Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:04 PM GMT

PDB ID	:	3SUC
Title	:	Crystal structure of the pre-mature bacteriophage phi29 gene product 12
Authors	:	Xiang, Y.; Rossmann, M.G.
Deposited on	:	2011-07-11
Resolution	:	2.15 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	Percentile Ranks	Value
Rfree		0.268
Clashscore		7
Ramachandran outliers		0.8%
Sidechain outliers		5.8%
RSRZ outliers		12.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
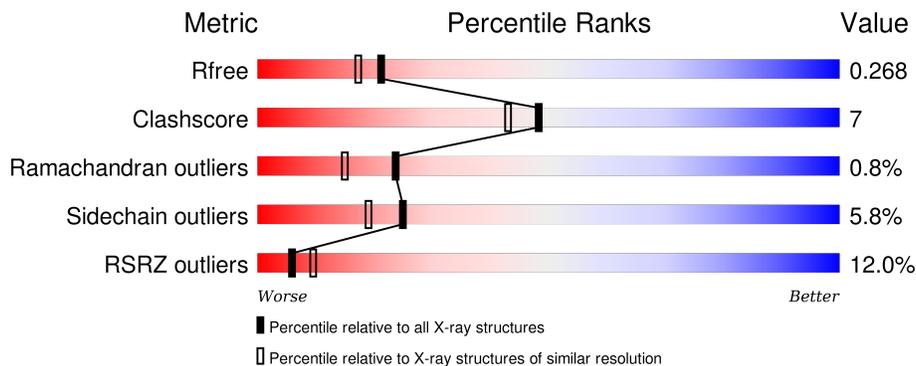
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 <=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	772	12% / 81% / 16% / ··

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5875 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 Preneck appendage protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	0	5	0
			5767	3587	1006	1159	15			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	HIS	-	EXPRESSION TAG	UNP B3VMP8
A	84	HIS	-	EXPRESSION TAG	UNP B3VMP8
A	85	HIS	-	EXPRESSION TAG	UNP B3VMP8
A	86	HIS	-	EXPRESSION TAG	UNP B3VMP8
A	87	HIS	-	EXPRESSION TAG	UNP B3VMP8
A	88	HIS	-	EXPRESSION TAG	UNP B3VMP8
A	166	ARG	LYS	Natural Variant	UNP B3VMP8
A	627	GLN	LYS	Natural Variant	UNP B3VMP8
A	695	GLN	GLU	ENGINEERED MUTATION	UNP B3VMP8
A	701	GLY	ASP	Natural Variant	UNP B3VMP8
A	817	SER	GLY	Natural Variant	UNP B3VMP8

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

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

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
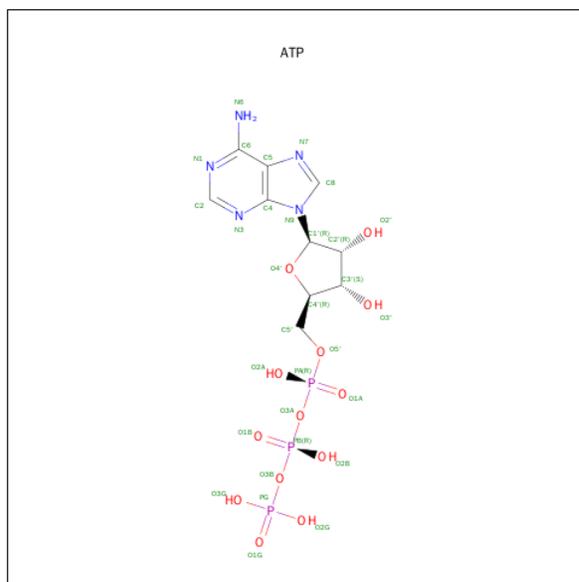
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	73	74	74	0	1

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: Preneck appendage protein
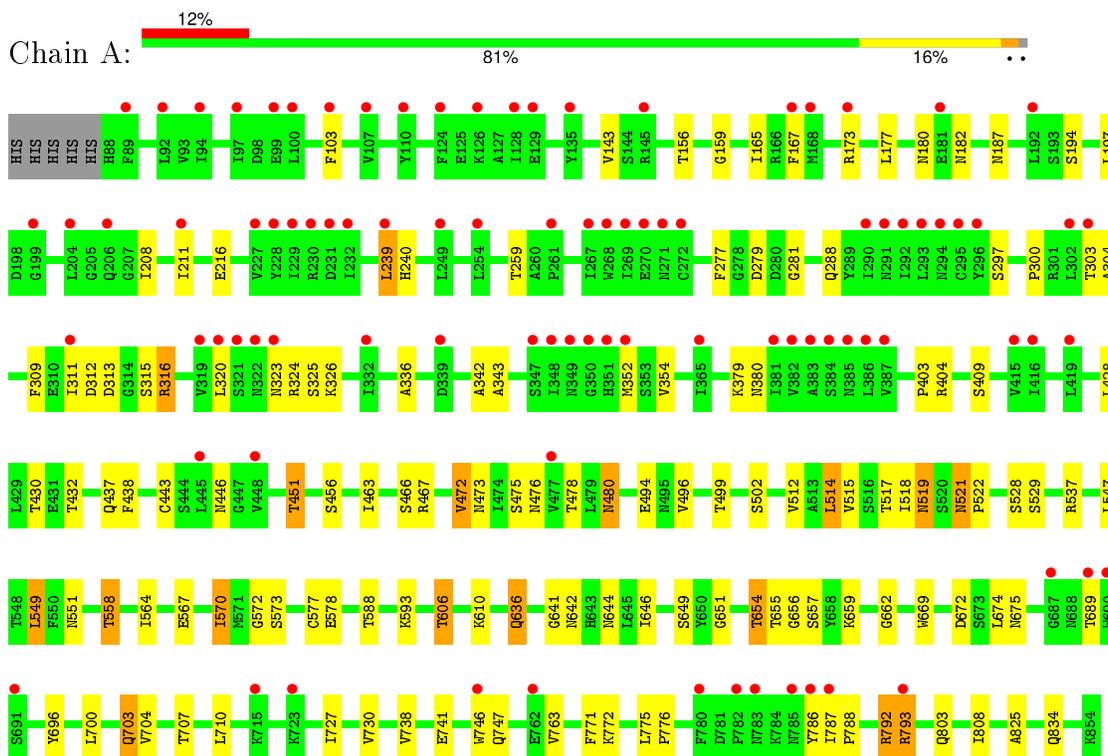
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	95.89Å 95.89Å 795.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 2.15 49.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	65.5 (49.27-2.15) 65.5 (49.26-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	15.88 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.291 0.238 , 0.268	Depositor DCC
R_{free} test set	2530 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.53, <L^2> = 0.37$	Xtriage
Outliers	17 of 50808 reflections (0.033%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ 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, 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	0.39	0/5882	0.54	1/7972 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	549	LEU	CA-CB-CG	5.59	128.16	115.30

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	5767	0	5628	84	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	31	0	12	0	0
5	A	74	0	0	3	0
All	All	5875	0	5640	84	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 7.

All (84) 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:644:ASN:HD21	1:A:654:THR:CG2	1.55	1.18
1:A:644:ASN:ND2	1:A:654:THR:HG22	1.66	1.11
1:A:644:ASN:HD21	1:A:654:THR:HG22	0.85	1.00
1:A:517:THR:HG22	1:A:519:ASN:O	1.78	0.82
1:A:558:THR:HG21	1:A:570:ILE:HG22	1.59	0.82
1:A:792:ARG:HH11	1:A:792:ARG:HG2	1.43	0.81
1:A:336:ALA:HB2	1:A:342:ALA:HA	1.65	0.79
1:A:496[B]:VAL:HG23	1:A:522:PRO:HB3	1.67	0.77
1:A:514:LEU:HG	1:A:529:SER:HB3	1.73	0.71
1:A:578:GLU:HB3	1:A:593:LYS:HG2	1.74	0.70
1:A:572:GLY:O	1:A:588:THR:HA	1.93	0.68
1:A:644:ASN:ND2	1:A:654:THR:CG2	2.39	0.65
1:A:517:THR:HG21	1:A:522:PRO:HG2	1.77	0.65
1:A:182:ASN:H	1:A:187:ASN:HD21	1.45	0.63
1:A:696:TYR:CE1	1:A:741:GLU:HG2	2.36	0.60
1:A:451:THR:HB	1:A:480:ASN:HB3	1.84	0.60
1:A:519:ASN:HD21	1:A:521:ASN:CG	2.05	0.60
1:A:641:GLY:H	1:A:644:ASN:HD22	1.49	0.59
1:A:792:ARG:NH1	1:A:792:ARG:HG2	2.15	0.58
1:A:521:ASN:HA	1:A:551:ASN:ND2	2.19	0.58
1:A:494:GLU:HG3	5:A:72:HOH:O	2.03	0.58
1:A:473[B]:ASN:ND2	5:A:12:HOH:O	2.38	0.56
1:A:656:GLY:HA3	1:A:659:LYS:HG3	1.86	0.56
1:A:517:THR:CG2	1:A:522:PRO:HG2	2.36	0.55
1:A:288:GLN:HE21	1:A:316:ARG:HE	1.52	0.55
1:A:696:TYR:HE1	1:A:741:GLU:HG2	1.70	0.55
1:A:512:VAL:HG12	1:A:537:ARG:HH12	1.71	0.54
1:A:502:SER:HA	1:A:528:SER:O	2.07	0.54
1:A:277:PHE:CE2	1:A:300:PRO:HB3	2.43	0.54
1:A:646:ILE:HD11	1:A:654:THR:HB	1.89	0.53
1:A:496[B]:VAL:CG2	1:A:522:PRO:HB3	2.36	0.53
1:A:564:ILE:HG12	1:A:570:ILE:CD1	2.39	0.53
1:A:521:ASN:N	1:A:522:PRO:CD	2.73	0.52
1:A:636:GLN:O	1:A:651:GLY:HA2	2.10	0.52
1:A:577:CYS:HB2	5:A:3:HOH:O	2.10	0.51
1:A:514:LEU:HD13	1:A:515:VAL:HG23	1.92	0.51
1:A:159:GLY:HA2	1:A:194:SER:HB3	1.92	0.51
1:A:517:THR:CG2	1:A:519:ASN:O	2.56	0.51
1:A:446:ASN:HD21	1:A:476:ASN:HD22	1.58	0.50
1:A:710:LEU:HD23	1:A:730:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASP:CG	1:A:313:ASP:H	2.15	0.49
1:A:803:GLN:HG2	1:A:834:GLN:HE22	1.77	0.49
1:A:521:ASN:HA	1:A:551:ASN:HD21	1.77	0.49
1:A:472:VAL:HG13	1:A:496[B]:VAL:HG12	1.95	0.48
1:A:475:SER:HA	1:A:499:THR:O	2.13	0.48
1:A:403:PRO:HG2	1:A:428:LEU:O	2.14	0.47
1:A:564:ILE:HG12	1:A:570:ILE:HD13	1.95	0.47
1:A:558:THR:HB	1:A:573:SER:O	2.15	0.46
1:A:315:SER:O	1:A:343:ALA:HA	2.15	0.46
1:A:704:VAL:HG22	1:A:793:ARG:HG2	1.97	0.46
1:A:336:ALA:CB	1:A:342:ALA:HA	2.41	0.46
1:A:239:LEU:HB3	1:A:240:HIS:H	1.55	0.46
1:A:288:GLN:NE2	1:A:316:ARG:HE	2.14	0.45
1:A:324:ARG:HG3	1:A:352:MET:HB3	1.98	0.45
1:A:404:ARG:HD3	1:A:432:THR:O	2.16	0.45
1:A:326:LYS:HA	1:A:354:VAL:O	2.16	0.45
1:A:808:ILE:HG22	1:A:825:ALA:HB3	1.99	0.45
1:A:662:GLY:HA3	1:A:669:TRP:CE2	2.52	0.45
1:A:763:VAL:HB	1:A:771:PHE:CE2	2.52	0.44
1:A:281:GLY:HA3	1:A:297[A]:SER:OG	2.16	0.44
1:A:326:LYS:HG3	1:A:354:VAL:HB	1.99	0.44
1:A:443[B]:CYS:HB3	1:A:472:VAL:HB	1.99	0.44
1:A:309:PHE:CZ	1:A:323:ASN:HB3	2.53	0.44
1:A:672:ASP:OD1	1:A:675:ASN:HB2	2.18	0.44
1:A:480:ASN:HD22	1:A:480:ASN:C	2.22	0.42
1:A:311:ILE:HD11	1:A:320:LEU:HD21	2.01	0.42
1:A:240:HIS:CE1	1:A:279:ASP:HB3	2.54	0.42
1:A:437:GLN:HB3	1:A:463:ILE:HD12	2.01	0.42
1:A:211:ILE:H	1:A:211:ILE:HG13	1.70	0.42
1:A:710:LEU:HD22	1:A:727:ILE:HG21	2.02	0.42
1:A:775:LEU:HA	1:A:776:PRO:HD3	1.92	0.42
1:A:642:ASN:HB3	1:A:657:SER:HB3	2.02	0.41
1:A:446:ASN:ND2	1:A:475:SER:OG	2.50	0.41
1:A:700:LEU:O	1:A:703:GLN:HG3	2.20	0.41
1:A:772:LYS:HE2	1:A:772:LYS:HB3	1.88	0.41
1:A:165:ILE:HB	1:A:197:LEU:HD23	2.02	0.41
1:A:649:SER:OG	1:A:662:GLY:HA2	2.21	0.41
1:A:409:SER:HB3	1:A:438:PHE:HB2	2.02	0.41
1:A:430:THR:O	1:A:456:SER:HA	2.21	0.41
1:A:303:THR:O	1:A:303:THR:HG22	2.20	0.40
1:A:173:ARG:HH12	1:A:208:ILE:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:ILE:HA	1:A:788:PRO:HD3	1.90	0.40
1:A:746:TRP:HA	1:A:786:TYR:CE2	2.57	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	770/772 (100%)	717 (93%)	47 (6%)	6 (1%)	24	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	THR
1	A	689	THR
1	A	304	ALA
1	A	380	ASN
1	A	216	GLU
1	A	521	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	629/630 (100%)	592 (94%)	37 (6%)	24	18

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	PHE
1	A	143	VAL
1	A	156	THR
1	A	167	PHE
1	A	177	LEU
1	A	180	ASN
1	A	239	LEU
1	A	259	THR
1	A	316	ARG
1	A	379	LYS
1	A	451	THR
1	A	466	SER
1	A	467	ARG
1	A	472	VAL
1	A	478	THR
1	A	480	ASN
1	A	514	LEU
1	A	518	ILE
1	A	519	ASN
1	A	547	LEU
1	A	549	LEU
1	A	558	THR
1	A	567[A]	GLU
1	A	567[B]	GLU
1	A	570	ILE
1	A	606	THR
1	A	610	LYS
1	A	636	GLN
1	A	654	THR
1	A	655	THR
1	A	674	LEU
1	A	703	GLN
1	A	707	THR
1	A	738	VAL
1	A	747	GLN
1	A	792	ARG
1	A	793	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	187	ASN
1	A	200	ASN
1	A	288	GLN
1	A	361	ASN
1	A	374	GLN
1	A	417	ASN
1	A	437	GLN
1	A	446	ASN
1	A	480	ASN
1	A	519	ASN
1	A	551	ASN
1	A	614	ASN
1	A	636	GLN
1	A	644	ASN
1	A	661	ASN
1	A	668	ASN
1	A	703	GLN
1	A	747	GLN
1	A	816	HIS
1	A	834	GLN

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, 3 are 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

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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	ATP	A	856	3	24,33,33	1.04	1 (4%)	31,52,52	1.87	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
4	ATP	A	856	3	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	856	ATP	C5-C4	3.37	1.48	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	856	ATP	N3-C2-N1	-6.80	123.69	128.89
4	A	856	ATP	PA-O3A-PB	-3.25	123.60	132.73
4	A	856	ATP	C4-C5-N7	-3.19	106.55	109.48
4	A	856	ATP	C2'-C1'-N9	-2.92	109.83	114.29
4	A	856	ATP	PB-O3B-PG	-2.66	123.75	132.67

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 (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	767/772 (99%)	0.65	92 (11%)	6	9	12, 42, 96, 155	3 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ASN	8.8
1	A	319	VAL	4.9
1	A	293	LEU	4.9
1	A	269	ILE	4.7
1	A	690	TRP	4.7
1	A	292	ILE	4.4
1	A	302	LEU	4.4
1	A	249	LEU	4.3
1	A	348	ILE	4.2
1	A	320	LEU	4.2
1	A	272	CYS	3.8
1	A	268	TRP	3.8
1	A	386	LEU	3.7
1	A	107	VAL	3.6
1	A	92	LEU	3.5
1	A	349	ASN	3.5
1	A	321	SER	3.5
1	A	204	LEU	3.4
1	A	322	ASN	3.4
1	A	384	SER	3.3
1	A	786	TYR	3.3
1	A	229	ILE	3.3
1	A	232	ILE	3.2
1	A	199	GLY	3.2
1	A	271	ASN	3.2
1	A	415	VAL	3.2
1	A	173	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	416	ILE	3.1
1	A	294	ASN	3.1
1	A	387	VAL	3.0
1	A	254	LEU	3.0
1	A	382	VAL	2.9
1	A	124	PHE	2.8
1	A	145	ARG	2.8
1	A	783	ASN	2.8
1	A	290	ILE	2.8
1	A	103	PHE	2.8
1	A	192	LEU	2.7
1	A	746	TRP	2.7
1	A	267	ILE	2.7
1	A	323	ASN	2.7
1	A	230	ARG	2.7
1	A	448	VAL	2.6
1	A	350	GLY	2.6
1	A	347	SER	2.5
1	A	227	VAL	2.5
1	A	126	LYS	2.5
1	A	723	LYS	2.5
1	A	181	GLU	2.5
1	A	206	GLN	2.5
1	A	383	ALA	2.5
1	A	291	ASN	2.5
1	A	99	GLU	2.5
1	A	211	ILE	2.5
1	A	89	PHE	2.4
1	A	445	LEU	2.4
1	A	168	MET	2.4
1	A	303	THR	2.4
1	A	687	GLY	2.4
1	A	261	PRO	2.4
1	A	782	PRO	2.4
1	A	296	TYR	2.4
1	A	365	ILE	2.3
1	A	419	LEU	2.3
1	A	477	VAL	2.3
1	A	691	SER	2.3
1	A	129	GLU	2.3
1	A	228	TYR	2.2
1	A	332	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	762	GLU	2.2
1	A	94	ILE	2.2
1	A	128	ILE	2.2
1	A	295	CYS	2.2
1	A	780	PHE	2.2
1	A	689	THR	2.1
1	A	785	ASN	2.1
1	A	97	ILE	2.1
1	A	381	ILE	2.1
1	A	100	LEU	2.1
1	A	270	GLU	2.1
1	A	239	LEU	2.1
1	A	339	ASP	2.1
1	A	311	ILE	2.1
1	A	793	ARG	2.1
1	A	787	ILE	2.1
1	A	352	MET	2.1
1	A	231	ASP	2.0
1	A	167	PHE	2.0
1	A	135	TYR	2.0
1	A	715	LYS	2.0
1	A	351	HIS	2.0
1	A	110	TYR	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(Å²)	Q<0.9
4	ATP	A	856	31/31	0.85	0.27	1.48	49,59,60,62	0
3	MG	A	857	1/1	0.87	0.07	-2.11	47,47,47,47	0
2	CA	A	1	1/1	0.90	0.04	-3.63	49,49,49,49	0
3	MG	A	855	1/1	0.96	0.09	-	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.