Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2016 – 02:57 PM EDT

PDB ID	:	4QEI
Title	:	Two distinct conformational states of GlyRS captured in crystal lattice
Authors	:	Xie, W.; Qin, X.; Deng, X.; Zhang, Q.; Li, Q.
Deposited on	:	2014-05-16
Resolution	:	2.88 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

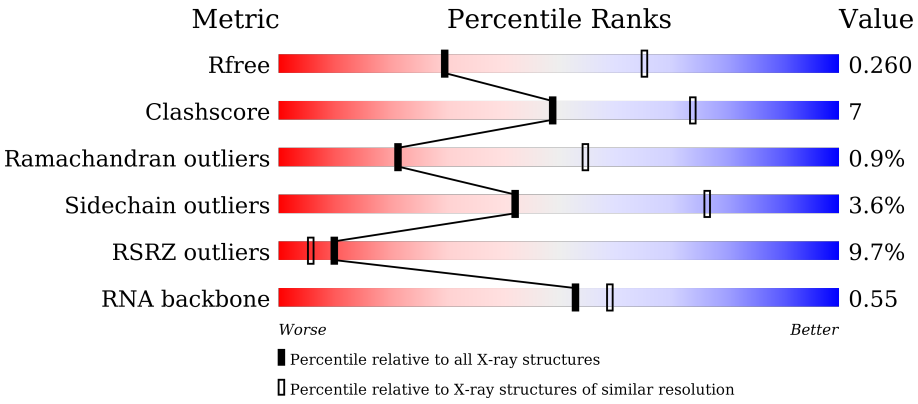
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)
RNA backbone	2183	1033 (3.26-2.50)

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	630	9% 71% 17% • 11%
2	C	69	3% 58% 33% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5764 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 Glycine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4232	2691	738	781	22			

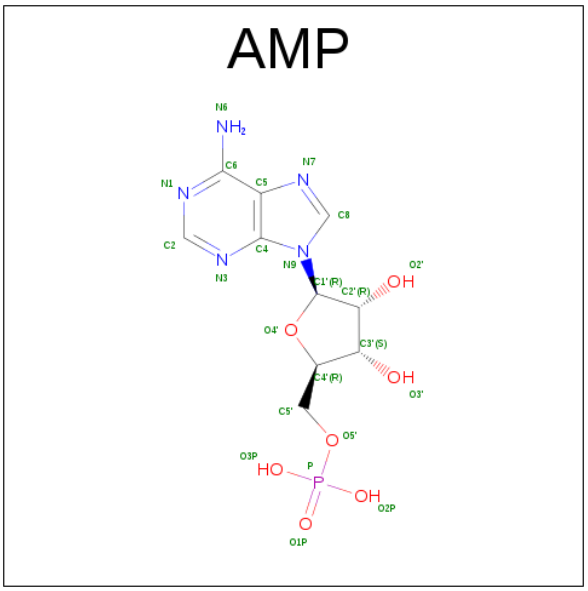
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	GLY	GLU	ENGINEERED MUTATION	UNP P41250
A	157	ARG	CYS	ENGINEERED MUTATION	UNP P41250
A	686	LEU	-	EXPRESSION TAG	UNP P41250
A	687	GLU	-	EXPRESSION TAG	UNP P41250
A	688	HIS	-	EXPRESSION TAG	UNP P41250
A	689	HIS	-	EXPRESSION TAG	UNP P41250
A	690	HIS	-	EXPRESSION TAG	UNP P41250
A	691	HIS	-	EXPRESSION TAG	UNP P41250
A	692	HIS	-	EXPRESSION TAG	UNP P41250
A	693	HIS	-	EXPRESSION TAG	UNP P41250

- Molecule 2 is a RNA chain called tRNA-Gly-CCC-2-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	69	Total	C	N	O	P	0	0	0
			1476	653	254	498	71			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

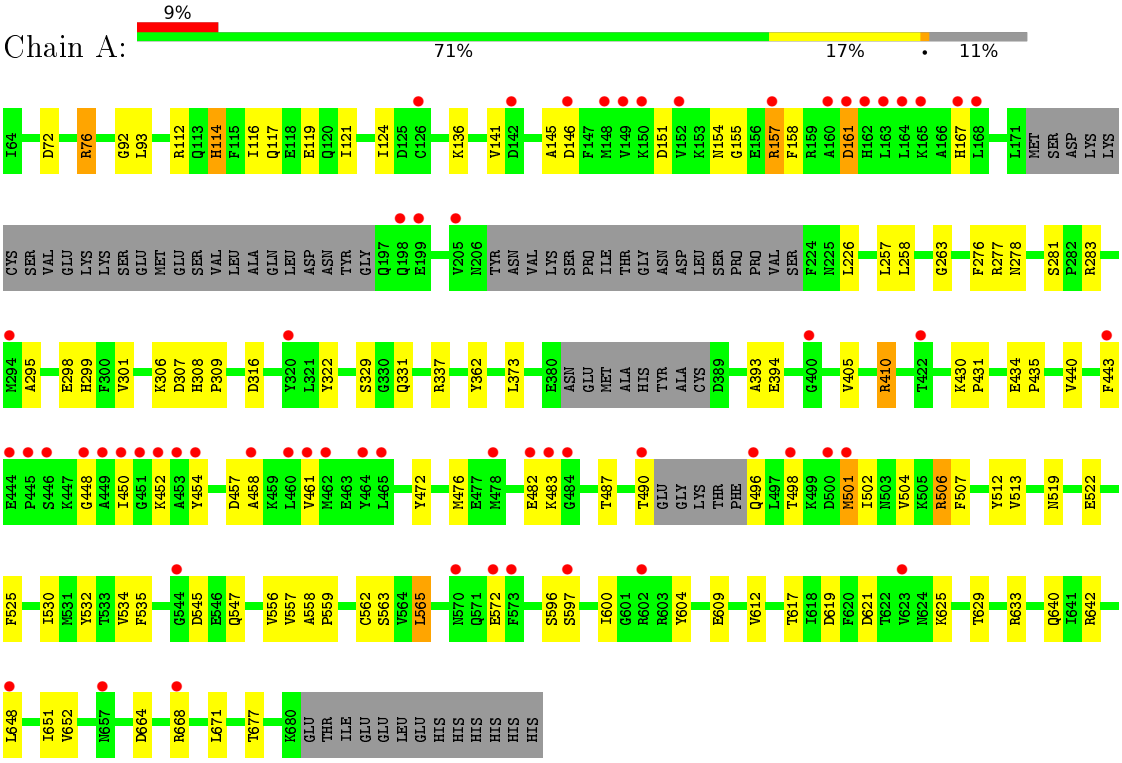
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	C	9	Total	O	0	0
			9	9		

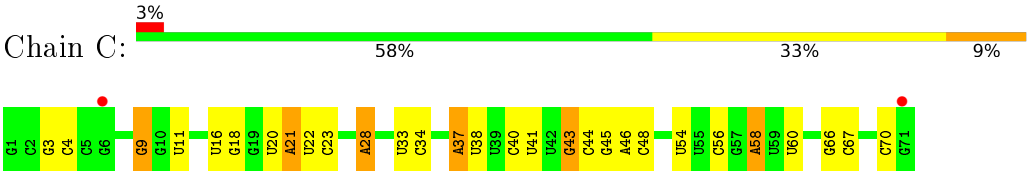
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Glycine–tRNA ligase



- Molecule 2: tRNA-Gly-CCC-2-2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.60Å 88.45Å 81.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.90 – 2.88 36.90 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.90-2.88) 97.7 (36.90-2.87)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.213 , 0.265 0.210 , 0.260	Depositor DCC
R_{free} test set	1126 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	1.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 22296 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5764	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.61	0/4322	0.89	2/5861 (0.0%)
2	C	0.65	0/1610	1.28	11/2507 (0.4%)
All	All	0.62	0/5932	1.02	13/8368 (0.2%)

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
1	A	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	GLU	N-CA-C	-8.54	87.94	111.00
2	C	21	A	C8-N9-C4	-8.49	102.40	105.80
2	C	21	A	N9-C4-C5	7.68	108.87	105.80
2	C	21	A	N1-C6-N6	-7.33	114.20	118.60
2	C	28	A	N1-C6-N6	-6.83	114.50	118.60
2	C	70	C	C6-N1-C2	-6.57	117.67	120.30
2	C	43	G	O5'-P-OP2	-6.51	99.84	105.70
2	C	34	C	C6-N1-C2	-5.84	117.96	120.30
2	C	58	A	N7-C8-N9	5.75	116.67	113.80
2	C	28	A	N9-C4-C5	5.50	108.00	105.80
2	C	21	A	C5-C6-N6	5.30	127.94	123.70
2	C	33	U	N3-C2-O2	-5.12	118.61	122.20
1	A	504	VAL	N-CA-C	-5.12	97.18	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ARG	Mainchain

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	4232	0	3955	63	0
2	C	1476	0	743	14	0
3	A	23	0	12	0	0
4	A	24	0	0	1	0
4	C	9	0	0	1	0
All	All	5764	0	4710	75	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 (75) 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)
2:C:54:U:H3	2:C:58:A:H2	1.21	0.86
1:A:112:ARG:HD2	4:A:807:HOH:O	1.84	0.75
1:A:155:GLY:O	1:A:157:ARG:NH1	2.24	0.70
1:A:664:ASP:HB3	1:A:668:ARG:NH2	2.10	0.67
1:A:498:THR:HG21	1:A:502:ILE:HG13	1.76	0.66
1:A:431:PRO:HA	1:A:513:VAL:HG12	1.78	0.66
1:A:393:ALA:HB3	1:A:405:VAL:HB	1.79	0.65
1:A:298:GLU:OE2	1:A:522:GLU:HG3	1.96	0.64
1:A:410:ARG:NH1	1:A:522:GLU:OE1	2.31	0.64
1:A:600:ILE:HG13	1:A:604:TYR:CE1	2.38	0.59
1:A:76:ARG:NH2	1:A:609:GLU:OE2	2.28	0.59
1:A:621:ASP:OD2	1:A:677:THR:OG1	2.16	0.59
1:A:664:ASP:O	1:A:668:ARG:HG3	2.02	0.59
1:A:619:ASP:OD2	1:A:642:ARG:NH2	2.37	0.58
1:A:295:ALA:HB3	1:A:525:PHE:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:TYR:HB2	1:A:458:ALA:HB2	1.89	0.55
1:A:450:ILE:HG22	1:A:458:ALA:HB1	1.90	0.54
1:A:556:VAL:HG23	1:A:557:VAL:HG13	1.88	0.54
1:A:458:ALA:HA	1:A:461:VAL:HB	1.90	0.53
1:A:226:LEU:O	1:A:278:ASN:N	2.41	0.52
1:A:72:ASP:O	1:A:76:ARG:HB2	2.08	0.52
1:A:151:ASP:HB3	1:A:154:ASN:O	2.08	0.52
1:A:648:LEU:HD23	1:A:651:ILE:HD12	1.92	0.52
2:C:9:G:H5"	4:C:201:HOH:O	2.10	0.50
1:A:487:THR:HG23	1:A:496:GLN:C	2.32	0.50
1:A:316:ASP:OD1	1:A:337:ARG:NH1	2.43	0.49
1:A:114:HIS:CD2	1:A:362:TYR:HB2	2.48	0.49
1:A:596:SER:OG	1:A:597:SER:N	2.46	0.49
1:A:299:HIS:CD2	1:A:301:VAL:HG22	2.48	0.48
1:A:329:SER:OG	1:A:331:GLN:NE2	2.37	0.48
1:A:532:TYR:O	1:A:535:PHE:HB2	2.14	0.47
1:A:158:PHE:CB	1:A:161:ASP:HB2	2.44	0.47
1:A:116:ILE:HA	1:A:121:ILE:HB	1.96	0.47
1:A:440:VAL:O	1:A:506:ARG:HA	2.15	0.47
1:A:141:VAL:O	1:A:145:ALA:HB3	2.15	0.46
1:A:448:GLY:O	1:A:452:LYS:HG3	2.16	0.46
1:A:565:LEU:O	1:A:617:THR:HA	2.15	0.46
1:A:558:ALA:HA	1:A:559:PRO:HD3	1.73	0.46
1:A:124:ILE:HG21	1:A:257:LEU:HD21	1.98	0.46
1:A:562:CYS:HB2	1:A:652:VAL:HG11	1.97	0.46
1:A:633:ARG:HB2	1:A:640:GLN:HE21	1.81	0.45
1:A:498:THR:HA	1:A:501:MET:HE2	1.99	0.45
1:A:472:TYR:O	1:A:476:MET:HG2	2.16	0.45
1:A:454:TYR:HB3	1:A:457:ASP:CB	2.47	0.45
2:C:44:C:O2'	2:C:45:G:H5'	2.17	0.45
1:A:430:LYS:HA	1:A:431:PRO:HD3	1.62	0.45
1:A:547:GLN:HB3	2:C:37:A:N7	2.32	0.44
2:C:58:A:H8	2:C:60:U:C6	2.36	0.44
1:A:633:ARG:HB2	1:A:640:GLN:HG2	1.99	0.44
1:A:530:ILE:O	1:A:534:VAL:HG23	2.18	0.44
1:A:119:GLU:HB2	1:A:121:ILE:HG13	1.99	0.43
1:A:276:PHE:C	1:A:277:ARG:HG2	2.38	0.43
1:A:629:THR:O	1:A:642:ARG:NH1	2.51	0.43
2:C:22:U:H2'	2:C:23:C:C6	2.54	0.43
1:A:92:GLY:O	1:A:93:LEU:HD23	2.19	0.43
2:C:58:A:H8	2:C:60:U:C5	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:THR:HG21	1:A:502:ILE:CG1	2.46	0.43
2:C:40:C:H2'	2:C:41:U:C6	2.54	0.43
1:A:512:TYR:CD2	1:A:512:TYR:N	2.87	0.42
2:C:21:A:H61	2:C:46:A:H2'	1.84	0.42
1:A:306:LYS:HE3	1:A:519:ASN:HD22	1.84	0.41
1:A:373:LEU:HD12	1:A:394:GLU:O	2.20	0.41
1:A:563:SER:HB3	1:A:612:VAL:HG11	2.03	0.41
1:A:671:LEU:N	1:A:671:LEU:HD12	2.35	0.41
2:C:16:U:H2'	2:C:60:U:O2	2.21	0.41
1:A:308:HIS:HA	1:A:309:PRO:HD2	1.88	0.41
1:A:506:ARG:O	1:A:507:PHE:HB3	2.21	0.41
2:C:66:G:C6	2:C:67:C:C4	3.09	0.41
1:A:434:GLU:HA	1:A:435:PRO:HD2	1.84	0.41
1:A:619:ASP:CG	1:A:642:ARG:HH22	2.23	0.41
2:C:28:A:C2	2:C:43:G:C4	3.09	0.41
2:C:3:G:H2'	2:C:4:C:C6	2.56	0.41
1:A:72:ASP:OD1	2:C:11:U:O2'	2.36	0.40
1:A:136:LYS:HB2	1:A:136:LYS:HE2	1.89	0.40
1:A:258:LEU:HG	1:A:263:GLY:HA2	2.02	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	552/630 (88%)	515 (93%)	32 (6%)	5 (1%)	21 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	114	HIS

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Mol	Chain	Res	Type
1	A	146	ASP
1	A	545	ASP
1	A	483	LYS

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	415/549 (76%)	400 (96%)	15 (4%)	42 76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	117	GLN
1	A	157	ARG
1	A	161	ASP
1	A	281	SER
1	A	307	ASP
1	A	322	TYR
1	A	410	ARG
1	A	443	PHE
1	A	490	THR
1	A	501	MET
1	A	506	ARG
1	A	565	LEU
1	A	572	GLU
1	A	625	LYS

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	481	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	67/69 (97%)	7 (10%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	9	G
2	C	18	G
2	C	20	U
2	C	37	A
2	C	38	U
2	C	48	C
2	C	56	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	GTP	C	1	2	26,34,34	2.65	10 (38%)	29,54,54	1.78	7 (24%)

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	GTP	C	1	2	-	0/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GTP	C8-N7	-5.29	1.24	1.34
2	C	1	GTP	C2'-C3'	-4.89	1.40	1.53
2	C	1	GTP	C2'-C1'	-3.33	1.48	1.53
2	C	1	GTP	O4'-C4'	-2.86	1.38	1.45
2	C	1	GTP	O3'-C3'	-2.27	1.37	1.43
2	C	1	GTP	PB-O2B	-2.13	1.46	1.55
2	C	1	GTP	C3'-C4'	-2.08	1.47	1.53
2	C	1	GTP	C5-C4	3.26	1.47	1.40
2	C	1	GTP	C2-N2	5.04	1.44	1.34
2	C	1	GTP	O6-C6	6.81	1.41	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GTP	N3-C2-N1	-3.87	122.29	127.56
2	C	1	GTP	C5-C6-N1	-3.37	119.12	123.52
2	C	1	GTP	C1'-N9-C4	-2.87	123.60	126.81
2	C	1	GTP	C6-C5-C4	-2.21	118.33	120.86
2	C	1	GTP	O2A-PA-O3A	2.12	114.35	105.27
2	C	1	GTP	O5'-C5'-C4'	2.96	119.78	109.09
2	C	1	GTP	C6-N1-C2	4.27	120.89	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
3	AMP	A	701	-	22,25,25	0.95	1 (4%)	22,38,38	1.69	3 (13%)

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	AMP	A	701	-	-	0/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	AMP	C5-C4	3.20	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	AMP	N3-C2-N1	-5.72	124.38	128.87
3	A	701	AMP	C1'-N9-C4	-2.25	124.30	126.81
3	A	701	AMP	N6-C6-N1	2.71	123.06	118.52

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	562/630 (89%)	0.74	59 (10%) 8 5	32, 53, 112, 128	0
2	C	68/69 (98%)	0.62	2 (2%) 55 50	44, 68, 122, 134	0
All	All	630/699 (90%)	0.73	61 (9%) 10 6	32, 55, 113, 134	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	LEU	9.5
1	A	444	GLU	6.8
1	A	165	LYS	6.2
1	A	443	PHE	6.1
1	A	483	LYS	5.4
1	A	449	ALA	5.0
1	A	501	MET	4.7
1	A	157	ARG	4.7
1	A	464	TYR	4.7
1	A	458	ALA	4.3
1	A	445	PRO	4.3
1	A	452	LYS	4.2
1	A	167	HIS	4.1
1	A	149	VAL	4.1
1	A	148	MET	4.0
1	A	162	HIS	4.0
1	A	460	LEU	4.0
1	A	161	ASP	3.9
1	A	446	SER	3.9
1	A	453	ALA	3.6
1	A	146	ASP	3.4
1	A	448	GLY	3.4
1	A	478	MET	3.3
1	A	623	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	3.2
1	A	168	LEU	3.2
1	A	461	VAL	3.2
1	A	484	GLY	3.2
1	A	199	GLU	3.1
1	A	160	ALA	3.1
1	A	198	GLN	3.1
1	A	668	ARG	3.0
1	A	657	ASN	3.0
1	A	152	VAL	3.0
1	A	544	GLY	2.9
1	A	150	LYS	2.9
1	A	451	GLY	2.8
2	C	6	G	2.7
1	A	462	MET	2.7
1	A	648	LEU	2.6
1	A	482	GLU	2.5
1	A	294	MET	2.5
1	A	498	THR	2.5
1	A	142	ASP	2.5
2	C	71	G	2.5
1	A	573	PHE	2.4
1	A	320	TYR	2.4
1	A	597	SER	2.4
1	A	602	ARG	2.3
1	A	454	TYR	2.3
1	A	500	ASP	2.3
1	A	450	ILE	2.3
1	A	465	LEU	2.2
1	A	570	ASN	2.2
1	A	205	VAL	2.2
1	A	126	CYS	2.2
1	A	496	GLN	2.1
1	A	400	GLY	2.0
1	A	490	THR	2.0
1	A	572	GLU	2.0
1	A	422	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
2	GTP	C	1	32/32	0.78	0.31	1.36	86,113,121,124	0

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, 95^{th} 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	AMP	A	701	23/23	0.93	0.16	-1.81	36,44,52,64	0

6.5 Other polymers (i)

There are no such residues in this entry.