Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:24 PM GMT

PDB ID	:	3ZD7
Title	:	Snapshot 3 of RIG-I scanning on RNA duplex
Authors	:	Luo, D.; Pyle, A.M.
Deposited on	:	2012-11-25
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

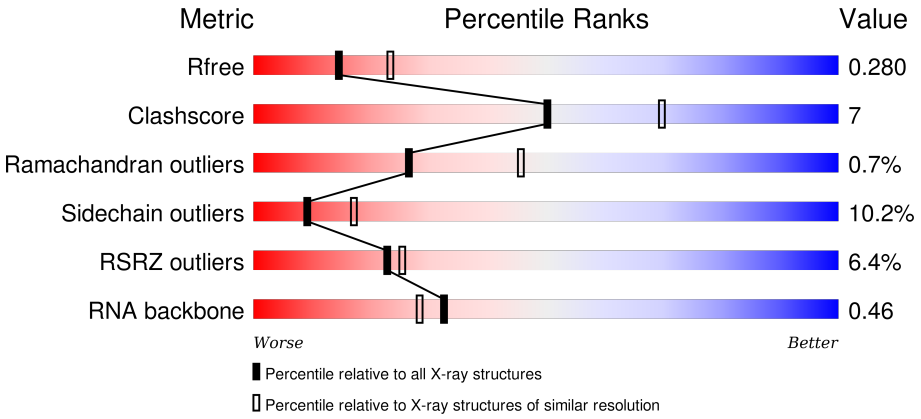
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	696	6%, 69%, 18%, •, 10%
2	C	10	80%, 10%, 10%
2	D	10	60%, 30%, 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5369 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 PROBABLE ATP-DEPENDENT RNA HELICASE DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	4	0	0
			4856	3114	814	899	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ASN	GLN	CONFLICT	UNP O95786
A	499	SER	ILE	CONFLICT	UNP O95786
A	696	LEU	ALA	CONFLICT	UNP O95786
A	828	ASP	GLU	CONFLICT	UNP O95786

- Molecule 2 is a RNA chain called RNA DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			
2	D	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

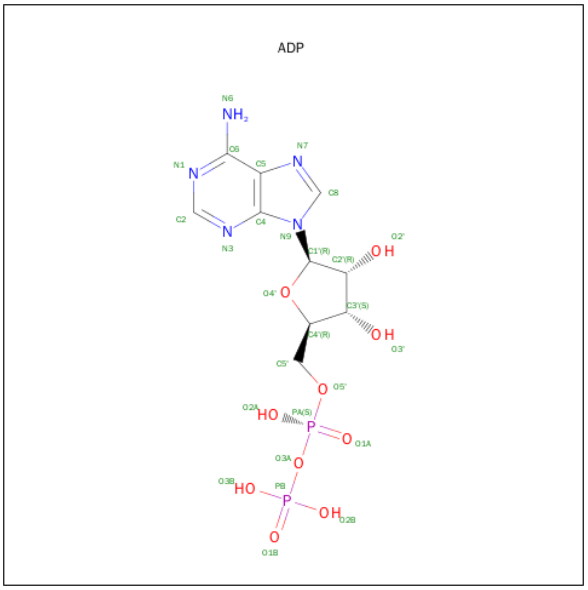
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total	O	0	0
			56	56		
6	C	1	Total	O	0	0
			1	1		
6	D	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

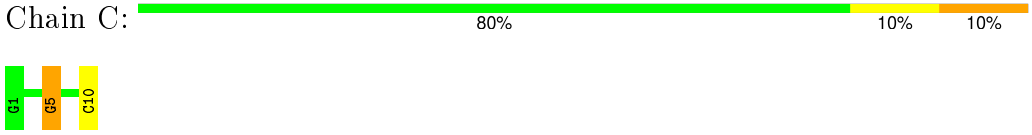
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PROBABLE ATP-DEPENDENT RNA HELICASE DDX58

Chain A:

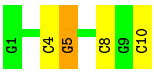
- Molecule 2: RNA DUPLEX

Chain C:



- Molecule 2: RNA DUPLEX

Chain D:


G1
C4
G5
C8
G9
C10

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.25Å 76.00Å 207.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.50) 98.0 (24.61-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.229 , 0.288 0.222 , 0.280	Depositor DCC
R_{free} test set	1343 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 26693 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5369	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.69	2/4953 (0.0%)	0.75	9/6702 (0.1%)
2	C	0.90	0/236	1.60	1/367 (0.3%)
2	D	0.81	0/236	1.50	2/367 (0.5%)
All	All	0.71	2/5425 (0.0%)	0.87	12/7436 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	807	LYS	CE-NZ	-18.10	1.03	1.49
1	A	914	GLU	CG-CD	-11.47	1.34	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	807	LYS	CD-CE-NZ	11.97	139.23	111.70
1	A	914	GLU	CG-CD-OE1	-10.49	97.31	118.30
1	A	914	GLU	CG-CD-OE2	10.20	138.69	118.30
1	A	914	GLU	CB-CG-CD	8.42	136.93	114.20
1	A	771	TRP	CA-CB-CG	6.62	126.29	113.70
2	D	10	C	C3'-C2'-C1'	6.40	106.62	101.50
1	A	768	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	446	LEU	CB-CG-CD1	-5.78	101.17	111.00
2	C	5	G	C8-N9-C4	-5.53	104.19	106.40
1	A	740	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	694	LEU	CA-CB-CG	5.27	127.42	115.30
2	D	8	C	O4'-C1'-N1	5.09	112.27	108.20

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	4856	0	4731	71	0
2	C	212	0	112	1	0
2	D	212	0	112	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	27	0	12	1	0
6	A	56	0	0	1	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
All	All	5369	0	4967	72	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 7.

All (72) 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:703:GLY:HA2	1:A:704:ILE:CB	1.86	1.05
1:A:478:LEU:O	1:A:482:THR:HG23	1.66	0.94
1:A:540:LEU:HD21	1:A:583:GLU:HG3	1.53	0.89
1:A:428:CYS:SG	1:A:779:LYS:NZ	2.50	0.85
1:A:483:GLU:OE2	1:A:502:ARG:NH1	2.13	0.80
1:A:265:PRO:HG2	1:A:453:VAL:HG21	1.65	0.79
1:A:379:LYS:O	1:A:380:GLN:HB2	1.82	0.79
1:A:315:GLU:O	1:A:316:ARG:CB	2.35	0.74
1:A:412:VAL:HG22	1:A:430:LEU:HD23	1.70	0.73
1:A:269:GLY:HA2	5:A:1924:ADP:O1A	1.89	0.71
1:A:661:LEU:HD23	1:A:696:LEU:HD22	1.74	0.70
1:A:357:LYS:HA	1:A:357:LYS:HE2	1.74	0.69
1:A:657:LYS:O	1:A:693:ILE:HG23	1.93	0.68
1:A:379:LYS:O	2:C:5:G:OP2	2.14	0.66
1:A:864:CYS:HB3	1:A:871:HIS:H	1.62	0.65
1:A:656:LEU:HA	1:A:694:LEU:HD23	1.78	0.64
1:A:580:ASP:HB2	1:A:583:GLU:HB2	1.79	0.63
1:A:630:THR:HB	1:A:695:ILE:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:HB2	1:A:583:GLU:H	1.65	0.61
1:A:483:GLU:CD	1:A:502:ARG:HH12	2.06	0.58
1:A:701:ASP:O	1:A:702:GLU:HB2	2.05	0.57
1:A:258:LYS:HE2	1:A:773:GLU:OE1	2.06	0.56
1:A:703:GLY:CA	1:A:704:ILE:CB	2.70	0.56
1:A:554:ILE:HD11	1:A:638:ALA:HB1	1.88	0.56
1:A:379:LYS:O	1:A:380:GLN:CB	2.49	0.56
1:A:412:VAL:CG1	1:A:427:ILE:HG12	2.36	0.56
1:A:412:VAL:HG22	1:A:430:LEU:CD2	2.35	0.54
1:A:889:ILE:HB	1:A:908:TRP:CE2	2.43	0.54
1:A:482:THR:OG1	1:A:545:LEU:HD21	2.07	0.54
1:A:485:LEU:O	1:A:488:ARG:HB2	2.08	0.54
1:A:826:ILE:HB	1:A:830:HIS:HB2	1.90	0.53
1:A:449:LEU:C	1:A:451:GLN:H	2.13	0.52
1:A:702:GLU:HA	1:A:704:ILE:CB	2.40	0.52
1:A:325:SER:HA	1:A:350:ILE:HD11	1.93	0.51
2:D:4:C:H2'	2:D:5:G:O4'	2.09	0.51
1:A:264:ALA:O	1:A:410:ALA:HA	2.10	0.51
1:A:653:LEU:HB3	1:A:656:LEU:HD22	1.93	0.51
1:A:508:LYS:O	1:A:511:GLN:N	2.43	0.51
1:A:412:VAL:HG11	1:A:427:ILE:HG12	1.93	0.50
1:A:653:LEU:O	1:A:656:LEU:HB2	2.12	0.50
1:A:864:CYS:HB3	1:A:871:HIS:N	2.27	0.49
1:A:888:LYS:HB2	1:A:890:GLU:HG2	1.94	0.49
1:A:768:LEU:C	1:A:768:LEU:HD12	2.33	0.49
1:A:399:SER:HA	1:A:400:GLY:HA3	1.70	0.48
1:A:477:GLN:HA	1:A:477:GLN:OE1	2.13	0.48
1:A:587:THR:HG22	1:A:591:GLU:OE2	2.14	0.48
1:A:852:GLN:HA	1:A:857:GLU:HG3	1.94	0.48
1:A:482:THR:OG1	1:A:545:LEU:CD2	2.62	0.47
1:A:824:ARG:HA	1:A:916:ILE:O	2.14	0.47
1:A:475:ILE:HB	1:A:552:LEU:HD11	1.97	0.47
1:A:477:GLN:OE1	1:A:480:ARG:NE	2.36	0.46
1:A:328:THR:O	1:A:329:ALA:HB3	2.14	0.46
1:A:348:PRO:HD2	6:A:2018:HOH:O	2.16	0.46
1:A:347:THR:OG1	1:A:350:ILE:HD12	2.15	0.46
1:A:300:ILE:HB	1:A:301:PRO:HD3	1.98	0.45
1:A:418:LYS:HE3	1:A:422:GLU:OE2	2.18	0.44
1:A:656:LEU:HA	1:A:694:LEU:CD2	2.46	0.44
1:A:252:LEU:HB3	1:A:253:PRO:HD3	1.99	0.44
1:A:702:GLU:HA	1:A:703:GLY:HA2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:HIS:HD1	1:A:610:LYS:NZ	2.16	0.43
1:A:740:LEU:HD12	1:A:748:ILE:HD13	2.01	0.43
1:A:325:SER:HA	1:A:350:ILE:CD1	2.48	0.43
1:A:323:GLY:HA2	1:A:345:ILE:O	2.20	0.42
1:A:449:LEU:C	1:A:451:GLN:N	2.73	0.41
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.88	0.41
1:A:836:ASP:N	1:A:836:ASP:OD1	2.53	0.41
1:A:475:ILE:HG21	1:A:552:LEU:HD13	2.03	0.41
1:A:469:ASP:OD1	1:A:471:PHE:HB3	2.21	0.41
1:A:655:PHE:O	1:A:694:LEU:HD21	2.21	0.41
1:A:281:HIS:O	1:A:284:LYS:HG2	2.21	0.40
1:A:650:ASN:HA	1:A:651:PRO:HD2	1.79	0.40
1:A:773:GLU:OE2	1:A:777:ARG:NH2	2.53	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	609/696 (88%)	567 (93%)	38 (6%)	4 (1%)	26 46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	702	GLU
1	A	704	ILE
1	A	316	ARG
1	A	452	VAL

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	518/625 (83%)	465 (90%)	53 (10%)	9 17

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	SER
1	A	242	LYS
1	A	248	LEU
1	A	266	THR
1	A	270	LYS
1	A	276	LEU
1	A	283	LYS
1	A	322	THR
1	A	328	THR
1	A	334	VAL
1	A	339	GLU
1	A	398	SER
1	A	412	VAL
1	A	418	LYS
1	A	420	THR
1	A	424	LEU
1	A	449	LEU
1	A	457	GLN
1	A	470	LYS
1	A	488	ARG
1	A	493	LEU
1	A	540	LEU
1	A	552	LEU
1	A	559	ARG
1	A	564	LEU
1	A	575	ARG
1	A	589	ARG
1	A	594	LEU
1	A	598	GLU
1	A	601	SER

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Mol	Chain	Res	Type
1	A	602	ARG
1	A	614	LEU
1	A	627	GLU
1	A	629	ILE
1	A	631	ILE
1	A	656	LEU
1	A	699	VAL
1	A	710	ASN
1	A	711	LEU
1	A	716	GLU
1	A	741	LEU
1	A	750	LYS
1	A	758	GLU
1	A	767	ARG
1	A	768	LEU
1	A	780	ILE
1	A	787	GLU
1	A	807	LYS
1	A	811	ARG
1	A	836	ASP
1	A	856	PHE
1	A	896	ASP
1	A	906	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/10 (90%)	1 (11%)	0
2	D	9/10 (90%)	1 (11%)	0
All	All	18/20 (90%)	2 (11%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	10	C

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Mol	Chain	Res	Type
2	D	5	G

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	ADP	A	1924	4	22,29,29	1.12	2 (9%)	27,45,45	1.99	4 (14%)

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	ADP	A	1924	4	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1924	ADP	O4'-C1'	2.21	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1924	ADP	C5-C4	3.65	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1924	ADP	N3-C2-N1	-7.37	123.25	128.89
5	A	1924	ADP	O3A-PA-O5'	-3.40	93.91	102.94
5	A	1924	ADP	PA-O3A-PB	-3.16	122.06	132.67
5	A	1924	ADP	C4-C5-N7	-2.92	106.80	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1924	ADP	1	0

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	623/696 (89%)	0.24	41 (6%) 22 24	23, 60, 111, 140	2 (0%)
2	C	10/10 (100%)	-0.26	0 100 100	62, 97, 124, 126	0
2	D	10/10 (100%)	-0.35	0 100 100	75, 106, 118, 123	0
All	All	643/716 (89%)	0.22	41 (6%) 23 25	23, 61, 113, 140	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	848	PRO	7.3
1	A	865	ALA	5.9
1	A	867	GLN	5.7
1	A	887	ILE	4.7
1	A	850	PRO	4.5
1	A	904	LEU	4.4
1	A	856	PHE	3.8
1	A	868	ASN	3.4
1	A	835	GLY	3.4
1	A	521	MET	3.4
1	A	886	VAL	3.2
1	A	849	LYS	3.1
1	A	906	SER	3.1
1	A	846	PRO	3.1
1	A	704	ILE	3.1
1	A	532	SER	3.0
1	A	703	GLY	3.0
1	A	705	ASP	2.9
1	A	577	ALA	2.9
1	A	294	VAL	2.9
1	A	702	GLU	2.8
1	A	813	CYS	2.8
1	A	662	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	399	SER	2.7
1	A	534	ILE	2.7
1	A	860	ALA	2.7
1	A	899	THR	2.6
1	A	866	ARG	2.6
1	A	836	ASP	2.5
1	A	875	ILE	2.4
1	A	370	ILE	2.4
1	A	910	ASP	2.4
1	A	881	THR	2.4
1	A	467	ILE	2.4
1	A	719	GLY	2.3
1	A	837	ALA	2.3
1	A	661	LEU	2.2
1	A	239	SER	2.2
1	A	874	GLY	2.2
1	A	452	VAL	2.1
1	A	575	ARG	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	ADP	A	1924	27/27	0.91	0.17	0.18	60,69,75,77	0
3	ZN	A	927	1/1	0.98	0.07	-2.33	82,82,82,82	0
4	MG	A	1923	1/1	0.78	0.33	-	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.