



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID : 3QKT  
Title : Rad50 ABC-ATPase with adjacent coiled-coil region in complex with AMP-PNP  
Authors : Williams, G.J.; Williams, R.S.; Arvai, A.; Moncalian, G.; Tainer, J.A.  
Deposited on : 2011-02-01  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

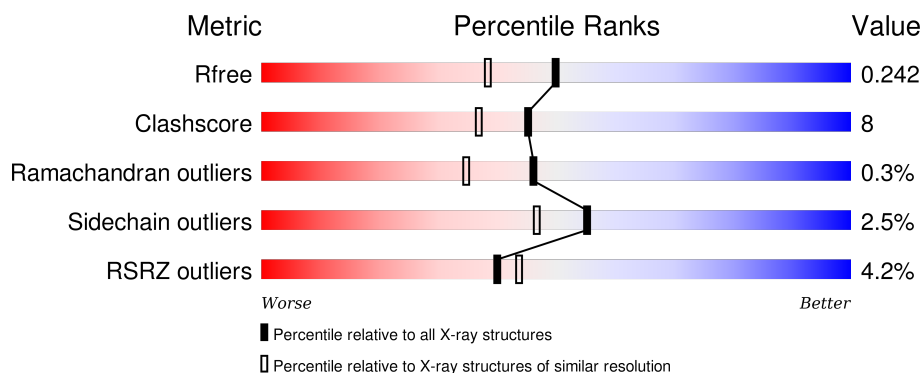
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	339	<div> <div>4%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	B	339	<div> <div>4%</div> <div>75%</div> <div>18%</div> <div>6%</div> <div>.</div> </div>
1	C	339	<div> <div>4%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	D	339	<div> <div>3%</div> <div>76%</div> <div>17%</div> <div>6%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11598 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.

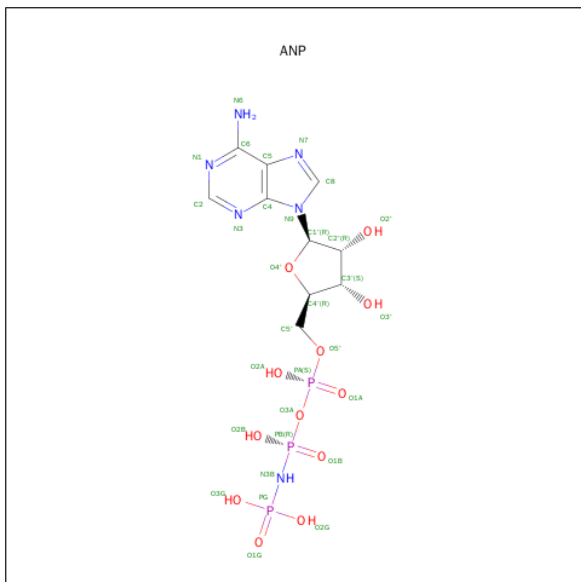
- Molecule 1 is a protein called DNA double-strand break repair rad50 ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2715	1740	464	506	5			
1	B	319	Total	C	N	O	S	0	0	0
			2550	1634	440	471	5			
1	C	339	Total	C	N	O	S	0	0	0
			2715	1740	464	506	5			
1	D	318	Total	C	N	O	S	0	0	0
			2555	1639	439	472	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	GLY	-	LINKER	UNP P58301
A	179	GLY	-	LINKER	UNP P58301
A	180	SER	-	LINKER	UNP P58301
A	181	GLY	-	LINKER	UNP P58301
A	182	GLY	-	LINKER	UNP P58301
B	721	GLY	-	LINKER	UNP P58301
B	722	GLY	-	LINKER	UNP P58301
B	723	SER	-	LINKER	UNP P58301
B	724	GLY	-	LINKER	UNP P58301
B	725	GLY	-	LINKER	UNP P58301
C	178	GLY	-	LINKER	UNP P58301
C	179	GLY	-	LINKER	UNP P58301
C	180	SER	-	LINKER	UNP P58301
C	181	GLY	-	LINKER	UNP P58301
C	182	GLY	-	LINKER	UNP P58301
D	721	GLY	-	LINKER	UNP P58301
D	722	GLY	-	LINKER	UNP P58301
D	723	SER	-	LINKER	UNP P58301
D	724	GLY	-	LINKER	UNP P58301
D	725	GLY	-	LINKER	UNP P58301

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

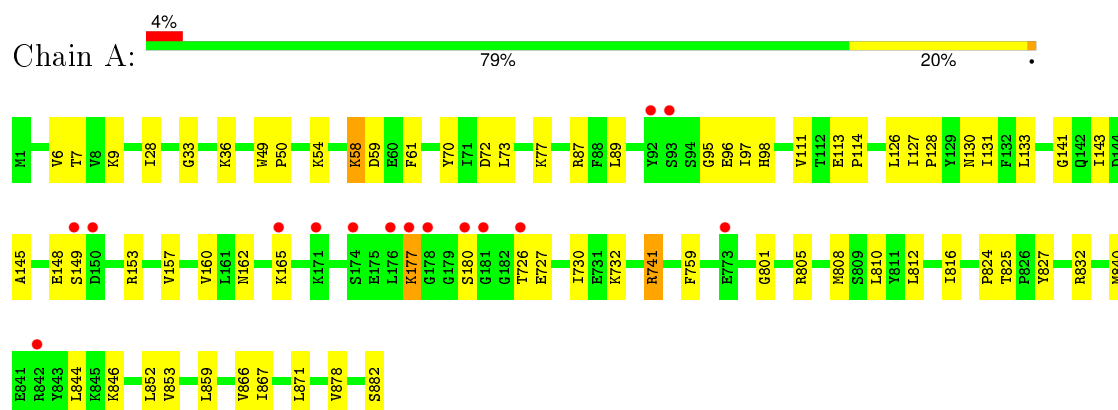
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	243	Total 243	O 243	0	0
4	B	234	Total 234	O 234	0	0
4	C	242	Total 242	O 242	0	0
4	D	216	Total 216	O 216	0	0

### 3 Residue-property plots [i](#)

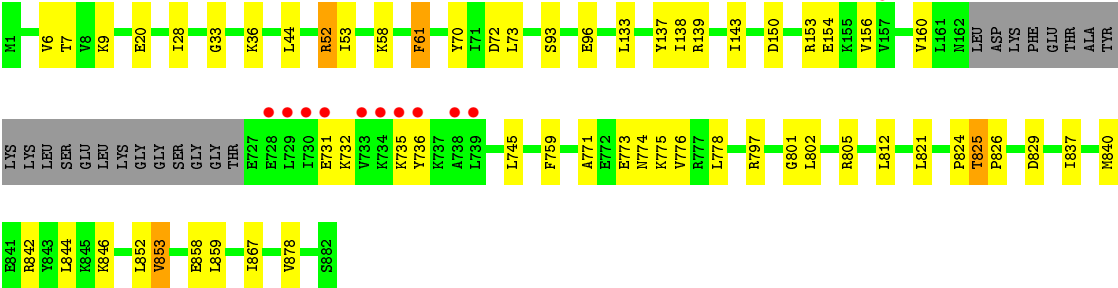
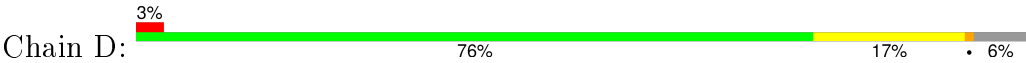
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA double-strand break repair rad50 ATPase





- Molecule 1: DNA double-strand break repair rad50 ATPase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.39Å 108.52Å 150.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 1.90 49.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.65-1.90) 97.5 (49.65-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.192 , 0.244 0.191 , 0.242	Depositor DCC
$R_{free}$ test set	5289 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 105235 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.1273e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ANP

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	0.29	0/2757	0.46	0/3701
1	B	0.30	0/2589	0.47	0/3478
1	C	0.28	0/2757	0.46	0/3701
1	D	0.28	0/2594	0.48	0/3484
All	All	0.29	0/10697	0.47	0/14364

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	2715	0	2813	52	0
1	B	2550	0	2628	44	0
1	C	2715	0	2813	40	0
1	D	2555	0	2648	35	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	243	0	0	7	0
4	B	234	0	0	4	0
4	C	242	0	0	2	0
4	D	216	0	0	3	0
All	All	11598	0	10954	169	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 8.

All (169) 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:128:PRO:HB2	1:A:131:ILE:HD13	1.61	0.82
1:C:180:SER:OG	1:C:726:THR:HG23	1.82	0.79
1:B:87:ARG:HB2	1:B:97:ILE:HG22	1.66	0.77
1:A:801:GLY:O	1:A:805:ARG:HG2	1.85	0.76
1:A:28:ILE:HB	1:A:853:VAL:HG22	1.67	0.74
1:C:148:GLU:HG2	1:C:149:SER:N	2.03	0.73
1:D:840:MET:HG2	1:D:844:LEU:HD12	1.71	0.73
1:A:157:VAL:HG22	1:A:808:MET:HE1	1.70	0.71
1:B:817:SER:OG	1:B:848:PRO:HG2	1.92	0.68
1:C:160:VAL:HG13	1:C:812:LEU:HD21	1.76	0.68
1:B:128:PRO:HB2	1:B:131:ILE:HD13	1.76	0.67
1:D:20:GLU:HG3	4:D:227:HOH:O	1.95	0.67
1:A:89:LEU:HD22	1:A:95:GLY:HA3	1.77	0.66
1:D:154:GLU:HG2	1:D:776:VAL:HG23	1.77	0.66
1:A:840:MET:HG2	1:A:844:LEU:HD22	1.77	0.65
1:C:830:GLU:HG2	1:C:833:ARG:NH2	2.10	0.65
1:D:7:THR:HB	1:D:72:ASP:HB3	1.77	0.65
1:D:801:GLY:O	1:D:805:ARG:HG2	1.96	0.64
1:C:113:GLU:HG2	1:C:114:PRO:HD2	1.79	0.64
1:B:49:TRP:CG	1:B:50:PRO:HA	2.33	0.64
1:A:160:VAL:HG13	1:A:812:LEU:HD21	1.81	0.61
1:B:745:LEU:HD12	1:B:771:ALA:HB2	1.83	0.61
1:A:824:PRO:HG3	1:A:852:LEU:HD11	1.83	0.60
1:B:840:MET:HG2	1:B:844:LEU:HD12	1.82	0.60
1:C:801:GLY:O	1:C:805:ARG:HG2	2.02	0.60
1:C:732:LYS:NZ	1:C:732:LYS:HB2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TRP:CG	1:A:50:PRO:HA	2.38	0.59
1:A:87:ARG:HB3	1:A:97:ILE:HG12	1.84	0.58
1:C:28:ILE:HB	1:C:853:VAL:HG22	1.84	0.58
1:A:162:ASN:OD1	1:A:741:ARG:NH2	2.36	0.57
1:D:52:ARG:HG3	1:D:52:ARG:O	2.03	0.57
1:C:19:VAL:HG13	1:C:867:ILE:HD13	1.87	0.57
1:A:180:SER:OG	1:A:726:THR:HG23	2.03	0.57
1:B:77:LYS:HE2	4:B:936:HOH:O	2.03	0.57
1:D:837:ILE:HD11	1:D:858:GLU:HG2	1.86	0.57
1:C:36:LYS:HD2	1:C:853:VAL:HG13	1.87	0.56
1:A:866:VAL:H	1:A:882:SER:HB2	1.70	0.56
1:B:49:TRP:CD2	1:B:50:PRO:HA	2.41	0.56
1:D:153:ARG:NE	1:D:778:LEU:HD13	2.20	0.56
1:C:157:VAL:HG11	1:C:745:LEU:HD21	1.88	0.56
1:D:93:SER:O	1:D:96:GLU:HG3	2.05	0.56
1:B:729:LEU:O	1:B:733:VAL:HG23	2.06	0.55
1:A:36:LYS:HB3	1:A:853:VAL:HG11	1.89	0.55
1:A:130:ASN:HB3	4:A:273:HOH:O	2.06	0.55
1:C:33:GLY:H	2:C:901:ANP:HNB1	1.55	0.55
1:A:871:LEU:HD21	4:A:890:HOH:O	2.06	0.55
1:D:842:ARG:O	1:D:846:LYS:HE3	2.07	0.54
1:A:832:ARG:HG2	4:B:957:HOH:O	2.07	0.54
1:D:731:GLU:O	1:D:735:LYS:HD3	2.06	0.54
1:D:745:LEU:HD12	1:D:771:ALA:HB2	1.90	0.53
1:A:36:LYS:HB3	1:A:853:VAL:CG1	2.39	0.53
1:B:131:ILE:HD11	1:B:159:GLU:HB3	1.90	0.53
1:C:25:ILE:HD11	1:C:844:LEU:HB3	1.91	0.53
1:D:867:ILE:HG23	1:D:878:VAL:HG13	1.91	0.52
1:B:732:LYS:HD3	1:B:735:LYS:HD2	1.91	0.52
1:A:6:VAL:HG13	1:A:73:LEU:CD2	2.40	0.52
1:A:727:GLU:O	1:A:730:ILE:HG12	2.10	0.51
1:C:830:GLU:HG2	1:C:833:ARG:HH22	1.73	0.51
1:A:867:ILE:CG2	1:A:878:VAL:HG13	2.40	0.51
1:C:70:TYR:HD1	1:C:87:ARG:HG2	1.75	0.51
1:B:6:VAL:HG23	1:B:73:LEU:CD2	2.41	0.51
1:B:731:GLU:O	1:B:735:LYS:HG3	2.11	0.51
1:A:96:GLU:HG2	1:A:98:HIS:HE2	1.76	0.51
1:B:824:PRO:C	1:B:826:PRO:HD2	2.32	0.50
1:A:113:GLU:CD	1:A:114:PRO:HD2	2.32	0.50
1:B:860:LYS:HG3	1:B:866:VAL:HG21	1.94	0.50
1:A:54:LYS:N	1:A:54:LYS:HE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:LEU:HD13	1:A:816:ILE:HD12	1.94	0.50
1:A:810:LEU:HD22	1:A:846:LYS:HZ1	1.76	0.50
1:B:59:ASP:O	1:B:90:LYS:HE2	2.12	0.49
1:D:732:LYS:HB3	1:D:736:TYR:CE2	2.48	0.49
1:A:840:MET:HA	1:A:844:LEU:HD13	1.95	0.49
1:B:143:ILE:HD11	1:B:824:PRO:HA	1.95	0.49
1:D:867:ILE:CG2	1:D:878:VAL:HG13	2.43	0.48
1:D:773:GLU:O	1:D:774:ASN:HB2	2.13	0.48
1:D:137:TYR:CZ	1:D:139:ARG:HG2	2.48	0.48
1:A:157:VAL:HG22	1:A:808:MET:CE	2.40	0.48
1:A:143:ILE:HD11	1:A:824:PRO:HA	1.96	0.48
1:B:824:PRO:HG3	1:B:852:LEU:HD11	1.95	0.48
1:D:150:ASP:HB3	1:D:775:LYS:HB3	1.95	0.48
1:D:824:PRO:HG3	1:D:852:LEU:HD11	1.96	0.48
1:A:77:LYS:HE3	4:A:691:HOH:O	2.13	0.47
1:A:145:ALA:O	1:A:148:GLU:HG2	2.14	0.47
1:B:92:TYR:CD1	1:B:93:SER:N	2.79	0.47
1:D:156:VAL:O	1:D:160:VAL:HB	2.14	0.47
1:A:49:TRP:CD2	1:A:50:PRO:HA	2.50	0.47
1:B:143:ILE:HG21	1:B:802:LEU:HD13	1.96	0.47
1:A:149:SER:HA	4:A:900:HOH:O	2.14	0.47
1:C:58:LYS:HA	1:C:61:PHE:CE2	2.49	0.47
1:B:7:THR:HB	1:B:72:ASP:HB3	1.97	0.47
1:D:28:ILE:HB	1:D:853:VAL:HG22	1.96	0.47
1:D:9:LYS:HB2	1:D:70:TYR:HB3	1.96	0.47
1:C:841:GLU:HB2	4:C:336:HOH:O	2.15	0.47
1:C:856:ASP:OD1	1:C:858:GLU:CG	2.64	0.46
1:C:36:LYS:HB3	1:C:853:VAL:CG1	2.46	0.46
1:C:126:LEU:C	1:C:127:ILE:HG13	2.36	0.46
1:C:812:LEU:HD13	1:C:816:ILE:HD12	1.96	0.46
1:B:840:MET:HA	1:B:844:LEU:HB2	1.97	0.46
1:B:46:GLY:HA3	1:B:73:LEU:HD11	1.96	0.46
1:A:153:ARG:O	1:A:157:VAL:HG23	2.16	0.46
1:B:160:VAL:HG12	1:B:161:LEU:HD12	1.97	0.46
1:A:128:PRO:CB	1:A:131:ILE:HD13	2.41	0.45
1:A:96:GLU:HG2	1:A:98:HIS:NE2	2.32	0.45
1:C:837:ILE:HG23	1:C:862:ALA:HB2	1.98	0.45
1:C:817:SER:HB3	1:C:848:PRO:HG2	1.96	0.45
1:A:810:LEU:HD22	1:A:846:LYS:NZ	2.30	0.45
1:D:36:LYS:HD2	1:D:853:VAL:HG13	1.99	0.45
1:A:36:LYS:HD2	1:A:853:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LEU:HD21	1:D:53:ILE:HD12	1.99	0.45
1:B:812:LEU:HD13	1:B:816:ILE:HD12	1.99	0.45
1:B:758:GLU:O	1:B:835:LYS:HE2	2.16	0.45
1:C:732:LYS:HZ3	1:C:732:LYS:HB2	1.80	0.45
1:A:96:GLU:CG	1:A:98:HIS:HE2	2.30	0.45
1:A:165:LYS:HG3	4:A:964:HOH:O	2.16	0.45
1:B:146:ILE:O	1:B:153:ARG:HD3	2.17	0.45
1:A:732:LYS:HD3	4:A:271:HOH:O	2.16	0.45
1:B:6:VAL:HG23	1:B:73:LEU:HD23	1.98	0.45
1:A:177:LYS:N	1:A:177:LYS:HD3	2.32	0.44
1:D:829:ASP:HB2	4:D:690:HOH:O	2.17	0.44
1:D:33:GLY:H	2:D:901:ANP:HNB1	1.66	0.44
1:A:9:LYS:HB2	1:A:70:TYR:HB3	1.99	0.44
1:A:840:MET:SD	1:A:859:LEU:HD22	2.58	0.44
1:B:59:ASP:N	1:B:59:ASP:OD1	2.43	0.44
1:C:822:ASP:OD1	1:C:823:GLU:HG2	2.18	0.44
1:C:36:LYS:HB3	1:C:853:VAL:HG11	2.00	0.43
1:D:58:LYS:HA	1:D:61:PHE:CE2	2.53	0.43
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.89	0.43
1:C:737:LYS:O	1:C:741:ARG:HG3	2.18	0.43
1:B:844:LEU:HD23	1:B:844:LEU:HA	1.87	0.43
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.85	0.43
1:A:33:GLY:H	2:A:901:ANP:HNB1	1.66	0.43
1:C:871:LEU:HD21	4:C:924:HOH:O	2.17	0.43
1:D:160:VAL:CG1	1:D:812:LEU:HD11	2.49	0.43
1:C:856:ASP:OD1	1:C:858:GLU:HG2	2.19	0.43
1:B:136:ILE:HG12	1:B:816:ILE:HG21	2.01	0.42
1:D:138:ILE:HB	1:D:821:LEU:HD12	2.00	0.42
1:D:825:THR:N	1:D:826:PRO:CD	2.82	0.42
1:B:33:GLY:H	2:B:901:ANP:HNB1	1.67	0.42
1:A:165:LYS:HE3	1:A:165:LYS:HB2	1.76	0.42
1:A:827:TYR:OH	1:B:141:GLY:HA2	2.19	0.42
1:C:754:GLU:HG2	1:C:843:TYR:OH	2.19	0.42
1:C:137:TYR:CZ	1:C:139:ARG:HG2	2.55	0.42
1:C:1:MET:SD	1:C:127:ILE:HD13	2.59	0.42
1:B:149:SER:HB3	1:B:152:ALA:HB3	2.00	0.42
1:C:133:LEU:HD23	1:C:133:LEU:HA	1.85	0.42
1:B:842:ARG:HD2	1:B:843:TYR:CE1	2.54	0.42
1:A:7:THR:HB	1:A:72:ASP:HB3	2.02	0.42
1:C:866:VAL:H	1:C:882:SER:HB3	1.85	0.42
1:B:822:ASP:HA	1:B:853:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:HA2	1:B:827:TYR:OH	2.19	0.42
1:D:797:ARG:HD2	4:D:549:HOH:O	2.20	0.42
1:C:157:VAL:O	1:C:161:LEU:HG	2.20	0.41
1:D:732:LYS:HB3	1:D:736:TYR:CD2	2.55	0.41
1:B:157:VAL:HG11	1:B:745:LEU:HD21	2.03	0.41
1:B:143:ILE:CG2	1:B:802:LEU:HD13	2.51	0.41
1:B:832:ARG:HD2	4:B:368:HOH:O	2.20	0.41
1:A:126:LEU:C	1:A:127:ILE:HG13	2.39	0.41
1:D:133:LEU:HA	1:D:133:LEU:HD23	1.78	0.41
1:D:143:ILE:HD11	1:D:824:PRO:HA	2.01	0.41
1:C:173:LEU:O	1:C:176:LEU:HG	2.20	0.41
1:D:6:VAL:HG13	1:D:73:LEU:CD2	2.50	0.41
1:C:49:TRP:CG	1:C:50:PRO:HA	2.55	0.41
1:A:58:LYS:HG2	4:A:934:HOH:O	2.21	0.41
1:C:106:ASN:N	1:C:106:ASN:OD1	2.52	0.40
1:B:137:TYR:CZ	1:B:139:ARG:HG2	2.56	0.40
1:A:36:LYS:HE3	1:A:36:LYS:HB2	1.92	0.40
1:B:842:ARG:HG3	4:B:447:HOH:O	2.20	0.40
1:C:113:GLU:HG2	1:C:114:PRO:CD	2.49	0.40
1:C:856:ASP:OD1	1:C:858:GLU:HG3	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	337/339 (99%)	326 (97%)	10 (3%)	1 (0%)	46	35
1	B	315/339 (93%)	307 (98%)	7 (2%)	1 (0%)	46	35
1	C	337/339 (99%)	326 (97%)	10 (3%)	1 (0%)	46	35
1	D	314/339 (93%)	305 (97%)	8 (2%)	1 (0%)	46	35
All	All	1303/1356 (96%)	1264 (97%)	35 (3%)	4 (0%)	46	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	825	THR
1	A	825	THR
1	C	825	THR
1	D	825	THR

### 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	293/294 (100%)	285 (97%)	8 (3%)	52	43
1	B	273/294 (93%)	265 (97%)	8 (3%)	50	40
1	C	293/294 (100%)	287 (98%)	6 (2%)	63	57
1	D	276/294 (94%)	270 (98%)	6 (2%)	60	53
All	All	1135/1176 (96%)	1107 (98%)	28 (2%)	55	47

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

Mol	Chain	Res	Type
1	A	58	LYS
1	A	59	ASP
1	A	61	PHE
1	A	111	VAL
1	A	133	LEU
1	A	177	LYS
1	A	741	ARG
1	A	759	PHE
1	B	59	ASP
1	B	61	PHE
1	B	160	VAL
1	B	746	SER
1	B	759	PHE
1	B	802	LEU
1	B	805	ARG
1	B	859	LEU

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Mol	Chain	Res	Type
1	C	61	PHE
1	C	76	GLU
1	C	106	ASN
1	C	148	GLU
1	C	759	PHE
1	C	858	GLU
1	D	52	ARG
1	D	61	PHE
1	D	759	PHE
1	D	802	LEU
1	D	853	VAL
1	D	859	LEU

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

Mol	Chain	Res	Type
1	D	31	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ANP	A	901	3	27,33,33	2.17	9 (33%)	30,52,52	2.37	5 (16%)
2	ANP	B	901	3	27,33,33	2.09	8 (29%)	30,52,52	2.48	6 (20%)
2	ANP	C	901	3	27,33,33	2.12	9 (33%)	30,52,52	2.48	8 (26%)
2	ANP	D	901	3	27,33,33	2.08	8 (29%)	30,52,52	2.42	8 (26%)

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	ANP	A	901	3	-	0/12/38/38	0/3/3/3
2	ANP	B	901	3	-	0/12/38/38	0/3/3/3
2	ANP	C	901	3	-	0/12/38/38	0/3/3/3
2	ANP	D	901	3	-	0/12/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ANP	O4'-C4'	-2.98	1.38	1.45
2	B	901	ANP	O4'-C4'	-2.93	1.38	1.45
2	D	901	ANP	O4'-C4'	-2.83	1.38	1.45
2	A	901	ANP	PG-O2G	-2.74	1.49	1.56
2	D	901	ANP	PA-O2A	-2.74	1.43	1.54
2	C	901	ANP	O4'-C4'	-2.72	1.38	1.45
2	C	901	ANP	C2'-C3'	-2.60	1.46	1.53
2	C	901	ANP	PG-O3G	-2.53	1.49	1.56
2	D	901	ANP	PG-O3G	-2.47	1.49	1.56
2	B	901	ANP	PG-O2G	-2.47	1.49	1.56
2	C	901	ANP	PA-O2A	-2.42	1.44	1.54
2	D	901	ANP	PG-O2G	-2.41	1.50	1.56
2	C	901	ANP	PG-O2G	-2.40	1.50	1.56
2	C	901	ANP	C3'-C4'	-2.34	1.46	1.53
2	B	901	ANP	C3'-C4'	-2.33	1.46	1.53
2	B	901	ANP	PG-O3G	-2.29	1.50	1.56
2	A	901	ANP	C2'-C3'	-2.29	1.47	1.53
2	B	901	ANP	PA-O2A	-2.26	1.45	1.54
2	D	901	ANP	C3'-C4'	-2.17	1.47	1.53
2	A	901	ANP	PA-O2A	-2.17	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ANP	C3'-C4'	-2.08	1.47	1.53
2	A	901	ANP	PG-O3G	-2.06	1.50	1.56
2	D	901	ANP	C6-N6	3.94	1.47	1.34
2	B	901	ANP	O4'-C1'	3.95	1.46	1.41
2	A	901	ANP	O4'-C1'	4.21	1.46	1.41
2	B	901	ANP	C6-N6	4.27	1.48	1.34
2	C	901	ANP	C6-N6	4.31	1.48	1.34
2	A	901	ANP	C6-N6	4.35	1.48	1.34
2	C	901	ANP	O4'-C1'	4.36	1.46	1.41
2	D	901	ANP	O4'-C1'	4.70	1.47	1.41
2	C	901	ANP	PG-O1G	5.46	1.52	1.46
2	D	901	ANP	PG-O1G	5.62	1.52	1.46
2	B	901	ANP	PG-O1G	6.22	1.53	1.46
2	A	901	ANP	PG-O1G	6.70	1.53	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ANP	N3-C2-N1	-9.91	121.31	128.89
2	D	901	ANP	N3-C2-N1	-9.90	121.31	128.89
2	C	901	ANP	N3-C2-N1	-9.81	121.39	128.89
2	B	901	ANP	N3-C2-N1	-9.73	121.44	128.89
2	B	901	ANP	C4'-O4'-C1'	-5.92	103.22	109.72
2	C	901	ANP	C4'-O4'-C1'	-5.37	103.82	109.72
2	A	901	ANP	C4'-O4'-C1'	-4.93	104.30	109.72
2	D	901	ANP	C4'-O4'-C1'	-4.67	104.59	109.72
2	D	901	ANP	O2G-PG-O1G	-2.48	106.90	113.49
2	B	901	ANP	O2G-PG-O1G	-2.27	107.45	113.49
2	C	901	ANP	O2B-PB-O1B	-2.19	105.44	110.00
2	C	901	ANP	C1'-N9-C4	-2.17	123.67	126.94
2	C	901	ANP	C4-C5-N7	-2.16	107.49	109.48
2	A	901	ANP	C1'-N9-C4	-2.15	123.70	126.94
2	D	901	ANP	O2B-PB-O1B	-2.09	105.64	110.00
2	C	901	ANP	O2G-PG-O1G	-2.07	107.99	113.49
2	B	901	ANP	C4-C5-N7	-2.05	107.59	109.48
2	D	901	ANP	C4-C5-N7	-2.02	107.62	109.48
2	D	901	ANP	C2'-C1'-N9	2.01	117.36	114.29
2	D	901	ANP	O5'-C5'-C4'	2.12	116.92	109.12
2	C	901	ANP	O5'-C5'-C4'	2.16	117.09	109.12
2	A	901	ANP	O5'-C5'-C4'	2.23	117.34	109.12
2	B	901	ANP	C2'-C1'-N9	2.86	118.66	114.29
2	A	901	ANP	O1B-PB-N3B	2.92	116.37	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	901	ANP	O1B-PB-N3B	3.46	117.20	111.90
2	B	901	ANP	O1B-PB-N3B	3.48	117.23	111.90
2	C	901	ANP	O1B-PB-N3B	4.45	118.72	111.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ANP	1	0
2	B	901	ANP	1	0
2	C	901	ANP	1	0
2	D	901	ANP	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	339/339 (100%)	0.21	15 (4%) 38 41	17, 37, 82, 130	0
1	B	319/339 (94%)	0.20	15 (4%) 35 38	17, 36, 87, 160	0
1	C	339/339 (100%)	0.20	14 (4%) 41 45	20, 38, 76, 124	0
1	D	318/339 (93%)	0.19	11 (3%) 48 51	19, 37, 77, 158	0
All	All	1315/1356 (96%)	0.20	55 (4%) 40 44	17, 37, 80, 160	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	730	ILE	12.1
1	B	730	ILE	8.8
1	D	729	LEU	8.1
1	D	733	VAL	7.0
1	B	736	TYR	5.5
1	D	736	TYR	5.5
1	B	726	THR	5.3
1	B	729	LEU	5.2
1	A	93	SER	4.9
1	A	176	LEU	4.9
1	D	728	GLU	4.8
1	A	178	GLY	4.3
1	D	735	LYS	4.0
1	A	177	LYS	3.5
1	B	106	ASN	3.5
1	C	166	PHE	3.5
1	C	165	LYS	3.4
1	D	734	LYS	3.4
1	A	174	SER	3.3
1	B	735	LYS	3.2
1	A	92	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	150	ASP	3.2
1	C	176	LEU	3.2
1	D	738	ALA	3.2
1	A	165	LYS	3.1
1	B	733	VAL	3.0
1	C	732	LYS	2.9
1	B	161	LEU	2.9
1	C	152	ALA	2.9
1	D	731	GLU	2.9
1	A	180	SER	2.8
1	D	739	LEU	2.7
1	A	171	LYS	2.7
1	A	773	GLU	2.7
1	B	734	LYS	2.5
1	D	157	VAL	2.4
1	A	149	SER	2.4
1	C	169	ALA	2.4
1	C	181	GLY	2.4
1	B	732	LYS	2.4
1	C	164	ASP	2.3
1	B	92	TYR	2.3
1	C	171	LYS	2.3
1	A	181	GLY	2.3
1	C	93	SER	2.2
1	A	842	ARG	2.2
1	B	160	VAL	2.2
1	B	728	GLU	2.2
1	B	731	GLU	2.2
1	B	107	GLU	2.1
1	C	149	SER	2.1
1	C	174	SER	2.1
1	A	726	THR	2.1
1	C	92	TYR	2.0
1	C	175	GLU	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 [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MG	B	902	1/1	0.98	0.11	0.89	19,19,19,19	0
3	MG	C	902	1/1	0.96	0.12	0.73	24,24,24,24	0
3	MG	A	902	1/1	0.99	0.10	0.25	20,20,20,20	0
2	ANP	D	901	31/31	0.98	0.09	-0.23	16,19,23,24	0
2	ANP	C	901	31/31	0.98	0.09	-0.49	17,23,28,31	0
2	ANP	B	901	31/31	0.99	0.09	-0.77	12,17,20,21	0
2	ANP	A	901	31/31	0.99	0.08	-0.89	15,21,25,26	0
3	MG	D	902	1/1	0.99	0.06	-2.63	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.