



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:03 AM GMT

PDB ID : 2O1V  
Title : Structure of full length GRP94 with ADP bound  
Authors : Dollins, D.E.; Warren, J.J.; Immormino, R.M.; Gewirth, D.T.  
Deposited on : 2006-11-29  
Resolution : 2.45 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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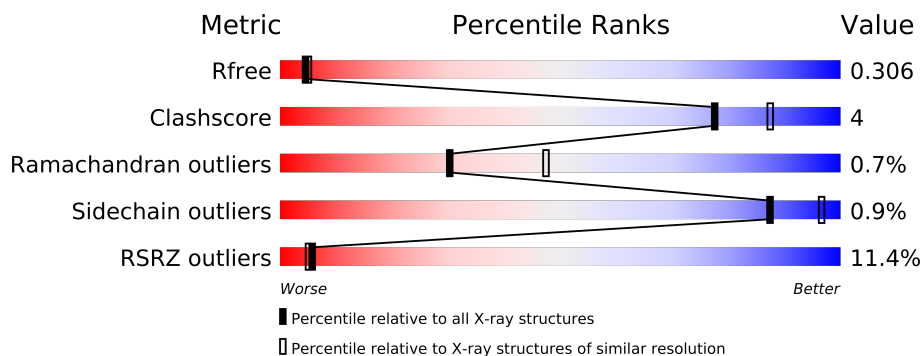
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.45 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))
$R_{free}$	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	666	
1	B	666	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	756	-	X
2	MG	B	756	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9607 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	13	0
			4666	2978	785	886	17			
1	B	575	Total	C	N	O	S	0	0	0
			4623	2946	776	885	16			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	EXPRESSION TAG	UNP P41148
A	53	GLY	-	EXPRESSION TAG	UNP P41148
A	54	SER	-	EXPRESSION TAG	UNP P41148
A	55	SER	-	EXPRESSION TAG	UNP P41148
A	56	HIS	-	EXPRESSION TAG	UNP P41148
A	57	HIS	-	EXPRESSION TAG	UNP P41148
A	58	HIS	-	EXPRESSION TAG	UNP P41148
A	59	HIS	-	EXPRESSION TAG	UNP P41148
A	60	HIS	-	EXPRESSION TAG	UNP P41148
A	61	HIS	-	EXPRESSION TAG	UNP P41148
A	62	SER	-	EXPRESSION TAG	UNP P41148
A	63	SER	-	EXPRESSION TAG	UNP P41148
A	64	GLY	-	EXPRESSION TAG	UNP P41148
A	65	LEU	-	EXPRESSION TAG	UNP P41148
A	66	VAL	-	EXPRESSION TAG	UNP P41148
A	67	PRO	-	EXPRESSION TAG	UNP P41148
A	68	ARG	-	EXPRESSION TAG	UNP P41148
A	69	GLY	-	EXPRESSION TAG	UNP P41148
A	70	SER	-	EXPRESSION TAG	UNP P41148
A	71	HIS	-	EXPRESSION TAG	UNP P41148
A	72	MET	-	EXPRESSION TAG	UNP P41148
A	287	GLY	-	see remark 999	UNP P41148
A	288	GLY	-	see remark 999	UNP P41148
A	289	GLY	-	see remark 999	UNP P41148
A	290	GLY	-	see remark 999	UNP P41148

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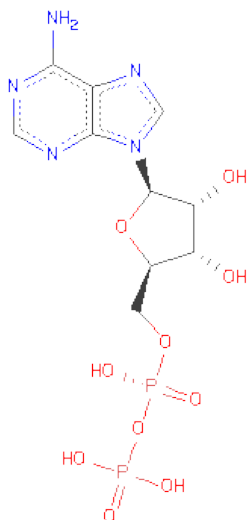
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Chain	Residue	Modelled	Actual	Comment	Reference
B	52	MET	-	EXPRESSION TAG	UNP P41148
B	53	GLY	-	EXPRESSION TAG	UNP P41148
B	54	SER	-	EXPRESSION TAG	UNP P41148
B	55	SER	-	EXPRESSION TAG	UNP P41148
B	56	HIS	-	EXPRESSION TAG	UNP P41148
B	57	HIS	-	EXPRESSION TAG	UNP P41148
B	58	HIS	-	EXPRESSION TAG	UNP P41148
B	59	HIS	-	EXPRESSION TAG	UNP P41148
B	60	HIS	-	EXPRESSION TAG	UNP P41148
B	61	HIS	-	EXPRESSION TAG	UNP P41148
B	62	SER	-	EXPRESSION TAG	UNP P41148
B	63	SER	-	EXPRESSION TAG	UNP P41148
B	64	GLY	-	EXPRESSION TAG	UNP P41148
B	65	LEU	-	EXPRESSION TAG	UNP P41148
B	66	VAL	-	EXPRESSION TAG	UNP P41148
B	67	PRO	-	EXPRESSION TAG	UNP P41148
B	68	ARG	-	EXPRESSION TAG	UNP P41148
B	69	GLY	-	EXPRESSION TAG	UNP P41148
B	70	SER	-	EXPRESSION TAG	UNP P41148
B	71	HIS	-	EXPRESSION TAG	UNP P41148
B	72	MET	-	EXPRESSION TAG	UNP P41148
B	287	GLY	-	see remark 999	UNP P41148
B	288	GLY	-	see remark 999	UNP P41148
B	289	GLY	-	see remark 999	UNP P41148
B	290	GLY	-	see remark 999	UNP P41148

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

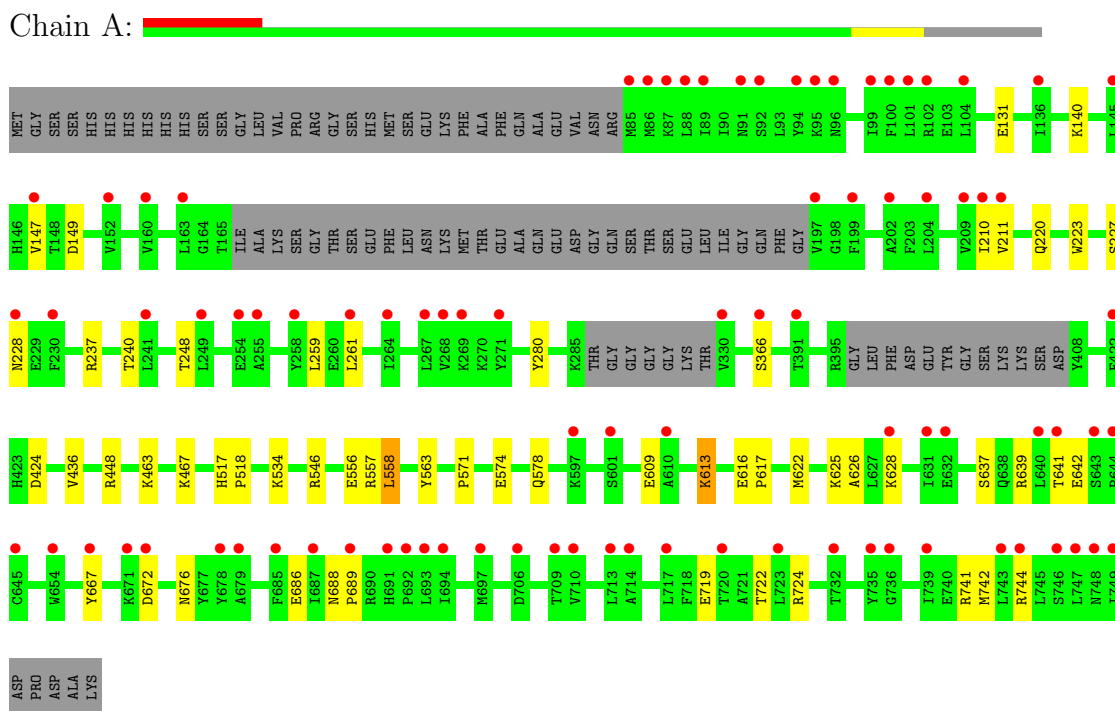
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	125	Total	O	0	0
			125	125		

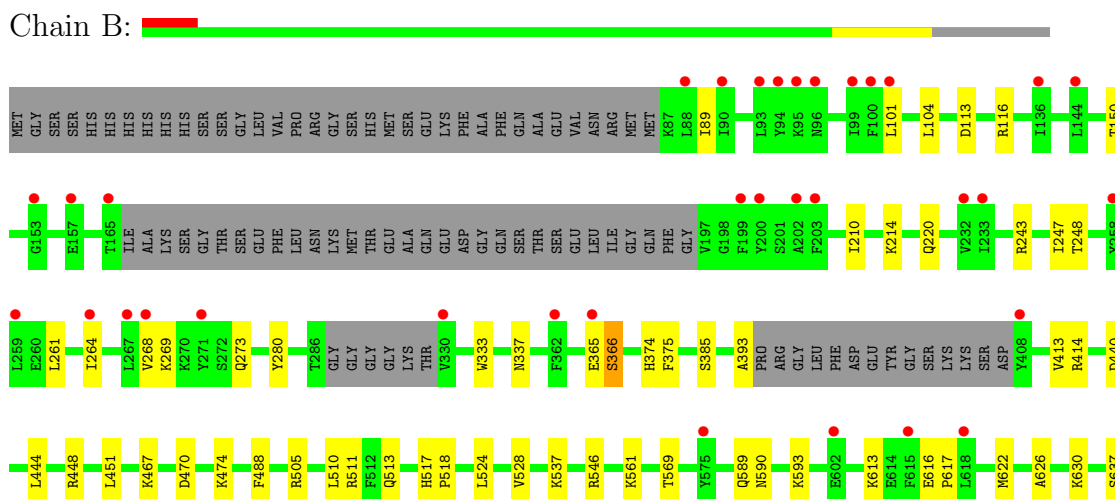
### 3 Residue-property plots

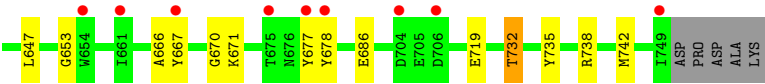
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 1: Endoplasmic





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.08Å 108.85Å 148.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 47.70 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.45) 99.6 (47.70-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.248 , 0.299 0.265 , 0.306	Depositor DCC
$R_{free}$ test set	2972 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 59633 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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	0.53	6/4792 (0.1%)	0.67	2/6465 (0.0%)
1	B	0.41	0/4708	0.64	1/6351 (0.0%)
All	All	0.47	6/9500 (0.1%)	0.66	3/12816 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CD-OE2	8.02	1.34	1.25
1	A	237	ARG	C-O	7.10	1.36	1.23
1	A	131	GLU	CD-OE1	6.67	1.32	1.25
1	A	147	VAL	C-O	6.33	1.35	1.23
1	A	237	ARG	C-N	6.07	1.44	1.33
1	A	280	TYR	C-O	5.67	1.34	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	LEU	CA-CB-CG	5.71	128.43	115.30
1	B	451	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	546	ARG	NE-CZ-NH1	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4666	0	4617	30	0
1	B	4623	0	4571	42	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	135	0	0	2	0
4	B	125	0	0	4	0
All	All	9607	0	9212	68	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (68) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:637:SER:HB2	1:B:686:GLU:HB3	1.62	0.82
1:A:724:ARG:HD2	1:B:732:THR:HG23	1.67	0.76
1:A:741[B]:ARG:CG	1:A:741[B]:ARG:HH11	2.03	0.71
1:A:210:ILE:HG13	1:A:248:THR:HB	1.76	0.67
1:A:741[B]:ARG:HG2	1:A:741[B]:ARG:HH11	1.59	0.66
1:A:556:GLU:HB3	1:A:641:THR:HB	1.81	0.63
1:A:625:LYS:HA	1:A:628:LYS:HD2	1.82	0.62
1:B:104:LEU:HD22	1:B:247:ILE:HD13	1.82	0.61
1:A:637:SER:HB2	1:A:686:GLU:HB3	1.82	0.61
1:B:470:ASP:OD2	1:B:505:ARG:NH2	2.35	0.58
1:B:590:ASN:HB3	1:B:593:LYS:HD2	1.87	0.57
1:B:653:GLY:HA2	1:B:678:TYR:HB2	1.88	0.56
1:A:140:LYS:HA	1:A:259:LEU:HD13	1.88	0.56
1:A:741[A]:ARG:HA	1:A:744[A]:ARG:HE	1.72	0.54
1:B:210:ILE:HB	1:B:248:THR:HB	1.90	0.54
1:B:414:ARG:HD2	1:B:444:LEU:HD22	1.89	0.53
1:B:413:VAL:HG23	1:B:444:LEU:HD13	1.91	0.52
1:B:666:ALA:O	1:B:671:LYS:N	2.39	0.52
1:B:474:LYS:HB2	4:B:872:HOH:O	2.10	0.52
1:B:517:HIS:CG	1:B:518:PRO:HD2	2.45	0.51
1:A:571:PRO:HG3	1:B:667:TYR:CE2	2.46	0.50
1:A:563:TYR:O	4:A:775:HOH:O	2.20	0.49
1:B:113:ASP:OD1	1:B:116:ARG:NH2	2.46	0.49
1:B:537:LYS:HD3	1:B:589:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:463:LYS:O	1:A:467:LYS:HG2	2.13	0.48
1:B:337:ASN:ND2	4:B:841:HOH:O	2.45	0.48
1:B:513:GLN:OE1	1:B:546:ARG:NH1	2.45	0.48
1:B:261:LEU:HA	1:B:264:ILE:HG22	1.96	0.47
1:B:719:GLU:OE2	1:B:735:TYR:HD1	1.97	0.47
1:A:667:TYR:HE1	1:B:569:THR:O	1.99	0.46
1:A:622:MET:HA	1:A:626:ALA:HB3	1.98	0.46
1:B:622:MET:HA	1:B:626:ALA:HB3	1.98	0.46
1:B:393:ALA:HA	1:B:488:PHE:HE2	1.80	0.46
1:B:719:GLU:OE1	1:B:738:ARG:NH2	2.46	0.45
1:A:220:GLN:HE22	1:A:240:THR:HB	1.81	0.45
1:B:647:LEU:HD23	1:B:647:LEU:HA	1.72	0.45
1:A:534:LYS:HD2	1:A:534:LYS:HA	1.84	0.45
1:A:517:HIS:CG	1:A:518:PRO:HD2	2.51	0.45
1:B:616:GLU:N	1:B:617:PRO:HD2	2.31	0.45
1:B:393:ALA:HA	1:B:488:PHE:CE2	2.51	0.45
1:B:375:PHE:CE1	1:B:467:LYS:HG3	2.51	0.44
1:A:719:GLU:O	1:A:722:THR:HB	2.18	0.44
1:B:524:LEU:O	1:B:528:VAL:HG23	2.16	0.44
1:B:269:LYS:O	1:B:273:GLN:NE2	2.51	0.44
1:A:616:GLU:N	1:A:617:PRO:HD2	2.33	0.44
1:B:150:THR:O	1:B:243:ARG:NH2	2.48	0.43
1:A:574:GLU:HB2	4:A:845:HOH:O	2.18	0.43
1:B:630:LYS:NZ	4:B:828:HOH:O	2.48	0.43
1:B:561:LYS:HD3	1:B:561:LYS:HA	1.82	0.43
1:B:101:LEU:HD21	1:B:268:VAL:HG12	2.00	0.43
1:A:688:ASN:HA	1:A:689:PRO:HD2	1.93	0.42
1:B:613:LYS:HD2	1:B:613:LYS:HA	1.92	0.42
1:A:211:VAL:HG22	1:A:223:TRP:HB3	2.00	0.42
1:A:557:ARG:HB2	1:A:639:ARG:HA	2.00	0.42
1:B:365:GLU:O	1:B:366:SER:HB3	2.19	0.42
1:A:574:GLU:O	1:A:578:GLN:HB2	2.20	0.42
1:A:424:ASP:OD1	1:A:424:ASP:N	2.53	0.42
1:B:505:ARG:HG3	4:B:779:HOH:O	2.19	0.41
1:B:666:ALA:HA	1:B:670:GLY:HA3	2.02	0.41
1:A:742:MET:SD	1:B:742:MET:HB3	2.61	0.41
1:A:641:THR:HG22	1:A:642:GLU:N	2.36	0.41
1:B:214:LYS:HD3	1:B:220:GLN:HB2	2.02	0.41
1:B:510:LEU:O	1:B:511:ARG:HD3	2.20	0.41
1:A:639:ARG:HD2	1:A:686:GLU:OE1	2.21	0.41
1:A:609:GLU:O	1:A:613:LYS:HD2	2.22	0.40
1:B:374:HIS:HA	1:B:385:SER:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:641:THR:HG22	1:A:642:GLU:HG3	2.03	0.40
1:B:280:TYR:HB3	1:B:333:TRP:HB3	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	583/666 (88%)	549 (94%)	29 (5%)	5 (1%)	25	39
1	B	565/666 (85%)	523 (93%)	39 (7%)	3 (0%)	38	57
All	All	1148/1332 (86%)	1072 (93%)	68 (6%)	8 (1%)	30	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	366	SER
1	B	366	SER
1	A	228	ASN
1	B	89	ILE
1	A	676	ASN
1	B	677	TYR
1	A	672	ASP

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/598 (85%)	502 (99%)	6 (1%)	82	94
1	B	504/598 (84%)	501 (99%)	3 (1%)	92	98
All	All	1012/1196 (85%)	1003 (99%)	9 (1%)	87	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	A	261	LEU
1	A	436	VAL
1	A	448	ARG
1	A	558	LEU
1	A	613	LYS
1	B	440	ASP
1	B	448	ARG
1	B	732	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	500	HIS
1	A	681	GLN
1	B	337	ASN
1	B	681	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 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	301	2	29,29,29	1.20	2 (6%)	45,45,45	1.84	6 (13%)
3	ADP	B	302	2	29,29,29	1.24	4 (13%)	45,45,45	1.96	7 (15%)

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	301	2	-	0/16/32/32	0/1/3/3
3	ADP	B	302	2	-	0/16/32/32	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	ADP	O4'-C1'	3.07	1.46	1.41
3	B	302	ADP	C4-N9	-3.05	1.33	1.37
3	A	301	ADP	C4-N9	-3.03	1.33	1.37
3	A	301	ADP	O4'-C1'	2.74	1.45	1.41
3	B	302	ADP	PB-O3B	2.34	1.63	1.54
3	B	302	ADP	PB-O2B	2.02	1.62	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	ADP	N3-C2-N1	-8.73	121.41	128.71
3	B	302	ADP	N3-C2-N1	-8.67	121.46	128.71
3	B	302	ADP	PA-O3A-PB	-4.78	117.67	131.68
3	A	301	ADP	N3-C4-N9	4.10	132.83	125.43
3	B	302	ADP	N3-C4-N9	4.05	132.75	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	ADP	O4'-C1'-N9	3.96	112.12	108.44
3	B	302	ADP	C5-C4-N3	-2.81	119.58	125.70
3	A	301	ADP	C5-C4-N3	-2.65	119.93	125.70
3	A	301	ADP	C4-C5-N7	-2.56	107.33	109.52
3	A	301	ADP	PA-O3A-PB	-2.49	124.39	131.68
3	B	302	ADP	C4-C5-N7	-2.39	107.47	109.52
3	B	302	ADP	C2-N3-C4	2.28	120.49	114.01
3	A	301	ADP	C2-N3-C4	2.18	120.22	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	578/666 (86%)	0.91	88 (15%) 3 3	13, 30, 43, 54	0
1	B	575/666 (86%)	0.55	43 (7%) 14 13	10, 30, 40, 51	0
All	All	1153/1332 (86%)	0.73	131 (11%) 6 5	10, 30, 42, 54	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	ASN	11.0
1	A	85	MET	8.4
1	A	96	ASN	7.0
1	B	94	TYR	5.8
1	B	99	ILE	5.8
1	B	100	PHE	5.4
1	A	160	VAL	5.3
1	B	200	TYR	5.3
1	A	258	TYR	5.3
1	A	87	LYS	5.3
1	B	202	ALA	5.2
1	B	267	LEU	5.1
1	A	86	MET	5.1
1	A	679	ALA	4.9
1	A	261	LEU	4.9
1	B	678	TYR	4.9
1	A	101	LEU	4.5
1	B	330	VAL	4.5
1	B	136	ILE	4.4
1	B	157	GLU	4.4
1	B	93	LEU	4.3
1	A	671	LYS	4.3
1	A	366	SER	4.2
1	A	713	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	95	LYS	4.1
1	B	199	PHE	4.0
1	A	88	LEU	4.0
1	A	99	ILE	3.9
1	B	88	LEU	3.9
1	A	330	VAL	3.8
1	A	209	VAL	3.8
1	B	259	LEU	3.8
1	A	268	VAL	3.8
1	B	706	ASP	3.7
1	A	739	ILE	3.7
1	A	271	TYR	3.7
1	B	95	LYS	3.7
1	B	661	ILE	3.7
1	A	210	ILE	3.6
1	B	165	THR	3.6
1	B	258	TYR	3.6
1	B	675	THR	3.5
1	A	717	LEU	3.5
1	B	677	TYR	3.5
1	A	749	ILE	3.5
1	B	264	ILE	3.5
1	A	678	TYR	3.4
1	A	202	ALA	3.4
1	A	645	CYS	3.3
1	A	100	PHE	3.3
1	B	101	LEU	3.3
1	A	94	TYR	3.3
1	A	694	ILE	3.3
1	B	233	ILE	3.3
1	A	199	PHE	3.2
1	B	144	LEU	3.2
1	A	710	VAL	3.2
1	A	228	ASN	3.1
1	A	746	SER	3.1
1	A	693	LEU	3.1
1	A	714	ALA	3.1
1	A	230	PHE	3.1
1	A	691	HIS	3.1
1	A	136	ILE	3.0
1	B	90	ILE	3.0
1	A	692	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	641	THR	3.0
1	A	601	SER	3.0
1	A	597	LYS	2.9
1	A	211	VAL	2.9
1	A	743	LEU	2.9
1	A	632[A]	GLU	2.9
1	A	267	LEU	2.9
1	A	654	TRP	2.9
1	A	89	ILE	2.8
1	A	264	ILE	2.8
1	A	255	ALA	2.8
1	A	152	VAL	2.8
1	B	203	PHE	2.8
1	A	163	LEU	2.8
1	A	147	VAL	2.8
1	A	145	LEU	2.7
1	A	254	GLU	2.7
1	A	91	ASN	2.6
1	B	153	GLY	2.6
1	A	92	SER	2.6
1	B	362	PHE	2.6
1	B	615	PHE	2.6
1	B	232	VAL	2.6
1	A	685	PHE	2.6
1	A	667	TYR	2.6
1	A	640	LEU	2.5
1	A	102	ARG	2.5
1	A	747	LEU	2.5
1	B	268	VAL	2.5
1	A	610	ALA	2.5
1	A	104	LEU	2.4
1	A	697	MET	2.4
1	B	704	ASP	2.4
1	A	689	PRO	2.4
1	A	249	LEU	2.3
1	A	732	THR	2.3
1	A	736	GLY	2.3
1	A	720	THR	2.3
1	A	672	ASP	2.3
1	B	654	TRP	2.3
1	A	735	TYR	2.3
1	A	706	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	575	TYR	2.2
1	A	687	ILE	2.2
1	A	269	LYS	2.2
1	B	602	GLU	2.2
1	A	748	ASN	2.2
1	A	631	ILE	2.2
1	A	744[A]	ARG	2.2
1	B	408	TYR	2.2
1	B	749	ILE	2.2
1	B	667	TYR	2.2
1	A	422	PHE	2.1
1	A	643	SER	2.1
1	A	644	PRO	2.1
1	A	241	LEU	2.1
1	A	391	THR	2.1
1	A	709	THR	2.1
1	B	365	GLU	2.1
1	A	204	LEU	2.1
1	B	271	TYR	2.1
1	A	628	LYS	2.0
1	A	723	LEU	2.0
1	B	618	LEU	2.0
1	A	197	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 carbohydrates 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. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	756	1/1	0.41	3.32	34,34,34,34	0
2	MG	A	756	1/1	0.35	3.18	42,42,42,42	0
2	MG	B	755	1/1	0.14	-0.52	37,37,37,37	0
3	ADP	B	302	27/27	0.09	-1.13	35,37,39,39	0
3	ADP	A	301	27/27	0.12	-1.45	29,32,34,34	0
2	MG	A	755	1/1	0.06	-4.85	12,12,12,12	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.