Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2026 – 07:29 pm BST

PDB ID	:	9QIL / pdb_00009qil
Title	:	Crystal Structure of human PMS1 N-terminal domain N309S with ADP
Authors	:	Thomsen, M.; Ganichkin, O.; Thieulin-Pardo, G.; Bandera, A.M.; Boudet, J.; Finley, M.; Felsenfeld, D.; Haque, T.; Prasad, B.C.; Monteagudo, E.; Vogt, T.; Stamford, A.
Deposited on	:	2025-03-17
Resolution	:	1.86 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

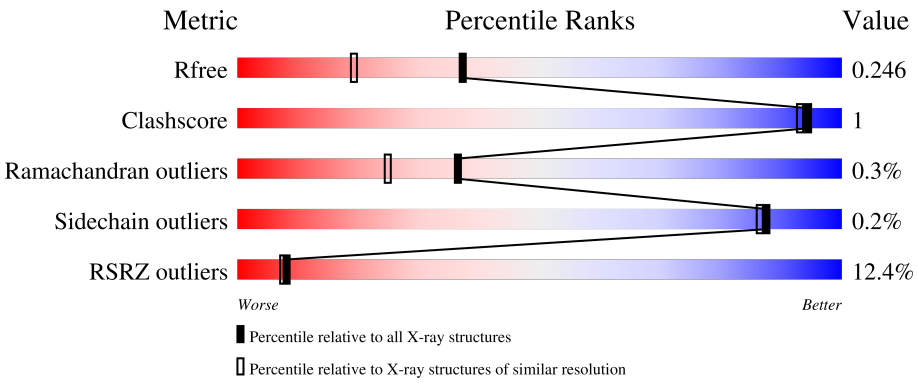
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 <=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	342	19% 97% •
1	B	342	14% 94% 5%
1	C	342	6% 96% •
1	D	342	10% 97% •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11868 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.

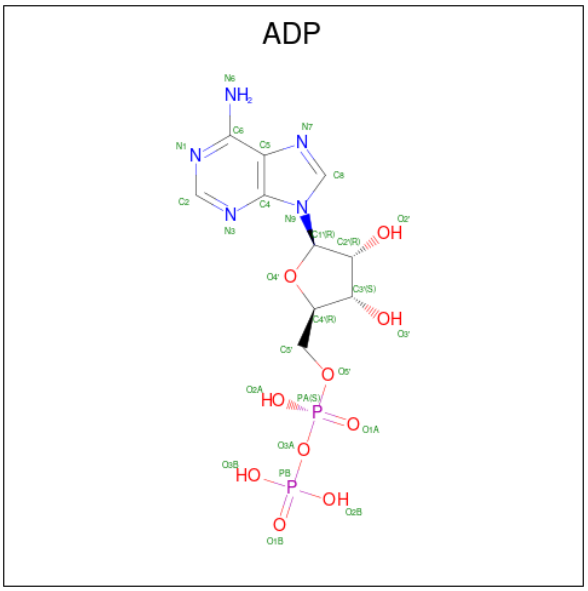
- Molecule 1 is a protein called PMS1 protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2708	1721	460	511	16	86	3	0
1	B	341	2730	1738	460	515	17	73	7	0
1	C	342	2712	1723	458	515	16	24	4	0
1	D	341	2683	1707	453	508	15	54	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P54277
A	309	SER	ASN	engineered mutation	UNP P54277
B	0	GLY	-	expression tag	UNP P54277
B	309	SER	ASN	engineered mutation	UNP P54277
C	0	GLY	-	expression tag	UNP P54277
C	309	SER	ASN	engineered mutation	UNP P54277
D	0	GLY	-	expression tag	UNP P54277
D	309	SER	ASN	engineered mutation	UNP P54277

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

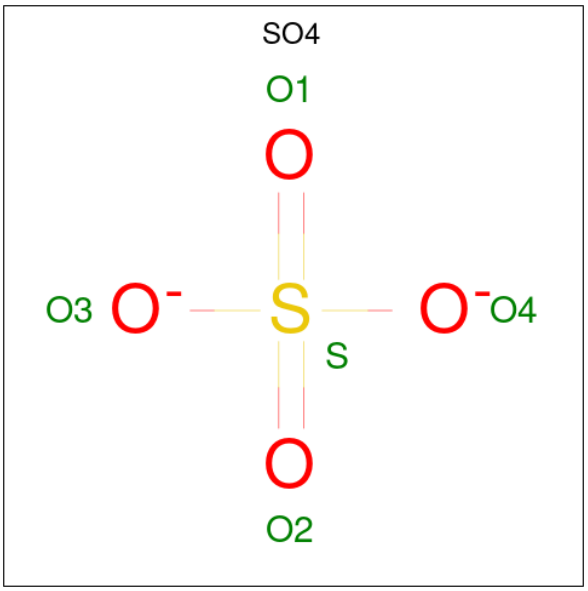


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

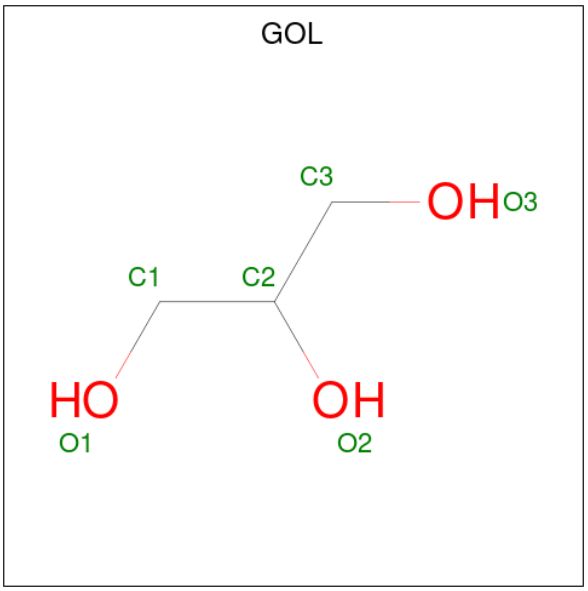


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	3	Total Cl 3 3	0	0
5	C	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

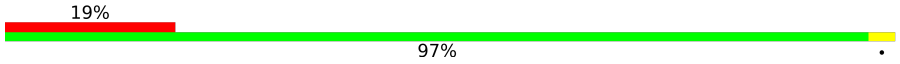
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	193	193	193	0	0
			Total	O		
7	B	189	189	189	0	0
			Total	O		
7	C	259	259	259	0	0
			Total	O		
7	D	215	215	215	0	0

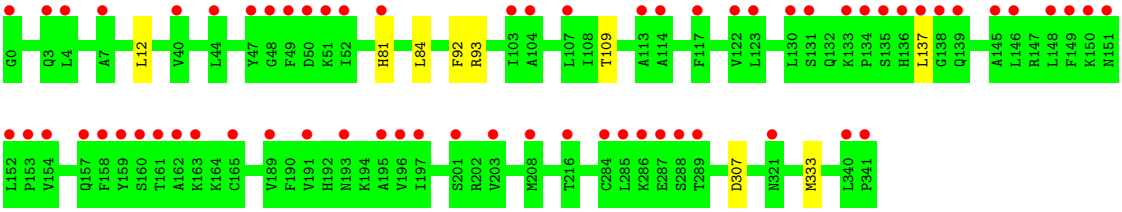
3 Residue-property plots (i)

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: PMS1 protein homolog 1

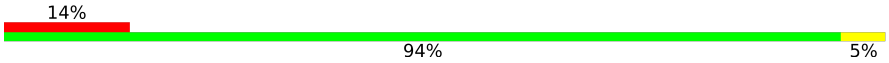
Chain A:

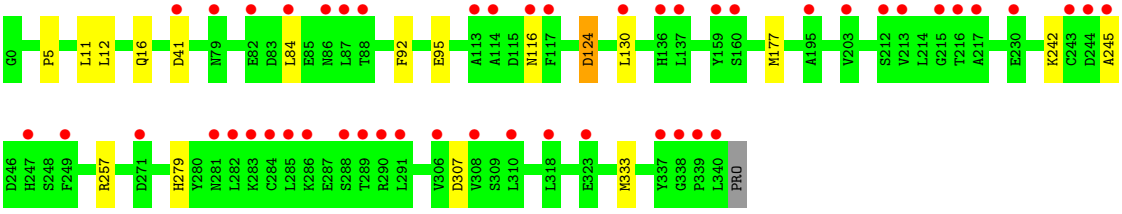




• Molecule 1: PMS1 protein homolog 1

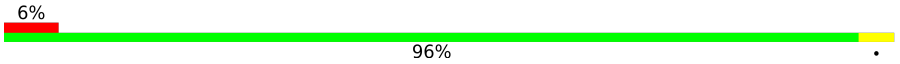
Chain B:

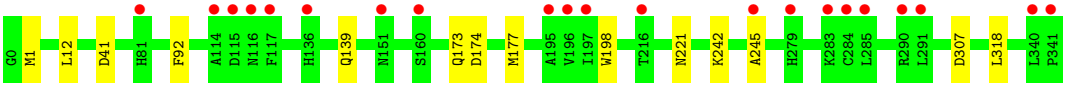




• Molecule 1: PMS1 protein homolog 1

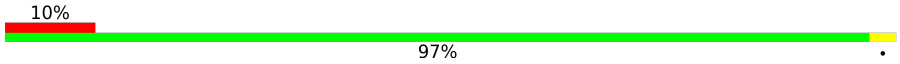
Chain C:

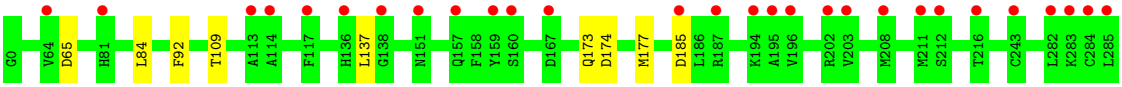


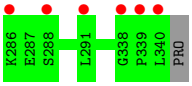


• Molecule 1: PMS1 protein homolog 1

Chain D:






K286
E287
S288
L291
G338
P339
L340
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	242.08Å 55.78Å 142.02Å 90.00° 124.07° 90.00°	Depositor
Resolution (Å)	117.64 – 1.86 117.64 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.9 (117.64-1.86) 98.9 (117.64-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.211 , 0.243 0.217 , 0.246	Depositor DCC
R_{free} test set	6620 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.029 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11868	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 64.34 % 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 8.4093e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ADP, MG, GOL, SO4, CL

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	0/2757	0.93	1/3726 (0.0%)
1	B	0.51	0/2778	0.93	4/3755 (0.1%)
1	C	0.50	0/2761	0.94	0/3732
1	D	0.50	0/2731	0.93	1/3692 (0.0%)
All	All	0.51	0/11027	0.93	6/14905 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	307	ASP	CA-CB-CG	6.24	118.84	112.60
1	D	185	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	116	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	307	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	124	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	95	GLU	CB-CG-CD	5.10	121.27	112.60

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	2708	0	2763	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2730	0	2787	10	0
1	C	2712	0	2760	13	0
1	D	2683	0	2738	6	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	0	0	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
6	A	12	0	16	0	0
6	B	12	0	16	1	0
6	C	12	0	16	0	0
6	D	12	0	16	0	0
7	A	193	0	0	0	0
7	B	189	0	0	1	0
7	C	259	0	0	0	0
7	D	215	0	0	0	0
All	All	11868	0	11160	29	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 1.

All (29) 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:C:139[B]:GLN:NE2	1:C:139[B]:GLN:HA	2.14	0.63
1:B:279:HIS:NE2	7:B:501:HOH:O	2.33	0.56
1:C:174:ASP:HA	1:C:177:MET:HE3	1.88	0.55
1:A:84:LEU:HD11	1:B:12:LEU:HD21	1.89	0.53
1:D:174:ASP:HA	1:D:177:MET:HE3	1.92	0.51
1:B:242:LYS:HB2	1:B:245:ALA:HB2	1.94	0.50
1:C:242:LYS:HB2	1:C:245:ALA:HB2	1.94	0.50
1:D:109:THR:HG21	1:D:137:LEU:HD12	1.95	0.48
1:C:12:LEU:HD21	1:D:84:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE3	1:D:65:ASP:HB3	1.95	0.47
1:A:333:MET:HA	1:A:333:MET:HE2	1.95	0.47
1:C:139[B]:GLN:NE2	1:C:139[B]:GLN:CA	2.74	0.46
1:C:177:MET:HG2	1:C:198:TRP:CZ2	2.52	0.45
1:B:177:MET:HE1	1:B:257:ARG:CZ	2.47	0.45
1:C:221:ASN:HB3	1:C:245:ALA:HB1	2.01	0.43
1:C:139[B]:GLN:HA	1:C:139[B]:GLN:HE21	1.80	0.43
1:A:81:HIS:CG	1:B:11:LEU:HD23	2.55	0.42
1:C:173:GLN:HG2	1:C:177:MET:HE2	2.00	0.42
1:D:174:ASP:HA	1:D:177:MET:CE	2.49	0.42
1:A:109:THR:HG21	1:A:137:LEU:HD12	2.00	0.42
1:A:93:ARG:HD2	1:B:16:GLN:HE22	1.85	0.41
1:C:174:ASP:HA	1:C:177:MET:CE	2.49	0.41
1:B:333:MET:HE2	1:B:333:MET:HA	2.02	0.41
1:A:12:LEU:HD21	1:B:84:LEU:HD11	2.01	0.41
1:B:5:PRO:HA	6:B:403:GOL:H2	2.03	0.41
1:C:307:ASP:HB3	1:C:318:LEU:HB3	2.02	0.41
1:C:139[B]:GLN:CA	1:C:139[B]:GLN:HE21	2.33	0.40
1:B:124:ASP:HB3	1:B:130:LEU:HG	2.02	0.40
1:D:173:GLN:HG2	1:D:177:MET:HE2	2.03	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	343/342 (100%)	335 (98%)	7 (2%)	1 (0%)	36	25
1	B	346/342 (101%)	338 (98%)	7 (2%)	1 (0%)	36	25
1	C	344/342 (101%)	339 (98%)	4 (1%)	1 (0%)	36	25
1	D	340/342 (99%)	333 (98%)	6 (2%)	1 (0%)	36	25
All	All	1373/1368 (100%)	1345 (98%)	24 (2%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	PHE
1	B	92	PHE
1	C	92	PHE
1	D	92	PHE

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	310/307 (101%)	310 (100%)	0	100	100
1	B	313/307 (102%)	312 (100%)	1 (0%)	86	85
1	C	311/307 (101%)	310 (100%)	1 (0%)	86	85
1	D	307/307 (100%)	307 (100%)	0	100	100
All	All	1241/1228 (101%)	1239 (100%)	2 (0%)	87	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	ASP
1	C	41	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	228	HIS
1	A	268	HIS
1	A	320	GLN
1	B	120	GLN
1	B	279	HIS
1	B	320	GLN
1	C	81	HIS
1	C	120	GLN

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Mol	Chain	Res	Type
1	C	228	HIS
1	C	321	ASN
1	C	331	ASN
1	D	79	ASN
1	D	81	HIS
1	D	132	GLN
1	D	268	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 13 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
6	GOL	C	405	-	5,5,5	0.11	0	5,5,5	0.39	0
6	GOL	D	403	-	5,5,5	0.12	0	5,5,5	0.39	0
4	SO4	A	406	-	4,4,4	0.38	0	6,6,6	0.05	0
6	GOL	B	403	-	5,5,5	0.11	0	5,5,5	0.32	0
6	GOL	A	408	-	5,5,5	0.12	0	5,5,5	0.45	0
2	ADP	A	401	3	27,29,29	0.35	0	42,45,45	0.46	0
2	ADP	B	401	3	27,29,29	0.40	0	42,45,45	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	B	404	-	5,5,5	0.11	0	5,5,5	0.38	0
6	GOL	C	403	-	5,5,5	0.13	0	5,5,5	0.35	0
6	GOL	D	405	-	5,5,5	0.10	0	5,5,5	0.31	0
4	SO4	A	403	-	4,4,4	0.39	0	6,6,6	0.05	0
2	ADP	D	401	3	27,29,29	0.40	0	42,45,45	0.52	0
2	ADP	C	401	3	27,29,29	0.41	0	42,45,45	0.50	0
6	GOL	A	405	-	5,5,5	0.09	0	5,5,5	0.34	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
6	GOL	C	405	-	-	2/4/4/4	-
6	GOL	D	403	-	-	2/4/4/4	-
6	GOL	B	403	-	-	2/4/4/4	-
6	GOL	A	408	-	-	2/4/4/4	-
2	ADP	A	401	3	-	3/16/32/32	0/3/3/3
2	ADP	B	401	3	-	3/16/32/32	0/3/3/3
6	GOL	B	404	-	-	2/4/4/4	-
6	GOL	C	403	-	-	0/4/4/4	-
6	GOL	D	405	-	-	2/4/4/4	-
2	ADP	D	401	3	-	3/16/32/32	0/3/3/3
2	ADP	C	401	3	-	3/16/32/32	0/3/3/3
6	GOL	A	405	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	PA-O3A-PB-O3B
2	B	401	ADP	PA-O3A-PB-O3B
2	C	401	ADP	PA-O3A-PB-O3B
2	D	401	ADP	PA-O3A-PB-O3B
6	B	403	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	404	GOL	O1-C1-C2-C3
6	C	405	GOL	C1-C2-C3-O3
6	D	403	GOL	C1-C2-C3-O3
6	D	405	GOL	C1-C2-C3-O3
6	A	408	GOL	C1-C2-C3-O3
6	D	405	GOL	O2-C2-C3-O3
6	B	404	GOL	O1-C1-C2-O2
6	C	405	GOL	O2-C2-C3-O3
6	D	403	GOL	O2-C2-C3-O3
6	B	403	GOL	O2-C2-C3-O3
2	A	401	ADP	PA-O3A-PB-O1B
2	B	401	ADP	PA-O3A-PB-O1B
2	C	401	ADP	PA-O3A-PB-O1B
2	D	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	PA-O3A-PB-O2B
2	B	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	PA-O3A-PB-O2B
2	D	401	ADP	PA-O3A-PB-O2B
6	A	408	GOL	O2-C2-C3-O3

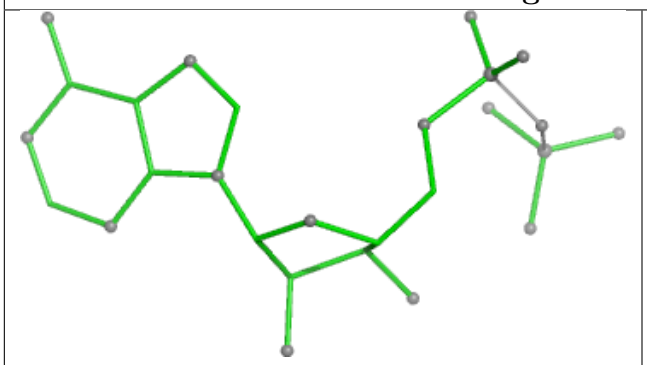
There are no ring outliers.

1 monomer is involved in 1 short contact:

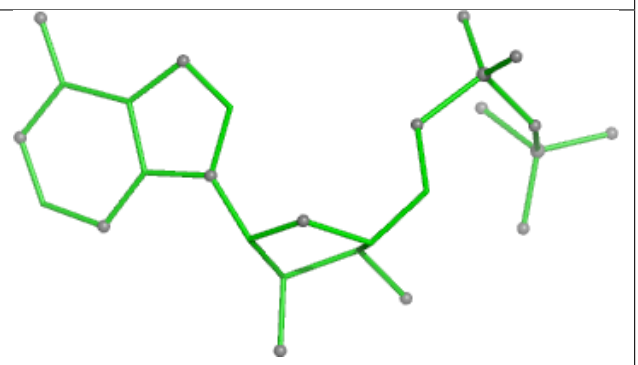
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	403	GOL	1	0

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.

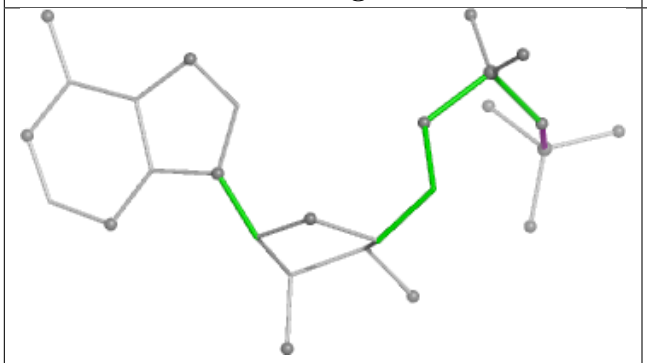
Ligand ADP A 401



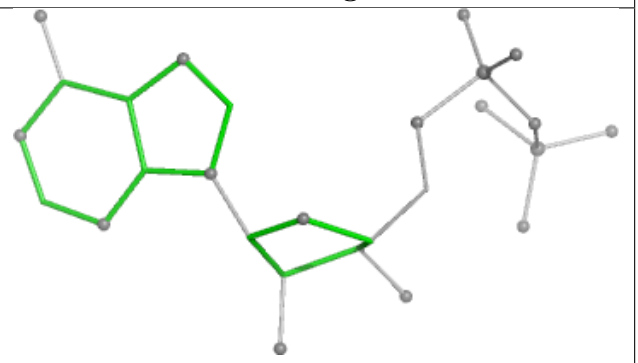
Bond lengths



Bond angles

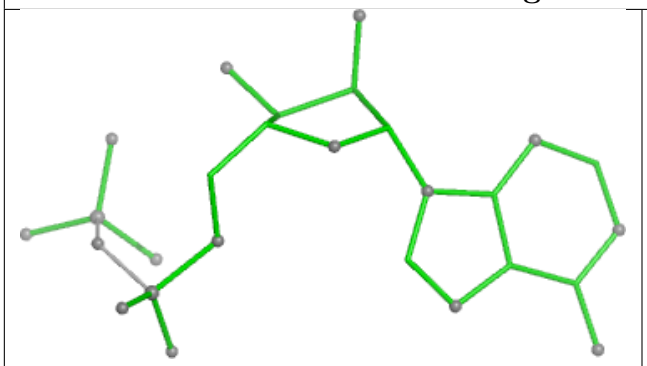


Torsions

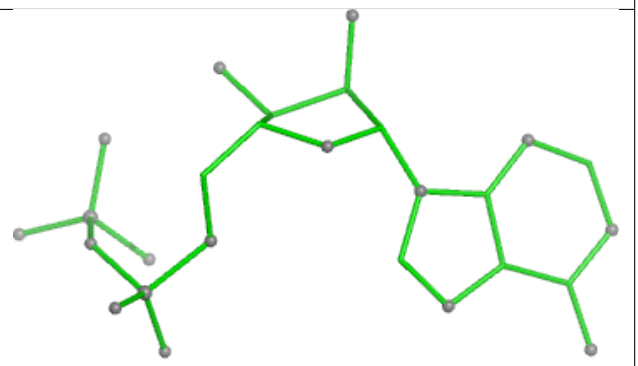


Rings

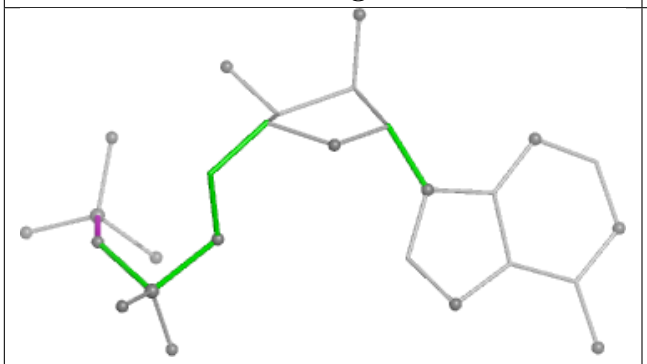
Ligand ADP B 401



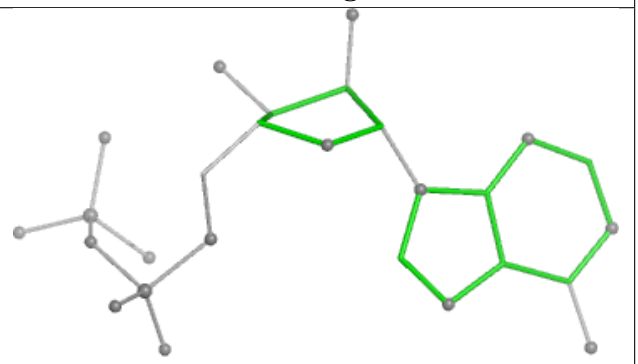
Bond lengths



Bond angles

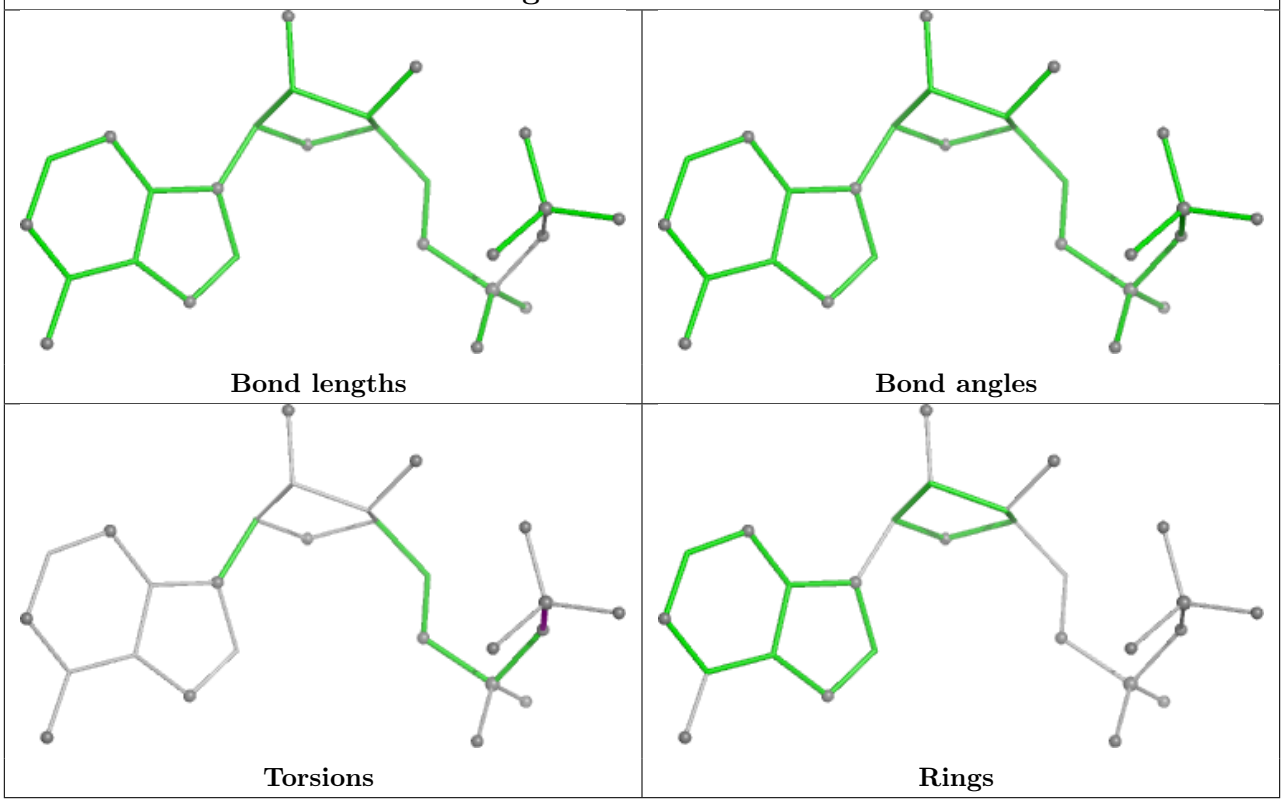


Torsions

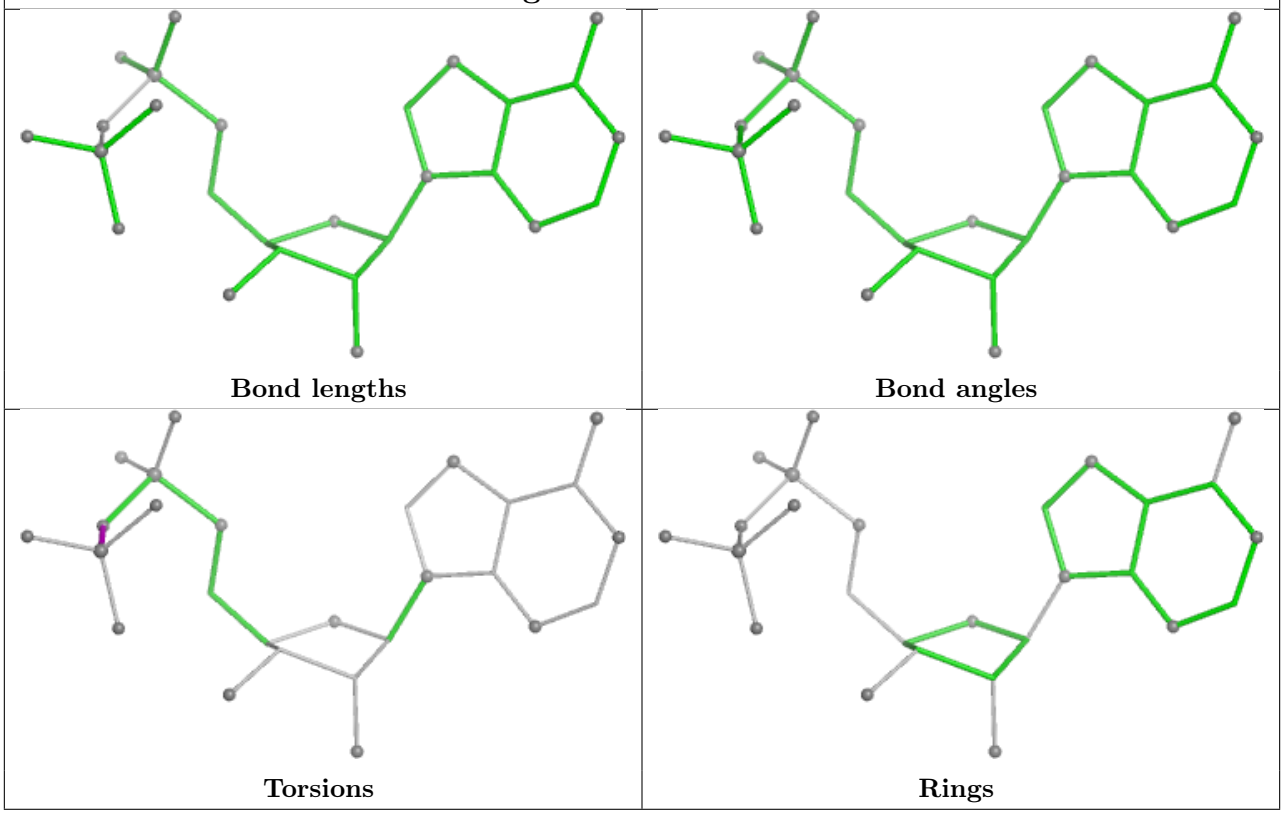


Rings

Ligand ADP D 401



Ligand ADP C 401



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(Å^2)	Q<0.9
1	A	342/342 (100%)	1.11	66 (19%)	3	2	14, 36, 62, 81	30 (8%)
1	B	341/342 (99%)	1.00	49 (14%)	6	6	13, 35, 58, 101	32 (9%)
1	C	342/342 (100%)	0.43	21 (6%)	27	29	11, 30, 48, 68	14 (4%)
1	D	341/342 (99%)	0.73	34 (9%)	12	12	19, 34, 52, 70	20 (5%)
All	All	1366/1368 (99%)	0.82	170 (12%)	8	7	11, 34, 57, 101	96 (7%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	LEU	5.7
1	B	340	LEU	5.5
1	B	339	PRO	5.0
1	A	149	PHE	4.8
1	A	114	ALA	4.8
1	B	282	LEU	4.7
1	D	285	LEU	4.6
1	A	152	LEU	4.5
1	C	340	LEU	4.5
1	C	341	PRO	4.5
1	A	154	VAL	4.4
1	B	245	ALA	4.4
1	A	117	PHE	4.3
1	A	130	LEU	4.2
1	A	134	PRO	4.2
1	B	284	CYS	4.1
1	B	216	THR	4.0
1	B	286	LYS	4.0
1	A	159	TYR	4.0
1	B	291	LEU	4.0
1	B	160	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	288	SER	4.0
1	A	47	TYR	3.9
1	A	137	LEU	3.9
1	A	146	LEU	3.9
1	C	285	LEU	3.9
1	A	341	PRO	3.9
1	A	162	ALA	3.9
1	D	339	PRO	3.9
1	A	284	CYS	3.9
1	A	150	LYS	3.8
1	A	136	HIS	3.7
1	B	289	THR	3.7
1	B	114	ALA	3.7
1	A	151	ASN	3.7
1	B	247	HIS	3.7
1	A	285	LEU	3.6
1	B	243[A]	CYS	3.6
1	A	131	SER	3.6
1	B	244	ASP	3.6
1	A	135	SER	3.5
1	B	283	LYS	3.5
1	D	338	GLY	3.5
1	B	290	ARG	3.4
1	A	48	GLY	3.4
1	A	287	GLU	3.4
1	B	159	TYR	3.4
1	D	340	LEU	3.4
1	A	153	PRO	3.4
1	C	117	PHE	3.4
1	B	230	GLU	3.3
1	D	114	ALA	3.3
1	A	104	ALA	3.3
1	B	338	GLY	3.3
1	A	133	LYS	3.2
1	A	122	VAL	3.2
1	A	158	PHE	3.2
1	C	114	ALA	3.1
1	D	195	ALA	3.1
1	D	203	VAL	3.1
1	B	337	TYR	3.1
1	A	40	VAL	3.1
1	A	138	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	148	LEU	3.1
1	D	284	CYS	3.1
1	D	113	ALA	3.1
1	C	279	HIS	3.0
1	C	160	SER	3.0
1	A	201	SER	3.0
1	D	288	SER	3.0
1	A	161	THR	3.0
1	D	157	GLN	3.0
1	A	107	LEU	2.9
1	B	130	LEU	2.9
1	A	196	VAL	2.9
1	A	0	GLY	2.9
1	B	84	LEU	2.9
1	B	116	ASN	2.9
1	D	196	VAL	2.8
1	A	52	ILE	2.8
1	B	136	HIS	2.8
1	A	208	MET	2.8
1	A	195	ALA	2.8
1	A	193	ASN	2.8
1	C	136	HIS	2.8
1	D	282	LEU	2.8
1	C	195	ALA	2.7
1	C	290	ARG	2.7
1	B	306	VAL	2.7
1	B	288	SER	2.7
1	D	160	SER	2.7
1	D	211	MET	2.6
1	A	50	ASP	2.6
1	D	202	ARG	2.6
1	C	216	THR	2.6
1	D	151	ASN	2.6
1	B	87	LEU	2.6
1	B	113	ALA	2.6
1	B	217	ALA	2.6
1	C	81	HIS	2.6
1	B	323[A]	GLU	2.6
1	A	160	SER	2.6
1	D	208	MET	2.5
1	A	123	LEU	2.5
1	A	145	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	81	HIS	2.5
1	A	289	THR	2.5
1	A	49	PHE	2.5
1	A	51	LYS	2.5
1	D	291	LEU	2.5
1	D	136	HIS	2.5
1	A	7	ALA	2.5
1	C	283	LYS	2.5
1	D	159	TYR	2.4
1	A	44	LEU	2.4
1	A	203	VAL	2.4
1	D	194	LYS	2.4
1	B	117	PHE	2.4
1	A	3	GLN	2.4
1	B	215	GLY	2.4
1	B	308	VAL	2.4
1	A	286	LYS	2.4
1	A	340	LEU	2.3
1	D	117	PHE	2.3
1	A	113	ALA	2.3
1	B	212	SER	2.3
1	A	165	CYS	2.3
1	B	310	LEU	2.3
1	C	291	LEU	2.3
1	B	249	PHE	2.3
1	B	86	ASN	2.3
1	D	283	LYS	2.3
1	B	82	GLU	2.3
1	B	318	LEU	2.3
1	D	216	THR	2.3
1	B	195	ALA	2.2
1	A	139	GLN	2.2
1	D	81	HIS	2.2
1	D	187	ARG	2.2
1	A	191	VAL	2.2
1	A	216	THR	2.2
1	B	88	THR	2.2
1	C	284	CYS	2.2
1	C	115	ASP	2.2
1	A	103	ILE	2.2
1	C	197	ILE	2.2
1	A	157	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	281	ASN	2.1
1	C	116	ASN	2.1
1	B	41	ASP	2.1
1	A	189	VAL	2.1
1	B	137	LEU	2.1
1	D	286	LYS	2.1
1	C	151	ASN	2.1
1	C	245	ALA	2.1
1	A	197	ILE	2.1
1	D	138	GLY	2.1
1	A	163	LYS	2.1
1	A	4	LEU	2.1
1	D	185	ASP	2.1
1	B	79	ASN	2.1
1	D	167	ASP	2.1
1	A	321[A]	ASN	2.0
1	B	213	VAL	2.0
1	D	243	CYS	2.0
1	B	271	ASP	2.0
1	D	212	SER	2.0
1	B	203	VAL	2.0
1	C	196	VAL	2.0
1	D	64	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.

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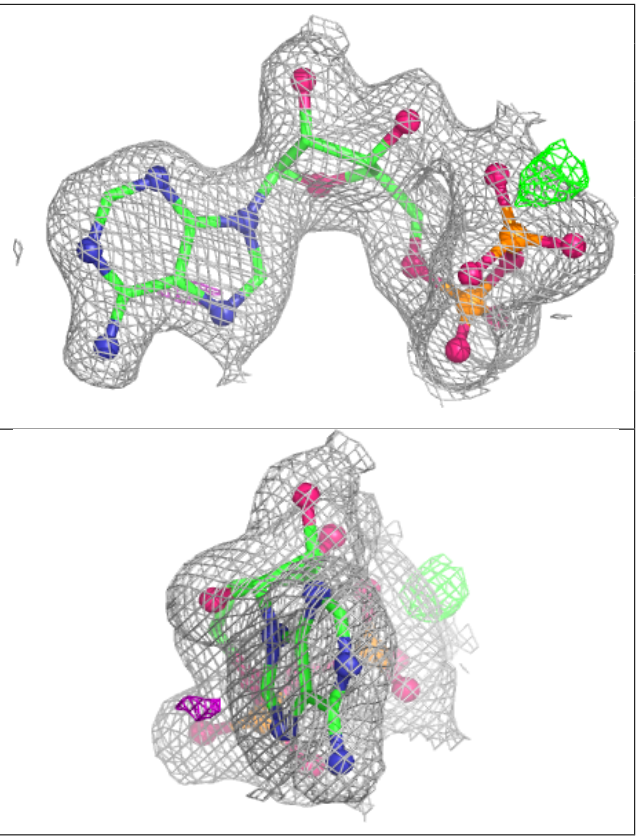
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	403	5/5	0.69	0.11	103,104,106,108	0
6	GOL	D	405	6/6	0.71	0.18	50,59,61,65	0
6	GOL	B	403	6/6	0.72	0.19	58,59,62,64	0
4	SO4	A	406	5/5	0.76	0.13	71,78,80,84	0
6	GOL	C	405	6/6	0.78	0.17	49,59,60,63	0
6	GOL	D	403	6/6	0.83	0.18	54,55,57,57	0
5	CL	C	407	1/1	0.83	0.14	76,76,76,76	0
5	CL	D	404	1/1	0.84	0.10	79,79,79,79	0
6	GOL	A	408	6/6	0.84	0.17	53,57,58,60	0
5	CL	B	406	1/1	0.84	0.12	83,83,83,83	0
5	CL	C	404	1/1	0.85	0.14	75,75,75,75	0
6	GOL	A	405	6/6	0.86	0.13	46,51,52,53	0
5	CL	B	407	1/1	0.87	0.16	73,73,73,73	0
5	CL	C	406	1/1	0.89	0.13	69,69,69,69	0
5	CL	A	404	1/1	0.89	0.12	67,67,67,67	0
6	GOL	C	403	6/6	0.89	0.18	49,53,55,57	0
5	CL	B	405	1/1	0.90	0.13	67,67,67,67	0
6	GOL	B	404	6/6	0.90	0.12	47,48,50,51	0
5	CL	A	407	1/1	0.95	0.10	52,52,52,52	0
3	MG	C	402	1/1	0.96	0.04	19,19,19,19	0
3	MG	A	402	1/1	0.96	0.05	23,23,23,23	0
3	MG	D	402	1/1	0.98	0.06	23,23,23,23	0
2	ADP	D	401	27/27	0.98	0.05	21,26,27,28	0
2	ADP	A	401	27/27	0.98	0.05	22,24,27,28	0
2	ADP	B	401	27/27	0.98	0.05	23,26,27,28	0
3	MG	B	402	1/1	0.99	0.06	23,23,23,23	0
2	ADP	C	401	27/27	0.99	0.04	18,19,20,21	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.

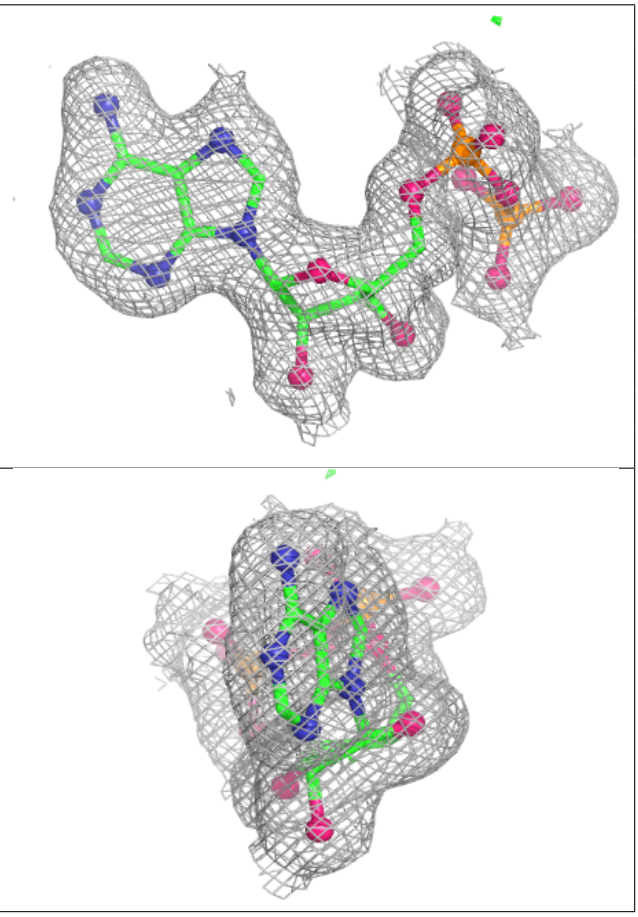
Electron density around ADP D 401:

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



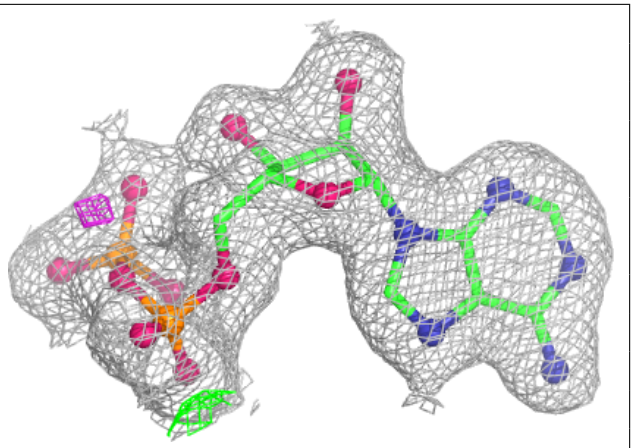
Electron density around ADP A 401:

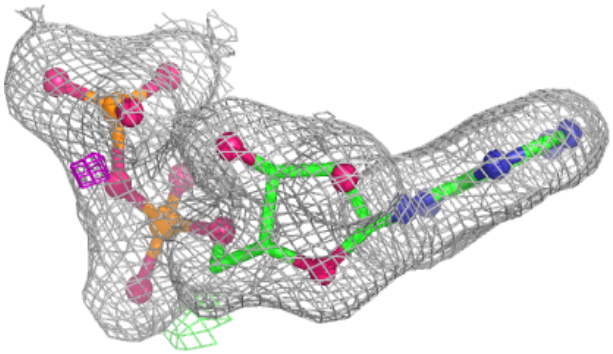
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

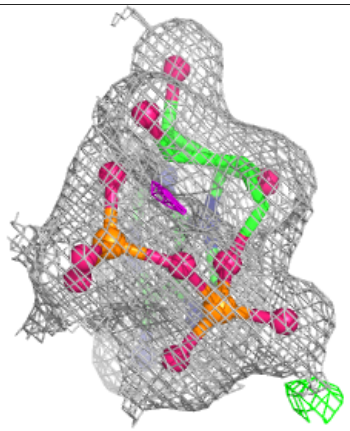


Electron density around ADP B 401:

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

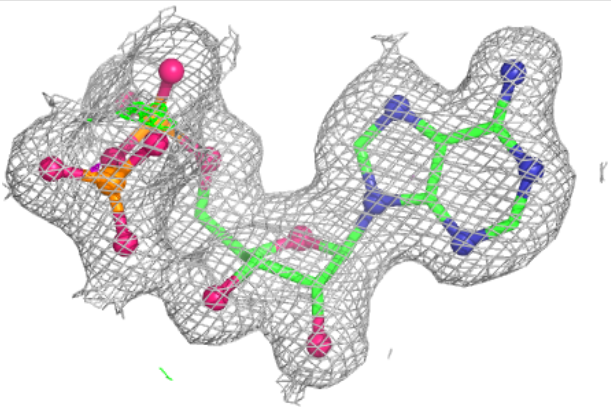


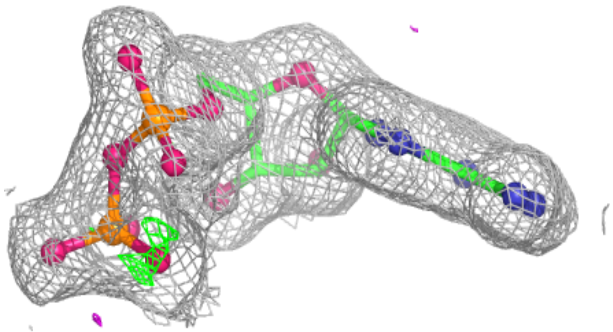


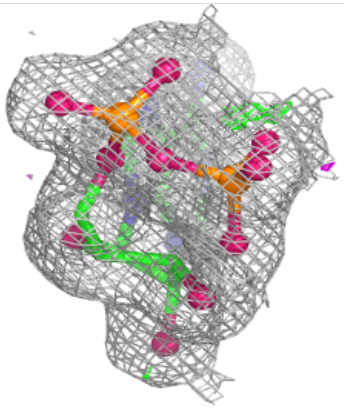


Electron density around ADP C 401:

$2mF_o$-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.