



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PX2
Title : Crystal Structure of Rat Synapsin I C Domain Complexed to Ca.ATP (Form 1)
Authors : Brautigam, C.A.; Chelliah, Y.; Deisenhofer, J.
Deposited on : 2003-07-02
Resolution : 2.23 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

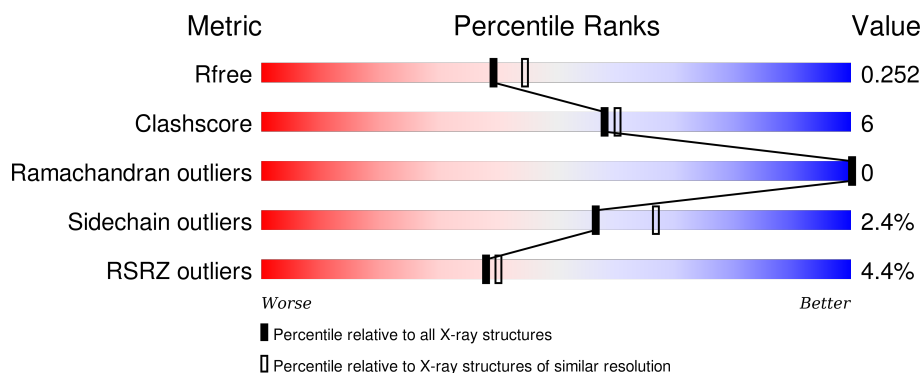
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	422	<div> <div>3%</div> <div>58%</div> <div>11%</div> <div>30%</div> </div>
1	B	422	<div> <div>4%</div> <div>61%</div> <div>8%</div> <div>30%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5139 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 Synapsin I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	4	0	0
			2338	1493	403	429	13			
1	B	294	Total	C	N	O	S	6	1	0
			2349	1499	404	433	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP P09951
A	1	SER	MET	CLONING ARTIFACT	UNP P09951
B	0	GLY	-	CLONING ARTIFACT	UNP P09951
B	1	SER	MET	CLONING ARTIFACT	UNP P09951

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 62	C 20	N 10	O 26	P 6	0	1
3	B	1	Total 62	C 20	N 10	O 26	P 6	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	B	170	Total	O	0	0
			170	170		

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 ($\text{RSRZ} > 2$). 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.

Chain A:

3% 58% 11% 30%

GLY SER ASN TYR LEU ARG ARG ARG LEU ASP ASN PHE MET ALA ASN LEU PRO GLY TYR ASP GLN ARG PRO GLN PRO PRO PRO PRO PRO PRO PRO ALA ALA ALA ALA ALA ALA ALA ALA GLU ARG SER THR ALA ALA PRO

VAL ALA SER PRO ALA PRO PRO GLY PHE GLY PHE SER LEU SER SER ALA VAL GLN THR THR ALA ALA ALA ALA THR PHE SER SER GLU THR VAL GLY GLY SER GLY ALA ARG GLY ALA ALA I112 I119 H123 T124 D125

K134 I135 H136 G137 E138 I139 D140 W135 A146 L153 V154 D164 M165 E166 V167 L168 R169 K173 K174 V175 L178 V183 N196 R199 S212 F222 H236 L239 F244 H255 K256 E257 T262 P265 H286 F307 D313 V316 Q317 K318

R328 T329 SER VAL SER GLY ASN W335 T336 THR ASN THR GLY SER ALA MET L344 R352 V357 D358 T359 A371 V372 E373 A374 L375 V388 M392 P393 F394 D402 K403 V407 E408 L409 Q416 A417 LEU PRO ARG GLN

Chain B:

Amino Acid	Frequency (%)
THR	4%
GLY	61%
SER	8%
MET	30%
L344	
D368	
E373	
A374	
L375	
E386	
V387	
M392	
L409	
A417	
LEU	
PRO	
ARG	
GLN	
VAL	
L133	
K134	
I135	
L136	
G137	
E138	
I139	
L153	
V154	
F161	
V167	
L168	
R169	
H170	
G171	
V172	
K173	
V174	
L178	
K179	
P180	
Q187	
R194	
N195	
I210	
F222	
V228	
Q231	
E257	
P265	
S275	
F307	
N322	
K328	
T329	
SER	
VAL	
SER	
GLY	
ASN	
K335	
K336	
T337	
ASN	

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.00 Å 96.00 Å 305.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.23 19.88 – 2.23	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.23) 97.2 (19.88-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.23 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.240 0.212 , 0.252	Depositor DCC
R_{free} test set	2033 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	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	0 of 41619 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5139	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: CA, ATP

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	0.35	0/2388	0.62	0/3225
1	B	0.37	0/2399	0.63	0/3240
All	All	0.36	0/4787	0.63	0/6465

There are no bond length outliers.

There are no bond angle outliers.

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	2338	0	2325	38	0
1	B	2349	0	2332	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	62	0	24	1	0
3	B	62	0	24	2	0
4	A	156	0	0	3	0
4	B	170	0	0	1	0
All	All	5139	0	4705	56	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 6.

All (56) 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:328:ARG:NH2	1:B:373[B]:GLU:OE2	2.27	0.68
1:A:318:LYS:HB2	1:A:357:VAL:HG11	1.77	0.65
1:A:239:LEU:HD11	1:A:359:THR:HG21	1.79	0.65
1:A:165:MET:HE3	1:A:178:LEU:HD11	1.78	0.64
1:A:167:VAL:HG12	1:A:168:LEU:N	2.15	0.61
1:A:183:VAL:CG1	1:A:212:SER:HB2	2.31	0.60
1:A:195:ASN:HA	4:A:882:HOH:O	2.02	0.59
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.67	0.59
1:A:265:PRO:HG2	1:A:307:PHE:HB3	1.83	0.58
1:B:161:PHE:CE2	1:B:210:ILE:HD11	2.38	0.58
1:B:169:ARG:O	1:B:172:VAL:HG12	2.04	0.58
1:B:168:LEU:O	1:B:169:ARG:HD3	2.04	0.57
1:A:409:LEU:O	1:A:409:LEU:HD12	2.05	0.56
1:A:255:HIS:HD2	4:A:920:HOH:O	1.89	0.55
1:A:165:MET:CE	1:A:178:LEU:HD11	2.37	0.55
1:B:178:LEU:HD12	1:B:180:PRO:HG3	1.89	0.54
1:A:154:VAL:HG22	1:B:257:GLU:HB3	1.89	0.54
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.73	0.54
1:A:169:ARG:HG2	1:A:169:ARG:NH1	2.23	0.53
1:A:236:HIS:HD2	1:A:244:PHE:O	1.93	0.52
1:A:167:VAL:CG1	1:A:168:LEU:N	2.73	0.51
1:A:257:GLU:HB3	1:B:154:VAL:HG22	1.92	0.51
1:A:403:LYS:O	1:A:407:VAL:HG23	2.11	0.50
1:B:265:PRO:HG2	1:B:307:PHE:HB3	1.94	0.50
1:B:153:LEU:HD12	1:B:153:LEU:C	2.32	0.50
1:A:239:LEU:CD1	1:A:359:THR:HG21	2.41	0.49
1:A:371:ALA:HB3	1:A:388:VAL:CG2	2.42	0.49
1:A:318:LYS:HB2	1:A:357:VAL:CG1	2.43	0.49
1:A:199:ARG:NH1	4:A:827:HOH:O	2.46	0.49
1:B:368:ASP:HB3	1:B:409:LEU:HD21	1.95	0.48
1:A:392:MET:HG3	1:A:392:MET:O	2.13	0.48
1:A:352:ARG:HG3	1:A:352:ARG:HH11	1.79	0.48
1:A:394:LEU:HD22	1:A:402:ASP:HB3	1.95	0.48
1:A:134:LYS:HE2	1:A:140:ASP:OD1	2.12	0.47
1:A:153:LEU:C	1:A:153:LEU:HD12	2.35	0.47
1:A:371:ALA:HB3	1:A:388:VAL:HG22	1.96	0.47
1:A:328:ARG:HB2	1:A:328:ARG:NH1	2.30	0.47
1:A:135:ILE:O	1:A:136:HIS:HB2	2.15	0.47
1:B:121:GLU:HB2	1:B:122:PRO:HD2	1.97	0.46
1:A:316:VAL:HG12	1:A:357:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLN:O	1:A:417:ALA:HB2	2.15	0.46
1:B:392:MET:HG3	1:B:392:MET:O	2.16	0.45
1:B:135:ILE:O	1:B:136:HIS:HB2	2.18	0.44
1:B:228:VAL:O	1:B:231:GLN:HB2	2.18	0.43
1:B:386:GLU:HG2	1:B:387:VAL:N	2.32	0.43
1:A:153:LEU:O	1:B:257:GLU:HG3	2.18	0.43
1:A:375:LEU:HD21	3:A:800[B]:ATP:H2'	2.01	0.42
1:A:183:VAL:HG13	1:A:212:SER:HB2	2.00	0.42
1:B:138:GLU:HG3	1:B:139:ILE:HG13	2.02	0.42
1:B:322:ASN:HB2	4:B:930:HOH:O	2.20	0.41
1:A:119:ILE:HA	1:A:146:ALA:O	2.20	0.41
1:B:169:ARG:HA	1:B:169:ARG:HD3	1.42	0.41
1:A:313:ASP:CB	1:A:375:LEU:HD23	2.51	0.41
1:B:375:LEU:HD21	3:B:800[B]:ATP:H2'	2.03	0.41
1:B:275:SER:HA	3:B:800[B]:ATP:O2G	2.21	0.41
1:A:164:ASP:HB3	1:A:175:VAL:CG1	2.52	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	288/422 (68%)	283 (98%)	5 (2%)	0	100	100
1	B	289/422 (68%)	287 (99%)	2 (1%)	0	100	100
All	All	577/844 (68%)	570 (99%)	7 (1%)	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	254/340 (75%)	249 (98%)	5 (2%)	63	73
1	B	256/340 (75%)	249 (97%)	7 (3%)	52	63
All	All	510/680 (75%)	498 (98%)	12 (2%)	57	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	A	222	PHE
1	A	329	THR
1	A	344	LEU
1	A	373	GLU
1	B	134	LYS
1	B	169	ARG
1	B	178	LEU
1	B	187	GLN
1	B	194	ARG
1	B	222	PHE
1	B	337	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS

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	$\# Z > 2$
3	ATP	A	800[A]	2	24,33,33	0.85	0	31,52,52	1.05	2 (6%)
3	ATP	A	800[B]	2	24,33,33	0.82	0	31,52,52	1.07	4 (12%)
3	ATP	B	800[A]	2	24,33,33	0.84	0	31,52,52	1.04	2 (6%)
3	ATP	B	800[B]	2	24,33,33	0.85	0	31,52,52	1.12	5 (16%)

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	ATP	A	800[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	A	800[B]	2	-	0/18/38/38	0/3/3/3
3	ATP	B	800[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	B	800[B]	2	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800[B]	ATP	O3G-PG-O2G	-2.38	98.30	107.38
3	B	800[B]	ATP	C2'-C1'-N9	-2.21	110.92	114.29
3	A	800[B]	ATP	O3A-PA-O5'	-2.19	97.13	102.94
3	A	800[B]	ATP	O3G-PG-O2G	-2.16	99.16	107.38
3	B	800[B]	ATP	O3A-PA-O5'	-2.09	97.38	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	800[A]	ATP	O2G-PG-O1G	2.42	118.38	110.58
3	B	800[B]	ATP	O2G-PG-O1G	2.48	118.57	110.58
3	B	800[A]	ATP	O3G-PG-O1G	2.49	118.60	110.58
3	A	800[A]	ATP	O2G-PG-O1G	2.50	118.63	110.58
3	A	800[B]	ATP	O2G-PG-O1G	2.51	118.66	110.58
3	A	800[A]	ATP	O3G-PG-O1G	2.54	118.75	110.58
3	A	800[B]	ATP	O3G-PG-O1G	2.54	118.77	110.58
3	B	800[B]	ATP	O3G-PG-O1G	2.58	118.90	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800[B]	ATP	1	0
3	B	800[B]	ATP	2	0

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	294/422 (69%)	-0.07	11 (3%) 45 47	21, 37, 65, 77	1 (0%)
1	B	294/422 (69%)	-0.09	15 (5%) 32 33	19, 34, 67, 80	1 (0%)
All	All	588/844 (69%)	-0.08	26 (4%) 38 40	19, 35, 65, 80	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	HIS	6.2
1	B	170	ASN	6.2
1	B	123	HIS	5.1
1	A	335	TRP	5.0
1	B	169	ARG	4.5
1	B	171	GLY	4.3
1	B	138	GLU	4.1
1	B	168	LEU	3.6
1	B	172	VAL	3.6
1	A	138	GLU	3.2
1	B	167	VAL	3.1
1	B	195	ASN	2.9
1	B	174	VAL	2.7
1	B	173	LYS	2.7
1	A	125	ASP	2.6
1	A	262	THR	2.6
1	B	137	GLY	2.4
1	A	112	ALA	2.3
1	A	168	LEU	2.2
1	B	417	ALA	2.2
1	A	344	LEU	2.1
1	A	372	VAL	2.1
1	B	132	GLY	2.1
1	B	136	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	286	HIS	2.1
1	A	173	LYS	2.1

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	ATP	A	800[A]	31/31	0.95	0.12	-0.12	25,36,41,43	31
3	ATP	A	800[B]	31/31	0.95	0.12	-0.15	38,45,52,53	31
3	ATP	B	800[A]	31/31	0.96	0.10	-0.68	16,26,31,32	31
3	ATP	B	800[B]	31/31	0.96	0.10	-0.81	36,42,48,48	31
2	CA	A	817	1/1	0.87	0.06	-	72,72,72,72	0
2	CA	B	817	1/1	0.99	0.03	-	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.