



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 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 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 ⓘ symbol.

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

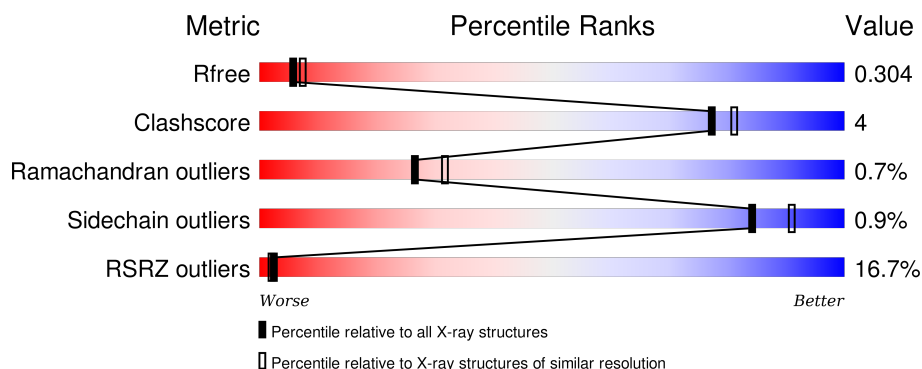
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (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 ≥ 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	666	<div> <div>20%</div> <div>78%</div> <div>8%</div> <div>13%</div> </div>
1	B	666	<div> <div>9%</div> <div>76%</div> <div>11%</div> <div>14%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9607 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 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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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: C₁₀H₁₅N₅O₁₀P₂).



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		

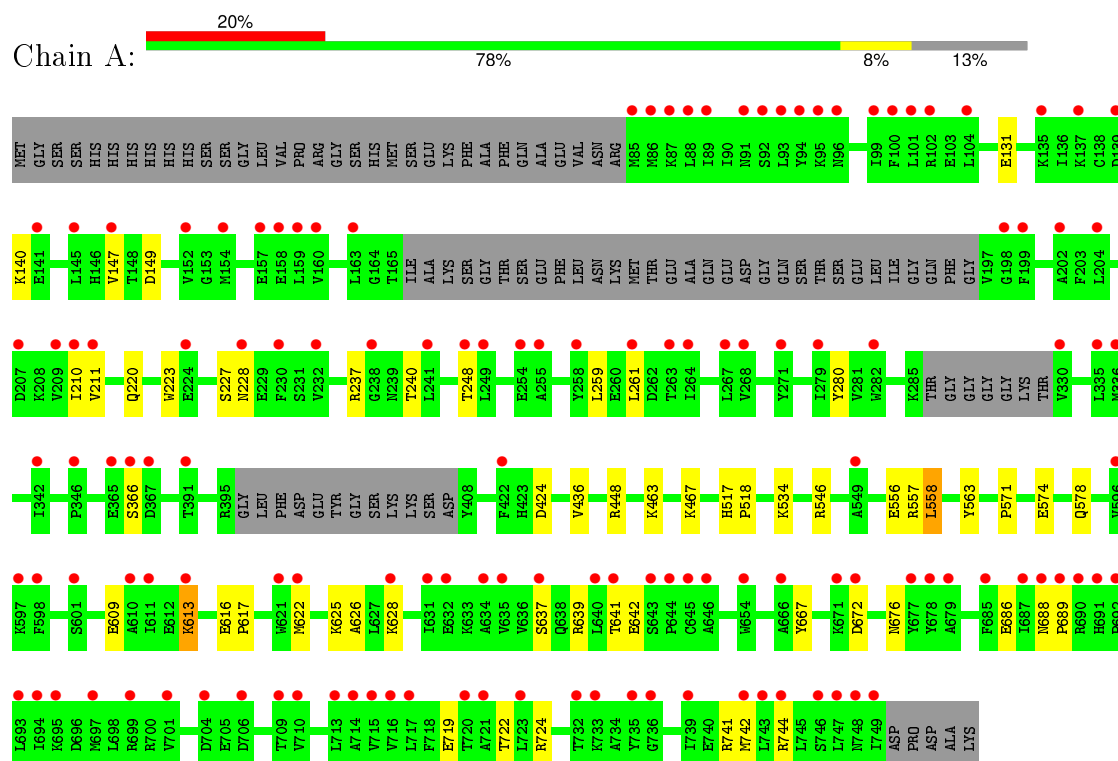
- Molecule 4 is water.

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

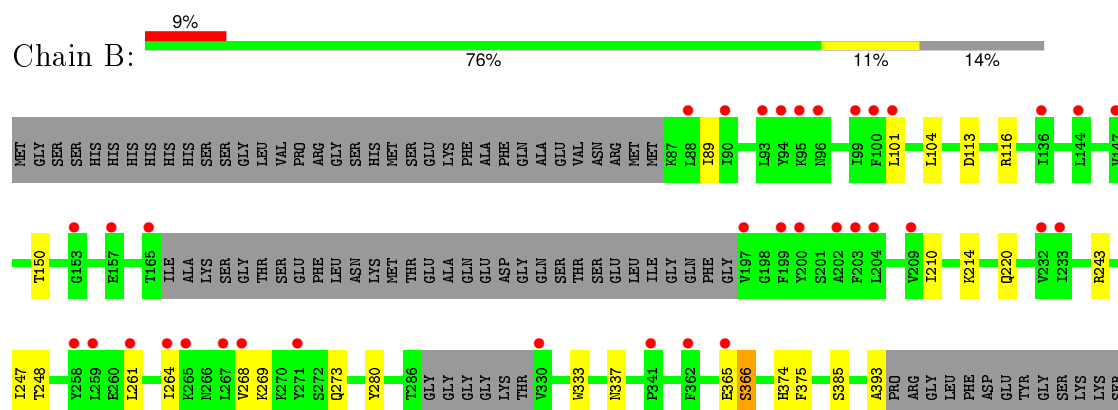
3 Residue-property plots

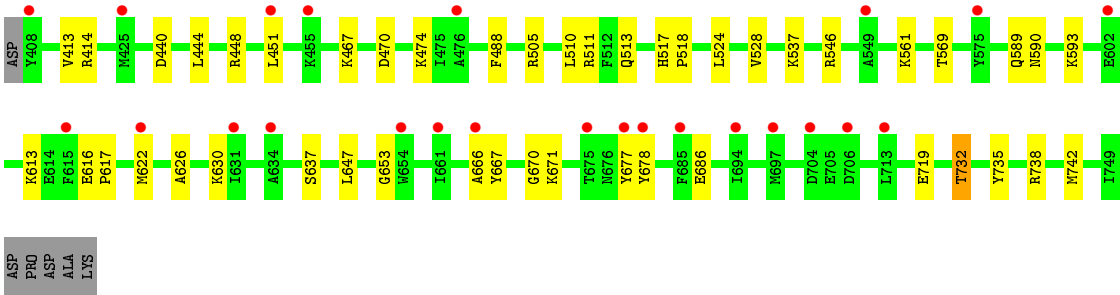
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.299 0.263 , 0.304	Depositor DCC
R_{free} test set	2970 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 59633 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9607	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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 Too-close contacts ⓘ

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	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

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 (68) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:HIS:HA	1:B:385:SER:O	2.22	0.40
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 [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	583/666 (88%)	549 (94%)	29 (5%)	5 (1%)	21	25
1	B	565/666 (85%)	523 (93%)	39 (7%)	3 (0%)	34	41
All	All	1148/1332 (86%)	1072 (93%)	68 (6%)	8 (1%)	26	32

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 [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	508/598 (85%)	502 (99%)	6 (1%)	78	87
1	B	504/598 (84%)	501 (99%)	3 (1%)	90	94
All	All	1012/1196 (85%)	1003 (99%)	9 (1%)	84	91

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 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 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	22,29,29	1.18	1 (4%)	27,45,45	2.23	4 (14%)
3	ADP	B	302	2	22,29,29	1.27	3 (13%)	27,45,45	2.26	3 (11%)

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	-	0/12/32/32	0/3/3/3
3	ADP	B	302	2	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	ADP	PB-O2B	2.06	1.62	1.54
3	B	302	ADP	PB-O3B	2.38	1.63	1.54
3	A	301	ADP	O4'-C1'	3.44	1.45	1.41
3	B	302	ADP	O4'-C1'	3.85	1.46	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	ADP	N3-C2-N1	-9.77	121.41	128.89
3	B	302	ADP	N3-C2-N1	-9.71	121.46	128.89
3	B	302	ADP	PA-O3A-PB	-4.47	117.67	132.67
3	A	301	ADP	PA-O3A-PB	-2.47	124.39	132.67
3	A	301	ADP	C2'-C1'-N9	-2.34	110.72	114.29
3	A	301	ADP	C4-C5-N7	-2.34	107.33	109.48
3	B	302	ADP	C4-C5-N7	-2.18	107.47	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	578/666 (86%)	1.25	132 (22%) 1 1	13, 30, 43, 54	0
1	B	575/666 (86%)	0.87	60 (10%) 8 8	10, 30, 40, 51	0
All	All	1153/1332 (86%)	1.06	192 (16%) 2 2	10, 30, 42, 54	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	ASN	12.5
1	B	200	TYR	7.2
1	A	85	MET	7.0
1	A	96	ASN	6.9
1	A	160	VAL	6.7
1	A	261	LEU	6.5
1	B	94	TYR	6.0
1	B	99	ILE	5.8
1	A	679	ALA	5.7
1	A	87	LYS	5.5
1	A	92	SER	5.4
1	A	210	ILE	5.3
1	A	94	TYR	5.3
1	B	267	LEU	5.1
1	A	330	VAL	5.0
1	B	199	PHE	5.0
1	B	144	LEU	4.9
1	B	157	GLU	4.8
1	B	232	VAL	4.8
1	A	713	LEU	4.7
1	A	209	VAL	4.6
1	A	255	ALA	4.6
1	A	86	MET	4.6
1	A	258	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	746	SER	4.5
1	B	330	VAL	4.4
1	A	88	LEU	4.4
1	A	366	SER	4.3
1	A	268	VAL	4.3
1	B	88	LEU	4.3
1	A	95	LYS	4.3
1	B	202	ALA	4.3
1	A	749	ILE	4.3
1	A	671	LYS	4.3
1	B	95	LYS	4.2
1	A	249	LEU	4.2
1	B	90	ILE	4.1
1	B	258	TYR	4.1
1	B	677	TYR	4.1
1	B	259	LEU	4.1
1	A	99	ILE	4.1
1	A	717	LEU	3.9
1	B	264	ILE	3.9
1	A	710	VAL	3.7
1	B	233	ILE	3.7
1	A	254	GLU	3.7
1	A	691	HIS	3.7
1	B	706	ASP	3.7
1	A	335	LEU	3.7
1	A	739	ILE	3.7
1	B	362	PHE	3.7
1	A	271	TYR	3.7
1	A	641	THR	3.6
1	B	153	GLY	3.6
1	B	261	LEU	3.6
1	A	199	PHE	3.6
1	A	694	ILE	3.5
1	B	365	GLU	3.5
1	A	93	LEU	3.5
1	A	645	CYS	3.5
1	B	678	TYR	3.4
1	B	100	PHE	3.4
1	A	89	ILE	3.3
1	A	342	ILE	3.3
1	B	575	TYR	3.3
1	A	267	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	692	PRO	3.3
1	A	714	ALA	3.3
1	A	693	LEU	3.3
1	A	211	VAL	3.2
1	B	93	LEU	3.2
1	B	675	THR	3.2
1	A	152	VAL	3.2
1	B	136	ILE	3.2
1	A	264	ILE	3.1
1	A	101	LEU	3.1
1	A	640	LEU	3.1
1	A	224	GLU	3.0
1	A	238	GLY	3.0
1	A	743	LEU	3.0
1	A	685	PHE	3.0
1	A	147	VAL	3.0
1	A	198	GLY	3.0
1	B	165	THR	2.9
1	B	661	ILE	2.9
1	A	601	SER	2.9
1	A	701	VAL	2.9
1	A	736	GLY	2.9
1	A	622	MET	2.9
1	A	628	LYS	2.8
1	A	732	THR	2.8
1	A	748	ASN	2.8
1	A	678	TYR	2.8
1	A	157	GLU	2.8
1	A	720	THR	2.8
1	A	697	MET	2.8
1	A	610	ALA	2.8
1	A	597	LYS	2.7
1	B	203	PHE	2.7
1	A	163	LEU	2.7
1	A	158	GLU	2.7
1	A	747	LEU	2.7
1	A	207	ASP	2.7
1	A	699	ARG	2.7
1	B	204	LEU	2.6
1	A	735	TYR	2.6
1	A	704	ASP	2.6
1	A	715	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	654	TRP	2.6
1	A	145	LEU	2.6
1	A	202	ALA	2.6
1	A	632[A]	GLU	2.6
1	A	634	ALA	2.6
1	A	644	PRO	2.6
1	A	391	THR	2.5
1	A	721	ALA	2.5
1	A	689	PRO	2.5
1	A	241	LEU	2.5
1	A	367	ASP	2.5
1	A	137	LYS	2.5
1	A	637	SER	2.5
1	A	232	VAL	2.5
1	A	706	ASP	2.5
1	B	549	ALA	2.5
1	A	100	PHE	2.5
1	A	635	VAL	2.5
1	A	228	ASN	2.5
1	B	408	TYR	2.5
1	A	549	ALA	2.5
1	A	104	LEU	2.4
1	A	687	ILE	2.4
1	B	425	MET	2.4
1	A	230	PHE	2.4
1	A	422	PHE	2.4
1	A	598	PHE	2.4
1	B	265	LYS	2.4
1	B	602	GLU	2.4
1	B	197	VAL	2.4
1	B	704	ASP	2.4
1	A	611	ILE	2.4
1	A	139	ASP	2.4
1	A	91	ASN	2.3
1	A	733	LYS	2.3
1	A	716	VAL	2.3
1	B	147	VAL	2.3
1	A	646	ALA	2.3
1	B	455	LYS	2.3
1	A	365	GLU	2.3
1	B	268	VAL	2.3
1	A	102	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	631	ILE	2.3
1	A	643	SER	2.3
1	B	615	PHE	2.3
1	B	101	LEU	2.3
1	A	596	VAL	2.3
1	A	666	ALA	2.2
1	B	622	MET	2.2
1	B	451	LEU	2.2
1	A	723	LEU	2.2
1	A	695	LYS	2.2
1	A	248	THR	2.2
1	A	677	TYR	2.2
1	B	341	PRO	2.2
1	A	613	LYS	2.2
1	A	159	LEU	2.2
1	B	209	VAL	2.2
1	B	476	ALA	2.2
1	B	697	MET	2.2
1	A	141	GLU	2.2
1	B	654	TRP	2.2
1	A	709	THR	2.2
1	A	688	ASN	2.2
1	B	634	ALA	2.1
1	A	135	LYS	2.1
1	A	744[A]	ARG	2.1
1	B	271	TYR	2.1
1	A	279	ILE	2.1
1	B	685	PHE	2.1
1	B	713	LEU	2.1
1	A	690	ARG	2.1
1	B	666	ALA	2.1
1	A	346	PRO	2.1
1	A	336	MET	2.1
1	A	621	TRP	2.1
1	A	742	MET	2.0
1	A	282	TRP	2.0
1	A	263	THR	2.0
1	A	672	ASP	2.0
1	B	631	ILE	2.0
1	B	694	ILE	2.0
1	A	154	MET	2.0
1	A	204	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	ADP	B	302	27/27	0.95	0.13	-0.90	35,37,39,39	0
3	ADP	A	301	27/27	0.92	0.16	-1.32	29,32,34,34	0
2	MG	B	756	1/1	0.83	0.23	-	34,34,34,34	0
2	MG	B	755	1/1	0.96	0.03	-	37,37,37,37	0
2	MG	A	755	1/1	0.98	0.08	-	12,12,12,12	0
2	MG	A	756	1/1	0.92	0.17	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.