



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:22 PM GMT

PDB ID : 5CNO
Title : Crystal structure of the EGFR kinase domain mutant V924R
Authors : Kovacs, E.; Das, R.; Mirza, A.; Jura, N.; Barros, T.; Kuriyan, J.
Deposited on : 2015-07-17
Resolution : 1.55 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

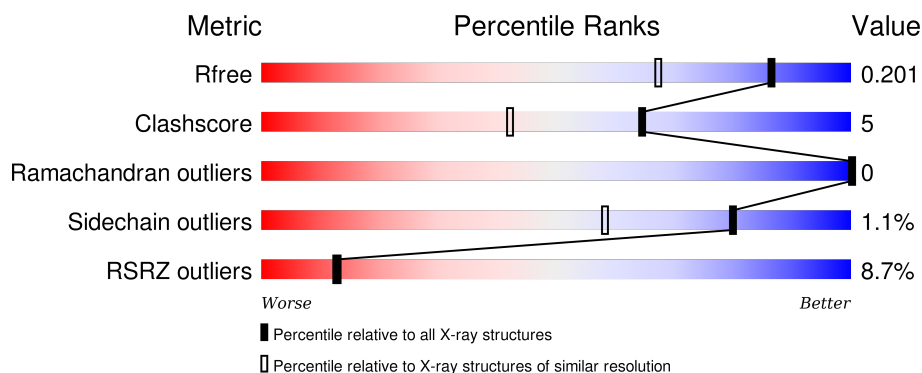
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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	330	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	B	330	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	X	330	<div> <div>2%</div> <div> <div></div> <div>97%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5579 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.

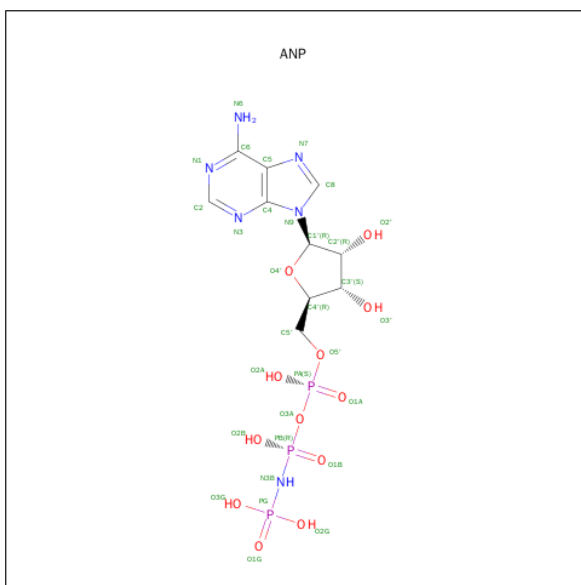
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	3	0
			2434	1563	411	440	20			
1	B	302	Total	C	N	O	S	0	5	0
			2461	1583	414	442	22			
1	X	10	Total	C	N	O		0	0	0
			79	50	12	17				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	669	GLY	-	expression tag	UNP P00533
A	670	ALA	-	expression tag	UNP P00533
A	671	MET	-	expression tag	UNP P00533
A	924	ARG	VAL	engineered mutation	UNP P00533
B	669	GLY	-	expression tag	UNP P00533
B	670	ALA	-	expression tag	UNP P00533
B	671	MET	-	expression tag	UNP P00533
B	924	ARG	VAL	engineered mutation	UNP P00533
X	669	GLY	-	expression tag	UNP P00533
X	670	ALA	-	expression tag	UNP P00533
X	671	MET	-	expression tag	UNP P00533
X	924	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	268	Total O 268 268	0	0
4	B	268	Total O 268 268	0	0
4	X	5	Total O 5 5	0	0

THR	ASP	SER	ASN	PHE	TYR	ARG	ALA	LEU	MET	ASP	GLU	GLU	ASP	MET	ASP	ASP	VAL	VAL	ASP	A989	D990	E991	Y992	I993	I994	P995	Q996	Q997	G998
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.40 Å 71.84 Å 76.40 Å 90.00° 113.27° 90.00°	Depositor
Resolution (Å)	38.56 – 1.55 43.66 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.56-1.55) 93.2 (43.66-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.55 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.175 , 0.203 0.173 , 0.201	Depositor DCC
R_{free} test set	5218 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 110975 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5579	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 53.19 % 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 4.3678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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	0.80	0/2493	0.84	3/3367 (0.1%)
1	B	0.81	0/2527	0.88	7/3412 (0.2%)
1	X	0.98	0/80	0.66	0/108
All	All	0.81	0/5100	0.86	10/6887 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	779	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	B	975	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	A	808	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	934	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	B	779	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	924	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	924	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	975	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	806	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	923	MET	CG-SD-CE	-5.22	91.84	100.20

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	2434	0	2484	23	0
1	B	2461	0	2524	29	0
1	X	79	0	71	4	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	268	0	0	5	2
4	B	268	0	0	15	2
4	X	5	0	0	0	0
All	All	5579	0	5105	52	2

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 5.

All (52) 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:740:TYR:OH	4:B:1101:HOH:O	1.82	0.96
1:B:836:LYS:NZ	4:B:1102:HOH:O	1.97	0.95
1:B:784:ASN:N	4:B:1109:HOH:O	2.20	0.73
1:A:747:ASN:HD21	1:X:989:ALA:HB1	1.53	0.73
1:B:780:GLU:OE1	4:B:1103:HOH:O	2.06	0.73
1:A:748:PRO:HD2	1:X:989:ALA:HA	1.70	0.72
1:B:943:GLU:OE1	4:B:1105:HOH:O	2.08	0.71
1:B:776:ASP:OD1	4:B:1104:HOH:O	2.08	0.71
1:B:675:PRO:HG2	4:B:1184:HOH:O	1.93	0.69
1:B:687:GLU:OE1	4:B:1106:HOH:O	2.10	0.68
1:B:692:LYS:HE2	1:X:990:ASP:HA	1.75	0.68
1:B:851:LYS:O	4:B:1107:HOH:O	2.11	0.67
1:B:925[B]:LYS:HG2	1:B:935:PRO:HD3	1.75	0.67
1:A:723:LEU:HD13	1:A:838:LEU:HD11	1.78	0.65
1:A:700:GLY:HA2	1:A:724:ARG:HG3	1.80	0.64
1:B:812:ARG:NH1	4:B:1108:HOH:O	2.12	0.62
1:A:902:ILE:HG23	1:A:907:GLU:HB2	1.81	0.61
1:B:779:ARG:HD3	1:B:887:GLY:O	2.03	0.59
1:A:720:ILE:HG12	1:A:765:ILE:CD1	2.33	0.58
1:B:989:ALA:HB1	1:B:991:GLU:HB2	1.87	0.56
1:B:949:ARG:NH2	4:B:1117:HOH:O	2.39	0.56
1:A:676:ASN:HD21	1:A:678:ALA:HB3	1.70	0.56
1:B:851:LYS:NZ	4:B:1110:HOH:O	2.21	0.55
1:A:949:ARG:NH1	4:A:1101:HOH:O	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:HIS:HB2	1:B:785:ILE:HD11	1.90	0.52
1:A:676:ASN:ND2	1:A:678:ALA:HB3	2.24	0.52
1:A:946[B]:LYS:HG3	4:A:1186:HOH:O	2.10	0.50
1:A:689:LYS:HE3	1:A:691:ILE:HD11	1.93	0.50
1:B:812:ARG:NE	4:B:1114:HOH:O	2.36	0.49
1:B:858:ALA:HA	1:B:874:TRP:CD2	2.48	0.49
1:A:748:PRO:CD	1:X:989:ALA:HA	2.40	0.48
1:B:902:ILE:HG23	1:B:907:GLU:HB2	1.96	0.47
1:A:858:ALA:HA	1:A:874:TRP:CD2	2.49	0.47
1:B:674:ALA:N	4:B:1121:HOH:O	2.47	0.46
1:A:720:ILE:HG12	1:A:765:ILE:HD13	1.96	0.46
1:B:779:ARG:HG2	1:B:887:GLY:HA3	1.97	0.46
1:B:745:VAL:HG11	1:B:832:PHE:CZ	2.51	0.46
1:A:825:GLN:NE2	4:A:1113:HOH:O	2.48	0.46
1:A:938:ARG:NH1	4:A:1102:HOH:O	2.24	0.45
1:A:946[B]:LYS:HG2	1:A:949:ARG:NH2	2.32	0.44
1:B:989:ALA:CB	1:B:991:GLU:HB2	2.47	0.44
1:B:730:LYS:NZ	1:B:836:LYS:O	2.48	0.43
1:A:699:PHE:CZ	1:A:835:ALA:HA	2.54	0.43
1:B:674:ALA:HA	1:B:675:PRO:HD3	1.89	0.42
1:B:779:ARG:HG2	1:B:886:PHE:O	2.20	0.42
1:B:947[A]:MET:HG2	1:B:954:TYR:CG	2.55	0.42
1:A:683:LEU:CD1	1:A:765:ILE:HG13	2.50	0.41
1:B:963:MET:C	4:B:1112:HOH:O	2.58	0.41
1:A:912:PRO:HA	1:A:913:PRO:HD3	1.98	0.41
1:A:946[A]:LYS:NZ	4:A:1105:HOH:O	2.31	0.41
1:A:852:VAL:HG12	1:A:857:MET:SD	2.61	0.40
1:A:944:PHE:HA	1:A:947[A]:MET:HE3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1290:HOH:O	4:B:1337:HOH:O[4_456]	1.69	0.51
4:A:1201:HOH:O	4:B:1272:HOH:O[4_456]	2.15	0.05

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	297/330 (90%)	291 (98%)	6 (2%)	0	100	100
1	B	301/330 (91%)	292 (97%)	9 (3%)	0	100	100
1	X	8/330 (2%)	6 (75%)	2 (25%)	0	100	100
All	All	606/990 (61%)	589 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	271/288 (94%)	267 (98%)	4 (2%)	72	44
1	B	275/288 (96%)	275 (100%)	0	100	100
1	X	8/288 (3%)	6 (75%)	2 (25%)	1	0
All	All	554/864 (64%)	548 (99%)	6 (1%)	80	58

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	725	GLU
1	A	852	VAL
1	A	958	GLN
1	A	974	TYR
1	X	990	ASP

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Mol	Chain	Res	Type
1	X	997	GLN

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 4 ligands modelled in this entry, 2 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$
2	ANP	A	1001	3	29,33,33	3.23	5 (17%)	26,52,52	0.88	1 (3%)
2	ANP	B	1001	3	29,33,33	1.88	4 (13%)	26,52,52	1.12	2 (7%)

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	1001	3	-	0/13/38/38	0/3/3/3
2	ANP	B	1001	3	-	0/13/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ANP	PB-O2B	-3.35	1.47	1.56
2	A	1001	ANP	PG-O3G	-2.95	1.48	1.56
2	A	1001	ANP	PB-O3A	-2.32	1.56	1.59
2	A	1001	ANP	PG-N3B	2.08	1.68	1.63
2	B	1001	ANP	PG-N3B	2.72	1.70	1.63
2	A	1001	ANP	PB-O1B	4.15	1.50	1.46
2	B	1001	ANP	PB-O1B	5.80	1.52	1.46
2	B	1001	ANP	PG-O1G	5.80	1.52	1.46
2	A	1001	ANP	PG-O1G	15.78	1.63	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ANP	O3G-PG-O1G	-2.77	106.28	113.58
2	B	1001	ANP	O3'-C3'-C4'	2.08	117.23	111.01
2	B	1001	ANP	O2B-PB-O1B	3.39	116.70	110.02

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	300/330 (90%)	0.25	19 (6%) 23 24	14, 25, 51, 87	0
1	B	302/330 (91%)	0.29	26 (8%) 13 13	13, 23, 55, 78	0
1	X	10/330 (3%)	3.13	8 (80%) 0 0	37, 49, 53, 66	0
All	All	612/990 (61%)	0.31	53 (8%) 13 13	13, 24, 54, 87	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	837	LEU	7.8
1	B	674	ALA	7.6
1	B	675	PRO	7.6
1	B	838	LEU	5.6
1	X	997	GLN	5.1
1	A	991	GLU	5.0
1	X	995	PRO	5.0
1	X	989	ALA	4.7
1	A	677	GLN	4.4
1	A	852	VAL	4.2
1	B	991	GLU	4.2
1	X	992	TYR	4.1
1	B	730	LYS	4.0
1	B	735	ILE	3.9
1	B	732	ASN	3.9
1	X	993	LEU	3.9
1	A	676	ASN	3.7
1	B	733	LYS	3.6
1	A	699	PHE	3.6
1	B	964	HIS	3.5
1	A	760	SER	3.5
1	B	989	ALA	3.5
1	A	839	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	734	GLU	3.4
1	A	731	ALA	3.4
1	A	838	LEU	3.4
1	B	677	GLN	3.3
1	A	724	ARG	3.3
1	B	740	TYR	3.3
1	A	837	LEU	3.3
1	A	725	GLU	3.2
1	B	760	SER	3.2
1	B	731	ALA	3.2
1	B	962	ARG	3.2
1	B	736	LEU	3.0
1	B	836	LYS	2.9
1	A	759	THR	2.7
1	B	734	GLU	2.6
1	B	783	ASP	2.6
1	B	678	ALA	2.6
1	B	759	THR	2.6
1	X	998	GLY	2.4
1	A	835	ALA	2.4
1	X	996	GLN	2.4
1	A	732	ASN	2.3
1	A	962	ARG	2.3
1	A	698	ALA	2.2
1	B	676	ASN	2.2
1	B	851	LYS	2.2
1	A	989	ALA	2.1
1	X	994	ILE	2.1
1	B	710	GLU	2.1
1	B	963	MET	2.1

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 [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
2	ANP	B	1001	31/31	0.99	0.08	-0.36	13,17,20,22	0
2	ANP	A	1001	31/31	0.98	0.08	-0.74	18,22,26,29	0
3	MG	A	1002	1/1	0.99	0.05	-	20,20,20,20	0
3	MG	B	1002	1/1	1.00	0.06	-	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.