



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:27 AM GMT

PDB ID : 2QRD
Title : Crystal Structure of the Adenylate Sensor from AMP-activated Protein Kinase
in complex with ADP and ATP
Authors : Jin, X.; Townley, R.; Shapiro, L.
Deposited on : 2007-07-28
Resolution : 2.41 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

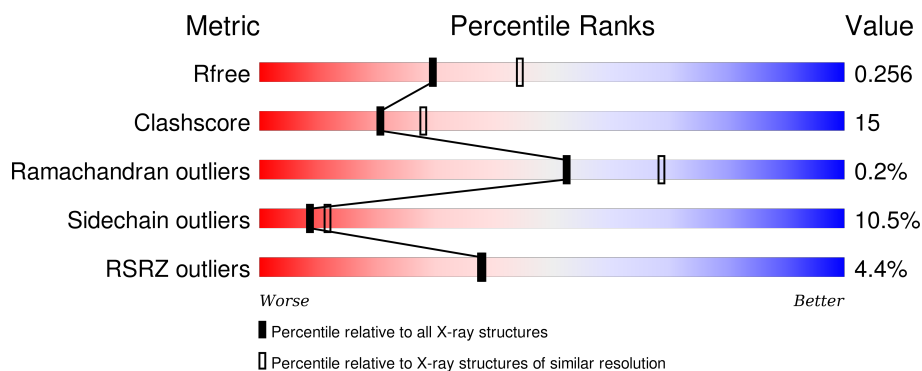
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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.



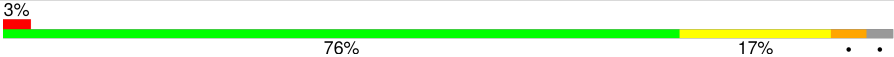
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 $\leq 5\%$. 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	137	<div> <div>4%</div> <div>64%</div> <div>18%</div> <div>•</div> <div>17%</div> </div>
1	C	137	<div> <div>9%</div> <div>55%</div> <div>23%</div> <div>5%</div> <div>17%</div> </div>
2	B	97	<div> <div>2%</div> <div>72%</div> <div>18%</div> <div>•</div> <div>6%</div> </div>
2	D	97	<div> <div>8%</div> <div>63%</div> <div>25%</div> <div>5%</div> <div>•</div> <div>5%</div> </div>
3	E	334	<div> <div>3%</div> <div>74%</div> <div>17%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	334	 A horizontal bar chart showing the quality of chain G. The bar is divided into four segments: a small red segment at the beginning labeled '3%', followed by a large green segment labeled '76%', then a yellow segment labeled '17%', and finally a small grey segment at the end. Two small black dots are visible at the far right end of the bar.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8951 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			916	593	154	160	9			
1	C	114	Total	C	N	O	S	0	0	0
			914	592	156	157	9			

- Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	S	0	0	0
			699	445	120	132	2			
2	D	92	Total	C	N	O	S	0	0	0
			727	464	124	137	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	MET	-	EXPRESSION TAG	UNP P78789
D	202	MET	-	EXPRESSION TAG	UNP P78789

- Molecule 3 is a protein called Protein C1556.08c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	325	Total	C	N	O	S	0	1	0
			2554	1631	425	483	15			
3	E	324	Total	C	N	O	S	0	1	0
			2551	1629	424	482	16			

There are 4 discrepancies between the modelled and reference sequences:

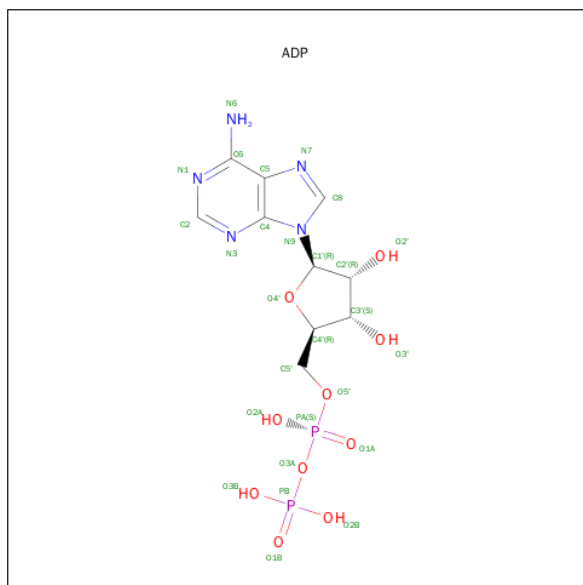
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	EXPRESSION TAG	UNP Q10343
G	2	MET	-	EXPRESSION TAG	UNP Q10343

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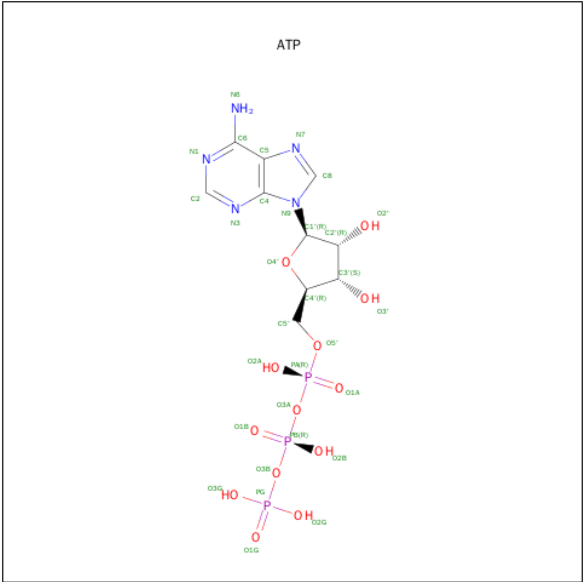
Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ALA	-	EXPRESSION TAG	UNP Q10343
E	2	MET	-	EXPRESSION TAG	UNP Q10343

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
5	E	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
5	E	1	Total	C	N	O	P	0	1
			31	10	5	13	3		

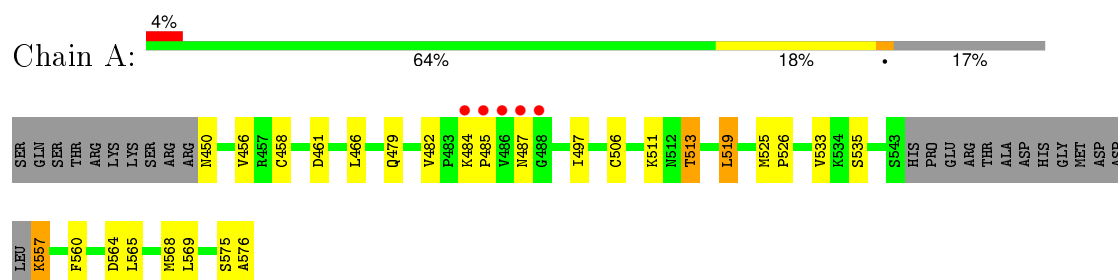
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		
6	B	39	Total	O	0	0
			39	39		
6	C	37	Total	O	0	0
			37	37		
6	D	41	Total	O	0	0
			41	41		
6	E	116	Total	O	0	0
			116	116		
6	G	133	Total	O	0	0
			133	133		

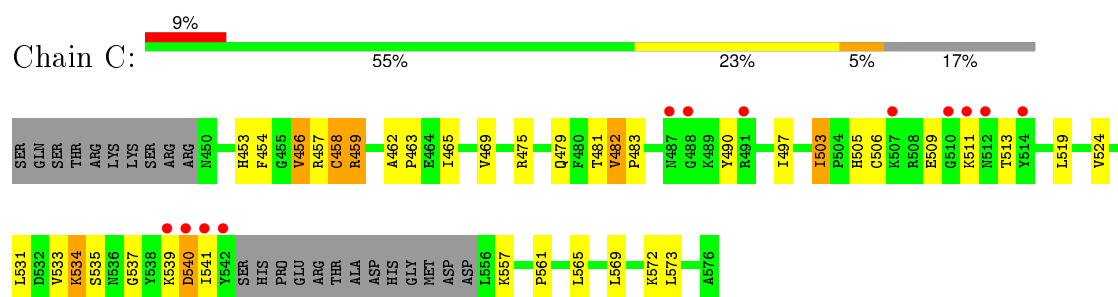
3 Residue-property plots

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.

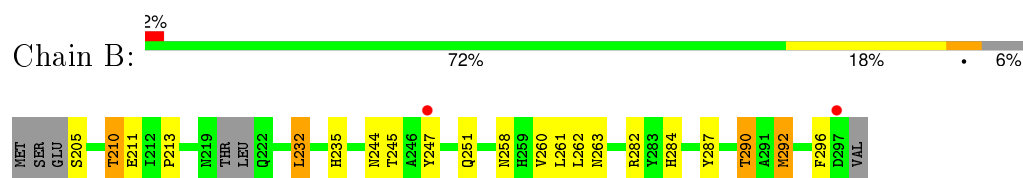
- Molecule 1: SNF1-like protein kinase ssp2



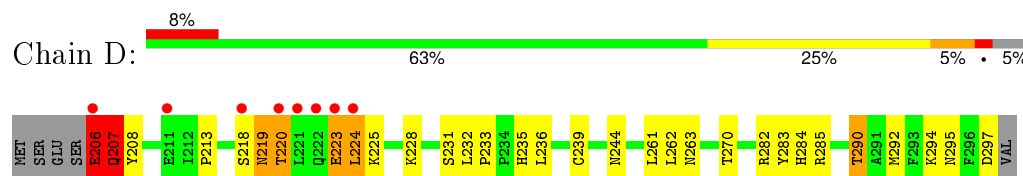
- Molecule 1: SNF1-like protein kinase ssp2



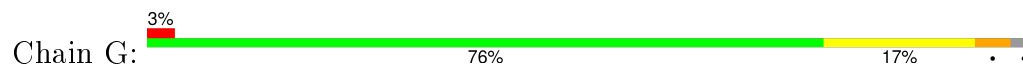
- Molecule 2: SPCC1919.03c protein

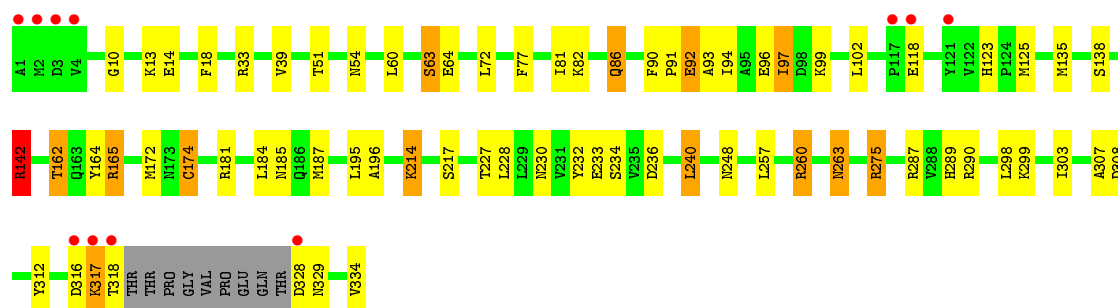


- Molecule 2: SPCC1919.03c protein

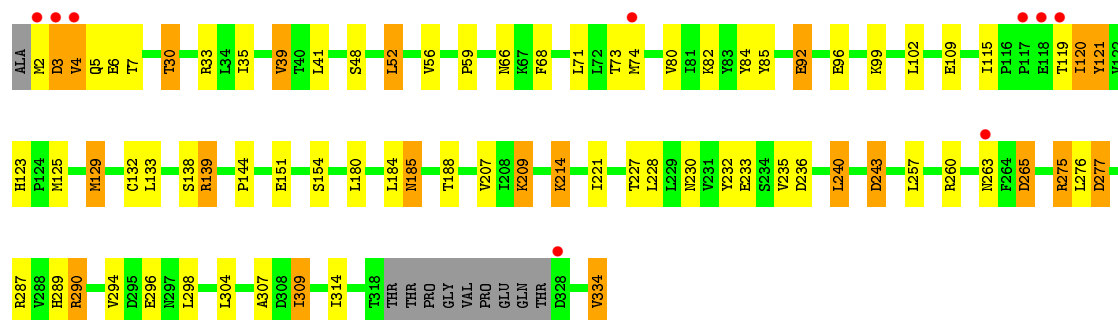
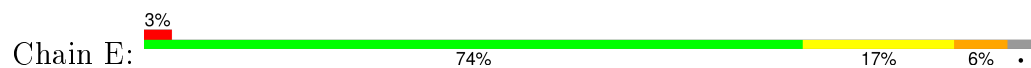


- Molecule 3: Protein C1556.08c





• Molecule 3: Protein C1556.08c



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.26Å 78.36Å 109.01Å 90.00° 124.18° 90.00°	Depositor
Resolution (Å)	35.94 – 2.41 35.94 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.94-2.41) 98.9 (35.94-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.262 0.190 , 0.256	Depositor DCC
R_{free} test set	2277 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 45179 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8951	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP

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	0.69	0/940	0.73	0/1266
1	C	0.65	0/937	0.74	0/1261
2	B	0.64	0/716	0.73	1/978 (0.1%)
2	D	0.74	3/745 (0.4%)	0.81	2/1018 (0.2%)
3	E	0.73	0/2596	0.78	2/3515 (0.1%)
3	G	0.74	1/2599 (0.0%)	0.84	2/3520 (0.1%)
All	All	0.71	4/8533 (0.0%)	0.79	7/11558 (0.1%)

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
2	B	0	1
2	D	0	4
3	G	0	1
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	239	CYS	CB-SG	-6.29	1.71	1.82
3	G	174	CYS	CB-SG	-6.19	1.71	1.82
2	D	297	ASP	CG-OD1	5.55	1.38	1.25
2	D	297	ASP	CB-CG	5.24	1.62	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	207	GLN	N-CA-C	5.95	127.07	111.00
3	G	260	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	D	297	ASP	N-CA-CB	5.67	120.81	110.60
3	E	290	ARG	NE-CZ-NH2	-5.48	117.56	120.30
3	E	39	VAL	CB-CA-C	-5.27	101.38	111.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	296	PHE	Peptide
2	D	206	GLU	Peptide
2	D	207	GLN	Peptide
2	D	219	ASN	Peptide
3	G	317	LYS	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	916	0	903	23	0
1	C	914	0	909	47	0
2	B	699	0	681	18	0
2	D	727	0	730	34	0
3	E	2551	0	2588	77	0
3	G	2554	0	2591	64	0
4	E	27	0	12	0	0
4	G	27	0	12	4	0
5	E	62	0	24	7	0
5	G	62	0	24	11	0
6	A	46	0	0	10	0
6	B	39	0	0	1	0
6	C	37	0	0	3	0
6	D	41	0	0	3	0
6	E	116	0	0	6	0
6	G	133	0	0	9	0
All	All	8951	0	8474	247	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 15.

The worst 5 of 247 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)
3:E:2:MET:CE	3:E:7:THR:HA	1.43	1.48
1:C:482:VAL:CG2	2:D:213:PRO:HG3	1.69	1.22
6:A:339:HOH:O	2:B:292:MET:HE2	1.37	1.20
3:E:307:ALA:HB3	5:E:1002[A]:ATP:O2A	1.42	1.18
2:D:219:ASN:HA	2:D:220:THR:HB	1.28	1.15

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	110/137 (80%)	109 (99%)	1 (1%)	0	100	100
1	C	110/137 (80%)	104 (94%)	6 (6%)	0	100	100
2	B	87/97 (90%)	82 (94%)	5 (6%)	0	100	100
2	D	90/97 (93%)	80 (89%)	9 (10%)	1 (1%)	17	24
3	E	321/334 (96%)	313 (98%)	8 (2%)	0	100	100
3	G	322/334 (96%)	311 (97%)	10 (3%)	1 (0%)	46	62
All	All	1040/1136 (92%)	999 (96%)	39 (4%)	2 (0%)	52	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	220	THR
3	G	263	ASN

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	97/120 (81%)	86 (89%)	11 (11%)	7	9
1	C	96/120 (80%)	85 (88%)	11 (12%)	7	9
2	B	77/88 (88%)	71 (92%)	6 (8%)	16	24
2	D	83/88 (94%)	73 (88%)	10 (12%)	6	7
3	E	286/296 (97%)	253 (88%)	33 (12%)	7	9
3	G	285/296 (96%)	259 (91%)	26 (9%)	12	16
All	All	924/1008 (92%)	827 (90%)	97 (10%)	8	11

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	456	VAL
2	D	206	GLU
3	E	257	LEU
1	C	459	ARG
1	C	534	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	263	ASN
1	C	453	HIS
3	E	66	ASN
3	G	311	ASN
1	C	505	HIS

5.3.3 RNA [i](#)

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 ⓘ

6 ligands are modelled in this entry.

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	$\# Z > 2$
5	ATP	E	1002[A]	-	24,33,33	0.98	1 (4%)	31,52,52	2.28	6 (19%)
4	ADP	E	1004	-	22,29,29	0.88	1 (4%)	27,45,45	2.19	4 (14%)
5	ATP	E	1502[B]	-	24,33,33	0.93	1 (4%)	31,52,52	2.30	5 (16%)
5	ATP	G	1001[A]	-	24,33,33	1.06	1 (4%)	31,52,52	2.17	7 (22%)
4	ADP	G	1003	-	22,29,29	1.01	1 (4%)	27,45,45	1.97	6 (22%)
5	ATP	G	1501[B]	-	24,33,33	1.04	1 (4%)	31,52,52	2.23	6 (19%)

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
5	ATP	E	1002[A]	-	-	0/18/38/38	0/3/3/3
4	ADP	E	1004	-	-	0/12/32/32	0/3/3/3
5	ATP	E	1502[B]	-	-	0/18/38/38	0/3/3/3
5	ATP	G	1001[A]	-	-	0/18/38/38	0/3/3/3
4	ADP	G	1003	-	-	0/12/32/32	0/3/3/3
5	ATP	G	1501[B]	-	-	0/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1004	ADP	C5-C4	2.26	1.45	1.40
5	E	1502[B]	ATP	C5-C4	3.03	1.47	1.40
5	E	1002[A]	ATP	C5-C4	3.09	1.47	1.40
5	G	1001[A]	ATP	C5-C4	3.38	1.48	1.40
4	G	1003	ADP	C5-C4	3.38	1.48	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1004	ADP	N3-C2-N1	-8.92	122.06	128.89
5	E	1502[B]	ATP	N3-C2-N1	-8.19	122.62	128.89
5	E	1002[A]	ATP	N3-C2-N1	-7.91	122.84	128.89
5	G	1001[A]	ATP	N3-C2-N1	-7.38	123.24	128.89
4	G	1003	ADP	N3-C2-N1	-7.02	123.52	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1002[A]	ATP	5	0
5	E	1502[B]	ATP	2	0
5	G	1001[A]	ATP	8	0
4	G	1003	ADP	4	0
5	G	1501[B]	ATP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	114/137 (83%)	0.17	5 (4%) 38 38	45, 52, 60, 64	0
1	C	114/137 (83%)	0.41	12 (10%) 8 7	45, 53, 58, 61	0
2	B	91/97 (93%)	0.46	2 (2%) 65 64	46, 52, 59, 66	0
2	D	92/97 (94%)	0.79	8 (8%) 13 12	24, 52, 60, 66	0
3	E	324/334 (97%)	0.04	9 (2%) 56 55	26, 52, 63, 77	0
3	G	325/334 (97%)	0.02	11 (3%) 49 48	24, 51, 61, 80	0
All	All	1060/1136 (93%)	0.19	47 (4%) 38 38	24, 52, 61, 80	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	542	TYR	7.6
1	A	486	VAL	6.6
2	B	247	TYR	6.4
3	G	2	MET	6.3
2	D	220	THR	6.1

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
5	ATP	E	1502[B]	31/31	0.95	0.12	-0.55	31,33,51,52	31
5	ATP	G	1001[A]	31/31	0.96	0.12	-0.77	36,54,56,57	31
5	ATP	E	1002[A]	31/31	0.96	0.11	-0.86	48,53,60,61	31
5	ATP	G	1501[B]	31/31	0.97	0.11	-0.88	27,31,48,49	31
4	ADP	G	1003	27/27	0.98	0.07	-3.29	36,38,42,45	0
4	ADP	E	1004	27/27	0.98	0.08	-4.75	33,40,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.