Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 11:52 PM UTC

PDB ID	:	7W78 / pdb_00007w78
Title	:	Heme exporter HrtBA in complex with Mg-AMPPNP
Authors	:	Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shirouzu, M.; Shiro, Y.
Deposited on	:	2021-12-04
Resolution	:	2.88 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:

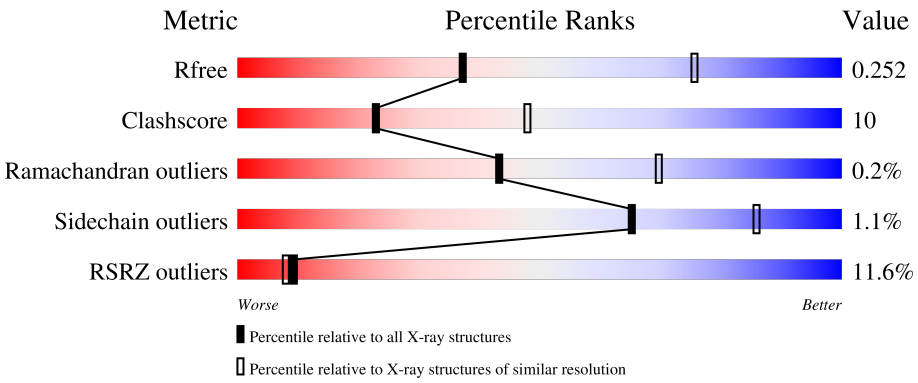
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	221	5% 77% 21% ·
2	B	344	16% 74% 26% ·

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4386 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 Putative ABC transport system, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1640	1023	299	315	3	4	1	0

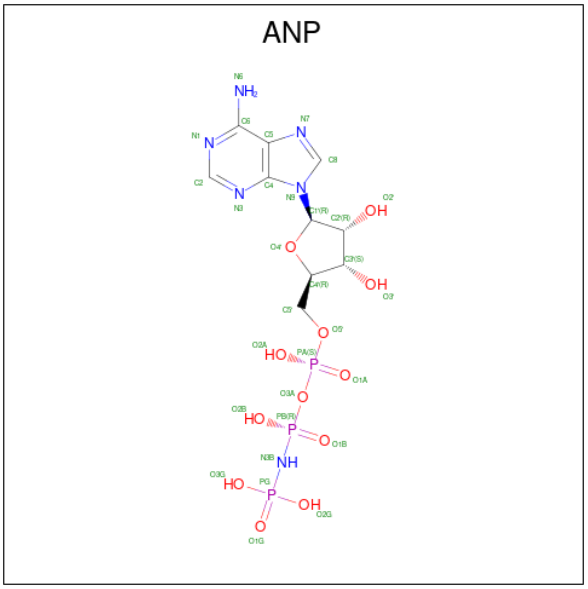
- Molecule 2 is a protein called Putative ABC transport system integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	344	2544	1637	426	476	5	20	2	0

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

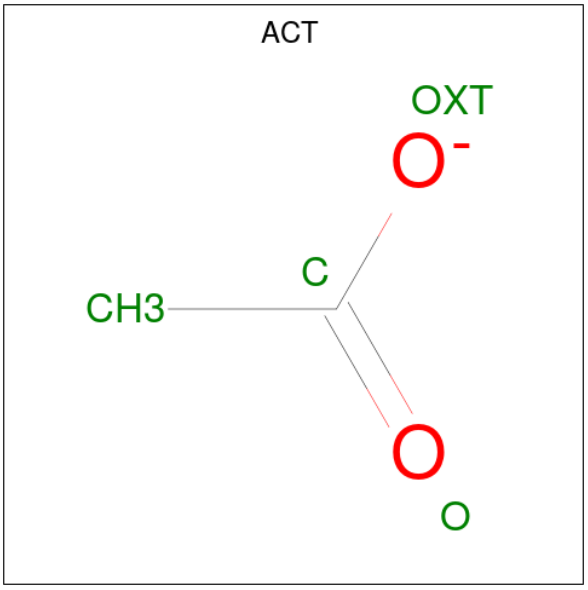
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



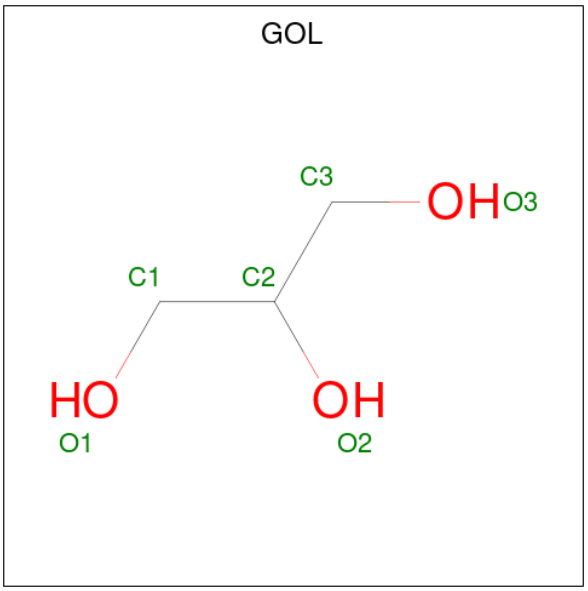
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	6	12	3	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



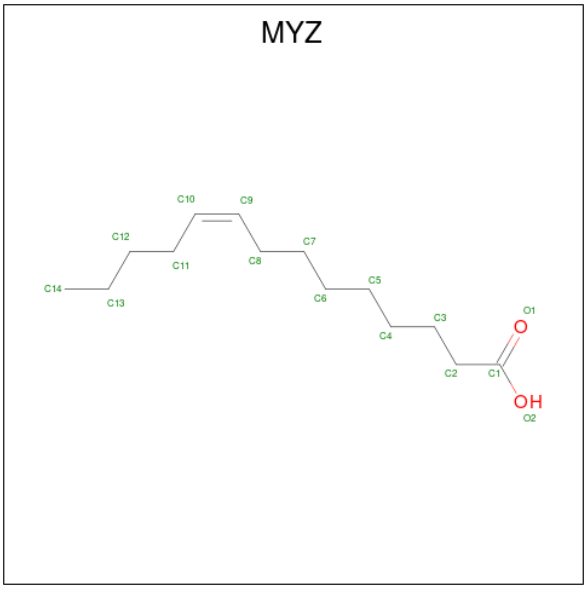
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	Total	C	O	0	0
			4	2	2		

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



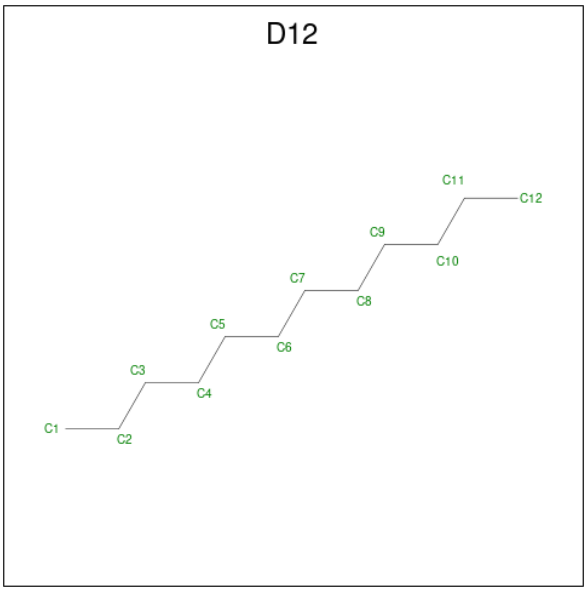
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	6	3	3	0	0

- Molecule 7 is Myristoleic acid (CCD ID: MYZ) (formula: $C_{14}H_{26}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
7	B	1	14	14	0	0
			Total	C		
7	B	1	14	14	0	0

- Molecule 8 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
8	B	1	12	12	0	0

- Molecule 9 is water.

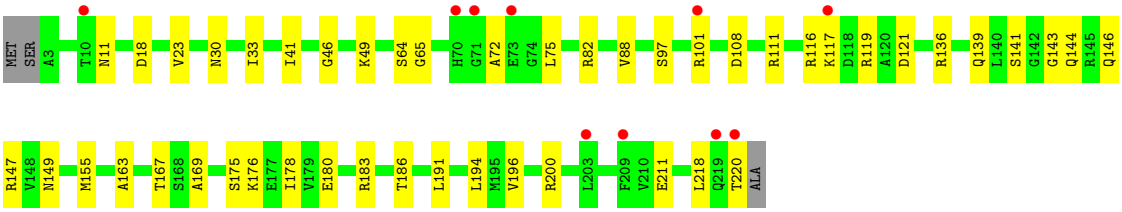
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	83	83	83	0	0
			Total	O		
9	B	33	33	33	0	0

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.

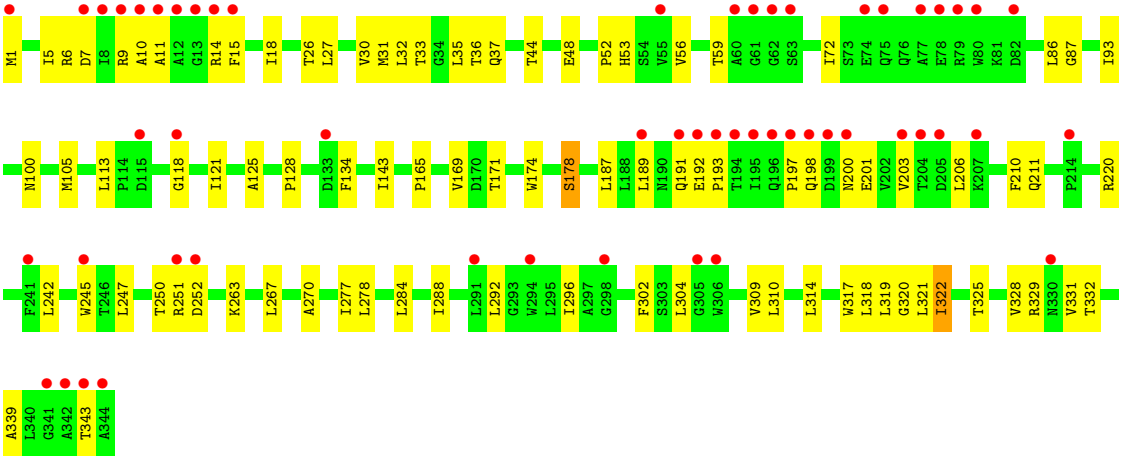
• Molecule 1: Putative ABC transport system, ATP-binding protein

Chain A:



• Molecule 2: Putative ABC transport system integral membrane protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	168.98Å 168.98Å 94.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.88 48.41 – 2.88	Depositor EDS
% Data completeness (in resolution range)	87.7 (48.41-2.88) 86.8 (48.41-2.88)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.221 , 0.251 0.220 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4386	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ACT, MYZ, D12, ANP, MG, GOL

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	0.36	0/1662	0.52	0/2249
2	B	0.30	0/2598	0.50	2/3553 (0.1%)
All	All	0.32	0/4260	0.51	2/5802 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	191	GLN	CA-C-N	-6.51	109.81	122.70
2	B	191	GLN	C-N-CA	-6.51	109.81	122.70

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	1640	0	1686	31	0
2	B	2544	0	2626	60	0
3	A	1	0	0	0	0
4	A	31	0	12	2	0
5	A	8	0	6	0	0
6	B	6	0	8	0	0
7	B	28	0	50	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	12	0	26	0	0
9	A	83	0	0	3	0
9	B	33	0	0	1	0
All	All	4386	0	4414	90	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 10.

All (90) 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)
2:B:251:ARG:NH1	2:B:252:ASP:OD2	2.03	0.90
1:A:136:ARG:H	1:A:139:GLN:HE21	1.19	0.86
1:A:146:GLN:HE22	1:A:169:ALA:H	1.29	0.80
2:B:329:ARG:NH2	9:B:501:HOH:O	2.16	0.78
1:A:167:THR:HB	1:A:175:SER:HB2	1.68	0.76
2:B:198:GLN:N	2:B:198:GLN:OE1	2.20	0.75
1:A:108:ASP:CG	1:A:116:ARG:HH21	1.97	0.73
2:B:309:VAL:HG12	2:B:310:LEU:HD23	1.72	0.72
1:A:30:ASN:ND2	9:A:401:HOH:O	2.21	0.71
1:A:108:ASP:OD1	1:A:116:ARG:NH2	2.20	0.71
2:B:15:PHE:HA	2:B:18:ILE:HG22	1.73	0.70
1:A:46:GLY:H	4:A:302:ANP:HNB1	1.39	0.70
2:B:53:HIS:CD2	2:B:192:GLU:HG2	2.27	0.69
2:B:44:THR:O	2:B:48:GLU:HG3	1.94	0.67
2:B:128:PRO:HG2	2:B:165:PRO:HB2	1.76	0.67
1:A:176:LYS:O	1:A:180:GLU:HG3	1.94	0.67
2:B:56:VAL:HG22	2:B:187:LEU:HB2	1.77	0.65
2:B:189:LEU:HD13	2:B:193:PRO:HD3	1.80	0.64
1:A:136:ARG:H	1:A:139:GLN:NE2	1.94	0.63
2:B:247:LEU:O	2:B:250:THR:HG23	2.00	0.62
1:A:141:SER:OG	1:A:144:GLN:HG3	2.00	0.61
1:A:200:ARG:NH2	1:A:211:GLU:OE1	2.34	0.61
2:B:6:ARG:O	2:B:9:ARG:HG2	2.01	0.60
2:B:197:PRO:HG3	2:B:203:VAL:HG23	1.84	0.60
2:B:174:TRP:O	2:B:178:SER:OG	2.20	0.60
2:B:15:PHE:HD2	2:B:277:ILE:HG13	1.67	0.59
2:B:304:LEU:CD2	2:B:309:VAL:HG23	2.32	0.59
1:A:41:ILE:HD11	1:A:194:LEU:HD22	1.86	0.58
2:B:27:LEU:O	2:B:31:MET:HG2	2.03	0.58
2:B:52:PRO:HD2	2:B:206:LEU:HD12	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101[B]:ARG:HD3	1:A:117:LYS:HE2	1.85	0.57
2:B:56:VAL:HG21	2:B:187:LEU:HD12	1.89	0.55
2:B:263:LYS:NZ	2:B:332:THR:O	2.39	0.55
1:A:82:ARG:HG3	1:A:111:ARG:HG2	1.89	0.54
2:B:72:ILE:HG12	2:B:187:LEU:HG	1.88	0.54
2:B:242:LEU:HD11	2:B:278:LEU:HD11	1.89	0.54
2:B:317:TRP:O	2:B:321:LEU:HG	2.07	0.54
2:B:125:ALA:HA	2:B:169:VAL:HG12	1.90	0.54
2:B:53:HIS:NE2	2:B:192:GLU:HG2	2.23	0.54
2:B:278:LEU:HD21	2:B:320:GLY:HA3	1.90	0.53
2:B:1:MET:O	2:B:5:ILE:HG22	2.09	0.53
2:B:302:PHE:CZ	2:B:304:LEU:HD12	2.45	0.52
1:A:33:ILE:HD11	1:A:194:LEU:HD21	1.92	0.51
1:A:143:GLY:O	1:A:147:ARG:HG3	2.09	0.51
2:B:250:THR:HG22	2:B:331:VAL:HG21	1.92	0.51
2:B:26:THR:O	2:B:30:VAL:HG23	2.09	0.51
1:A:49:LYS:N	4:A:302:ANP:O1B	2.38	0.50
2:B:304:LEU:HD22	2:B:309:VAL:HG23	1.92	0.50
1:A:211:GLU:HG2	1:A:218:LEU:HD12	1.94	0.49
1:A:146:GLN:O	1:A:149:ASN:HB3	2.12	0.49
1:A:186:THR:HA	1:A:191:LEU:HB2	1.95	0.49
1:A:101[B]:ARG:NE	1:A:121:ASP:OD1	2.40	0.49
2:B:304:LEU:HD21	2:B:309:VAL:HG23	1.95	0.48
2:B:339:ALA:O	2:B:343:THR:HG23	2.12	0.48
1:A:49:LYS:HD2	1:A:196:VAL:HG13	1.97	0.47
1:A:88:VAL:HB	1:A:163:ALA:HA	1.97	0.47
1:A:18:ASP:HB2	1:A:23:VAL:HG23	1.95	0.47
2:B:87:GLY:O	2:B:105:MET:HA	2.14	0.47
1:A:183:ARG:NH1	9:A:407:HOH:O	2.37	0.46
2:B:314:LEU:HD21	2:B:318:LEU:HD11	1.98	0.46
1:A:11:ASN:O	1:A:65:GLY:HA3	2.15	0.46
1:A:119:ARG:NH1	1:A:155:MET:O	2.48	0.46
1:A:101[A]:ARG:HD3	1:A:117:LYS:HE2	1.97	0.46
2:B:288:ILE:O	2:B:292:LEU:HB2	2.16	0.46
1:A:220:THR:HA	9:A:458:HOH:O	2.16	0.45
2:B:319:LEU:O	2:B:322:ILE:HG13	2.17	0.45
2:B:189:LEU:CD1	2:B:193:PRO:HD3	2.46	0.45
2:B:32:LEU:O	2:B:36:THR:HG23	2.17	0.45
2:B:270:ALA:CB	2:B:328:VAL:HG21	2.47	0.45
2:B:284:LEU:C	2:B:284:LEU:HD23	2.42	0.45
2:B:113:LEU:HD21	2:B:121:ILE:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:LEU:HD21	2:B:105:MET:HE3	1.99	0.44
1:A:97:SER:OG	2:B:7:ASP:OD1	2.28	0.44
2:B:9:ARG:HG3	2:B:10:ALA:N	2.26	0.44
2:B:15:PHE:CE2	2:B:245:TRP:HZ2	2.35	0.44
2:B:211:GLN:HE22	2:B:220:ARG:NH1	2.16	0.44
2:B:59:THR:O	2:B:200:ASN:HB2	2.18	0.44
2:B:33:THR:O	2:B:37:GLN:HG3	2.18	0.43
2:B:15:PHE:HA	2:B:18:ILE:CG2	2.45	0.43
2:B:267:LEU:HD11	2:B:325:THR:HG23	2.00	0.43
2:B:100:ASN:HB2	2:B:134:PHE:HE2	1.83	0.42
2:B:319:LEU:HD23	2:B:319:LEU:HA	1.89	0.42
2:B:15:PHE:CD2	2:B:277:ILE:HG13	2.50	0.42
2:B:197:PRO:HB2	2:B:201:GLU:HB2	2.01	0.42
2:B:93:ILE:HD11	2:B:143:ILE:HD12	2.02	0.42
2:B:11:ALA:HB1	2:B:14:ARG:HG2	2.02	0.42
2:B:296:ILE:HG12	2:B:296:ILE:O	2.21	0.41
2:B:35:LEU:HD23	2:B:302:PHE:HD2	1.86	0.41
2:B:210:PHE:N	2:B:210:PHE:CD1	2.85	0.41
1:A:72:ALA:O	1:A:75:LEU:HB2	2.21	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	217/221 (98%)	211 (97%)	6 (3%)	0	100 100
2	B	344/344 (100%)	328 (95%)	15 (4%)	1 (0%)	36 62
All	All	561/565 (99%)	539 (96%)	21 (4%)	1 (0%)	43 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	GLY

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	174/176 (99%)	172 (99%)	2 (1%)	65	86
2	B	267/265 (101%)	264 (99%)	3 (1%)	65	86
All	All	441/441 (100%)	436 (99%)	5 (1%)	65	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	178	ILE
2	B	171	THR
2	B	178	SER
2	B	322	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	146	GLN
1	A	157	ASN
1	A	159	GLN
2	B	163	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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
7	MYZ	B	402	-	13,13,15	0.40	0	12,12,15	0.62	0
5	ACT	A	304	-	3,3,3	0.81	0	3,3,3	1.41	0
4	ANP	A	302	3	33,33,33	3.21	17 (51%)	45,52,52	2.11	13 (28%)
7	MYZ	B	403	-	13,13,15	0.43	0	12,12,15	0.57	0
6	GOL	B	401	-	5,5,5	0.37	0	5,5,5	0.30	0
8	D12	B	404	-	11,11,11	0.38	0	10,10,10	0.68	0
5	ACT	A	303	-	3,3,3	0.81	0	3,3,3	1.36	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
7	MYZ	B	402	-	-	1/11/11/13	-
4	ANP	A	302	3	-	4/18/38/38	0/3/3/3
7	MYZ	B	403	-	-	6/11/11/13	-
6	GOL	B	401	-	-	4/4/4/4	-
8	D12	B	404	-	-	3/9/9/9	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	ANP	O4'-C1'	8.66	1.62	1.42
4	A	302	ANP	C2'-C1'	-7.19	1.30	1.53
4	A	302	ANP	O4'-C4'	-6.36	1.30	1.45
4	A	302	ANP	PA-O3A	5.50	1.65	1.59
4	A	302	ANP	PB-O3A	4.97	1.65	1.59
4	A	302	ANP	C6-N6	4.40	1.45	1.34
4	A	302	ANP	PB-O1B	3.23	1.51	1.46
4	A	302	ANP	PG-O1G	3.20	1.51	1.46
4	A	302	ANP	O2'-C2'	2.86	1.50	1.43
4	A	302	ANP	C5-C4	-2.85	1.34	1.39
4	A	302	ANP	O3'-C3'	-2.79	1.36	1.43
4	A	302	ANP	C5-N7	-2.78	1.34	1.39
4	A	302	ANP	PB-N3B	2.57	1.70	1.63
4	A	302	ANP	PG-N3B	2.47	1.69	1.63
4	A	302	ANP	C8-N9	-2.25	1.33	1.37
4	A	302	ANP	PG-O2G	-2.10	1.51	1.56
4	A	302	ANP	PG-O3G	-2.02	1.51	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	302	ANP	N3-C2-N1	-5.45	120.33	128.58
4	A	302	ANP	C5-C4-N3	-5.41	119.26	126.72
4	A	302	ANP	N6-C6-N1	-4.20	109.02	118.38
4	A	302	ANP	N9-C8-N7	-3.96	108.32	113.94
4	A	302	ANP	N3-C4-N9	3.87	133.74	127.17
4	A	302	ANP	O1B-PB-N3B	-3.67	106.37	111.77
4	A	302	ANP	C2-N3-C4	3.38	120.09	111.83
4	A	302	ANP	C5-C6-N6	3.08	130.91	123.29
4	A	302	ANP	C5-N7-C8	2.69	107.68	103.45
4	A	302	ANP	O1G-PG-N3B	-2.63	107.90	111.77
4	A	302	ANP	C6-C5-C4	2.47	120.55	117.18
4	A	302	ANP	C4-N9-C8	2.37	108.22	105.74
4	A	302	ANP	C1'-N9-C8	-2.05	122.54	127.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	ANP	PB-N3B-PG-O1G
4	A	302	ANP	PG-N3B-PB-O1B
6	B	401	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	401	GOL	O1-C1-C2-C3
6	B	401	GOL	C1-C2-C3-O3
8	B	404	D12	C4-C5-C6-C7
7	B	403	MYZ	C4-C5-C6-C7
8	B	404	D12	C5-C6-C7-C8
6	B	401	GOL	O2-C2-C3-O3
7	B	403	MYZ	C1-C2-C3-C4
7	B	403	MYZ	C2-C3-C4-C5
4	A	302	ANP	O4'-C4'-C5'-O5'
7	B	403	MYZ	C7-C8-C9-C10
7	B	403	MYZ	C5-C6-C7-C8
7	B	402	MYZ	C7-C8-C9-C10
7	B	403	MYZ	C9-C10-C11-C12
8	B	404	D12	C1-C2-C3-C4
4	A	302	ANP	PG-N3B-PB-O3A

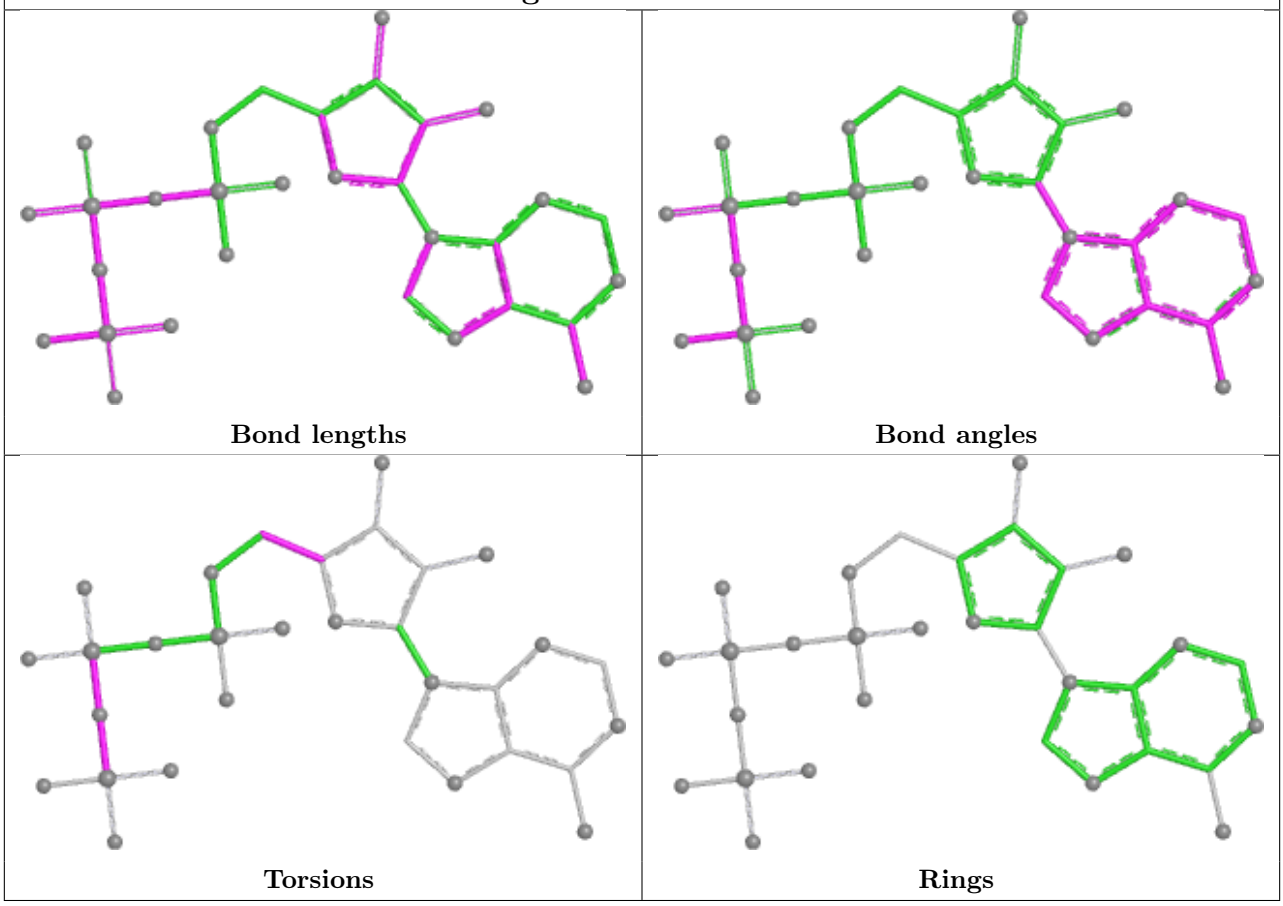
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	ANP	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 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 ANP A 302



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	218/221 (98%)	0.42	10 (4%)	37	29	21, 35, 54, 67	2 (0%)
2	B	344/344 (100%)	0.90	55 (15%)	5	4	21, 43, 75, 103	7 (2%)
All	All	562/565 (99%)	0.71	65 (11%)	9	8	21, 41, 68, 103	9 (1%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	342	ALA	6.5
1	A	220	THR	5.9
2	B	344	ALA	5.6
1	A	219	GLN	5.3
2	B	306[A]	TRP	5.3
2	B	191	GLN	5.1
2	B	78	GLU	5.0
2	B	195	ILE	4.8
2	B	10	ALA	4.4
2	B	79	ARG	4.4
2	B	14	ARG	4.1
2	B	198	GLN	4.0
2	B	74	GLU	4.0
2	B	194	THR	4.0
1	A	71	GLY	3.9
2	B	252	ASP	3.9
2	B	341	GLY	3.8
2	B	196	GLN	3.8
1	A	117	LYS	3.7
2	B	7	ASP	3.7
2	B	291[A]	LEU	3.7
2	B	15	PHE	3.7
2	B	193	PRO	3.6
2	B	245	TRP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	204	THR	3.5
2	B	75	GLN	3.4
2	B	200	ASN	3.3
2	B	9	ARG	3.2
2	B	207	LYS	3.2
2	B	80	TRP	3.2
2	B	343	THR	3.1
1	A	209	PHE	3.1
2	B	77	ALA	3.0
2	B	241	PHE	3.0
2	B	251	ARG	3.0
2	B	330	ASN	2.9
2	B	61	GLY	2.9
2	B	13	GLY	2.8
2	B	82	ASP	2.6
2	B	197	PRO	2.6
2	B	12	ALA	2.6
2	B	8	ILE	2.6
1	A	70	HIS	2.5
2	B	298	GLY	2.5
2	B	133	ASP	2.5
2	B	62	GLY	2.5
2	B	63	SER	2.4
1	A	101[A]	ARG	2.3
2	B	1	MET	2.3
2	B	115	ASP	2.3
2	B	214	PRO	2.3
2	B	192	GLU	2.2
2	B	11	ALA	2.2
2	B	203	VAL	2.2
1	A	73	GLU	2.2
1	A	203	LEU	2.2
2	B	205	ASP	2.1
2	B	118	GLY	2.1
2	B	199	ASP	2.1
2	B	294	TRP	2.0
2	B	189	LEU	2.0
2	B	305	GLY	2.0
1	A	10	THR	2.0
2	B	60	ALA	2.0
2	B	55	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

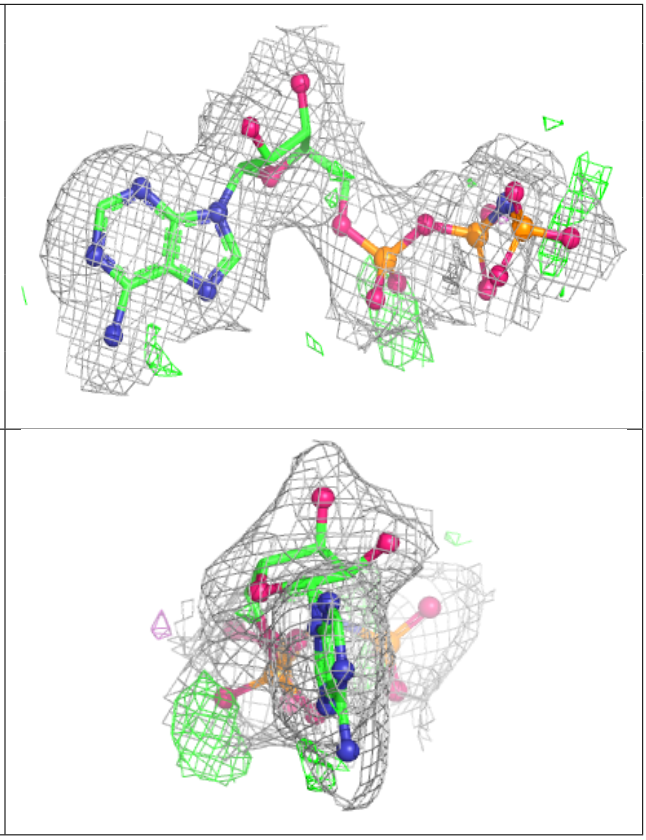
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	401	6/6	0.47	0.27	65,65,65,65	0
8	D12	B	404	12/12	0.69	0.33	51,51,51,51	0
7	MYZ	B	403	14/16	0.74	0.29	49,49,49,49	0
7	MYZ	B	402	14/16	0.75	0.28	51,51,51,51	0
5	ACT	A	304	4/4	0.89	0.18	49,49,49,49	0
5	ACT	A	303	4/4	0.97	0.10	31,31,31,31	0
4	ANP	A	302	31/31	0.98	0.06	23,23,23,23	0
3	MG	A	301	1/1	0.99	0.04	24,24,24,24	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 ANP A 302:

$2mF_o$-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.