Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:44 AM GMT

PDB ID	:	2O1U
Title	:	Structure of full length GRP94 with AMP-PNP bound
Authors	:	Dollins, D.E.; Warren, J.J.; Immormino, R.M.; Gewirth, D.T.
Deposited on	:	2006-11-29
Resolution	:	2.40 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:

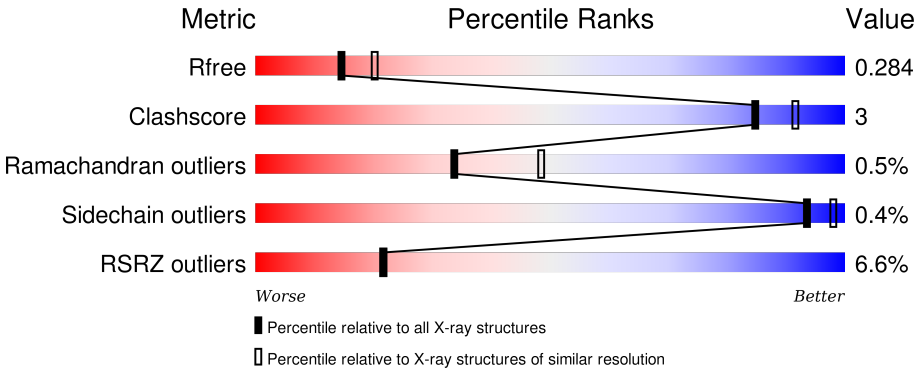
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	666	6% 79% 8% 13%
1	B	666	5% 78% 8% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9559 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	2	0
			4645	2962	780	886	17			
1	B	575	Total	C	N	O	S	0	0	0
			4611	2938	773	884	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

Continued on next page...

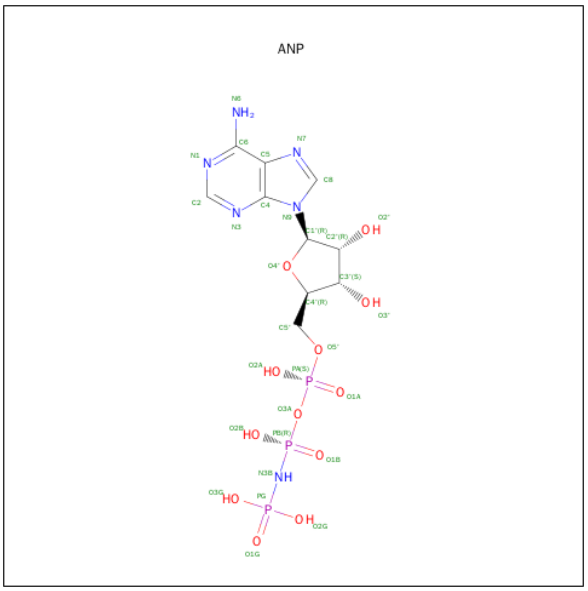
Continued from previous page...

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	3	Total Mg 3 3	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is water.

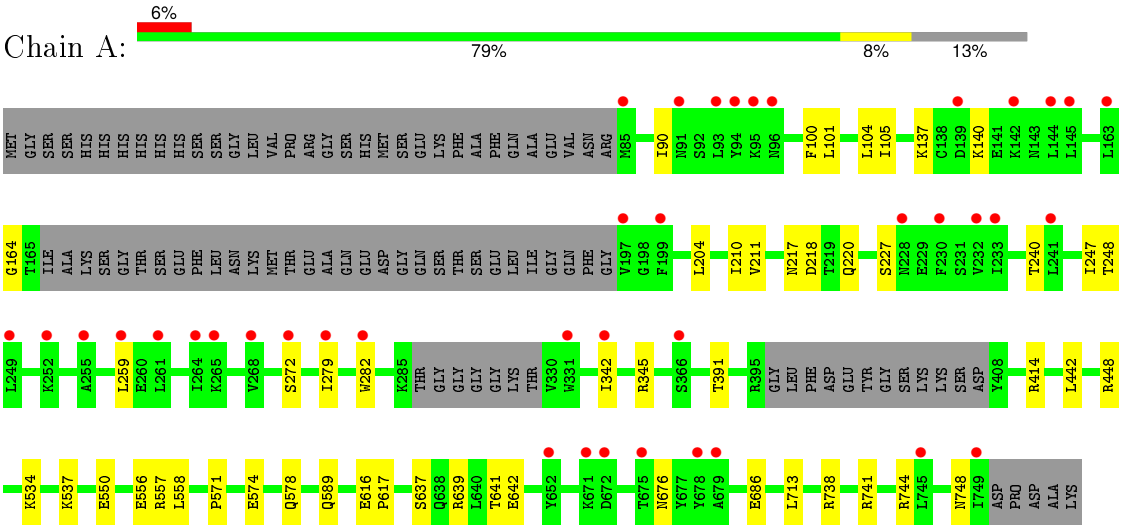
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	104	Total	O	0	0
			104	104		

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.

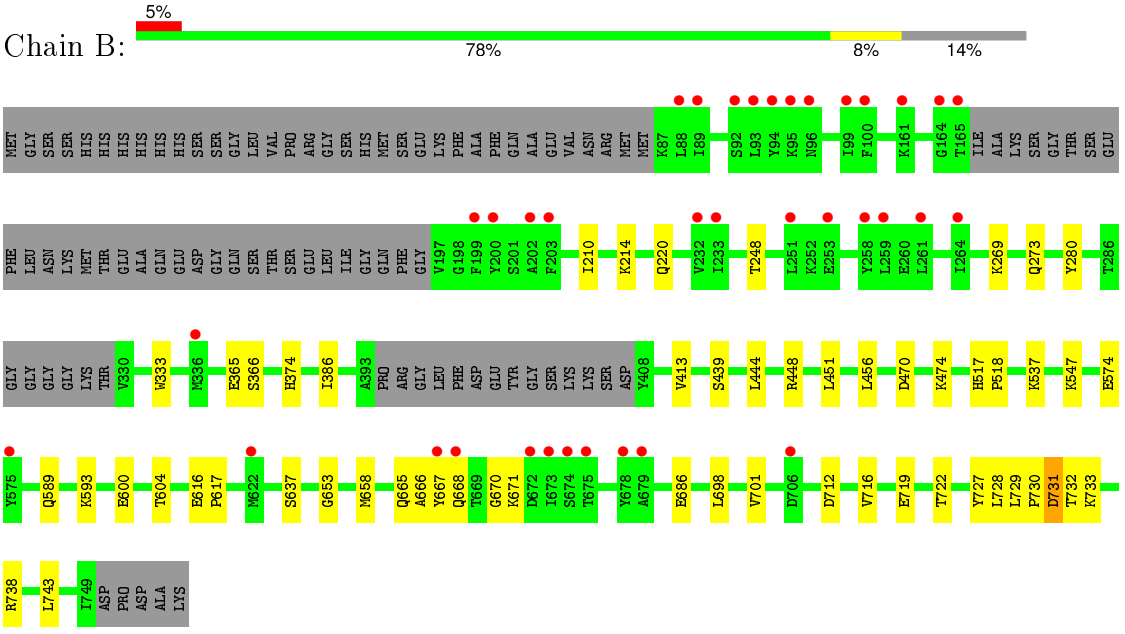
- Molecule 1: Endoplasmin

Chain A:



- Molecule 1: Endoplasmin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.33Å 109.26Å 148.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.89 – 2.40 47.87 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.89-2.40) 99.5 (47.87-2.23)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.289 0.238 , 0.284	Depositor DCC
R_{free} test set	3196 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.2	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 79295 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9559	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: 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	0.40	0/4739	0.64	0/6394
1	B	0.39	0/4696	0.64	3/6338 (0.0%)
All	All	0.39	0/9435	0.64	3/12732 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	451	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	728	LEU	CA-CB-CG	5.82	128.68	115.30
1	B	731	ASP	CB-CG-OD1	-5.42	113.42	118.30

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	4645	0	4583	26	0
1	B	4611	0	4543	30	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	132	0	0	2	0
4	B	104	0	0	2	0
All	All	9559	0	9152	54	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 3.

All (54) 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	1.66	0.78
1:A:637:SER:HB2	1:A:686:GLU:HB3	1.72	0.72
1:A:556:GLU:HB3	1:A:641:THR:HB	1.74	0.69
1:B:439:SER:HB2	4:B:764:HOH:O	1.96	0.65
1:B:593:LYS:NZ	1:B:653:GLY:O	2.29	0.65
1:A:414:ARG:NH1	1:A:442:LEU:O	2.30	0.64
1:A:272:SER:HB2	1:A:279:ILE:HD12	1.80	0.63
1:A:101:LEU:O	1:A:105:ILE:HG12	1.99	0.61
1:B:731:ASP:OD1	1:B:731:ASP:C	2.39	0.61
1:B:470:ASP:O	1:B:474:LYS:HG2	2.05	0.56
1:A:574:GLU:O	1:A:578:GLN:HB2	2.05	0.56
1:A:537:LYS:HE2	1:A:589:GLN:HB2	1.89	0.55
1:B:210:ILE:HB	1:B:248:THR:HB	1.89	0.55
1:A:210:ILE:HG13	1:A:248:THR:HB	1.88	0.55
1:B:547:LYS:HG2	4:B:758:HOH:O	2.09	0.53
1:A:713:LEU:HG	1:B:743:LEU:HD22	1.92	0.51
1:B:280:TYR:HB3	1:B:333:TRP:HB3	1.93	0.50
1:A:217:ASN:O	1:A:218:ASP:HB2	2.11	0.49
1:B:719:GLU:OE1	1:B:738:ARG:NH2	2.43	0.48
1:B:600:GLU:HB2	1:B:604:THR:HB	1.95	0.48
1:A:741:ARG:HA	1:A:744:ARG:HE	1.79	0.48
1:B:616:GLU:N	1:B:617:PRO:HD2	2.28	0.47
1:A:738:ARG:HG2	1:A:741:ARG:HH21	1.79	0.47
1:B:214:LYS:HD3	1:B:220:GLN:HB2	1.97	0.47
1:B:716:VAL:HG22	1:B:738:ARG:HB3	1.97	0.46
1:A:211:VAL:HG12	1:A:247:ILE:HA	1.98	0.45
1:A:550:GLU:O	4:A:792:HOH:O	2.21	0.45
1:B:666:ALA:O	1:B:671:LYS:N	2.47	0.45
1:A:100:PHE:O	1:A:104:LEU:HG	2.16	0.45
1:A:641:THR:HG22	1:A:642:GLU:N	2.32	0.45
1:A:140:LYS:HA	1:A:259:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HA	1:A:204:LEU:HD22	1.97	0.45
1:B:574:GLU:HG2	1:B:658:MET:SD	2.57	0.44
1:A:557:ARG:HB2	1:A:639:ARG:HA	2.00	0.44
1:A:342:ILE:HA	1:A:345:ARG:HD3	1.98	0.44
1:B:413:VAL:HG23	1:B:444:LEU:HD13	1.99	0.44
1:B:269:LYS:O	1:B:273:GLN:NE2	2.51	0.43
1:B:374:HIS:CD2	1:B:386:ILE:HG12	2.53	0.43
1:A:571:PRO:HG3	1:B:667:TYR:CE2	2.54	0.43
1:A:137:LYS:HG2	1:A:282:TRP:HB2	2.01	0.42
1:B:537:LYS:HD3	1:B:589:GLN:HB2	2.00	0.42
1:B:665:GLN:HA	1:B:668:GLN:HB3	2.01	0.42
1:B:517:HIS:CG	1:B:518:PRO:HD2	2.54	0.42
1:B:712:ASP:O	1:B:716:VAL:HG23	2.19	0.42
1:B:698:LEU:O	1:B:701:VAL:HG12	2.19	0.41
1:B:732:THR:CG2	1:B:733:LYS:N	2.83	0.41
1:B:732:THR:HG23	1:B:733:LYS:N	2.34	0.41
1:A:558:LEU:HD22	4:A:778:HOH:O	2.18	0.41
1:B:365:GLU:O	1:B:366:SER:HB3	2.20	0.41
1:B:729:LEU:HA	1:B:729:LEU:HD23	1.89	0.41
1:A:534:LYS:HD2	1:A:534:LYS:HA	1.84	0.40
1:A:616:GLU:N	1:A:617:PRO:HD2	2.36	0.40
1:B:722:THR:HG23	1:B:727:TYR:HB2	2.03	0.40
1:A:220:GLN:HE22	1:A:240:THR:HB	1.85	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	572/666 (86%)	533 (93%)	35 (6%)	4 (1%)	26	38
1	B	565/666 (85%)	528 (94%)	35 (6%)	2 (0%)	39	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1137/1332 (85%)	1061 (93%)	70 (6%)	6 (0%)	34 48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	748	ASN
1	B	670	GLY
1	A	676	ASN
1	B	730	PRO
1	A	164	GLY

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	505/598 (84%)	503 (100%)	2 (0%)	93 98
1	B	501/598 (84%)	499 (100%)	2 (0%)	93 98
All	All	1006/1196 (84%)	1002 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	THR
1	A	448	ARG
1	B	448	ARG
1	B	456	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 7 ligands modelled in this entry, 5 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	ANP	A	755	2	27,33,33	2.07	6 (22%)	30,52,52	2.14	6 (20%)
3	ANP	B	755	2	27,33,33	2.13	8 (29%)	30,52,52	2.15	7 (23%)

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	ANP	A	755	2	-	0/12/38/38	0/3/3/3
3	ANP	B	755	2	-	0/12/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	ANP	PB-O2B	-2.04	1.51	1.56
3	B	755	ANP	PG-O3G	-2.01	1.51	1.56
3	B	755	ANP	O4'-C1'	2.05	1.43	1.41
3	B	755	ANP	PB-O3A	2.11	1.61	1.59
3	A	755	ANP	C5-C4	3.14	1.47	1.40
3	B	755	ANP	C5-C4	3.25	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	ANP	PG-O1G	4.26	1.51	1.46
3	B	755	ANP	PB-N3B	4.39	1.75	1.63
3	B	755	ANP	PG-N3B	4.39	1.75	1.63
3	A	755	ANP	PB-N3B	4.53	1.75	1.63
3	B	755	ANP	PB-O1B	4.57	1.51	1.46
3	A	755	ANP	PG-N3B	4.66	1.75	1.63
3	A	755	ANP	PB-O1B	4.67	1.51	1.46
3	B	755	ANP	PG-O1G	4.84	1.51	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	755	ANP	N3-C2-N1	-7.41	123.22	128.89
3	A	755	ANP	N3-C2-N1	-7.18	123.40	128.89
3	B	755	ANP	O1G-PG-N3B	-4.71	104.67	111.90
3	A	755	ANP	C2'-C1'-N9	-4.62	107.23	114.29
3	A	755	ANP	O1G-PG-N3B	-3.68	106.25	111.90
3	A	755	ANP	C4-C5-N7	-3.18	106.56	109.48
3	B	755	ANP	C2'-C1'-N9	-3.10	109.56	114.29
3	B	755	ANP	C4-C5-N7	-2.99	106.73	109.48
3	B	755	ANP	PA-O3A-PB	-2.51	124.26	132.67
3	A	755	ANP	O3G-PG-O2G	2.18	114.05	107.58
3	B	755	ANP	O3G-PG-O2G	2.23	114.20	107.58
3	B	755	ANP	O2B-PB-O1B	3.96	118.26	110.00
3	A	755	ANP	O2B-PB-O1B	4.27	118.91	110.00

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 (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^{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	578/666 (86%)	0.44	40 (6%)	20	19	11, 35, 54, 66	0
1	B	575/666 (86%)	0.37	36 (6%)	23	24	2, 35, 59, 68	0
All	All	1153/1332 (86%)	0.40	76 (6%)	22	22	2, 35, 56, 68	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	9.2
1	A	675	THR	8.9
1	A	749	ILE	8.6
1	B	93	LEU	7.5
1	A	96	ASN	6.7
1	B	89	ILE	6.1
1	B	99	ILE	5.7
1	A	261	LEU	5.7
1	B	232	VAL	5.5
1	B	96	ASN	5.5
1	B	94	TYR	5.3
1	A	671	LYS	5.0
1	A	95	LYS	4.9
1	A	233	ILE	4.7
1	B	200	TYR	4.6
1	A	331	TRP	4.6
1	A	139	ASP	4.4
1	B	674	SER	4.1
1	B	667	TYR	4.0
1	B	672	ASP	3.9
1	B	202	ALA	3.8
1	B	199	PHE	3.7
1	A	197	VAL	3.7
1	B	233	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	249	LEU	3.6
1	B	165	THR	3.5
1	A	94	TYR	3.4
1	B	678	TYR	3.4
1	B	261	LEU	3.3
1	A	144	LEU	3.3
1	A	342	ILE	3.3
1	A	163	LEU	3.2
1	B	253	GLU	3.2
1	A	672	ASP	3.2
1	B	92	SER	3.2
1	B	95	LYS	3.2
1	A	241	LEU	3.1
1	A	745	LEU	3.1
1	A	199	PHE	3.0
1	A	268	VAL	2.9
1	A	145	LEU	2.8
1	A	232	VAL	2.8
1	B	164	GLY	2.8
1	A	678	TYR	2.7
1	A	366	SER	2.7
1	A	259	LEU	2.7
1	A	255	ALA	2.7
1	A	91	ASN	2.5
1	A	252	LYS	2.5
1	A	228	ASN	2.5
1	A	230	PHE	2.5
1	B	259	LEU	2.5
1	B	100	PHE	2.4
1	A	679	ALA	2.4
1	B	264	ILE	2.4
1	B	668	GLN	2.3
1	A	282	TRP	2.3
1	B	706	ASP	2.3
1	A	272	SER	2.3
1	A	265	LYS	2.3
1	B	251	LEU	2.3
1	A	264	ILE	2.2
1	B	673	ILE	2.2
1	B	203	PHE	2.2
1	A	93	LEU	2.2
1	A	142	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	85	MET	2.1
1	B	622	MET	2.1
1	B	575	TYR	2.1
1	A	279	ILE	2.1
1	B	679	ALA	2.1
1	B	336	MET	2.1
1	A	652	TYR	2.1
1	B	675	THR	2.1
1	B	161	LYS	2.1
1	B	258	TYR	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, 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
3	ANP	B	755	31/31	0.95	0.11	-0.80	40,42,44,44	0
3	ANP	A	755	31/31	0.91	0.14	-0.91	39,42,46,47	0
2	MG	B	305	1/1	0.71	0.09	-2.57	31,31,31,31	0
2	MG	B	304	1/1	0.85	0.60	-	27,27,27,27	0
2	MG	A	302	1/1	0.94	0.20	-	32,32,32,32	0
2	MG	A	303	1/1	0.32	0.60	-	48,48,48,48	0
2	MG	B	301	1/1	0.90	0.27	-	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.