



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:19 AM UTC

PDB ID : 5XDR / pdb_00005xdr
Title : Crystal structure of human DEAH-box RNA helicase DHX15 in complex with ADP
Authors : Murakami, K.; Nakano, K.; Shimizu, T.; Ohto, U.
Deposited on : 2017-03-29
Resolution : 2.00 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 Phenix2.0
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

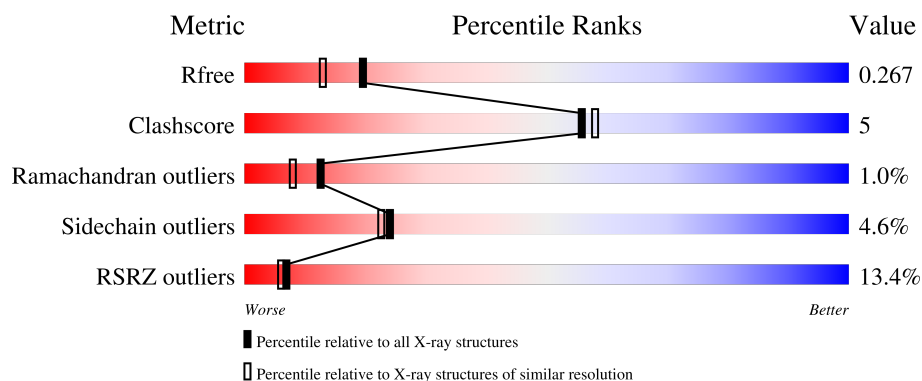
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	690	13% 83% 13% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5586 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.

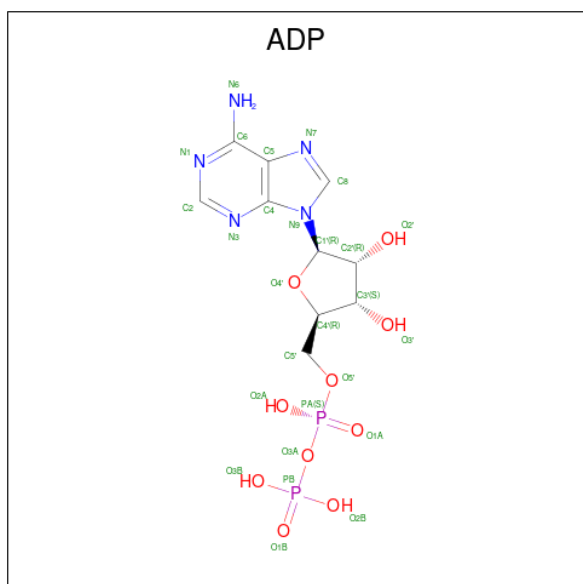
- Molecule 1 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	679	5458	3467	941	1014	36	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

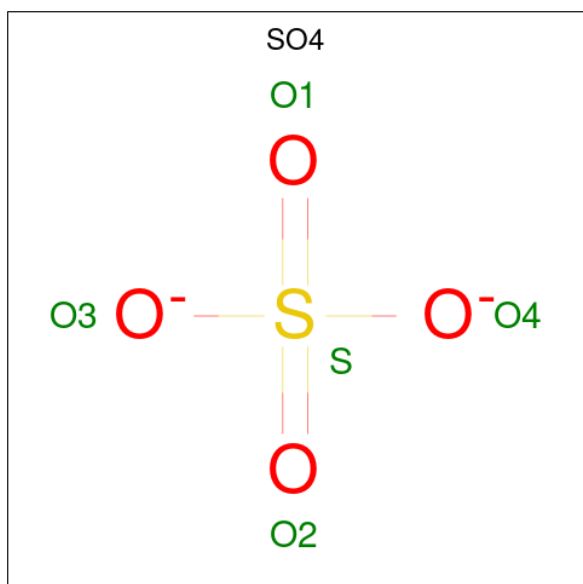
Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP O43143
A	107	PRO	-	expression tag	UNP O43143
A	108	GLU	-	expression tag	UNP O43143
A	109	PHE	-	expression tag	UNP O43143
A	678	SER	THR	engineered mutation	UNP O43143

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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

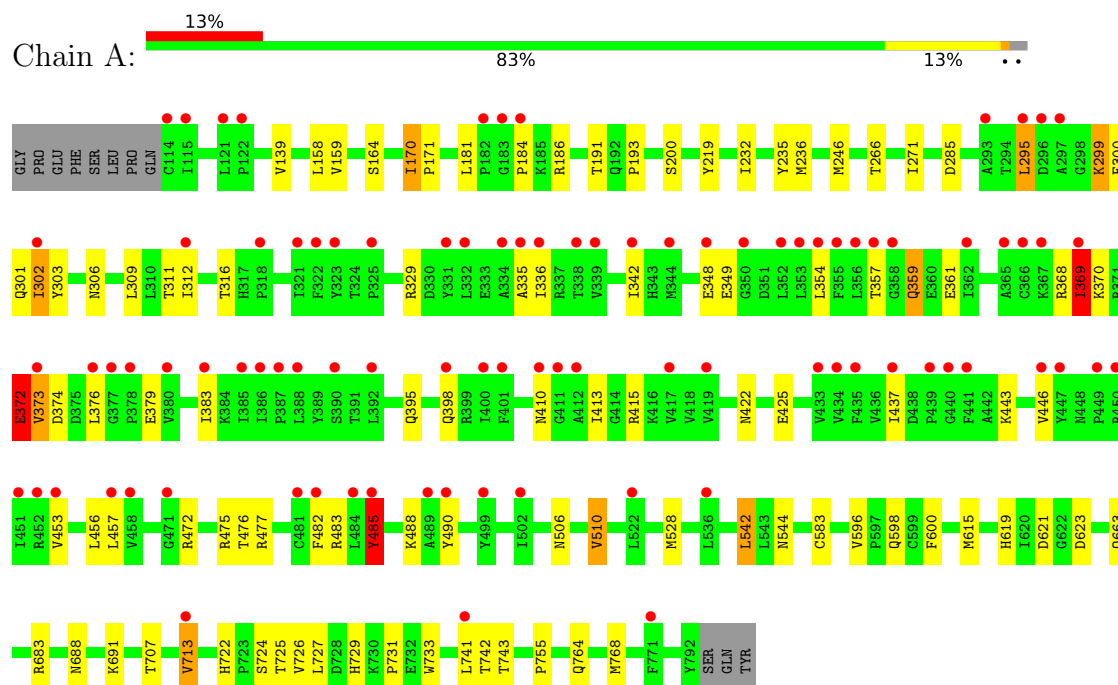
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		

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: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX15



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.92Å 89.38Å 211.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.54 – 2.00 105.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (105.54-2.00) 100.0 (105.54-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.223 , 0.269 0.229 , 0.267	Depositor DCC
R_{free} test set	2649 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5586	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: MG, ADP, SO4

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	0.93	3/5573 (0.1%)	1.04	11/7553 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	583	CYS	C-O	5.66	1.29	1.24
1	A	688	ASN	CG-ND2	5.22	1.44	1.33
1	A	691	LYS	N-CA	5.05	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	VAL	CA-C-N	-5.99	113.80	119.85
1	A	596	VAL	C-N-CA	-5.99	113.80	119.85
1	A	372	GLU	N-CA-C	-5.92	101.72	110.48
1	A	713	VAL	N-CA-C	5.87	116.33	110.23
1	A	359	GLN	N-CA-C	5.71	119.33	112.93
1	A	170	ILE	CB-CA-C	-5.65	108.36	114.35
1	A	707	THR	N-CA-C	5.34	119.64	113.18
1	A	485	TYR	CA-CB-CG	5.24	123.33	113.90
1	A	379	GLU	N-CA-C	5.19	119.89	111.37
1	A	713	VAL	CA-C-N	-5.07	113.02	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	VAL	C-N-CA	-5.07	113.02	122.09

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5458	0	5480	52	0
2	A	27	0	12	1	0
3	A	10	0	0	0	0
4	A	1	0	0	0	0
5	A	90	0	0	0	1
All	All	5586	0	5492	52	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (52) 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:598:GLN:HE21	1:A:600:PHE:H	1.20	0.90
1:A:725:THR:HG22	1:A:727:LEU:H	1.48	0.79
1:A:615:MET:HE1	1:A:726:VAL:HG12	1.63	0.78
1:A:623:ASP:OD2	1:A:725:THR:HG23	1.90	0.71
1:A:139:VAL:HG12	1:A:312:ILE:HD13	1.77	0.67
1:A:544:ASN:ND2	1:A:764:GLN:HE22	1.96	0.62
1:A:544:ASN:HD21	1:A:764:GLN:HE22	1.50	0.60
1:A:619:HIS:HD2	1:A:621:ASP:H	1.48	0.60
1:A:369:ILE:HD12	1:A:369:ILE:N	2.20	0.56
1:A:271:ILE:CD1	1:A:510:VAL:HG22	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:NH1	1:A:285:ASP:OD2	2.36	0.55
1:A:619:HIS:CD2	1:A:621:ASP:H	2.26	0.54
1:A:768:MET:HA	1:A:768:MET:HE2	1.91	0.53
1:A:299:LYS:HG2	1:A:302:ILE:HD13	1.89	0.52
1:A:200:SER:HB2	1:A:398:GLN:HE22	1.75	0.52
1:A:370:LYS:N	1:A:372:GLU:O	2.44	0.51
1:A:425:GLU:O	1:A:472:ARG:NH1	2.43	0.51
1:A:159:VAL:HG23	1:A:311:THR:HG23	1.93	0.50
1:A:193:PRO:HB3	1:A:266:THR:HG21	1.93	0.49
1:A:733:TRP:CE2	1:A:755:PRO:HB3	2.47	0.49
1:A:369:ILE:O	1:A:369:ILE:HG22	2.13	0.49
1:A:542:LEU:C	1:A:542:LEU:HD23	2.37	0.48
1:A:200:SER:CB	1:A:398:GLN:HE22	2.25	0.48
1:A:369:ILE:C	1:A:372:GLU:O	2.56	0.47
1:A:336:ILE:HG21	1:A:369:ILE:HD11	1.96	0.47
1:A:139:VAL:HG13	1:A:164:SER:O	2.15	0.47
1:A:159:VAL:HG22	1:A:309:LEU:HD11	1.95	0.47
1:A:299:LYS:O	1:A:301:GLN:N	2.48	0.46
1:A:303:TYR:CB	1:A:528:MET:HE2	2.45	0.46
1:A:372:GLU:HG2	1:A:373:VAL:HA	1.97	0.46
1:A:219:TYR:HA	1:A:235:TYR:O	2.16	0.46
1:A:446:VAL:HG22	1:A:457:LEU:HD23	1.98	0.46
1:A:349:GLU:HA	1:A:413:ILE:HG21	1.99	0.45
1:A:768:MET:HE2	1:A:768:MET:CA	2.47	0.45
1:A:335:ALA:HB1	1:A:354:LEU:HD11	1.99	0.44
1:A:302:ILE:HG13	1:A:306:ASN:HD21	1.81	0.44
1:A:722:HIS:HD2	1:A:724:SER:OG	2.00	0.44
1:A:598:GLN:HE21	1:A:600:PHE:N	2.01	0.44
1:A:742:THR:HG22	1:A:743:THR:H	1.83	0.43
1:A:348:GLU:O	1:A:415:ARG:NH2	2.51	0.43
1:A:729:HIS:O	1:A:731:PRO:HD3	2.19	0.43
1:A:170:ILE:HB	1:A:171:PRO:HD3	2.01	0.42
1:A:295:LEU:CD1	1:A:295:LEU:N	2.82	0.42
1:A:342:ILE:HD11	1:A:482:PHE:CD2	2.54	0.42
1:A:303:TYR:HB2	1:A:528:MET:HE2	2.02	0.42
1:A:475:ARG:NH2	2:A:801:ADP:O3'	2.53	0.41
1:A:476:THR:HG21	1:A:477:ARG:HH21	1.85	0.41
1:A:483:ARG:HB3	1:A:485:TYR:CD2	2.55	0.41
1:A:357:THR:HG22	1:A:361:GLU:OE1	2.20	0.41
1:A:598:GLN:HE22	1:A:600:PHE:HD2	1.69	0.41
1:A:357:THR:OG1	1:A:443:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:HA	1:A:236:MET:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:989:HOH:O	5:A:989:HOH:O[3_555]	1.65	0.55

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	677/690 (98%)	630 (93%)	40 (6%)	7 (1%)	12 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	LEU
1	A	422	ASN
1	A	490	TYR
1	A	300	PHE
1	A	395	GLN
1	A	184	PRO
1	A	369	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	606/616 (98%)	578 (95%)	28 (5%)	24	22

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LEU
1	A	181	LEU
1	A	232	ILE
1	A	246	MET
1	A	295	LEU
1	A	299	LYS
1	A	302	ILE
1	A	316	THR
1	A	329	ARG
1	A	359	GLN
1	A	368	ARG
1	A	369	ILE
1	A	372	GLU
1	A	373	VAL
1	A	383	ILE
1	A	410	ASN
1	A	437	ILE
1	A	453	VAL
1	A	456	LEU
1	A	485	TYR
1	A	488	LYS
1	A	506	ASN
1	A	510	VAL
1	A	542	LEU
1	A	663	GLN
1	A	683	ARG
1	A	713	VAL
1	A	741	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	317	HIS
1	A	398	GLN

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Mol	Chain	Res	Type
1	A	497	ASN
1	A	506	ASN
1	A	544	ASN
1	A	570	GLN
1	A	582	ASN
1	A	598	GLN
1	A	619	HIS
1	A	647	ASN
1	A	663	GLN
1	A	700	GLN
1	A	709	HIS
1	A	716	ASN
1	A	717	GLN
1	A	722	HIS
1	A	729	HIS
1	A	764	GLN
1	A	770	ASN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
2	ADP	A	801	4	28,29,29	1.47	4 (14%)	43,45,45	1.81	8 (18%)
3	SO4	A	803	-	4,4,4	0.45	0	6,6,6	0.22	0
3	SO4	A	802	-	4,4,4	0.46	0	6,6,6	0.13	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
2	ADP	A	801	4	-	6/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ADP	C5-C4	4.91	1.47	1.39
2	A	801	ADP	C5-C6	2.72	1.48	1.41
2	A	801	ADP	C5-N7	-2.52	1.34	1.39
2	A	801	ADP	C8-N7	2.07	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	C5-C4-N3	-5.94	118.53	126.72
2	A	801	ADP	N3-C4-N9	4.96	135.61	127.17
2	A	801	ADP	C2-N3-C4	3.90	121.35	111.83
2	A	801	ADP	N3-C2-N1	-3.83	122.78	128.58
2	A	801	ADP	C4-C5-N7	-3.03	107.12	110.58
2	A	801	ADP	C4-N9-C8	2.50	108.36	105.74
2	A	801	ADP	C5-N7-C8	2.44	107.28	103.45
2	A	801	ADP	C2-N1-C6	2.04	122.09	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O3B
2	A	801	ADP	C5'-O5'-PA-O2A
2	A	801	ADP	C5'-O5'-PA-O3A
2	A	801	ADP	O4'-C4'-C5'-O5'
2	A	801	ADP	C3'-C4'-C5'-O5'

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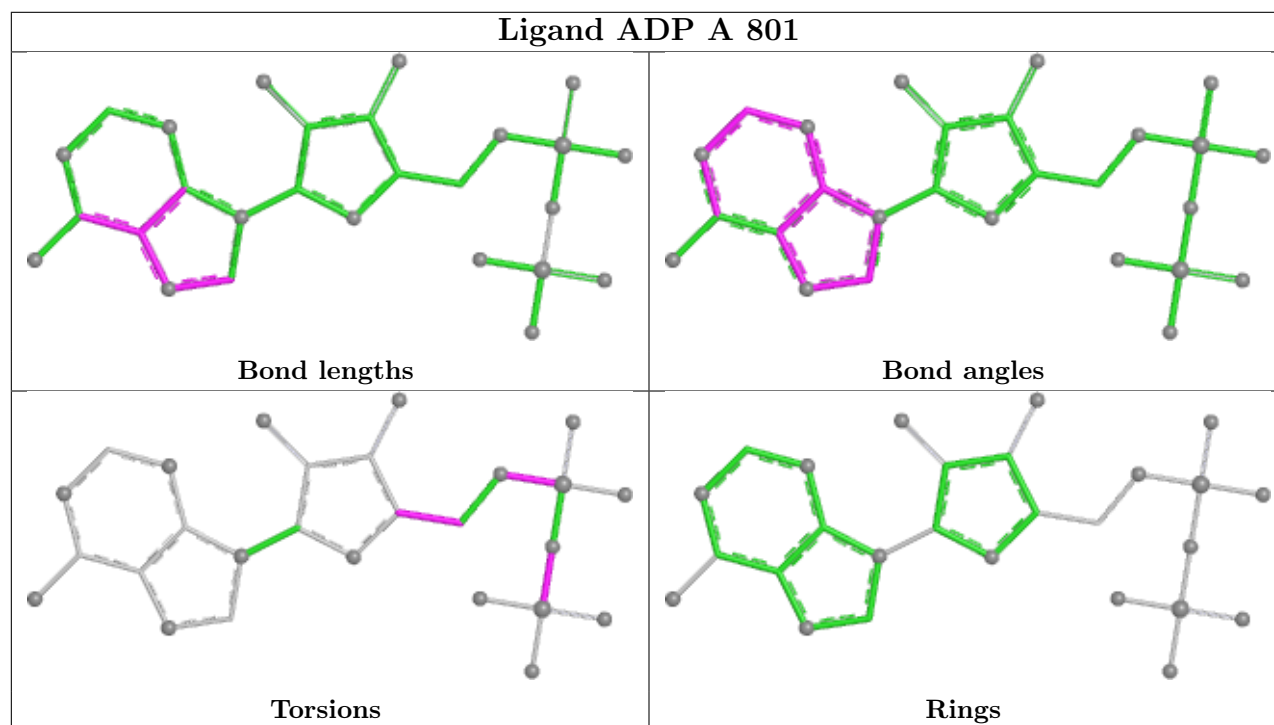
Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	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 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 [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 ⓘ

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	679/690 (98%)	0.81	91 (13%) 7 6	27, 60, 105, 126	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	PRO	5.5
1	A	297	ALA	4.8
1	A	451	ILE	4.4
1	A	356	LEU	4.2
1	A	376	LEU	4.2
1	A	322	PHE	4.2
1	A	369	ILE	4.1
1	A	115	ILE	3.8
1	A	357	THR	3.8
1	A	338	THR	3.8
1	A	385	ILE	3.8
1	A	457	LEU	3.7
1	A	386	ILE	3.7
1	A	365	ALA	3.7
1	A	332	LEU	3.6
1	A	489	ALA	3.5
1	A	446	VAL	3.5
1	A	440	GLY	3.4
1	A	354	LEU	3.4
1	A	481	CYS	3.3
1	A	295	LEU	3.3
1	A	366	CYS	3.3
1	A	417	VAL	3.3
1	A	373	VAL	3.3
1	A	485	TYR	3.3
1	A	342	ILE	3.3
1	A	114	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	336	ILE	3.1
1	A	522	LEU	3.1
1	A	435	PHE	3.1
1	A	184	PRO	3.1
1	A	453	VAL	3.1
1	A	321	ILE	3.1
1	A	482	PHE	3.0
1	A	484	LEU	3.0
1	A	387	PRO	3.0
1	A	437	ILE	2.9
1	A	325	PRO	2.9
1	A	458	VAL	2.9
1	A	335	ALA	2.9
1	A	412	ALA	2.9
1	A	447	TYR	2.9
1	A	331	TYR	2.8
1	A	411	GLY	2.8
1	A	367	LYS	2.8
1	A	392	LEU	2.8
1	A	439	PRO	2.8
1	A	471	GLY	2.7
1	A	378	PRO	2.7
1	A	400	ILE	2.7
1	A	380	VAL	2.7
1	A	419	VAL	2.7
1	A	401	PHE	2.6
1	A	490	TYR	2.6
1	A	339	VAL	2.6
1	A	121	LEU	2.6
1	A	713	VAL	2.6
1	A	355	PHE	2.5
1	A	344	MET	2.5
1	A	350	GLY	2.5
1	A	353	LEU	2.5
1	A	358	GLY	2.5
1	A	398	GLN	2.4
1	A	388	LEU	2.4
1	A	450	ARG	2.4
1	A	334	ALA	2.4
1	A	536	LEU	2.4
1	A	183	GLY	2.4
1	A	452	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	182	PRO	2.4
1	A	741	LEU	2.3
1	A	352	LEU	2.3
1	A	348	GLU	2.3
1	A	318	PRO	2.3
1	A	433	VAL	2.3
1	A	383	ILE	2.2
1	A	410	ASN	2.2
1	A	323	TYR	2.2
1	A	499	TYR	2.2
1	A	362	ILE	2.2
1	A	122	PRO	2.1
1	A	502	ILE	2.1
1	A	302	ILE	2.1
1	A	771	PHE	2.1
1	A	434	VAL	2.1
1	A	312	ILE	2.1
1	A	441	PHE	2.1
1	A	293	ALA	2.1
1	A	390	SER	2.1
1	A	296	ASP	2.0
1	A	377	GLY	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.

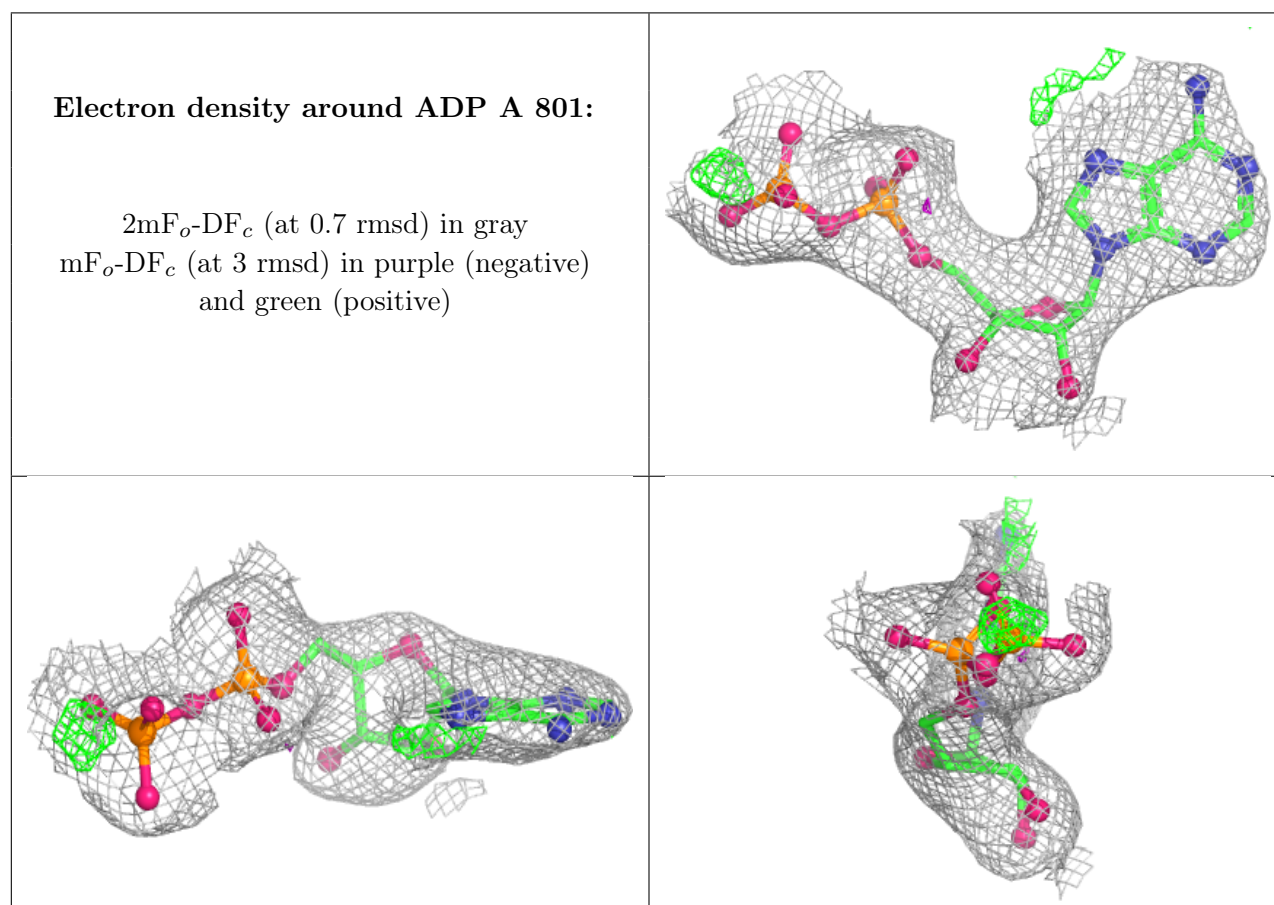
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	802	5/5	0.63	0.12	85,96,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	803	5/5	0.81	0.10	80,80,82,84	0
2	ADP	A	801	27/27	0.93	0.10	57,77,81,84	0
4	MG	A	804	1/1	0.99	0.06	53,53,53,53	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.