



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:03 am GMT

PDB ID : 1U6R
Title : Transition state analog complex of muscle creatine kinase (R134K) mutant
Authors : Ohren, J.F.; Kundracik, M.L.; Borders, C.L.; Edmiston, P.; Viola, R.E.
Deposited on : 2004-07-30
Resolution : 1.65 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

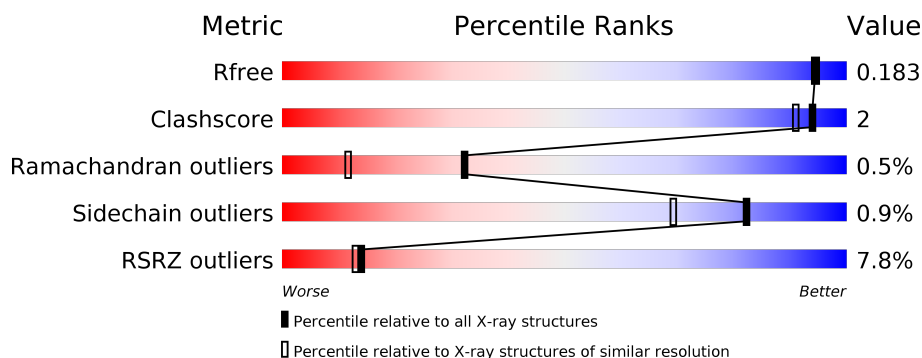
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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	380	<div> <div>14%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	380	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	B	1701	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7294 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 Creatine kinase, M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	1	0
			3028	1911	532	571	14			
1	B	380	Total	C	N	O	S	0	5	0
			3042	1918	533	577	14			

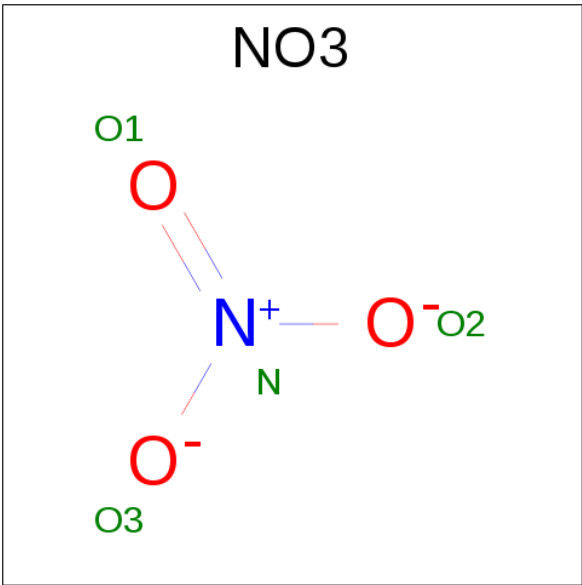
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	LYS	ARG	ENGINEERED	UNP P00563
B	134	LYS	ARG	ENGINEERED	UNP P00563

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

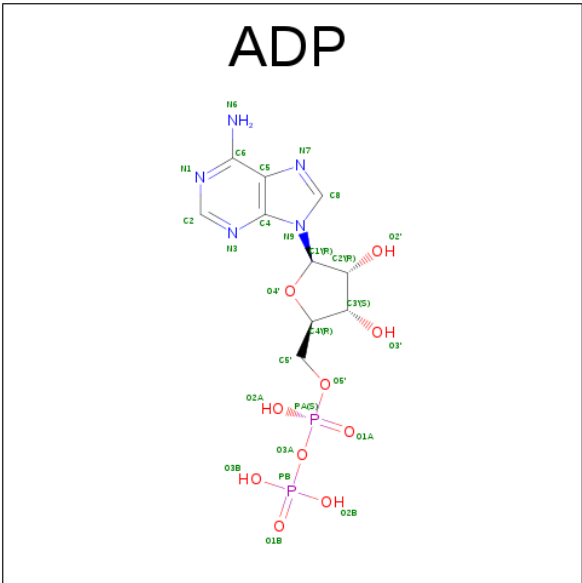
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



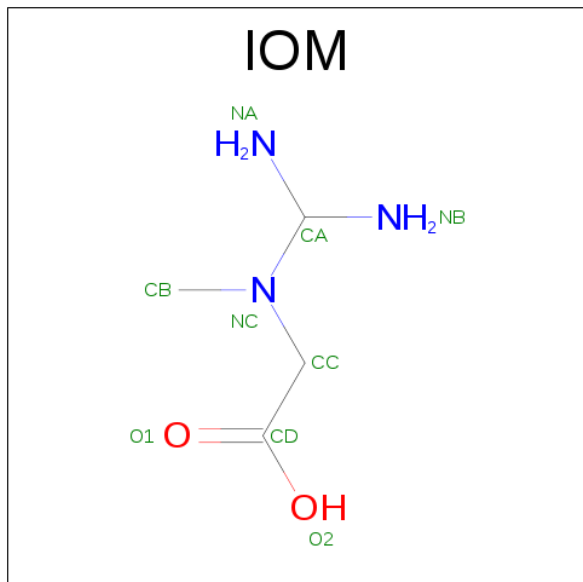
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	N	O		0	0
			4	1	3			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is (DIAMINOMETHYL-METHYL-AMINO)-ACETIC ACID (three-letter code: IOM) (formula: $C_4H_{11}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			9	4	3	2		

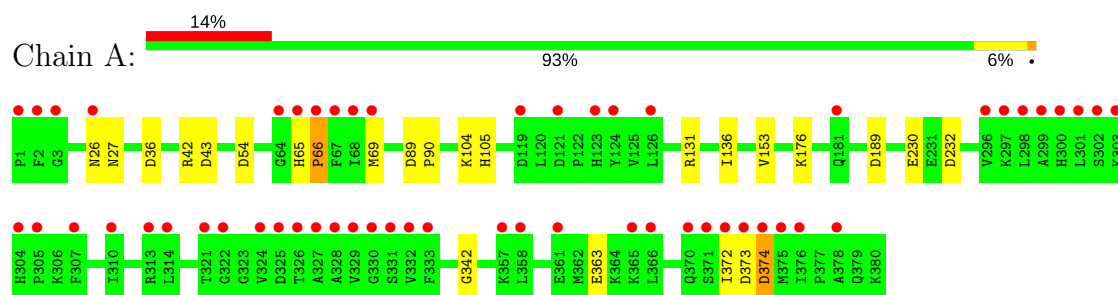
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	484	Total	O	0	0
			484	484		
6	B	671	Total	O	0	0
			671	671		

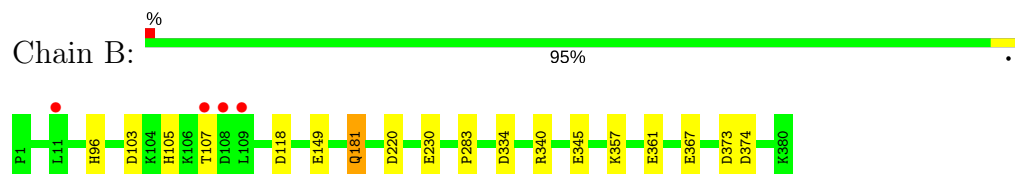
3 Residue-property plots [i](#)

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: Creatine kinase, M chain



- Molecule 1: Creatine kinase, M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.69Å 92.57Å 165.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 1.65 38.22 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.00-1.65) 97.9 (38.22-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.165 , 0.200 0.178 , 0.183	Depositor DCC
R_{free} test set	4457 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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, IOM, ADP, NO3

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	0.38	0/3102	0.72	7/4179 (0.2%)
1	B	0.44	0/3136	0.76	7/4224 (0.2%)
All	All	0.41	0/6238	0.74	14/8403 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	220	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	36	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	374[A]	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	374[B]	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	54	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	232	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	189	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	103	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	118	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	42	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	43	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	374	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	373	ASP	CB-CG-OD2	5.16	122.94	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	3028	0	2995	11	0
1	B	3042	0	3006	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	4	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	B	9	0	10	0	0
6	A	484	0	0	2	0
6	B	671	0	0	3	0
All	All	7294	0	6035	20	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 2.

All (20) 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:105:HIS:HD2	1:A:342:GLY:H	1.30	0.79
1:A:26:ASN:HD21	1:A:65:HIS:N	1.93	0.67
1:A:65:HIS:HB2	1:A:66:PRO:CD	2.25	0.67
1:B:96:HIS:HD2	1:B:340:ARG:H	1.54	0.55
1:B:96:HIS:HE1	1:B:283:PRO:O	1.91	0.54
1:B:107:THR:HG22	1:B:345:GLU:OE1	2.08	0.53
1:A:104:LYS:NZ	6:A:1965:HOH:O	2.44	0.50
1:A:65:HIS:HB2	1:A:66:PRO:HD2	1.93	0.49
1:B:361:GLU:HG2	6:B:1948:HOH:O	2.13	0.48
1:B:96:HIS:CD2	1:B:340:ARG:H	2.33	0.47
1:B:181:GLN:NE2	6:B:2032:HOH:O	2.48	0.46
1:A:89:ASP:HB2	1:A:90:PRO:HD3	1.98	0.45
1:B:367:GLU:OE2	6:B:1850:HOH:O	2.21	0.45
1:B:105:HIS:CE1	1:B:107:THR:HG23	2.52	0.44
1:A:27:ASN:HA	1:A:69:MET:HG3	2.01	0.43
1:A:131:ARG:C	1:A:131:ARG:HD2	2.40	0.42
1:B:357:LYS:O	1:B:361:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HD12	1:A:153:VAL:HG13	2.02	0.41
1:A:105:HIS:HE1	6:A:1824:HOH:O	2.02	0.41
1:A:65:HIS:HB2	1:A:66:PRO:HD3	1.99	0.41

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	379/380 (100%)	364 (96%)	12 (3%)	3 (1%)	22	5
1	B	383/380 (101%)	376 (98%)	6 (2%)	1 (0%)	44	23
All	All	762/760 (100%)	740 (97%)	18 (2%)	4 (0%)	32	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASP
1	B	230	GLU
1	A	230	GLU
1	A	66	PRO

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	335/334 (100%)	331 (99%)	4 (1%)	75	57
1	B	339/334 (102%)	337 (99%)	2 (1%)	89	79
All	All	674/668 (101%)	668 (99%)	6 (1%)	82	69

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

Mol	Chain	Res	Type
1	A	176	LYS
1	A	363	GLU
1	A	372	ILE
1	A	373	ASP
1	B	149	GLU
1	B	181	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	57	GLN
1	A	93	GLN
1	A	105	HIS
1	A	162	ASN
1	A	184	GLN
1	B	57	GLN
1	B	96	HIS
1	B	181	GLN
1	B	183	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, 2 are monoatomic - leaving 4 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$
4	ADP	A	1801	2	25,29,29	1.66	4 (16%)	24,45,45	2.25	6 (25%)
4	ADP	B	1501	2	25,29,29	1.53	3 (12%)	24,45,45	2.13	7 (29%)
5	IOM	B	1601	-	2,8,8	1.20	0	4,10,10	3.87	2 (50%)
3	NO3	B	1701	2	1,3,3	3.46	1 (100%)	0,3,3	0.00	-

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
4	ADP	A	1801	2	-	0/12/32/32	0/3/3/3
4	ADP	B	1501	2	-	0/12/32/32	0/3/3/3
5	IOM	B	1601	-	-	0/2/8/8	0/0/0/0
3	NO3	B	1701	2	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	PA-O5'	-2.19	1.49	1.59
4	B	1501	ADP	C2-N3	2.07	1.35	1.32
4	A	1801	ADP	C2-N3	2.08	1.35	1.32
4	B	1501	ADP	O4'-C1'	2.51	1.44	1.41
4	A	1801	ADP	O4'-C1'	3.11	1.45	1.41
3	B	1701	NO3	O1-N	3.46	1.36	1.23
4	B	1501	ADP	PB-O3A	5.47	1.68	1.60
4	A	1801	ADP	PB-O3A	5.84	1.69	1.60

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-8.40	121.54	128.86
4	B	1501	ADP	N3-C2-N1	-7.24	122.55	128.86
4	A	1801	ADP	C1'-N9-C4	-3.11	121.27	126.64
4	B	1501	ADP	C1'-N9-C4	-2.81	121.78	126.64
4	B	1501	ADP	O3'-C3'-C2'	-2.41	104.12	111.83
4	B	1501	ADP	C4'-O4'-C1'	-2.25	107.37	109.77
5	B	1601	IOM	CD-CC-NC	-2.02	108.77	111.73
4	B	1501	ADP	C5-C6-N6	2.10	124.76	120.47
4	A	1801	ADP	C2-N1-C6	2.16	122.55	118.77
4	A	1801	ADP	O5'-PA-O1A	2.55	119.55	109.25
4	A	1801	ADP	C5-C6-N6	2.59	125.76	120.47
4	B	1501	ADP	O2'-C2'-C1'	2.60	119.76	111.61
4	B	1501	ADP	C2'-C3'-C4'	2.82	108.12	102.62
4	A	1801	ADP	C2'-C3'-C4'	3.05	108.56	102.62
5	B	1601	IOM	CB-NC-CC	7.19	119.73	109.97

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	380/380 (100%)	0.72	55 (14%) 3 2	8, 18, 49, 57	0
1	B	380/380 (100%)	-0.27	4 (1%) 80 84	6, 11, 19, 30	0
All	All	760/760 (100%)	0.23	59 (7%) 14 13	6, 13, 44, 57	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	PHE	18.0
1	A	372	ILE	9.7
1	A	324	VAL	9.4
1	A	68	ILE	9.2
1	A	65	HIS	9.0
1	A	66	PRO	8.8
1	A	330	GLY	8.8
1	A	329	VAL	7.8
1	A	327	ALA	7.2
1	A	2	PHE	6.7
1	A	373	ASP	6.2
1	A	366	LEU	5.8
1	A	1	PRO	5.7
1	A	326	THR	5.6
1	A	375	MET	5.3
1	A	305	PRO	5.3
1	A	123	HIS	5.3
1	A	297	LYS	5.0
1	A	299	ALA	4.8
1	A	328	ALA	4.6
1	A	376	ILE	4.5
1	A	124	TYR	4.5
1	A	378	ALA	4.5
1	A	64	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	333	PHE	4.3
1	A	371	SER	4.3
1	A	322	GLY	4.2
1	A	300	HIS	4.1
1	A	331	SER	4.0
1	A	325	ASP	3.9
1	A	321	THR	3.9
1	B	11	LEU	3.5
1	A	26	ASN	3.5
1	A	304	HIS	3.4
1	A	307	PHE	3.4
1	B	107	THR	3.3
1	A	374	ASP	3.3
1	A	119	ASP	3.2
1	A	296	VAL	3.2
1	A	361	GLU	3.0
1	A	126	LEU	3.0
1	B	109	LEU	2.8
1	A	121	ASP	2.8
1	A	298	LEU	2.7
1	A	332	VAL	2.7
1	A	181	GLN	2.6
1	A	69	MET	2.6
1	A	310	ILE	2.6
1	A	3	GLY	2.5
1	A	303	LYS	2.4
1	A	370	GLN	2.4
1	B	108	ASP	2.4
1	A	358	LEU	2.3
1	A	357	LYS	2.2
1	A	365	LYS	2.2
1	A	302	SER	2.1
1	A	313	ARG	2.1
1	A	301	LEU	2.1
1	A	314	LEU	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 [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	NO3	B	1701	4/4	0.88	0.13	4.75	13,15,15,16	0
2	MG	B	1502	1/1	1.00	0.09	0.84	5,5,5,5	0
4	ADP	A	1801	27/27	0.90	0.16	-0.17	31,41,42,43	0
4	ADP	B	1501	27/27	0.98	0.06	-0.88	6,8,9,11	0
5	IOM	B	1601	9/9	0.98	0.07	-1.23	7,9,10,10	0
2	MG	A	1802	1/1	0.90	0.11	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.