Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 04:08 PM EDT

PDB ID	:	9MFS / pdb_00009mfs
Title	:	Cat DHX9 in Complex with ATX968 and ADP
Authors	:	Lockbaum, G.J.; Lee, Y.-T.; Sickmier, E.A.; Boriack-Sjodin, P.A.; Grigoriu, S.
Deposited on	:	2024-12-10
Resolution	:	2.43 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

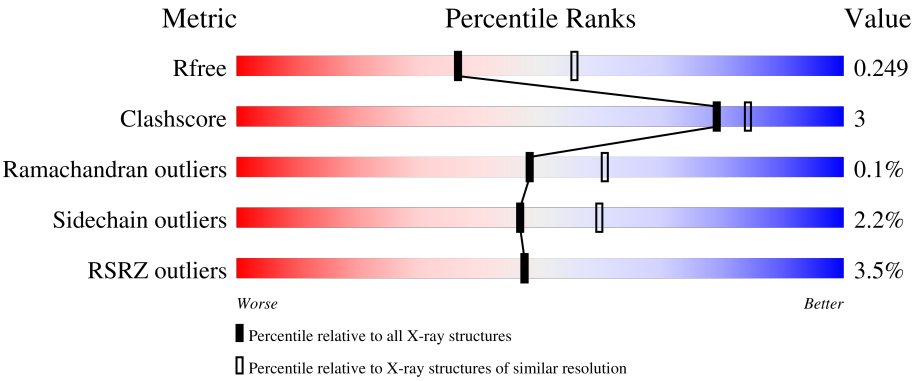
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.43 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	1010	3% 77% 7% 15%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7297 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.

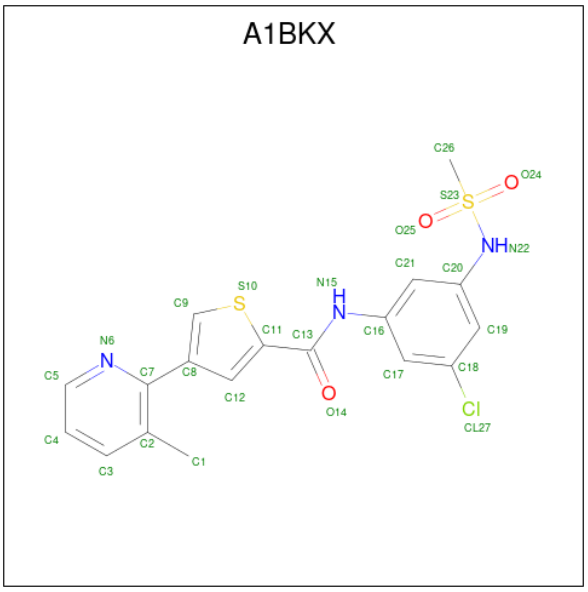
- Molecule 1 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	857	6834	4358	1176	1255	45	0	5	0

There are 9 discrepancies between the modelled and reference sequences:

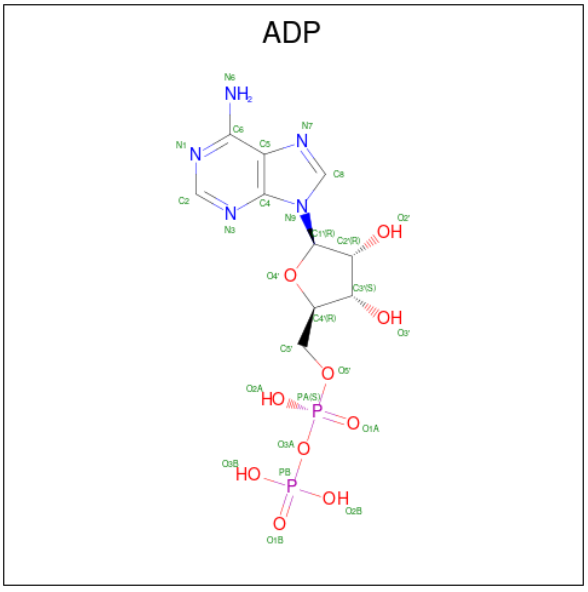
Chain	Residue	Modelled	Actual	Comment	Reference
A	150	MET	-	initiating methionine	UNP M3WPI7
A	1152	ASP	-	expression tag	UNP M3WPI7
A	1153	TYR	-	expression tag	UNP M3WPI7
A	1154	LYS	-	expression tag	UNP M3WPI7
A	1155	ASP	-	expression tag	UNP M3WPI7
A	1156	ASP	-	expression tag	UNP M3WPI7
A	1157	ASP	-	expression tag	UNP M3WPI7
A	1158	ASP	-	expression tag	UNP M3WPI7
A	1159	LYS	-	expression tag	UNP M3WPI7

- Molecule 2 is (4M)-N-[3-chloro-5-(methanesulfonamido)phenyl]-4-(3-methylpyridin-2-yl)thiophene-2-carboxamide (CCD ID: A1BKX) (formula: $C_{18}H_{16}ClN_3O_3S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			27	18	1	3	3	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

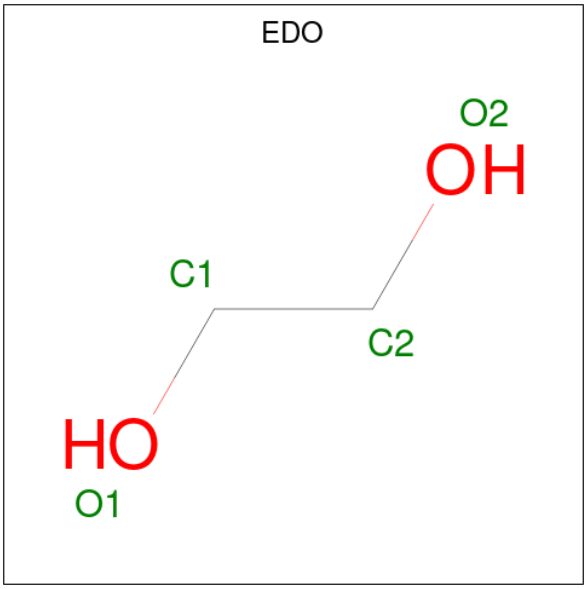


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

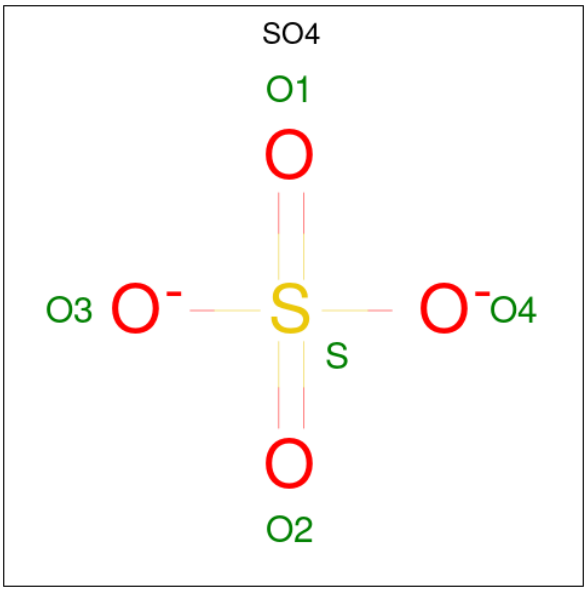
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is water.

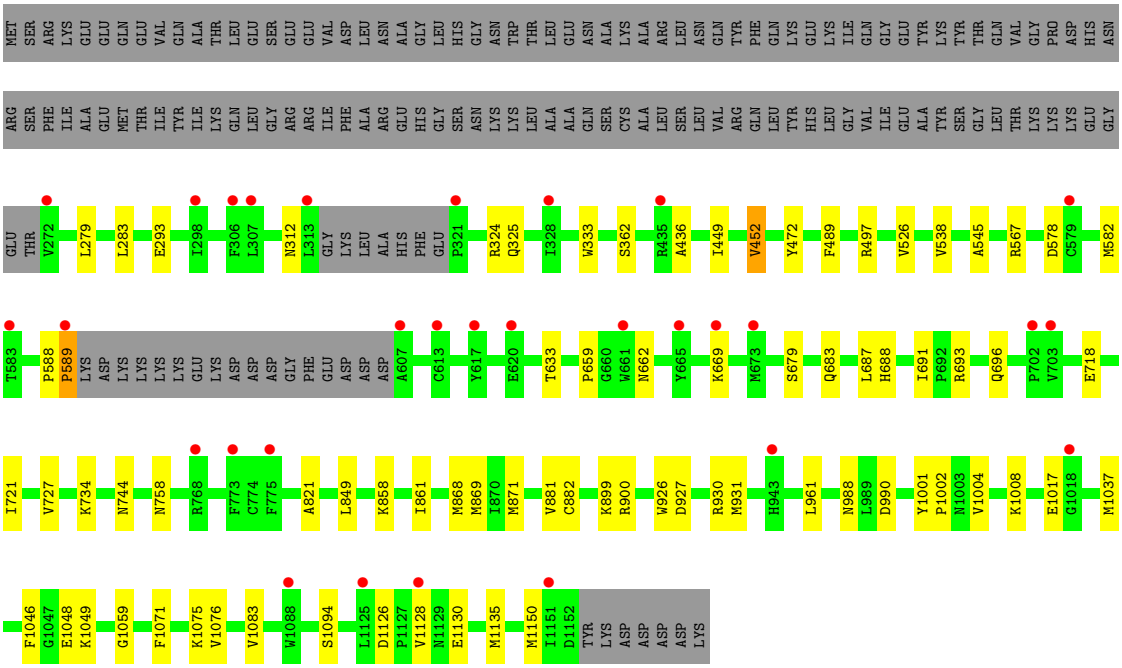
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	359	Total O 359 359	0	3

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: RNA helicase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.45Å 86.45Å 351.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.50 – 2.43 54.50 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.50-2.43) 100.0 (54.50-2.43)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.246 0.198 , 0.249	Depositor DCC
R_{free} test set	2496 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7297	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, A1BKX, MG, CL, SO4, EDO

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	1.02	0/6996	1.37	5/9500 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	633	THR	CB-CA-C	5.55	116.14	109.31
1	A	990	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	452	VAL	CA-C-N	5.29	127.68	120.54
1	A	452	VAL	C-N-CA	5.29	127.68	120.54
1	A	727	VAL	N-CA-C	-5.06	108.57	113.53

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	6834	0	6876	36	0
2	A	27	0	0	0	0
3	A	27	0	12	0	0
4	A	1	0	0	0	0
5	A	28	0	42	3	0
6	A	20	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	A	359	0	0	2	0
All	All	7297	0	6930	36	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 (36) 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:688:HIS:CE1	1:A:691:ILE:HG23	2.36	0.61
1:A:472:TYR:HA	1:A:489:PHE:O	2.02	0.59
1:A:1126:ASP:OD1	1:A:1128:VAL:HG12	2.04	0.58
1:A:1135:MET:HA	1:A:1135:MET:HE2	1.86	0.58
1:A:683:GLN:HA	1:A:683:GLN:OE1	2.06	0.54
1:A:333:TRP:NE1	1:A:538:VAL:HG23	2.21	0.54
1:A:988:ASN:OD1	5:A:1210:EDO:H22	2.08	0.54
1:A:871:MET:HE1	1:A:1071:PHE:CE1	2.43	0.52
1:A:497:ARG:NH2	8:A:1309:HOH:O	2.42	0.52
1:A:687:LEU:HD21	1:A:721:ILE:HD11	1.92	0.51
1:A:900:ARG:H	5:A:1208:EDO:H22	1.77	0.50
1:A:869:MET:HE1	1:A:961:LEU:HB3	1.93	0.49
1:A:868:MET:HE3	1:A:881[A]:VAL:HG13	1.94	0.49
1:A:312:ASN:HD21	1:A:1076:VAL:H	1.60	0.49
1:A:1001:TYR:CD1	1:A:1002:PRO:HA	2.47	0.49
1:A:1001:TYR:CG	1:A:1002:PRO:HA	2.48	0.49
1:A:718:GLU:OE2	1:A:758:ASN:ND2	2.44	0.48
1:A:588:PRO:O	1:A:589:PRO:C	2.55	0.48
1:A:449:ILE:HD11	1:A:696:GLN:OE1	2.13	0.47
1:A:900:ARG:HH11	5:A:1208:EDO:H21	1.79	0.47
1:A:1046:PHE:HA	1:A:1059:GLY:O	2.15	0.46
1:A:362:SER:HA	1:A:436:ALA:HB3	1.97	0.46
1:A:324:ARG:HG2	1:A:325:GLN:N	2.31	0.45
1:A:869:MET:HE3	1:A:882:CYS:SG	2.56	0.45
1:A:744:ASN:O	1:A:1049:LYS:NZ	2.49	0.45
1:A:858:LYS:NZ	8:A:1314:HOH:O	2.50	0.45
1:A:926:TRP:CZ2	1:A:930:ARG:HD3	2.51	0.44
1:A:927:ASP:OD1	1:A:930:ARG:NH1	2.40	0.43
1:A:659:PRO:HG3	1:A:734:LYS:HB2	1.99	0.43
1:A:279:LEU:CD1	1:A:283:LEU:HD23	2.49	0.42
1:A:849:LEU:HD12	1:A:849:LEU:HA	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:HD21	1:A:1075:LYS:HA	1.86	0.41
1:A:452:VAL:HG11	1:A:693:ARG:CZ	2.50	0.41
1:A:567:ARG:HH11	1:A:567:ARG:HG3	1.85	0.41
1:A:526:VAL:HG22	1:A:821:ALA:HA	2.03	0.41
1:A:578:ASP:O	1:A:582:MET:HG2	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	856/1010 (85%)	826 (96%)	29 (3%)	1 (0%)	48 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	ALA

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	765/891 (86%)	748 (98%)	17 (2%)	47 60

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	GLU
1	A	589	PRO
1	A	662	ASN
1	A	669	LYS
1	A	679	SER
1	A	861	ILE
1	A	899	LYS
1	A	931	MET
1	A	1004	VAL
1	A	1008	LYS
1	A	1017	GLU
1	A	1037	MET
1	A	1048	GLU
1	A	1083	VAL
1	A	1094	SER
1	A	1130	GLU
1	A	1150	MET

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	289	ASN
1	A	325	GLN
1	A	662	ASN
1	A	688	HIS
1	A	776	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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	EDO	A	1206	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	A	1209	-	3,3,3	0.20	0	2,2,2	0.27	0
5	EDO	A	1207	-	3,3,3	0.23	0	2,2,2	0.34	0
6	SO4	A	1211	-	4,4,4	0.32	0	6,6,6	0.13	0
2	A1BKX	A	1201	-	27,29,29	0.95	2 (7%)	34,42,42	2.09	9 (26%)
3	ADP	A	1202	4	24,29,29	0.79	0	29,45,45	0.91	0
5	EDO	A	1205	-	3,3,3	0.10	0	2,2,2	0.09	0
6	SO4	A	1212	-	4,4,4	0.35	0	6,6,6	0.22	0
6	SO4	A	1214	-	4,4,4	0.32	0	6,6,6	0.07	0
5	EDO	A	1210	-	3,3,3	0.24	0	2,2,2	0.08	0
5	EDO	A	1204	-	3,3,3	0.12	0	2,2,2	0.14	0
6	SO4	A	1213	-	4,4,4	0.30	0	6,6,6	0.13	0
5	EDO	A	1208	-	3,3,3	0.16	0	2,2,2	0.18	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	EDO	A	1206	-	-	1/1/1/1	-
5	EDO	A	1209	-	-	0/1/1/1	-
5	EDO	A	1207	-	-	1/1/1/1	-
2	A1BKX	A	1201	-	-	1/12/17/17	0/3/3/3
3	ADP	A	1202	4	-	2/12/32/32	0/3/3/3
5	EDO	A	1205	-	-	1/1/1/1	-
5	EDO	A	1210	-	-	1/1/1/1	-
5	EDO	A	1204	-	-	1/1/1/1	-
5	EDO	A	1208	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1BKX	C20-N22	-2.66	1.39	1.43
2	A	1201	A1BKX	C11-S10	2.07	1.74	1.72

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	A1BKX	C2-C7-N6	-4.96	118.93	123.08
2	A	1201	A1BKX	C3-C2-C7	4.70	118.84	116.98
2	A	1201	A1BKX	C8-C9-S10	-4.08	109.66	112.29
2	A	1201	A1BKX	C11-C13-N15	3.98	120.14	114.03
2	A	1201	A1BKX	C5-N6-C7	3.21	123.11	116.84
2	A	1201	A1BKX	C26-S23-N22	-2.78	103.44	106.56
2	A	1201	A1BKX	O25-S23-C26	2.66	112.46	108.26
2	A	1201	A1BKX	C8-C7-C2	2.52	126.44	123.52
2	A	1201	A1BKX	C16-C17-C18	2.34	120.63	118.72

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	A1BKX	C2-C7-C8-C12
5	A	1204	EDO	O1-C1-C2-O2
5	A	1206	EDO	O1-C1-C2-O2
5	A	1210	EDO	O1-C1-C2-O2
3	A	1202	ADP	PA-O3A-PB-O1B
5	A	1207	EDO	O1-C1-C2-O2
3	A	1202	ADP	PA-O3A-PB-O3B
5	A	1208	EDO	O1-C1-C2-O2
5	A	1205	EDO	O1-C1-C2-O2

There are no ring outliers.

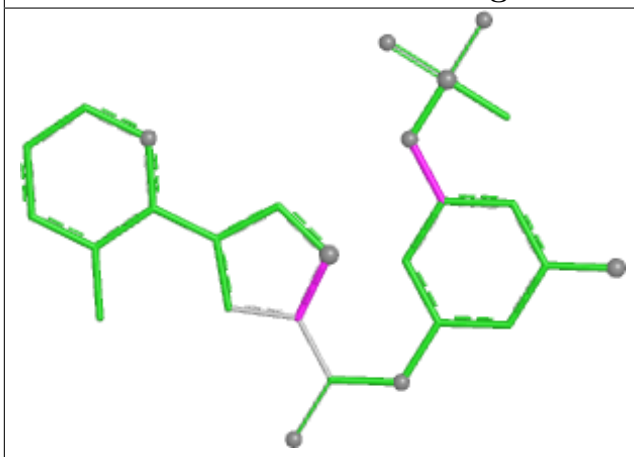
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1210	EDO	1	0
5	A	1208	EDO	2	0

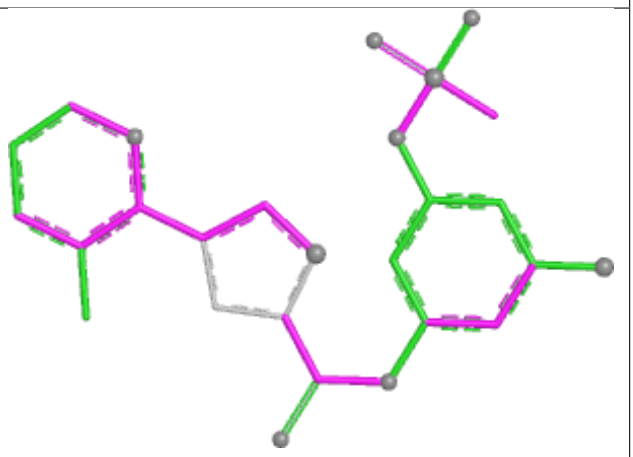
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

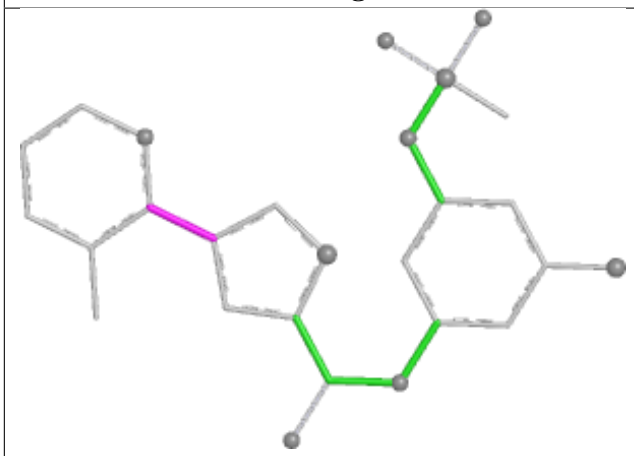
Ligand A1BKX A 1201



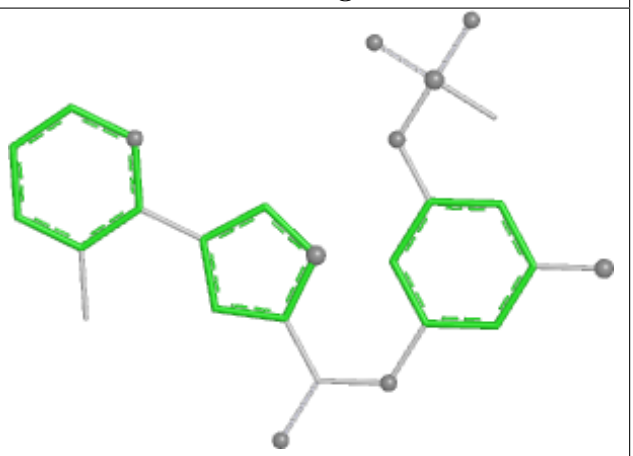
Bond lengths



Bond angles

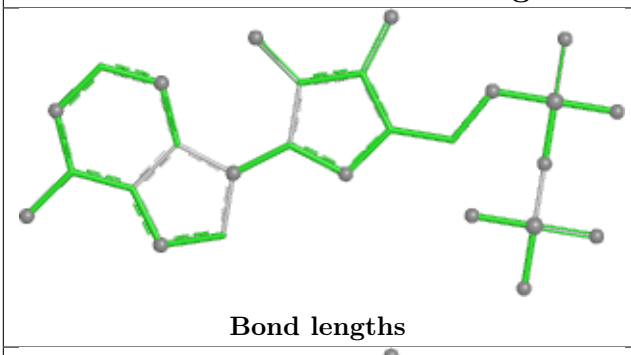


Torsions

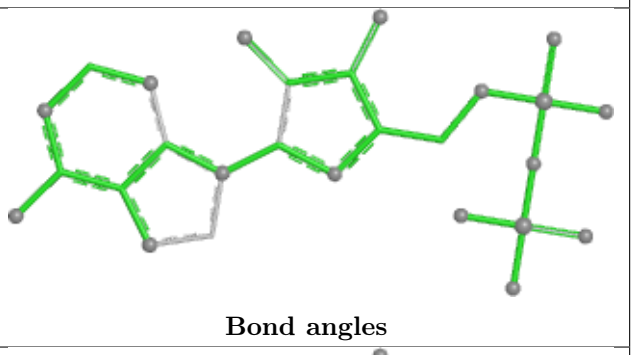


Rings

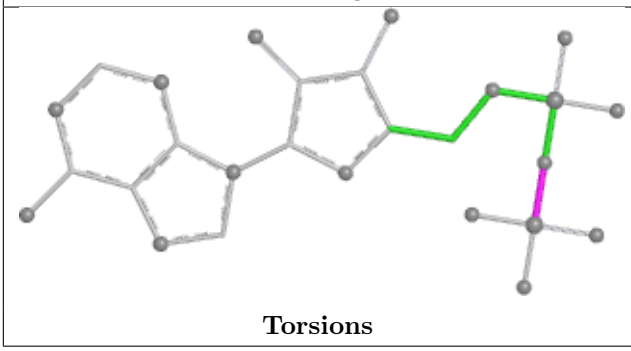
Ligand ADP A 1202



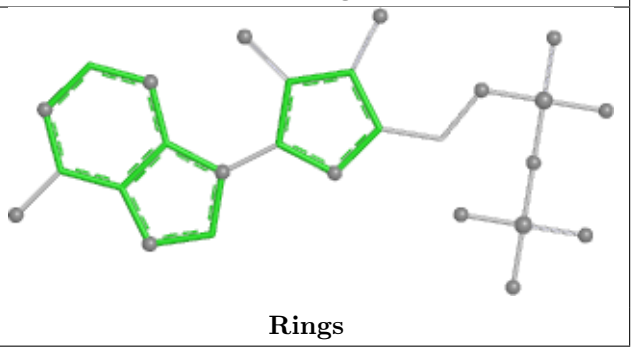
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	857/1010 (84%)	0.09	30 (3%) 47 47	23, 55, 93, 148	5 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ILE	4.3
1	A	1151	ILE	3.9
1	A	321	PRO	3.7
1	A	579	CYS	3.6
1	A	589	PRO	3.5
1	A	661	TRP	3.4
1	A	613	CYS	3.0
1	A	775	PHE	2.9
1	A	703	VAL	2.9
1	A	306	PHE	2.8
1	A	607	ALA	2.8
1	A	313	LEU	2.7
1	A	943[A]	HIS	2.6
1	A	673	MET	2.6
1	A	1018	GLY	2.5
1	A	773	PHE	2.4
1	A	620	GLU	2.4
1	A	669	LYS	2.4
1	A	1125	LEU	2.4
1	A	1128	VAL	2.4
1	A	768[A]	ARG	2.4
1	A	702	PRO	2.3
1	A	665	TYR	2.3
1	A	307	LEU	2.2
1	A	617	TYR	2.2
1	A	435	ARG	2.2
1	A	272	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	583	THR	2.1
1	A	1088	TRP	2.0
1	A	298	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

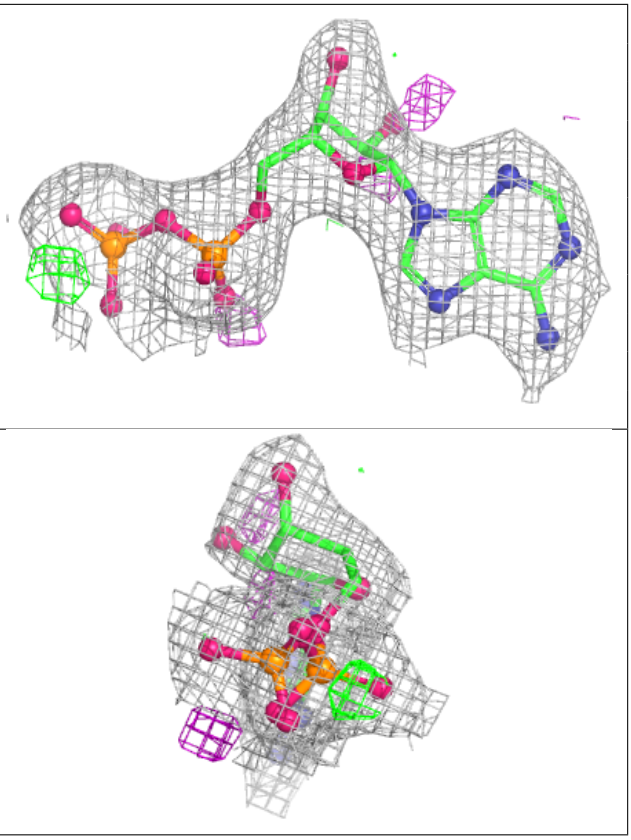
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	EDO	A	1205	4/4	0.77	0.17	78,83,86,86	0
5	EDO	A	1208	4/4	0.81	0.19	68,70,74,78	0
6	SO4	A	1211	5/5	0.85	0.12	84,98,105,109	0
5	EDO	A	1204	4/4	0.90	0.18	74,75,78,79	0
5	EDO	A	1206	4/4	0.91	0.19	69,73,74,75	0
6	SO4	A	1212	5/5	0.91	0.13	62,68,75,86	0
6	SO4	A	1214	5/5	0.91	0.14	106,106,117,117	5
5	EDO	A	1207	4/4	0.94	0.13	66,66,66,76	0
5	EDO	A	1210	4/4	0.95	0.13	66,66,70,80	0
7	CL	A	1215	1/1	0.95	0.19	89,89,89,89	0
5	EDO	A	1209	4/4	0.97	0.08	44,48,51,52	0
6	SO4	A	1213	5/5	0.97	0.07	59,62,66,68	0
3	ADP	A	1202	27/27	0.97	0.06	40,54,61,68	0
2	A1BKX	A	1201	27/27	0.97	0.06	34,42,54,56	0
4	MG	A	1203	1/1	0.99	0.04	42,42,42,42	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.

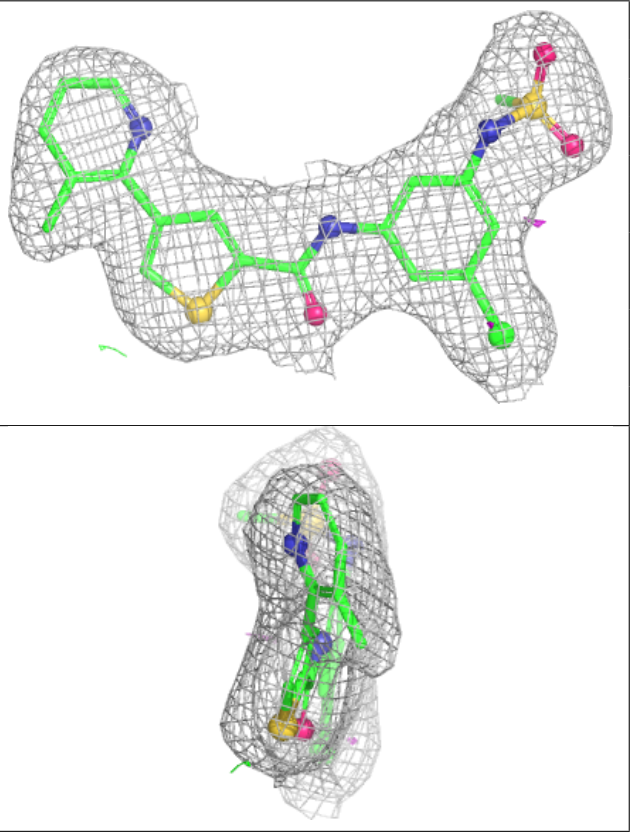
Electron density around ADP A 1202:

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



Electron density around A1BKX A 1201:

$2mF_o$-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.