42
1:A:73:LEU:O	1:A:77:ILE:HG12	2.20	0.42
1:A:178:ILE:HA	1:A:181:ARG:HG3	2.02	0.41
1:B:426:THR:HG22	1:B:430:HIS:CE1	2.55	0.41
1:B:479:LYS:HE3	1:B:655:LEU:CD1	2.50	0.41
1:B:172:TYR:O	1:B:220:VAL:HG23	2.19	0.41
1:B:780:LEU:HA	1:B:780:LEU:HD23	1.83	0.41
1:A:260:ARG:HH21	1:A:260:ARG:HG2	1.85	0.41
1:B:178:ILE:HA	1:B:181:ARG:HB2	2.03	0.41
1:B:104:PRO:O	1:B:105:LYS:HB2	2.20	0.41
1:B:364:LEU:HD22	1:B:372:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:GLU:HB2	1:B:648:LYS:HD2	2.02	0.41
1:B:671:PRO:HA	1:B:685:ILE:HD11	2.03	0.41
1:B:142:LYS:NZ	7:B:972:HOH:O	2.54	0.41
1:A:174:THR:HG23	1:A:176:GLN:N	2.30	0.41
1:A:260:ARG:HG3	1:A:265:LEU:HB2	2.02	0.41
1:B:92:ASN:HB3	1:B:763:PHE:CZ	2.56	0.41
1:A:558:SER:HB2	1:A:578:ILE:HB	2.03	0.41
1:A:22:VAL:HG23	1:A:30:THR:HB	2.02	0.41
1:A:439:VAL:O	1:A:442[B]:CYS:HB2	2.21	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.91	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	756/798 (95%)	734 (97%)	17 (2%)	5 (1%)	22	21
1	B	745/798 (93%)	718 (96%)	25 (3%)	2 (0%)	41	46
All	All	1501/1596 (94%)	1452 (97%)	42 (3%)	7 (0%)	29	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	B	229	LEU
1	B	176	GLN
1	A	40	THR
1	A	176	GLN
1	A	357	SER
1	A	26	PRO

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	646/705 (92%)	638 (99%)	8 (1%)	71	80
1	B	628/705 (89%)	622 (99%)	6 (1%)	76	84
All	All	1274/1410 (90%)	1260 (99%)	14 (1%)	76	82

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

Mol	Chain	Res	Type
1	A	109	SER
1	A	408	LYS
1	A	442[A]	CYS
1	A	442[B]	CYS
1	A	443	PHE
1	A	577	PHE
1	A	710	SER
1	A	747	ILE
1	B	389	SER
1	B	442	CYS
1	B	443	PHE
1	B	449	SER
1	B	599	ASP
1	B	708	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	B	549	GLN
1	B	712	HIS

5.3.3 RNA

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, 2 are monoatomic - leaving 11 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	GOL	A	807	-	5,5,5	0.21	0	5,5,5	0.61	0
3	VO4	B	802	2,4	1,4,4	5.33	1 (100%)	-		
5	GOL	B	806	-	5,5,5	0.29	0	5,5,5	0.28	0
6	PO4	B	804	-	4,4,4	0.98	0	6,6,6	0.44	0
2	ADP	A	801	3,4	24,29,29	1.03	1 (4%)	29,45,45	1.29	3 (10%)
5	GOL	A	806	-	5,5,5	0.48	0	5,5,5	0.22	0
5	GOL	A	805	-	5,5,5	0.33	0	5,5,5	0.31	0
5	GOL	B	805	-	5,5,5	0.34	0	5,5,5	0.59	0
2	ADP	B	801	3,4	24,29,29	1.03	2 (8%)	29,45,45	1.34	3 (10%)
3	VO4	A	802	2,4	1,4,4	5.24	1 (100%)	-		
5	GOL	A	804	-	5,5,5	0.36	0	5,5,5	0.48	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
5	GOL	A	807	-	-	4/4/4/4	-
5	GOL	B	805	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	806	-	-	2/4/4/4	-
2	ADP	A	801	3,4	-	3/12/32/32	0/3/3/3
5	GOL	A	806	-	-	2/4/4/4	-
5	GOL	A	805	-	-	2/4/4/4	-
2	ADP	B	801	3,4	-	3/12/32/32	0/3/3/3
5	GOL	A	804	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	VO4	O1-V	5.33	1.94	1.63
3	A	802	VO4	O1-V	5.24	1.93	1.63
2	A	801	ADP	C5-C4	2.49	1.47	1.40
2	B	801	ADP	C5-C4	2.12	1.46	1.40
2	B	801	ADP	O4'-C1'	2.09	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ADP	N3-C2-N1	-3.44	123.31	128.68
2	A	801	ADP	N3-C2-N1	-3.10	123.83	128.68
2	A	801	ADP	C4-C5-N7	-2.99	106.28	109.40
2	B	801	ADP	C4-C5-N7	-2.70	106.59	109.40
2	B	801	ADP	PA-O3A-PB	-2.24	125.13	132.83
2	A	801	ADP	O2A-PA-O1A	2.14	122.81	112.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	807	GOL	C1-C2-C3-O3
5	B	806	GOL	C1-C2-C3-O3
5	B	805	GOL	O1-C1-C2-C3
5	B	805	GOL	C1-C2-C3-O3
5	A	807	GOL	O1-C1-C2-C3
5	A	806	GOL	C1-C2-C3-O3
5	A	805	GOL	O1-C1-C2-C3
5	B	806	GOL	O2-C2-C3-O3
5	B	805	GOL	O2-C2-C3-O3
5	A	807	GOL	O2-C2-C3-O3

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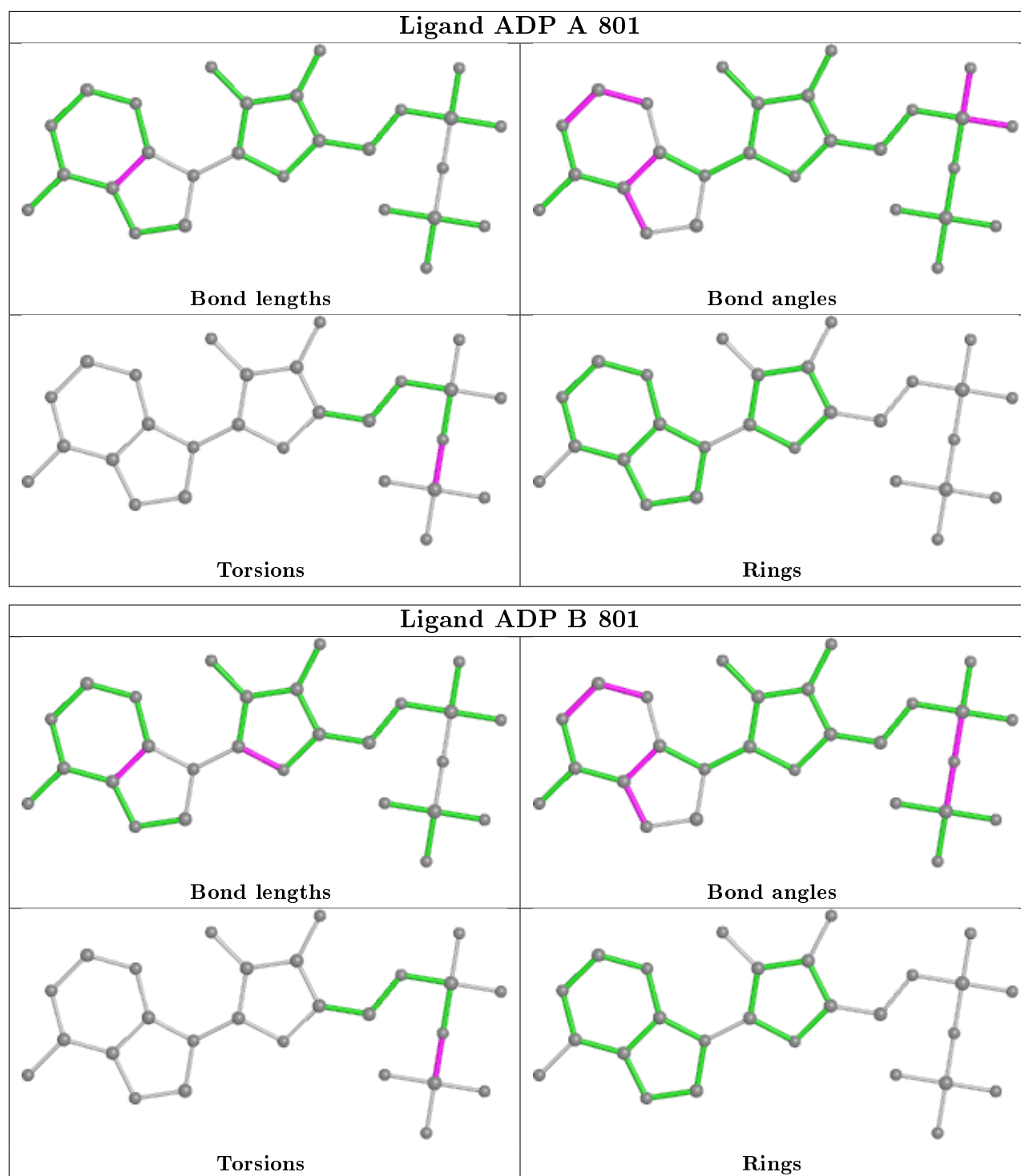
Mol	Chain	Res	Type	Atoms
5	B	805	GOL	O1-C1-C2-O2
2	A	801	ADP	PA-O3A-PB-O1B
2	B	801	ADP	PA-O3A-PB-O1B
5	A	806	GOL	O2-C2-C3-O3
5	A	807	GOL	O1-C1-C2-O2
2	A	801	ADP	PA-O3A-PB-O2B
2	A	801	ADP	PA-O3A-PB-O3B
2	B	801	ADP	PA-O3A-PB-O2B
2	B	801	ADP	PA-O3A-PB-O3B
5	A	805	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	807	GOL	3	0
5	B	806	GOL	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 ⓘ

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	762/798 (95%)	-0.15	31 (4%) 37 40	32, 47, 73, 115	0
1	B	752/798 (94%)	-0.10	25 (3%) 46 48	36, 52, 82, 124	0
All	All	1514/1596 (94%)	-0.12	56 (3%) 41 44	32, 49, 79, 124	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	LEU	8.6
1	A	359	SER	7.3
1	B	358	THR	5.8
1	A	396	LEU	5.7
1	B	356	GLY	5.4
1	B	355	ALA	5.3
1	A	394	VAL	4.9
1	B	357	SER	4.9
1	A	395	MET	4.6
1	A	406	VAL	4.3
1	B	787	TRP	4.3
1	A	358	THR	4.2
1	A	3	ASP	4.1
1	B	409	VAL	4.0
1	A	407	ILE	3.9
1	B	788	LEU	3.5
1	B	724	ASP	3.3
1	A	178	ILE	3.1
1	B	564	LYS	3.1
1	A	38	GLY	3.1
1	A	247	ILE	3.0
1	B	410	PRO	3.0
1	B	344	VAL	2.9
1	B	361	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	623	SER	2.8
1	B	35	ASN	2.7
1	B	174	THR	2.7
1	B	447	THR	2.6
1	A	408	LYS	2.6
1	A	179	ASP	2.5
1	B	37	LYS	2.5
1	A	40	THR	2.5
1	A	245	TYR	2.5
1	A	25	GLY	2.4
1	B	641	ILE	2.4
1	A	26	PRO	2.4
1	B	175	GLY	2.4
1	A	23	ARG	2.4
1	B	38	GLY	2.4
1	A	393	ARG	2.4
1	A	4	GLY	2.3
1	A	177	ASP	2.3
1	B	177	ASP	2.3
1	B	247	ILE	2.3
1	A	248	PHE	2.2
1	B	408	LYS	2.2
1	B	248	PHE	2.2
1	A	569	GLU	2.2
1	A	94	LEU	2.2
1	A	192	PHE	2.1
1	A	604	SER	2.1
1	B	341	VAL	2.1
1	B	414	GLU	2.1
1	A	39	LYS	2.0
1	A	191	ALA	2.0
1	A	679	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

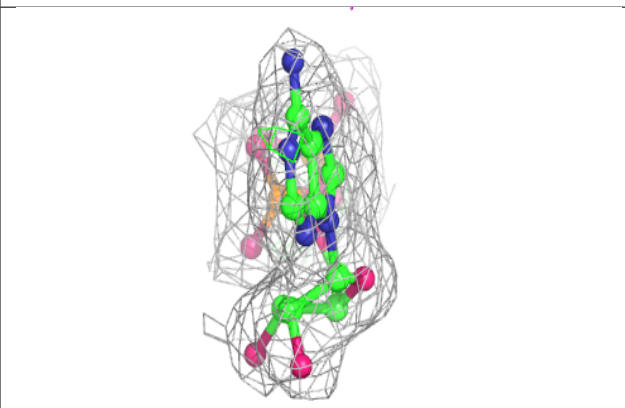
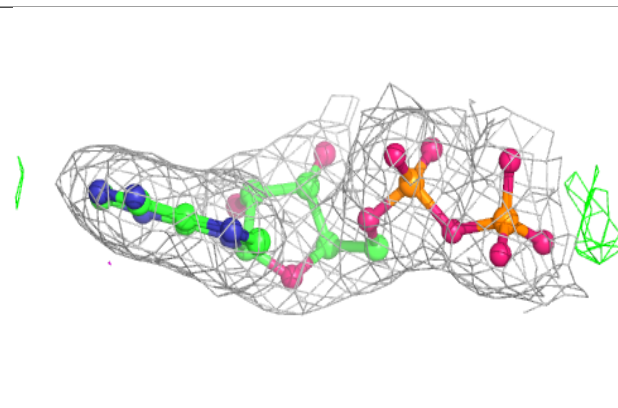
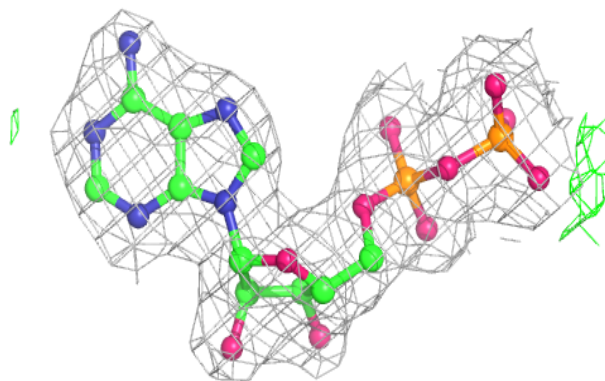
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	806	6/6	0.72	0.26	57,61,65,68	0
5	GOL	A	805	6/6	0.85	0.17	63,65,68,72	0
5	GOL	A	807	6/6	0.92	0.12	50,51,55,60	0
5	GOL	B	805	6/6	0.92	0.13	49,53,56,62	0
5	GOL	B	806	6/6	0.94	0.17	57,62,65,71	0
5	GOL	A	804	6/6	0.94	0.21	60,63,64,65	0
6	PO4	B	804	5/5	0.97	0.14	38,52,58,61	5
4	MG	A	803	1/1	0.97	0.20	37,37,37,37	0
2	ADP	B	801	27/27	0.98	0.12	30,39,44,44	0
3	VO4	A	802	5/5	0.99	0.19	35,35,37,39	0
3	VO4	B	802	5/5	0.99	0.20	35,35,36,38	0
4	MG	B	803	1/1	0.99	0.20	35,35,35,35	0
2	ADP	A	801	27/27	0.99	0.13	30,36,42,43	0

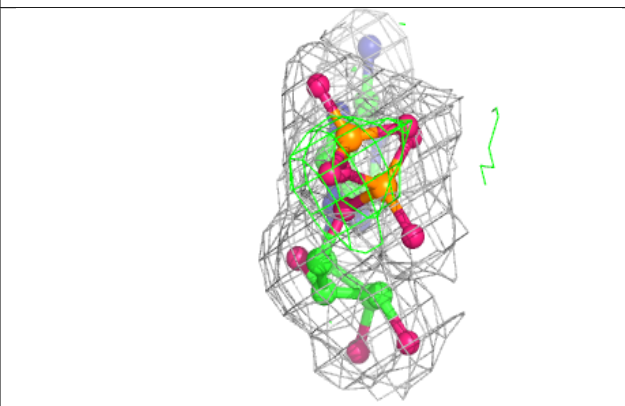
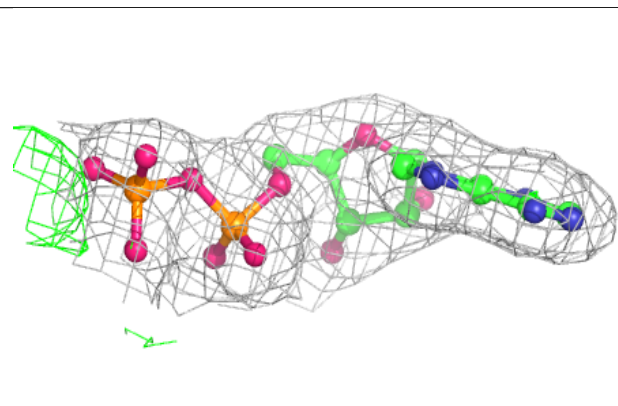
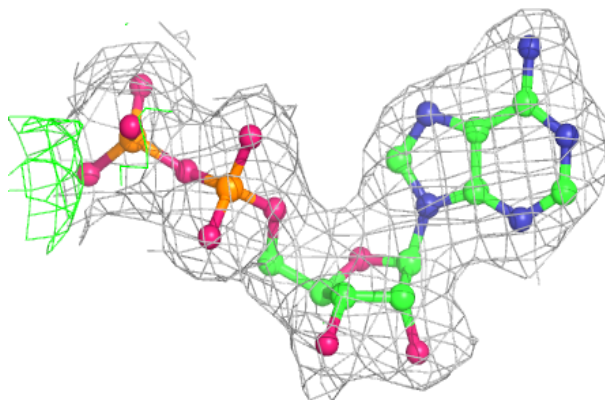
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 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 ADP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.