Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 07:31 pm GMT

PDB ID	:	6RMC
Title	:	Crystal structure of the DEAH-box ATPase Prp2 in complex with Spp2 and ADP
Authors	:	Hamann, F.; Neumann, P.; Schmitt, A.; Ficner, R.
Deposited on	:	2019-05-06
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
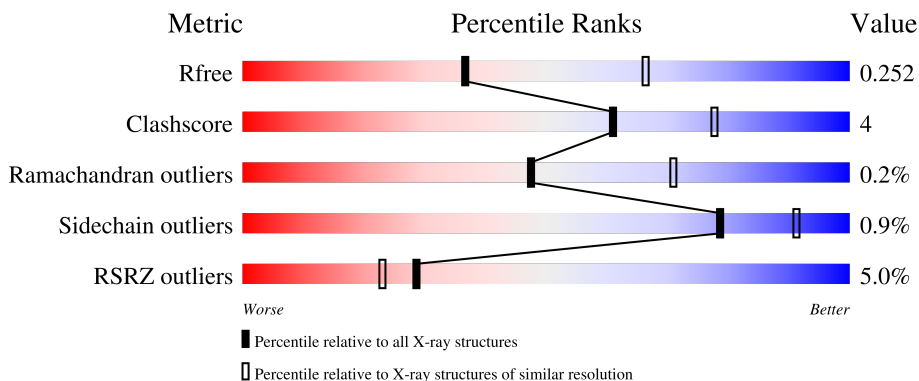
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	655	3% / 85% / 12% / · ·
1	B	655	7% / 88% / 10% / ·
2	C	47	83% / 11% / 6%
2	D	47	6% / 77% / 13% / · / 6%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10938 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 mRNA splicing factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total 5022	C 3179	N 874	O 945	S 24	0	0	0
1	B	645	Total 5039	C 3188	N 877	O 950	S 24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLY	-	expression tag	UNP G0SEG4
A	268	PRO	-	expression tag	UNP G0SEG4
A	269	MET	-	expression tag	UNP G0SEG4
B	267	GLY	-	expression tag	UNP G0SEG4
B	268	PRO	-	expression tag	UNP G0SEG4
B	269	MET	-	expression tag	UNP G0SEG4

- Molecule 2 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	44	Total 347	C 216	N 65	O 65	S 1	0	0	0
2	D	44	Total 358	C 222	N 69	O 66	S 1	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	208	GLY	-	expression tag	UNP G0SFN3
C	209	PRO	-	expression tag	UNP G0SFN3
C	210	MET	-	expression tag	UNP G0SFN3
D	208	GLY	-	expression tag	UNP G0SFN3
D	209	PRO	-	expression tag	UNP G0SFN3
D	210	MET	-	expression tag	UNP G0SFN3

- Molecule 3 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
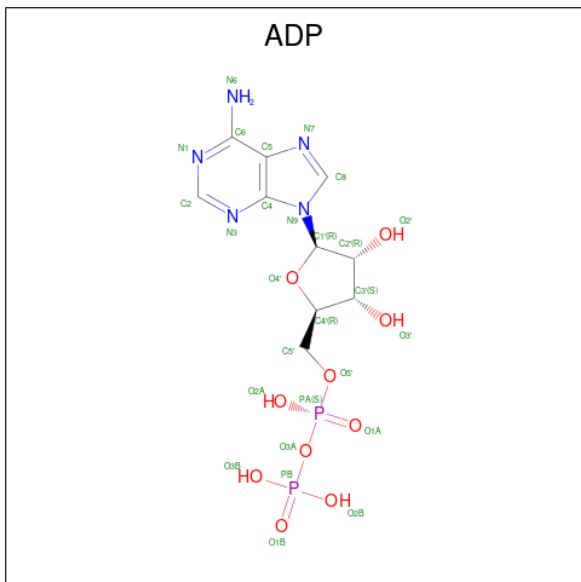
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total 56	O 56	0	0
5	B	51	Total 51	O 51	0	0
5	C	5	Total 5	O 5	0	0
5	D	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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 mRNA splicing factor
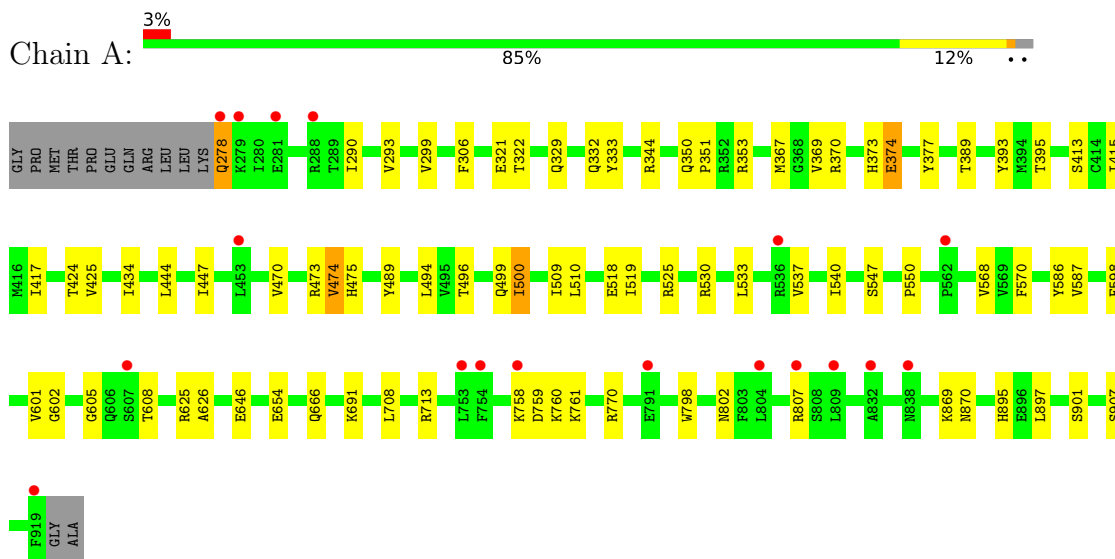
• Molecule 1: Putative mRNA splicing factor
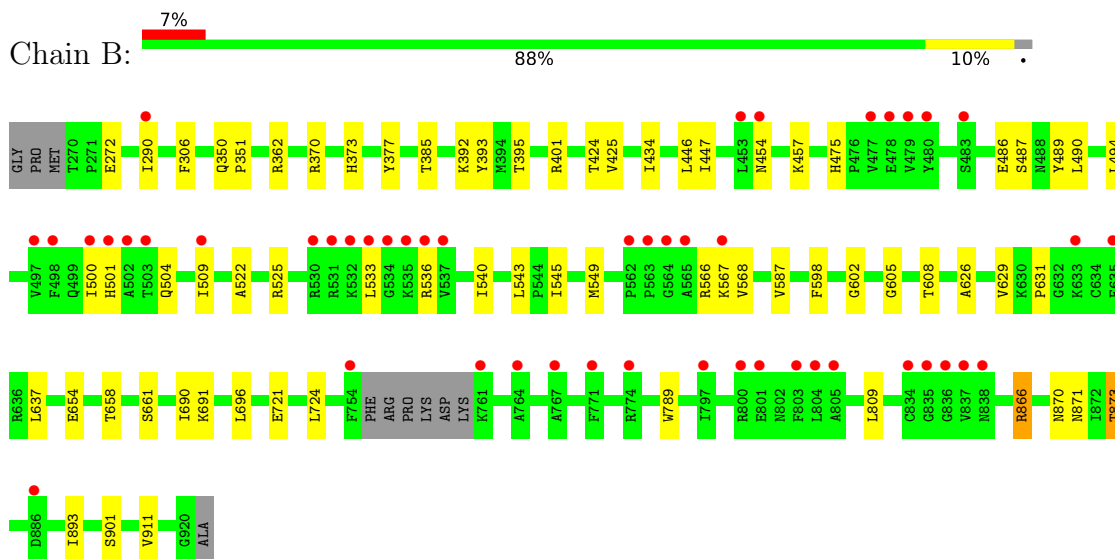
• Molecule 2: Putative pre-mRNA splicing protein

Chain C:

83% 11% 6%

GLY PRO MET V211 D212 V232 V235 E251 A252 E253 D254

• Molecule 2: Putative pre-mRNA splicing protein

6%

Chain D:

77% 13% • 6%

GLY PRO MET V211 D212 D213 F214 G215 E216 K231 R237 K250 E251 D254

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.73Å 113.69Å 191.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.60 48.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.90-2.60) 99.6 (48.90-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.222 , 0.250 0.224 , 0.252	Depositor DCC
R_{free} test set	2549 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å²)	62.0	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 42.2	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	0.94	EDS
Total number of atoms	10938	wwPDB-VP
Average B, all atoms (Å²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.25	0/5119	0.42	0/6947
1	B	0.25	0/5134	0.42	0/6967
2	C	0.26	0/351	0.40	0/466
2	D	0.25	0/362	0.42	0/480
All	All	0.25	0/10966	0.42	0/14860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	5022	0	5077	51	0
1	B	5039	0	5096	42	0
2	C	347	0	343	4	0
2	D	358	0	355	8	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	56	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	51	0	0	1	0
5	C	5	0	0	1	0
5	D	4	0	0	0	0
All	All	10938	0	10895	97	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 4.

All (97) 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:B:901:SER:HA	2:D:251:GLU:HA	1.63	0.79
1:B:500:ILE:HG13	1:B:504:GLN:HG3	1.68	0.75
1:A:425:VAL:HG23	1:A:654:GLU:HB3	1.74	0.69
1:B:425:VAL:HG23	1:B:654:GLU:HB3	1.78	0.65
1:A:901:SER:HA	2:C:251:GLU:HA	1.82	0.62
1:A:496:THR:O	1:A:500:ILE:HG22	2.00	0.61
1:A:601:VAL:HB	1:A:870:ASN:HD21	1.64	0.60
1:B:866:ARG:NH2	2:C:253:GLU:O	2.35	0.59
1:A:494:LEU:HD13	1:A:525:ARG:HG2	1.84	0.58
1:A:510:LEU:HB3	1:A:587:VAL:HG12	1.86	0.58
1:A:500:ILE:HD11	1:A:586:TYR:CG	2.38	0.57
1:B:866:ARG:NH1	1:B:873:THR:HG23	2.21	0.56
1:B:454:ASN:HD21	1:B:457:LYS:HB2	1.71	0.56
1:A:533:LEU:HD13	1:A:537:VAL:HG11	1.88	0.55
1:A:509:ILE:HD12	1:A:568:VAL:HG22	1.89	0.55
1:A:417:ILE:HD11	1:A:434:ILE:HD12	1.89	0.54
1:A:370:ARG:HB3	1:A:373:HIS:HD2	1.72	0.54
1:B:866:ARG:HH12	1:B:873:THR:HG23	1.73	0.54
1:A:377:TYR:HA	1:A:393:TYR:O	2.09	0.53
1:A:350:GLN:O	1:A:395:THR:HA	2.08	0.53
1:B:494:LEU:HD13	1:B:525:ARG:HG2	1.91	0.53
1:B:489:TYR:OH	2:D:250:LYS:NZ	2.42	0.53
1:A:415:ILE:HG21	1:A:434:ILE:HD13	1.91	0.52
1:B:370:ARG:HB2	1:B:373:HIS:HD2	1.73	0.52
1:B:385:THR:HG21	1:B:392:LYS:HE3	1.92	0.52
1:B:434:ILE:HG21	1:B:446:LEU:HD13	1.92	0.52
1:A:550:PRO:HG3	1:A:807:ARG:HD3	1.92	0.51
2:D:213:ASP:OD2	2:D:213:ASP:N	2.43	0.51
1:A:489:TYR:OH	1:A:518:GLU:OE2	2.22	0.50
1:A:758:LYS:HA	1:A:761:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:GLN:NE2	5:A:1105:HOH:O	2.43	0.50
1:A:332:GLN:HG2	1:A:367:MET:HE3	1.94	0.50
1:B:306:PHE:HZ	1:B:447:ILE:HD13	1.77	0.50
1:B:377:TYR:HA	1:B:393:TYR:O	2.11	0.50
1:A:344:ARG:HD3	1:A:413:SER:HB3	1.93	0.49
1:B:533:LEU:HB3	1:B:536:ARG:HB2	1.94	0.49
1:A:500:ILE:HD11	1:A:586:TYR:CD2	2.48	0.49
1:B:509:ILE:HD12	1:B:568:VAL:HG22	1.94	0.49
1:A:608:THR:HG22	1:A:897:LEU:HD23	1.95	0.48
1:A:369:VAL:HG11	1:A:374:GLU:HG3	1.95	0.48
1:A:798:TRP:O	1:A:802:ASN:ND2	2.33	0.47
1:A:601:VAL:HB	1:A:870:ASN:ND2	2.30	0.47
1:A:496:THR:HA	1:A:499:GLN:HG2	1.96	0.47
1:B:545:ILE:HA	1:B:549:MET:SD	2.55	0.47
1:A:321:GLU:OE2	1:A:625:ARG:NH2	2.42	0.47
1:A:474:VAL:HG23	1:A:475:HIS:CD2	2.50	0.47
1:B:602:GLY:O	1:B:691:LYS:HE3	2.15	0.46
1:A:321:GLU:HG3	1:A:322:THR:N	2.30	0.46
1:B:351:PRO:HB3	1:B:424:THR:HG21	1.97	0.46
1:B:350:GLN:O	1:B:395:THR:HA	2.16	0.46
1:A:602:GLY:O	1:A:691:LYS:HE3	2.16	0.45
1:B:602:GLY:HA3	1:B:870:ASN:HD21	1.81	0.45
2:C:212:ASP:O	5:C:301:HOH:O	2.21	0.45
1:B:543:LEU:HD12	1:B:567:LYS:HD3	1.99	0.45
1:A:415:ILE:HG12	1:A:444:LEU:HD11	1.98	0.45
1:B:721:GLU:HB2	1:B:724:LEU:HD13	1.99	0.44
1:B:893:ILE:HD12	1:B:911:VAL:HG11	1.99	0.44
1:B:401:ARG:NH1	5:B:1107:HOH:O	2.48	0.44
1:B:598:PHE:CZ	1:B:605:GLY:HA3	2.52	0.44
1:B:866:ARG:HG2	1:B:871:ASN:HA	1.99	0.44
1:B:690:ILE:HD13	2:D:216:GLU:HG2	1.99	0.44
1:A:540:ILE:HD11	1:A:568:VAL:HG21	2.00	0.44
1:A:587:VAL:HG22	1:A:626:ALA:HB2	1.99	0.44
1:B:661:SER:HB3	1:B:696:LEU:HD21	1.99	0.43
1:B:370:ARG:HB2	1:B:373:HIS:CD2	2.53	0.43
1:B:490:LEU:HD11	1:B:522:ALA:HB2	2.00	0.43
3:A:1001:ADP:H5'1	3:A:1001:ADP:H8	1.83	0.43
1:A:329:GLN:HB3	1:A:333:TYR:CZ	2.54	0.43
1:B:540:ILE:HD11	1:B:568:VAL:HG21	2.00	0.43
1:B:789:TRP:CG	1:B:809:LEU:HD13	2.53	0.43
1:A:605:GLY:O	1:A:869:LYS:NZ	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ASP:OD1	1:A:760:LYS:N	2.52	0.42
1:A:299:VAL:HG22	1:A:470:VAL:HG11	2.01	0.42
1:A:278:GLN:HE21	1:A:278:GLN:HB2	1.61	0.42
1:A:290:ILE:HA	1:A:293:VAL:HG12	2.00	0.42
1:A:598:PHE:CZ	1:A:605:GLY:HA3	2.54	0.42
1:B:654:GLU:O	1:B:658:THR:HG22	2.20	0.42
2:D:212:ASP:N	2:D:212:ASP:OD1	2.52	0.42
1:A:306:PHE:HZ	1:A:447:ILE:HD13	1.83	0.42
1:B:690:ILE:HG23	2:D:215:GLY:HA3	2.01	0.42
1:B:608:THR:OG1	2:D:237[B]:ARG:NH1	2.53	0.42
1:A:646:GLU:OE2	2:D:231:LYS:NZ	2.46	0.42
1:B:587:VAL:HG12	1:B:626:ALA:HB2	2.02	0.42
1:A:351:PRO:HB3	1:A:424:THR:HG21	2.02	0.41
1:A:530:ARG:NH2	1:A:540:ILE:O	2.53	0.41
1:B:475:HIS:ND1	1:B:631:PRO:HD3	2.35	0.41
1:B:501:HIS:ND1	1:B:566:ARG:HD2	2.35	0.41
1:B:290:ILE:HD11	1:B:362:ARG:NH2	2.36	0.41
1:A:708:LEU:HD23	1:A:713:ARG:HG2	2.03	0.41
1:B:486:GLU:OE1	1:B:487:SER:N	2.54	0.40
1:A:550:PRO:HG3	1:A:807:ARG:HH21	1.85	0.40
1:A:598:PHE:O	2:C:232:VAL:HG11	2.21	0.40
1:A:519:ILE:HG23	1:A:570:PHE:HB2	2.02	0.40
1:B:789:TRP:CD1	1:B:809:LEU:HD13	2.57	0.40
1:A:373:HIS:O	1:A:389:THR:HA	2.22	0.40
1:A:353:ARG:NH1	1:A:547:SER:O	2.49	0.40
1:A:895:HIS:HB3	1:A:907:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	640/655 (98%)	617 (96%)	22 (3%)	1 (0%)	47	71
1	B	641/655 (98%)	617 (96%)	22 (3%)	2 (0%)	41	64
2	C	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
2	D	43/47 (92%)	41 (95%)	2 (5%)	0	100	100
All	All	1366/1404 (97%)	1316 (96%)	47 (3%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ARG
1	B	637	LEU
1	B	629	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	546/556 (98%)	541 (99%)	5 (1%)	78	91
1	B	548/556 (99%)	545 (100%)	3 (0%)	88	96
2	C	34/36 (94%)	33 (97%)	1 (3%)	42	68
2	D	35/36 (97%)	33 (94%)	2 (6%)	20	41
All	All	1163/1184 (98%)	1152 (99%)	11 (1%)	78	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	374	GLU
1	A	474	VAL
1	A	500	ILE
1	A	770	ARG
1	B	272	GLU
1	B	866	ARG
1	B	873	THR

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Mol	Chain	Res	Type
2	C	235	VAL
2	D	212	ASP
2	D	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	373	HIS
1	B	314	GLN
1	B	373	HIS
1	B	499	GLN
1	B	802	ASN
1	B	870	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	ADP	A	1001	4	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
3	ADP	B	1001	4	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)

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
3	ADP	A	1001	4	-	2/12/32/32	0/3/3/3
3	ADP	B	1001	4	-	7/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ADP	C5-C4	2.53	1.47	1.40
3	B	1001	ADP	C5-C4	2.46	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	ADP	C3'-C2'-C1'	3.36	106.04	100.98
3	B	1001	ADP	C3'-C2'-C1'	3.26	105.89	100.98
3	A	1001	ADP	N3-C2-N1	-3.21	123.66	128.68
3	B	1001	ADP	N3-C2-N1	-3.16	123.74	128.68
3	A	1001	ADP	PA-O3A-PB	-2.98	122.60	132.83
3	B	1001	ADP	C4-C5-N7	-2.86	106.42	109.40
3	B	1001	ADP	PA-O3A-PB	-2.84	123.07	132.83
3	A	1001	ADP	C4-C5-N7	-2.62	106.67	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	ADP	PA-O3A-PB-O2B
3	B	1001	ADP	PA-O3A-PB-O3B
3	B	1001	ADP	C5'-O5'-PA-O1A
3	B	1001	ADP	C5'-O5'-PA-O2A
3	B	1001	ADP	C5'-O5'-PA-O3A
3	B	1001	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	B	1001	ADP	C3'-C4'-C5'-O5'
3	A	1001	ADP	C5'-O5'-PA-O1A
3	A	1001	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	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 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 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 1001

Bond lengths

Bond angles

Torsions

Rings
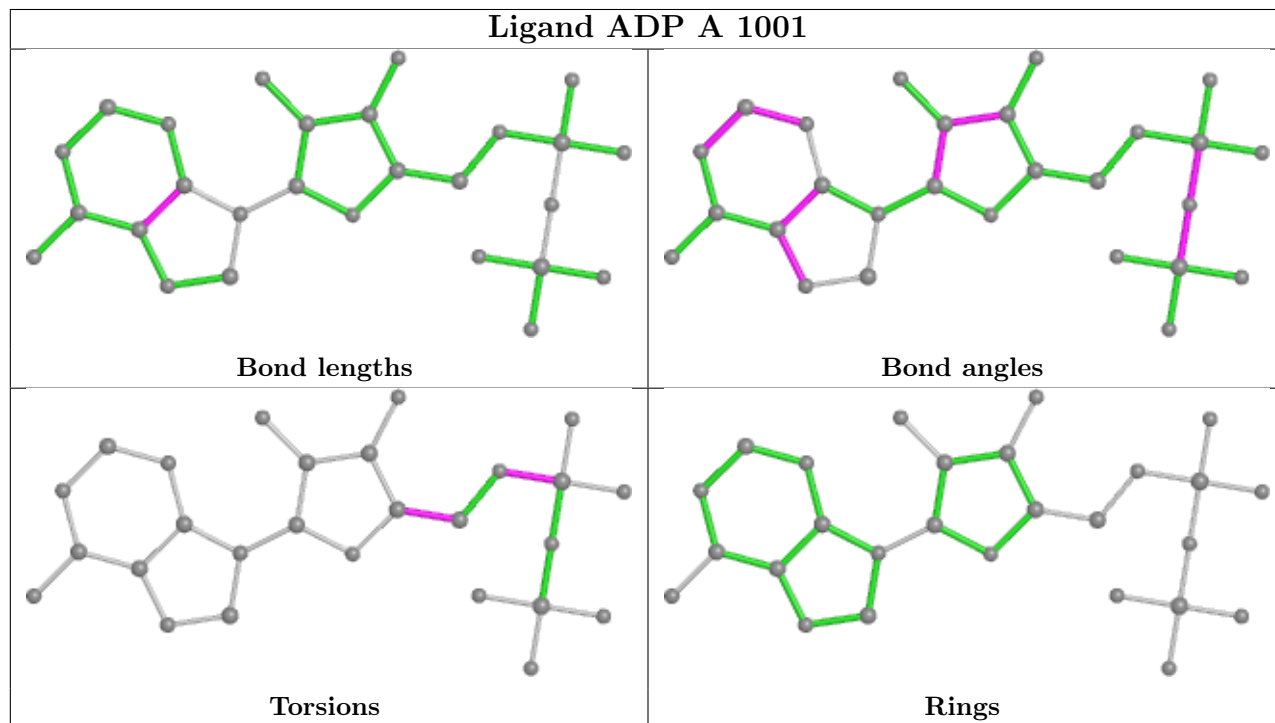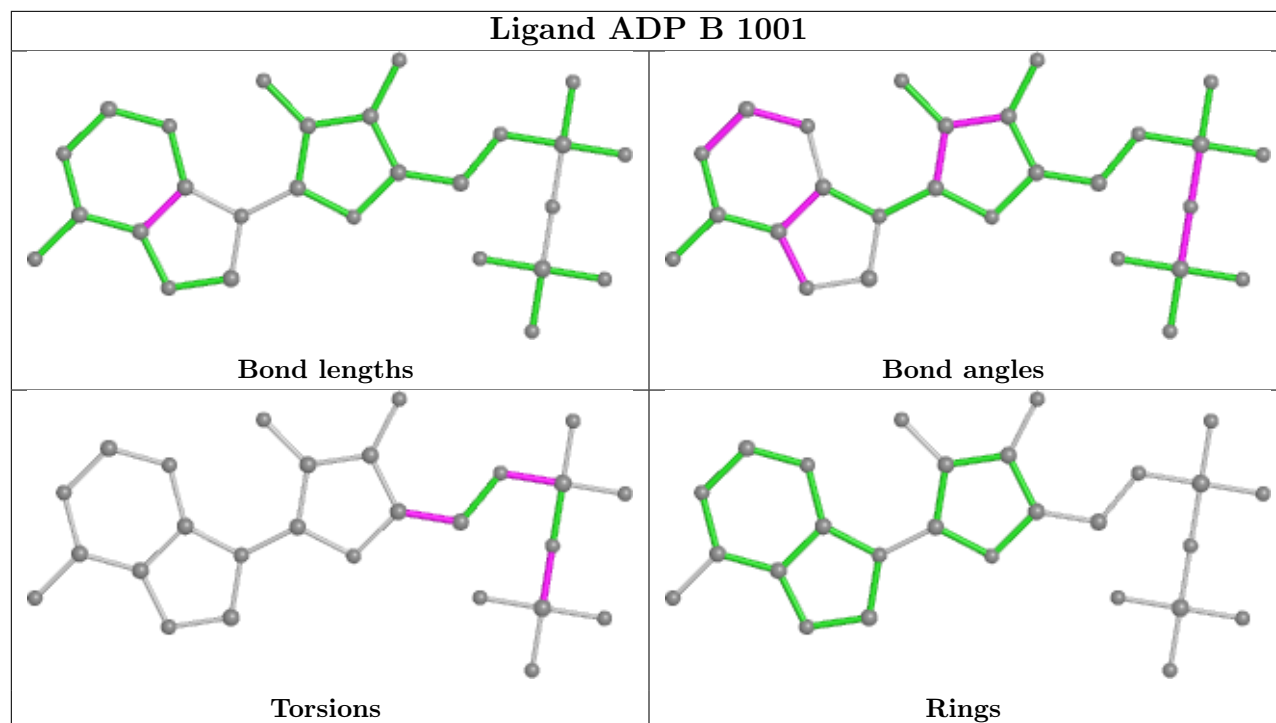
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	642/655 (98%)	0.26	18 (2%)	53	46	35, 64, 99, 151	0
1	B	645/655 (98%)	0.38	48 (7%)	14	10	39, 67, 114, 141	0
2	C	44/47 (93%)	0.33	0	100	100	45, 62, 83, 93	0
2	D	44/47 (93%)	0.41	3 (6%)	17	12	50, 71, 92, 115	0
All	All	1375/1404 (97%)	0.32	69 (5%)	28	23	35, 65, 106, 151	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	531	ARG	6.1
1	B	835	GLY	5.9
2	D	211	VAL	4.9
1	B	635	PHE	4.9
1	B	502	ALA	4.8
1	B	480	TYR	4.7
1	B	797	ILE	4.3
1	B	477	VAL	3.8
1	B	535	LYS	3.7
1	B	536	ARG	3.6
1	B	530	ARG	3.6
1	B	803	PHE	3.5
1	B	774	ARG	3.5
1	B	771	PHE	3.4
1	B	532	LYS	3.4
1	B	534	GLY	3.4
1	B	836	GLY	3.4
1	A	919	PHE	3.3
1	A	281	GLU	3.3
1	A	278	GLN	3.3
1	A	279	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	805	ALA	3.2
1	B	633	LYS	3.0
1	B	500	ILE	3.0
1	B	483	SER	3.0
1	B	533	LEU	3.0
1	B	838	ASN	2.9
2	D	212	ASP	2.9
1	A	758	LYS	2.9
1	B	801	GLU	2.8
1	B	837	VAL	2.8
1	A	536	ARG	2.8
1	A	832	ALA	2.8
1	A	809	LEU	2.8
1	B	498	PHE	2.7
1	B	834	CYS	2.7
1	B	453	LEU	2.6
1	A	288	ARG	2.6
1	B	804	LEU	2.6
1	B	886	ASP	2.6
1	A	804	LEU	2.5
1	A	607	SER	2.5
1	A	807	ARG	2.5
1	B	509	ILE	2.5
1	B	501	HIS	2.5
1	B	478	GLU	2.4
1	A	453	LEU	2.4
1	B	537	VAL	2.4
1	B	800	ARG	2.4
1	B	567	LYS	2.4
1	A	753	LEU	2.3
1	B	565	ALA	2.3
1	B	454	ASN	2.3
1	B	503	THR	2.3
1	B	479	VAL	2.3
1	A	754	PHE	2.3
1	B	761	LYS	2.3
1	B	562	PRO	2.2
1	B	764	ALA	2.2
1	A	838	ASN	2.2
1	A	791	GLU	2.2
1	B	767	ALA	2.1
2	D	237[A]	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	562	PRO	2.0
1	B	290	ILE	2.0
1	B	754	PHE	2.0
1	B	563	PRO	2.0
1	B	564	GLY	2.0
1	B	497	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

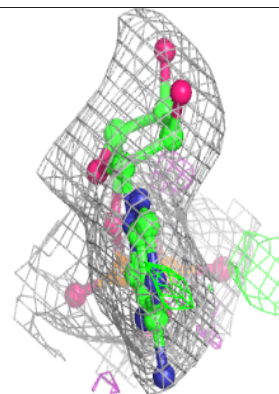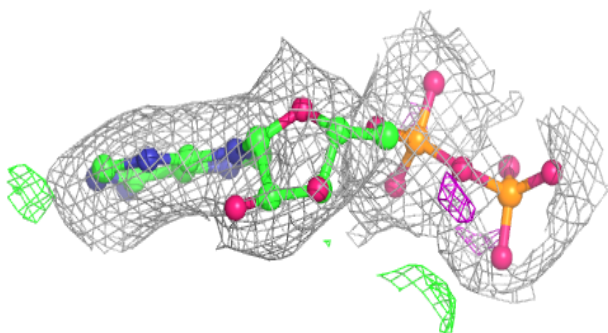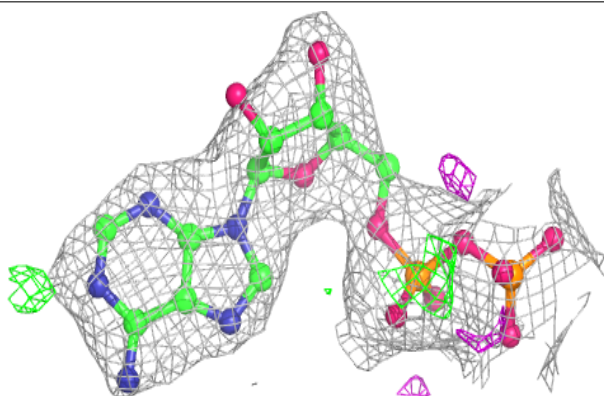| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1002	1/1	0.91	0.16	53,53,53,53	0
3	ADP	A	1001	27/27	0.93	0.20	63,86,93,94	0
4	MG	B	1002	1/1	0.93	0.10	65,65,65,65	0
3	ADP	B	1001	27/27	0.96	0.17	55,73,94,95	0

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 1001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
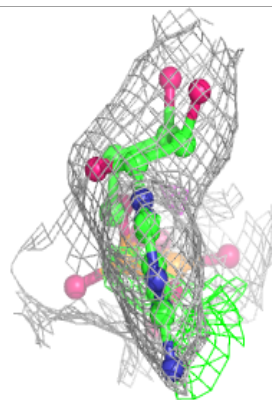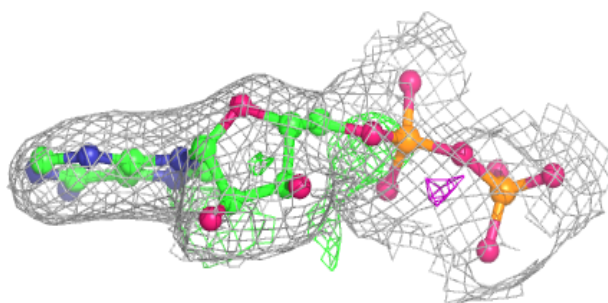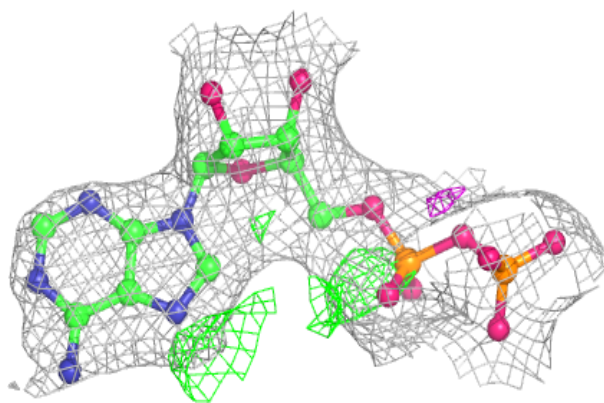
Electron density around ADP B 1001:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.