



wwPDB X-ray Structure Validation Summary Report i

Nov 20, 2014 – 06:42 PM EST

PDB ID : 4V0N
Title : Crystal structure of BBS1N in complex with ARL6DN, soaked with mercury
Authors : Mourao, A.; Lorentzen, E.
Deposited on : 2014-09-17
Resolution : 3.13 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

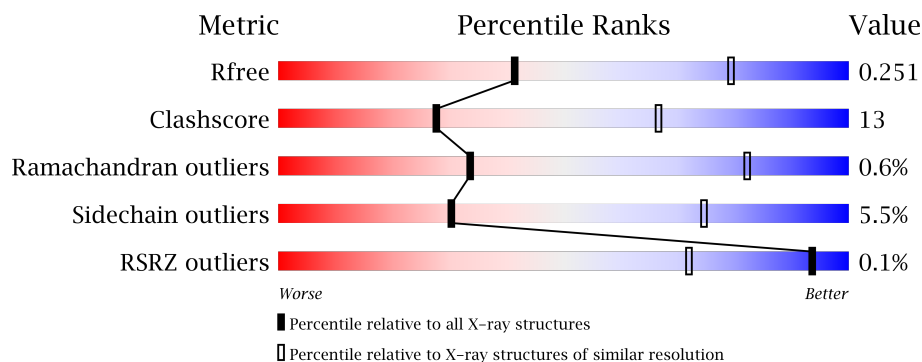
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24195
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 3.13 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}	66092	1337 (3.20-3.08)
Clashscore	79885	1656 (3.20-3.08)
Ramachandran outliers	78287	1614 (3.20-3.08)
Sidechain outliers	78261	1613 (3.20-3.08)
RSRZ outliers	66119	1338 (3.20-3.08)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	169	
1	C	169	
1	E	169	
1	G	169	
2	B	425	
2	D	425	
2	F	425	
2	H	425	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	601	-	X
4	MG	C	601	-	X
5	HG	B	1426	-	X
5	HG	B	1431	-	X
5	HG	B	1432	-	X
5	HG	B	1435	-	X
5	HG	B	1437	-	X
5	HG	F	1430	-	X
5	HG	H	1434	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14532 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ARF-LIKE SMALL GTPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1263	807	215	235	6			
1	C	166	Total	C	N	O	S	0	0	0
			1287	820	222	239	6			
1	E	166	Total	C	N	O	S	0	0	0
			1282	819	220	237	6			
1	G	166	Total	C	N	O	S	0	0	0
			1286	822	221	237	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	EXPRESSION TAG	UNP A8JF99
A	13	ALA	-	EXPRESSION TAG	UNP A8JF99
A	14	ALA	-	EXPRESSION TAG	UNP A8JF99
A	15	SER	-	EXPRESSION TAG	UNP A8JF99
C	12	GLY	-	EXPRESSION TAG	UNP A8JF99
C	13	ALA	-	EXPRESSION TAG	UNP A8JF99
C	14	ALA	-	EXPRESSION TAG	UNP A8JF99
C	15	SER	-	EXPRESSION TAG	UNP A8JF99
E	12	GLY	-	EXPRESSION TAG	UNP A8JF99
E	13	ALA	-	EXPRESSION TAG	UNP A8JF99
E	14	ALA	-	EXPRESSION TAG	UNP A8JF99
E	15	SER	-	EXPRESSION TAG	UNP A8JF99
G	12	GLY	-	EXPRESSION TAG	UNP A8JF99
G	13	ALA	-	EXPRESSION TAG	UNP A8JF99
G	14	ALA	-	EXPRESSION TAG	UNP A8JF99
G	15	SER	-	EXPRESSION TAG	UNP A8JF99

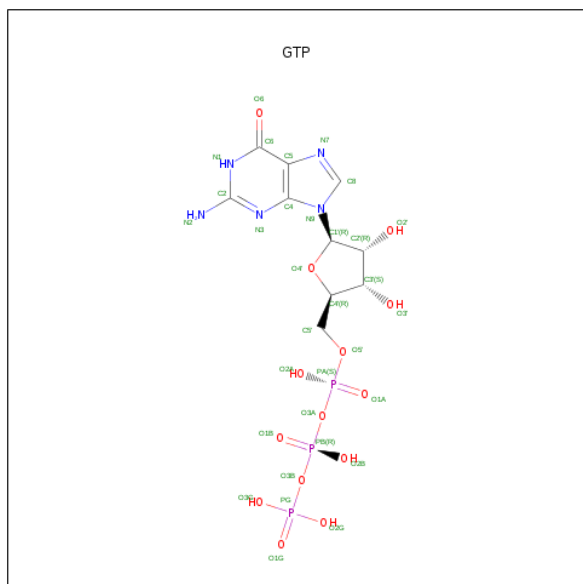
- Molecule 2 is a protein called BARDET-BIEDL SYNDROME 1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2442	1561	423	445	13			
2	D	304	Total	C	N	O	S	0	0	0
			2197	1399	383	403	12			
2	F	304	Total	C	N	O	S	0	0	0
			2200	1405	379	403	13			
2	H	325	Total	C	N	O	S	0	0	0
			2386	1526	410	437	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ARG	LYS	CONFLICT	UNP A8JEA1
D	37	ARG	LYS	CONFLICT	UNP A8JEA1
F	37	ARG	LYS	CONFLICT	UNP A8JEA1
H	37	ARG	LYS	CONFLICT	UNP A8JEA1

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

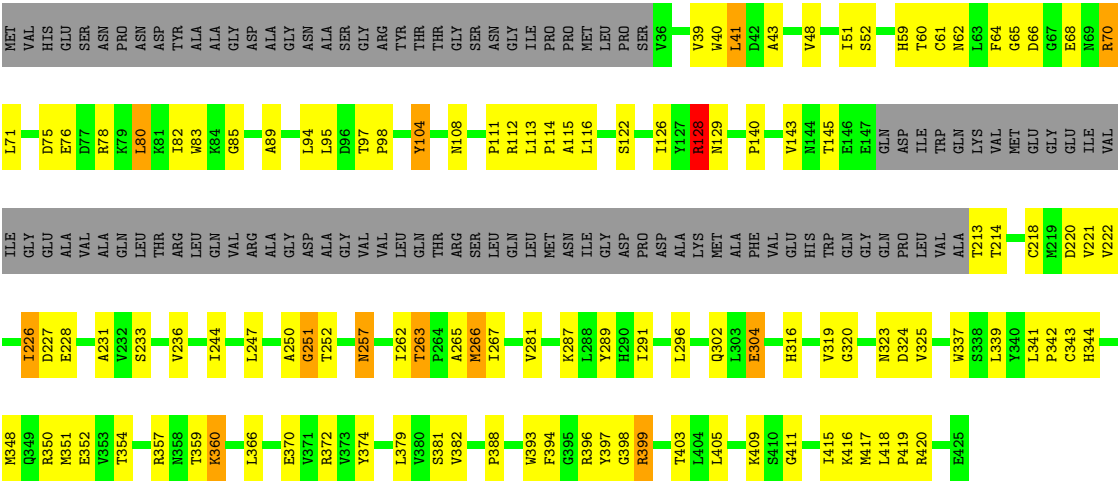
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Hg	0	0
			1	1		
5	D	12	Total	Hg	0	0
			12	12		
5	E	1	Total	Hg	0	0
			1	1		
5	H	14	Total	Hg	0	0
			14	14		
5	B	13	Total	Hg	0	0
			13	13		
5	C	1	Total	Hg	0	0
			1	1		
5	A	1	Total	Hg	0	0
			1	1		
5	F	14	Total	Hg	0	0
			14	14		

● Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.75Å 123.75Å 443.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	96.50 – 3.13 96.50 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.0 (96.50-3.13) 99.3 (96.50-3.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.13Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.249 0.213 , 0.251	Depositor DCC
R_{free} test set	3508 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	104.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.0	EDS
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 70045 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14532	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 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.44	0/1289	0.62	0/1755
1	C	0.59	0/1313	0.75	0/1784
1	E	0.62	0/1308	0.77	0/1777
1	G	0.46	0/1312	0.65	0/1781
2	B	0.54	0/2494	0.76	1/3412 (0.0%)
2	D	0.44	0/2240	0.66	0/3066
2	F	0.47	0/2244	0.68	0/3071
2	H	0.54	0/2437	0.79	3/3339 (0.1%)
All	All	0.51	0/14637	0.72	4/19985 (0.0%)

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	H	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	LEU	CA-CB-CG	6.97	131.34	115.30
2	B	80	LEU	CA-CB-CG	6.23	129.62	115.30
2	H	41	LEU	CA-CB-CG	5.71	128.44	115.30
2	H	128	ARG	N-CA-C	-5.20	96.96	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	226	ILE	Peptide
2	H	145	THR	Peptide
2	H	226	ILE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1263	0	1241	22	0
1	C	1287	0	1285	31	0
1	E	1282	0	1283	37	0
1	G	1286	0	1294	31	0
2	B	2442	0	2400	70	0
2	D	2197	0	2087	60	0
2	F	2200	0	2111	57	0
2	H	2386	0	2324	83	0
3	A	32	0	12	2	0
3	C	32	0	12	3	0
3	E	32	0	12	2	0
3	G	32	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	B	13	0	0	0	0
5	C	1	0	0	0	0
5	D	12	0	0	0	0
5	E	1	0	0	0	0
5	F	14	0	0	0	0
5	G	1	0	0	0	0
5	H	14	0	0	0	0
All	All	14532	0	14073	365	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 365 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:350:ARG:NH2	2:B:352:GLU:OE1	2.12	0.81
2:H:350:ARG:NH2	2:H:352:GLU:OE1	2.19	0.76
2:B:39:VAL:HG13	2:B:381:SER:HB2	1.67	0.76
1:E:101:ARG:NH1	2:F:399:ARG:HB2	2.01	0.75
2:D:247:LEU:HD22	2:D:254:ILE:HA	1.68	0.75

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	164/169 (97%)	155 (94%)	9 (6%)	0	100	100
1	C	164/169 (97%)	158 (96%)	6 (4%)	0	100	100
1	E	164/169 (97%)	155 (94%)	9 (6%)	0	100	100
1	G	164/169 (97%)	154 (94%)	10 (6%)	0	100	100
2	B	326/425 (77%)	290 (89%)	32 (10%)	4 (1%)	19	68
2	D	294/425 (69%)	269 (92%)	24 (8%)	1 (0%)	50	90
2	F	296/425 (70%)	271 (92%)	23 (8%)	2 (1%)	30	79
2	H	321/425 (76%)	288 (90%)	28 (9%)	5 (2%)	14	61
All	All	1893/2376 (80%)	1740 (92%)	141 (7%)	12 (1%)	33	82

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	65	GLY
2	B	113	LEU
2	B	130	LEU
2	F	65	GLY

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Mol	Chain	Res	Type
2	D	65	GLY

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	131/142 (92%)	129 (98%)	2 (2%)	76	95
1	C	137/142 (96%)	131 (96%)	6 (4%)	39	81
1	E	136/142 (96%)	129 (95%)	7 (5%)	33	77
1	G	137/142 (96%)	137 (100%)	0	100	100
2	B	250/352 (71%)	232 (93%)	18 (7%)	21	63
2	D	214/352 (61%)	202 (94%)	12 (6%)	30	74
2	F	218/352 (62%)	205 (94%)	13 (6%)	27	71
2	H	242/352 (69%)	219 (90%)	23 (10%)	12	45
All	All	1465/1976 (74%)	1384 (94%)	81 (6%)	30	74

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	356	GLN
2	F	59	HIS
2	H	304	GLU
2	D	421	THR
1	E	75	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	356	GLN
2	F	69	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 65 ligands modelled in this entry, 61 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	GTP	A	600	4	34,34,34	1.09	1 (2%)	52,54,54	2.20	9 (17%)
3	GTP	C	600	4	34,34,34	1.16	2 (5%)	52,54,54	2.51	10 (19%)
3	GTP	E	600	4	34,34,34	1.12	1 (2%)	52,54,54	1.73	12 (23%)
3	GTP	G	600	4	34,34,34	1.10	1 (2%)	52,54,54	2.17	10 (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
3	GTP	A	600	4	-	0/22/38/38	0/3/3/3
3	GTP	C	600	4	-	0/22/38/38	0/3/3/3
3	GTP	E	600	4	-	0/22/38/38	0/3/3/3
3	GTP	G	600	4	-	0/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	600	GTP	C2-N3	4.31	1.38	1.33
3	A	600	GTP	C2-N3	4.25	1.38	1.33
3	G	600	GTP	C2-N3	4.07	1.38	1.33
3	C	600	GTP	C2-N3	3.78	1.38	1.33
3	C	600	GTP	C5-N7	-2.34	1.35	1.38

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	600	GTP	C6-C5-N7	-12.43	132.47	134.14
3	A	600	GTP	C6-C5-N7	-11.07	132.65	134.14
3	G	600	GTP	C6-C5-N7	-10.71	132.70	134.14
3	C	600	GTP	PA-O3A-PB	-5.36	117.08	131.93
3	A	600	GTP	PA-O3A-PB	-4.84	118.54	131.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	166/169 (98%)	0.02	0	100 100	37, 62, 88, 105	0
1	C	166/169 (98%)	-0.02	0	100 100	19, 31, 56, 74	0
1	E	166/169 (98%)	-0.04	0	100 100	20, 35, 68, 83	0
1	G	166/169 (98%)	0.01	0	100 100	32, 51, 70, 80	0
2	B	330/425 (77%)	0.07	0	100 100	21, 43, 77, 101	0
2	D	304/425 (71%)	-0.10	0	100 100	23, 67, 106, 118	0
2	F	304/425 (71%)	-0.07	1 (0%)	91 56	23, 66, 110, 120	0
2	H	325/425 (76%)	0.06	0	100 100	24, 44, 79, 106	0
All	All	1927/2376 (81%)	-0.01	1 (0%)	93 72	19, 48, 101, 120	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	235	LEU	2.5

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

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	HG	B	1426	1/1	0.89	10.34	38,38,38,38	1
5	HG	B	1432	1/1	0.62	9.72	69,69,69,69	1
5	HG	B	1435	1/1	1.36	8.20	40,40,40,40	1
5	HG	B	1437	1/1	0.76	6.36	39,39,39,39	1
5	HG	H	1434	1/1	0.41	3.98	79,79,79,79	1
4	MG	C	601	1/1	0.32	3.98	27,27,27,27	0
5	HG	F	1430	1/1	0.21	3.20	82,82,82,82	1
5	HG	B	1431	1/1	0.26	2.26	43,43,43,43	1
4	MG	A	601	1/1	0.25	2.08	58,58,58,58	0
5	HG	F	1439	1/1	0.20	1.90	68,68,68,68	1
4	MG	E	601	1/1	0.24	1.69	31,31,31,31	0
4	MG	G	601	1/1	0.28	1.69	45,45,45,45	0
5	HG	D	1434	1/1	0.18	1.62	80,80,80,80	1
5	HG	H	1431	1/1	0.23	1.60	43,43,43,43	1
5	HG	H	1435	1/1	0.23	1.36	42,42,42,42	1
5	HG	E	1181	1/1	0.23	1.21	51,51,51,51	1
5	HG	F	1434	1/1	0.14	1.07	113,113,113,113	1
5	HG	D	1430	1/1	0.22	0.94	98,98,98,98	1
5	HG	D	1427	1/1	0.25	0.89	85,85,85,85	1
5	HG	C	1181	1/1	0.23	0.88	53,53,53,53	1
5	HG	B	1429	1/1	0.27	0.87	64,64,64,64	1
5	HG	D	1429	1/1	0.23	0.73	82,82,82,82	1
5	HG	D	1428	1/1	0.24	0.69	96,96,96,96	1
5	HG	B	1436	1/1	0.25	0.67	51,51,51,51	1
5	HG	H	1438	1/1	0.22	0.62	60,60,60,60	1
5	HG	F	1437	1/1	0.20	0.42	122,122,122,122	1
5	HG	F	1428	1/1	0.25	0.42	102,102,102,102	1
5	HG	B	1428	1/1	0.26	0.38	61,61,61,61	1
5	HG	F	1427	1/1	0.23	0.30	66,66,66,66	1
5	HG	F	1436	1/1	0.19	0.27	73,73,73,73	1
3	GTP	C	600	32/32	0.25	0.27	27,31,37,39	0
5	HG	H	1430	1/1	0.25	0.25	62,62,62,62	1
5	HG	H	1429	1/1	0.23	0.18	68,68,68,68	1
5	HG	F	1431	1/1	0.22	0.16	108,108,108,108	1
5	HG	F	1426	1/1	0.25	0.03	57,57,57,57	1
5	HG	F	1429	1/1	0.20	0.03	78,78,78,78	1
5	HG	D	1431	1/1	0.17	0.02	109,109,109,109	1
5	HG	H	1427	1/1	0.23	-0.01	41,41,41,41	1
3	GTP	E	600	32/32	0.22	-0.06	26,32,40,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	HG	B	1427	1/1	0.25	-0.08	42,42,42,42	1
5	HG	D	1426	1/1	0.23	-0.09	63,63,63,63	1
5	HG	B	1434	1/1	0.22	-0.13	45,45,45,45	1
5	HG	H	1432	1/1	0.23	-0.15	41,41,41,41	1
5	HG	H	1426	1/1	0.26	-0.16	41,41,41,41	1
5	HG	H	1436	1/1	0.21	-0.19	46,46,46,46	1
3	GTP	A	600	32/32	0.19	-0.22	55,60,67,72	0
5	HG	F	1435	1/1	0.15	-0.26	80,80,80,80	1
5	HG	D	1435	1/1	0.17	-0.31	109,109,109,109	1
5	HG	D	1432	1/1	0.19	-0.39	62,62,62,62	1
5	HG	B	1430	1/1	0.25	-0.42	45,45,45,45	1
5	HG	B	1438	1/1	0.24	-0.42	23,23,23,23	1
3	GTP	G	600	32/32	0.20	-0.48	40,44,47,50	0
5	HG	B	1433	1/1	0.24	-0.49	48,48,48,48	1
5	HG	H	1428	1/1	0.24	-0.54	49,49,49,49	1
5	HG	D	1437	1/1	0.20	-0.65	87,87,87,87	1
5	HG	H	1437	1/1	0.22	-0.65	30,30,30,30	1
5	HG	H	1439	1/1	0.19	-0.68	41,41,41,41	1
5	HG	F	1433	1/1	0.15	-0.91	118,118,118,118	1
5	HG	F	1438	1/1	0.15	-0.95	76,76,76,76	1
5	HG	H	1433	1/1	0.18	-1.13	43,43,43,43	1
5	HG	A	1181	1/1	0.12	-1.14	54,54,54,54	1
5	HG	F	1432	1/1	0.15	-1.19	73,73,73,73	1
5	HG	D	1436	1/1	0.07	-1.88	100,100,100,100	1
5	HG	D	1433	1/1	0.12	-1.89	82,82,82,82	1
5	HG	G	1181	1/1	0.13	-2.27	50,50,50,50	1

6.5 Other polymers ⓘ

There are no such residues in this entry.