



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:35 pm GMT

PDB ID : 2GJK
Title : Structural and functional insights into the human Upf1 helicase core
Authors : Cheng, Z.; Muhlrads, D.; Parker, R.; Song, H.
Deposited on : 2006-03-31
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

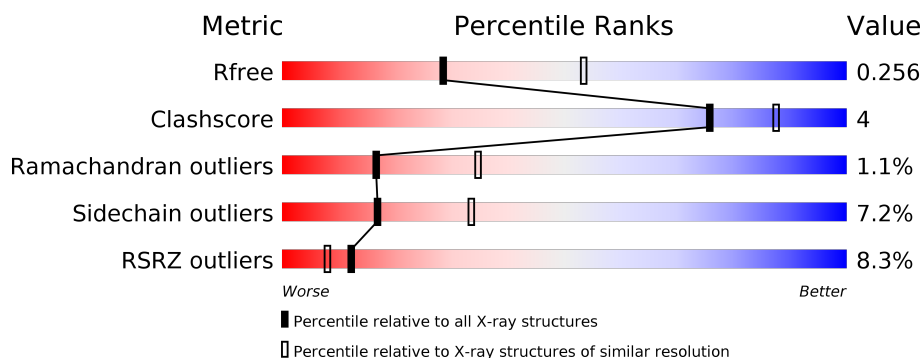
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	624	<div> <div>8%</div> <div>81%</div> <div>15%</div> <div>••</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4986 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 Regulator of nonsense transcripts 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			4844	3075	849	897	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	PRO	-	CLONING ARTIFACT	UNP Q92900
A	292	LEU	-	CLONING ARTIFACT	UNP Q92900
A	293	GLY	-	CLONING ARTIFACT	UNP Q92900
A	294	SER	-	CLONING ARTIFACT	UNP Q92900

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

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

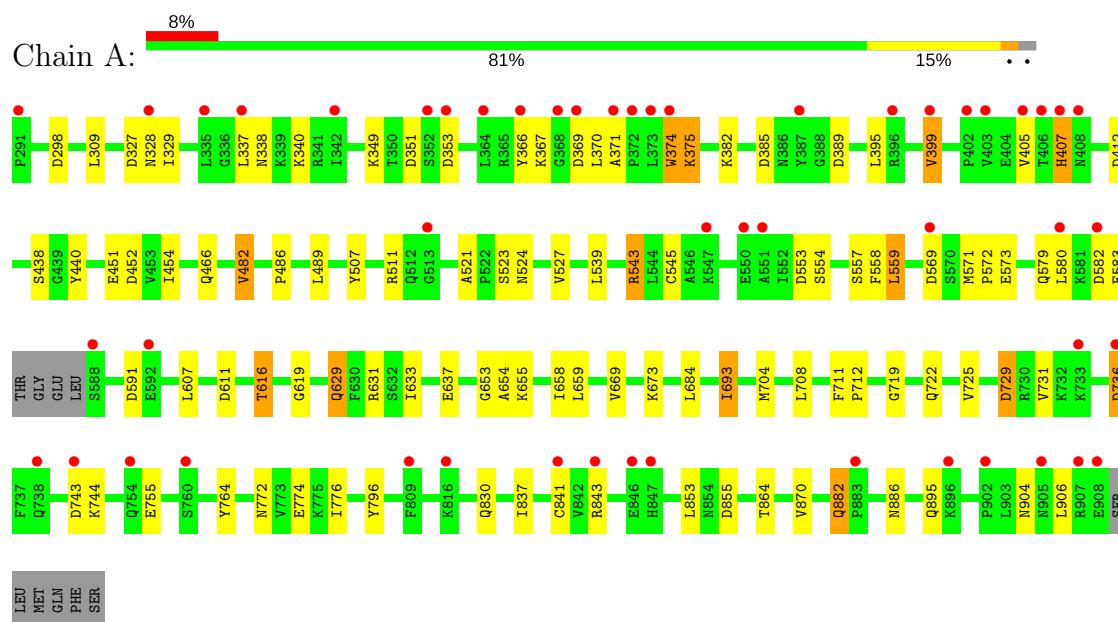
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		

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 the various outlier classes 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: Regulator of nonsense transcripts 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.98Å 188.98Å 44.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.60) 98.8 (19.95-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.245 , 0.271 0.242 , 0.256	Depositor DCC
R_{free} test set	1227 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4986	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.31	0/4939	0.66	18/6682 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	385	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	743	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	855	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	353	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	369	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	736	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	729	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	452	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	591	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	553	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	389	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	611	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	327	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	412	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	298	ASP	CB-CG-OD2	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	582	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	371	ALA	Peptide

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	4844	0	4910	35	0
2	A	1	0	0	0	0
3	A	31	0	13	0	0
4	A	110	0	0	1	0
All	All	4986	0	4923	35	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 (35) 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:796:TYR:OH	1:A:843:ARG:HD2	1.50	1.11
1:A:843:ARG:HG3	1:A:853:LEU:CD1	2.12	0.80
1:A:843:ARG:HG3	1:A:853:LEU:HD13	1.71	0.73
1:A:616:THR:HG22	1:A:619:GLY:H	1.54	0.72
1:A:796:TYR:OH	1:A:843:ARG:CD	2.35	0.70
1:A:796:TYR:HH	1:A:843:ARG:HD2	1.61	0.65
1:A:744:LYS:HE2	1:A:895:GLN:HE21	1.64	0.62
1:A:558:PHE:CE1	1:A:559:LEU:HD13	2.38	0.58
1:A:482:VAL:HG13	1:A:658:ILE:HD12	1.87	0.56
1:A:523:SER:OG	1:A:830:GLN:NE2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LEU:HD22	1:A:870:VAL:HG12	1.88	0.55
1:A:524:ASN:HD22	1:A:543:ARG:HH22	1.54	0.55
1:A:489:LEU:HG	1:A:693:ILE:HD11	1.88	0.55
1:A:571:MET:N	1:A:572:PRO:HD3	2.23	0.54
1:A:843:ARG:HB2	4:A:26:HOH:O	2.07	0.54
1:A:507:TYR:HA	1:A:539:LEU:HD11	1.92	0.52
1:A:719:GLY:O	1:A:722:GLN:NE2	2.41	0.52
1:A:579:GLN:O	1:A:583:GLU:HG2	2.10	0.51
1:A:772:ASN:O	1:A:776:ILE:HG12	2.13	0.49
1:A:755:GLU:OE1	1:A:843:ARG:CZ	2.61	0.48
1:A:438:SER:HB3	1:A:655:LYS:HA	1.96	0.47
1:A:507:TYR:O	1:A:511:ARG:HG2	2.15	0.47
1:A:725:VAL:HG13	1:A:729:ASP:HB2	1.97	0.46
1:A:704:MET:HE3	1:A:864:THR:HA	1.98	0.46
1:A:629:GLN:HG3	1:A:653:GLY:HA3	1.97	0.45
1:A:521:ALA:HB3	1:A:527:VAL:HG23	1.99	0.44
1:A:374:TRP:CG	1:A:375:LYS:N	2.86	0.44
1:A:633:ILE:HD12	1:A:654:ALA:HB2	2.00	0.44
1:A:764:TYR:CD2	1:A:843:ARG:NH1	2.69	0.43
1:A:440:TYR:CE2	1:A:486:PRO:HG2	2.54	0.43
1:A:731:VAL:HG13	1:A:731:VAL:O	2.19	0.43
1:A:454:ILE:N	1:A:454:ILE:HD12	2.34	0.42
1:A:554:SER:H	1:A:557:SER:HB3	1.85	0.42
1:A:711:PHE:HB3	1:A:712:PRO:HD3	2.01	0.40
1:A:489:LEU:HD22	1:A:659:LEU:HB2	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	610/624 (98%)	563 (92%)	40 (7%)	7 (1%)	17	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	LEU
1	A	399	VAL
1	A	407	HIS
1	A	573	GLU
1	A	405	VAL
1	A	882	GLN
1	A	906	LEU

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	531/540 (98%)	493 (93%)	38 (7%)	17	33

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LEU
1	A	328	ASN
1	A	329	ILE
1	A	337	LEU
1	A	338	ASN
1	A	340	LYS
1	A	349	LYS
1	A	366	TYR
1	A	367	LYS
1	A	374	TRP
1	A	375	LYS
1	A	382	LYS
1	A	395	LEU
1	A	399	VAL
1	A	407	HIS
1	A	451	GLU
1	A	466	GLN
1	A	482	VAL

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Mol	Chain	Res	Type
1	A	543	ARG
1	A	545	CYS
1	A	559	LEU
1	A	580	LEU
1	A	607	LEU
1	A	616	THR
1	A	629	GLN
1	A	631	ARG
1	A	637	GLU
1	A	669	VAL
1	A	673	LYS
1	A	684	LEU
1	A	693	ILE
1	A	736	ASP
1	A	774	GLU
1	A	837	ILE
1	A	841	CYS
1	A	882	GLN
1	A	886	ASN
1	A	904	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	ASN
1	A	475	GLN
1	A	629	GLN
1	A	738	GLN
1	A	830	GLN
1	A	860	ASN
1	A	895	GLN
1	A	904	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ANP	A	990	2	29,33,33	3.33	7 (24%)	28,52,52	1.99	5 (17%)

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	990	2	-	0/13/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	990	ANP	PA-O1A	2.04	1.58	1.50
3	A	990	ANP	C5-C4	2.12	1.45	1.40
3	A	990	ANP	PG-N3B	3.62	1.72	1.63
3	A	990	ANP	PB-N3B	3.86	1.73	1.63
3	A	990	ANP	C4-N3	6.01	1.44	1.35
3	A	990	ANP	PB-O1B	10.32	1.57	1.46
3	A	990	ANP	PG-O1G	11.18	1.58	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	990	ANP	N3-C2-N1	-7.29	122.51	128.86
3	A	990	ANP	C4-C5-N7	-3.89	105.65	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	990	ANP	PA-O3A-PB	-2.85	122.33	132.38
3	A	990	ANP	O1G-PG-N3B	-2.68	107.78	111.79
3	A	990	ANP	C2-N1-C6	2.83	123.72	118.77

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, 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	614/624 (98%)	0.25	51 (8%) 12 8	15, 40, 69, 77	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	LEU	8.2
1	A	371	ALA	5.4
1	A	843	ARG	4.7
1	A	551	ALA	4.5
1	A	291	PRO	4.3
1	A	368	GLY	4.3
1	A	369	ASP	4.3
1	A	406	THR	3.9
1	A	743	ASP	3.9
1	A	754	GLN	3.8
1	A	399	VAL	3.8
1	A	547	LYS	3.5
1	A	738	GLN	3.4
1	A	760	SER	3.2
1	A	408	ASN	3.2
1	A	902	PRO	3.1
1	A	328	ASN	3.1
1	A	841	CYS	3.1
1	A	580	LEU	3.1
1	A	905	ASN	3.0
1	A	366	TYR	3.0
1	A	405	VAL	2.9
1	A	736	ASP	2.9
1	A	352	SER	2.8
1	A	588	SER	2.8
1	A	847	HIS	2.8
1	A	373	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	569	ASP	2.7
1	A	883	PRO	2.7
1	A	907	ARG	2.6
1	A	809	PHE	2.6
1	A	374	TRP	2.5
1	A	372	PRO	2.4
1	A	402	PRO	2.4
1	A	816	LYS	2.4
1	A	908	GLU	2.4
1	A	364	LEU	2.3
1	A	353	ASP	2.3
1	A	896	LYS	2.3
1	A	846	GLU	2.2
1	A	335	LEU	2.2
1	A	733	LYS	2.2
1	A	550	GLU	2.2
1	A	396	ARG	2.1
1	A	592	GLU	2.1
1	A	387	TYR	2.1
1	A	403	VAL	2.0
1	A	342	ILE	2.0
1	A	513	GLY	2.0
1	A	582	ASP	2.0
1	A	407	HIS	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(\AA^2)	Q<0.9
3	ANP	A	990	31/31	0.89	0.22	1.36	38,49,51,52	0
2	MG	A	1000	1/1	0.85	0.38	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.