Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 PM GMT

PDB ID	:	4H1V
Title	:	GMP-PNP bound dynamin-1-like protein GTPase-GED fusion
Authors	:	Wenger, J.; Klinglmayr, E.; Eibl, C.; Hessenberger, M.; Goettig, P.
Deposited on	:	2012-09-11
Resolution	:	2.30 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 (i)

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

The reported resolution of this entry is 2.30 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		0.278
Clashscore		21
Ramachandran outliers		0.6%
Sidechain outliers		9.9%
RSRZ outliers		14.2%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
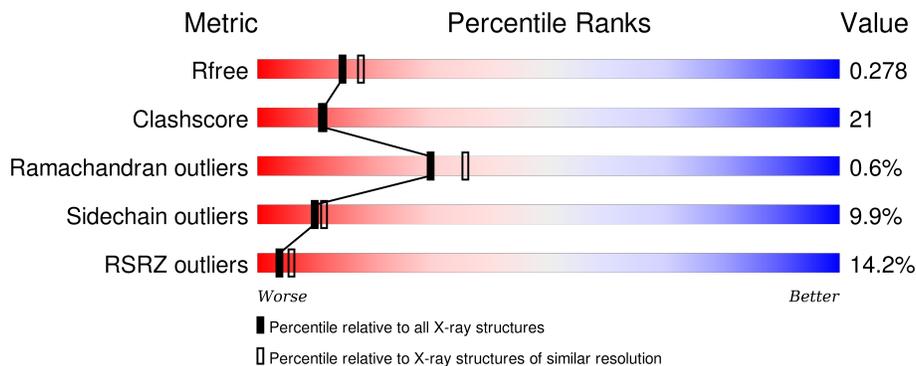
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	369	14% — 70% — 21% — 5% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2920 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 Dynamin-1-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2766	1731	489	537	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	703	GLY	-	LINKER	UNP O00429
A	704	SER	-	LINKER	UNP O00429
A	705	GLY	-	LINKER	UNP O00429
A	706	SER	-	LINKER	UNP O00429
A	707	GLY	-	LINKER	UNP O00429
A	708	SER	-	LINKER	UNP O00429
A	709	GLY	-	LINKER	UNP O00429
A	710	SER	-	LINKER	UNP O00429
A	737	LEU	-	EXPRESSION TAG	UNP O00429
A	738	GLU	-	EXPRESSION TAG	UNP O00429
A	739	HIS	-	EXPRESSION TAG	UNP O00429
A	740	HIS	-	EXPRESSION TAG	UNP O00429
A	741	HIS	-	EXPRESSION TAG	UNP O00429
A	742	HIS	-	EXPRESSION TAG	UNP O00429
A	743	HIS	-	EXPRESSION TAG	UNP O00429
A	744	HIS	-	EXPRESSION TAG	UNP O00429

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).
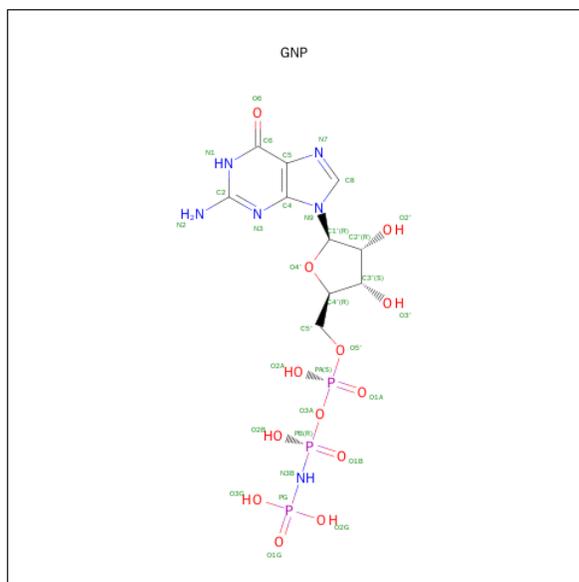
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total 122	O 122	0	0

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: Dynamin-1-like protein
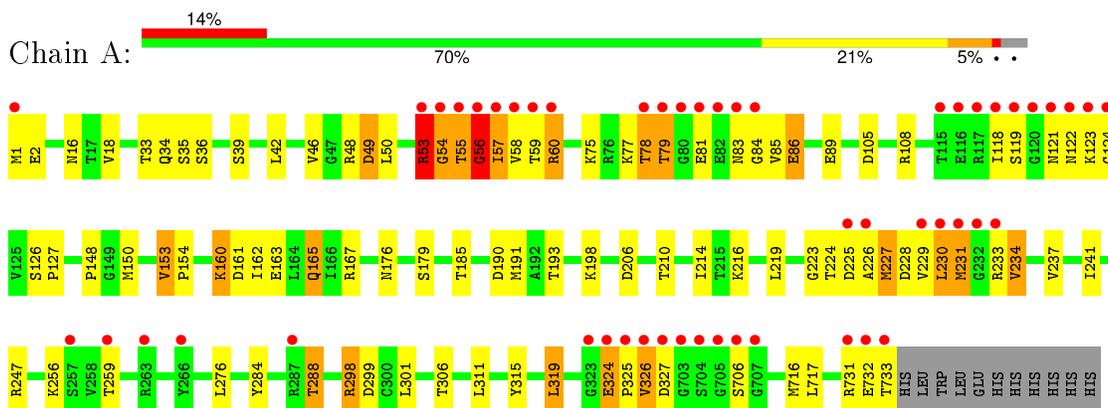
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	53.42Å 151.31Å 43.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.30 19.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.97-2.30) 97.8 (19.97-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.227 , 0.278 0.226 , 0.278	Depositor DCC
R_{free} test set	786 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	1 of 15823 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2920	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: GNP

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	0.49	0/2800	0.55	0/3789

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	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLY	Peptide
1	A	224	THR	Peptide
1	A	53	ARG	Peptide
1	A	54	GLY	Peptide
1	A	55	THR	Peptide
1	A	56	GLY	Peptide

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	2766	0	2860	116	0
2	A	32	0	13	1	0
3	A	122	0	0	2	0
All	All	2920	0	2873	117	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 21.

All (117) 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:226:ALA:HB1	1:A:229:VAL:CG2	1.62	1.27
1:A:230:LEU:HB3	1:A:276:LEU:CD2	1.69	1.20
1:A:53:ARG:HG2	1:A:54:GLY:CA	1.72	1.19
1:A:226:ALA:HB1	1:A:229:VAL:HG23	1.25	1.16
1:A:230:LEU:HB3	1:A:276:LEU:HD23	1.16	1.15
1:A:57:ILE:HD12	1:A:57:ILE:H	1.16	1.07
1:A:191:MET:HE1	1:A:229:VAL:HG21	1.42	1.01
1:A:324:GLU:CB	1:A:325:PRO:HA	1.90	0.99
1:A:77:LYS:HE2	1:A:84:GLY:CA	1.91	0.99
1:A:53:ARG:CG	1:A:54:GLY:HA3	1.94	0.97
1:A:57:ILE:CD1	1:A:57:ILE:H	1.79	0.95
1:A:53:ARG:CG	1:A:54:GLY:CA	2.45	0.95
1:A:77:LYS:CE	1:A:84:GLY:HA2	1.99	0.93
1:A:324:GLU:HB3	1:A:325:PRO:HA	1.45	0.93
1:A:191:MET:CE	1:A:229:VAL:HG21	2.00	0.91
1:A:53:ARG:HG2	1:A:54:GLY:N	1.80	0.90
1:A:230:LEU:CB	1:A:276:LEU:HD23	2.02	0.90
1:A:57:ILE:N	1:A:57:ILE:HD12	1.87	0.89
1:A:230:LEU:CB	1:A:276:LEU:CD2	2.51	0.89
1:A:226:ALA:CB	1:A:229:VAL:CG2	2.48	0.88
1:A:57:ILE:O	1:A:58:VAL:HG13	1.72	0.88
1:A:53:ARG:HG3	1:A:54:GLY:HA3	1.55	0.87
1:A:77:LYS:HE2	1:A:84:GLY:HA3	1.54	0.86
1:A:57:ILE:O	1:A:58:VAL:CG1	2.26	0.82
1:A:226:ALA:CB	1:A:229:VAL:HG23	2.09	0.82
1:A:226:ALA:HB1	1:A:229:VAL:CB	2.11	0.81
1:A:230:LEU:CD1	1:A:276:LEU:HD23	2.10	0.81
1:A:60:ARG:O	1:A:148:PRO:CG	2.28	0.81
1:A:77:LYS:HE2	1:A:84:GLY:HA2	1.58	0.78
1:A:324:GLU:HB3	1:A:325:PRO:CA	2.12	0.77
1:A:230:LEU:HD12	1:A:276:LEU:CD2	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:O	1:A:148:PRO:HG2	1.87	0.73
1:A:53:ARG:CG	1:A:54:GLY:N	2.52	0.72
1:A:324:GLU:CB	1:A:325:PRO:CA	2.69	0.71
1:A:60:ARG:O	1:A:148:PRO:HG3	1.92	0.70
1:A:247:ARG:NH1	1:A:256:LYS:O	2.23	0.70
1:A:324:GLU:CG	1:A:325:PRO:HA	2.21	0.70
1:A:325:PRO:O	1:A:326:VAL:HB	1.90	0.70
1:A:214:ILE:HG13	1:A:229:VAL:CG1	2.25	0.67
1:A:230:LEU:HB3	1:A:276:LEU:HD21	1.72	0.66
1:A:226:ALA:HB1	1:A:229:VAL:HG21	1.71	0.66
1:A:1:MET:N	1:A:732:GLU:OE1	2.26	0.65
1:A:53:ARG:HG2	1:A:54:GLY:C	2.16	0.65
1:A:160:LYS:HD2	1:A:161:ASP:N	2.11	0.65
1:A:57:ILE:C	1:A:58:VAL:HG13	2.16	0.65
1:A:214:ILE:HG13	1:A:229:VAL:HG12	1.77	0.65
1:A:191:MET:CE	1:A:229:VAL:CG2	2.76	0.64
1:A:325:PRO:HG2	1:A:327:ASP:HB2	1.80	0.64
1:A:298:ARG:NH1	1:A:299:ASP:OD1	2.31	0.64
1:A:230:LEU:CD1	1:A:276:LEU:CD2	2.74	0.63
1:A:16:ASN:HA	3:A:976:HOH:O	1.96	0.63
1:A:326:VAL:O	1:A:326:VAL:HG13	1.97	0.63
1:A:230:LEU:HD12	1:A:276:LEU:HD22	1.81	0.62
1:A:77:LYS:CE	1:A:84:GLY:CA	2.63	0.62
1:A:226:ALA:HB1	1:A:229:VAL:HB	1.82	0.61
1:A:58:VAL:O	1:A:59:THR:HG22	2.00	0.60
1:A:58:VAL:C	1:A:59:THR:HG22	2.22	0.60
1:A:56:GLY:O	1:A:58:VAL:HG13	2.02	0.60
1:A:226:ALA:CB	1:A:229:VAL:HG21	2.28	0.60
1:A:48:ARG:NH1	1:A:89:GLU:OE1	2.35	0.59
1:A:326:VAL:CG1	1:A:326:VAL:O	2.49	0.58
1:A:198:LYS:HG3	3:A:1003:HOH:O	2.03	0.58
1:A:58:VAL:O	1:A:59:THR:CG2	2.51	0.58
1:A:60:ARG:HD3	1:A:124:GLY:O	2.04	0.58
1:A:33:THR:HG22	1:A:36:SER:HB3	1.86	0.58
1:A:49:ASP:OD1	1:A:247:ARG:NH2	2.36	0.57
1:A:324:GLU:OE1	1:A:324:GLU:HA	2.05	0.57
1:A:231:MET:SD	1:A:233:ARG:NH2	2.77	0.56
1:A:731:ARG:O	1:A:731:ARG:HD2	2.05	0.56
1:A:77:LYS:NZ	1:A:84:GLY:HA2	2.22	0.55
1:A:153:VAL:HG22	1:A:154:PRO:HD2	1.90	0.54
2:A:801:GNP:H8	2:A:801:GNP:H5'2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG11	1:A:50:LEU:HD23	1.89	0.53
1:A:230:LEU:HD13	1:A:276:LEU:HD23	1.89	0.52
1:A:176:ASN:HB3	1:A:179:SER:HB3	1.92	0.52
1:A:229:VAL:O	1:A:241:ILE:HG21	2.10	0.51
1:A:77:LYS:CD	1:A:84:GLY:HA2	2.40	0.51
1:A:78:THR:HG22	1:A:85:VAL:O	2.11	0.51
1:A:325:PRO:HG2	1:A:327:ASP:CB	2.41	0.51
1:A:34:GLN:N	1:A:150:MET:O	2.41	0.47
1:A:190:ASP:OD2	1:A:193:THR:HG23	2.14	0.47
1:A:57:ILE:O	1:A:58:VAL:HG12	2.12	0.47
1:A:163:GLU:O	1:A:167:ARG:HG2	2.14	0.47
1:A:53:ARG:HD3	1:A:55:THR:H	1.81	0.46
1:A:165:GLN:O	1:A:165:GLN:HG3	2.15	0.46
1:A:59:THR:O	1:A:59:THR:OG1	2.31	0.46
1:A:731:ARG:O	1:A:731:ARG:CG	2.64	0.46
1:A:324:GLU:CD	1:A:325:PRO:HA	2.37	0.45
1:A:225:ASP:OD1	1:A:227:MET:SD	2.74	0.45
1:A:225:ASP:OD1	1:A:227:MET:HB2	2.16	0.45
1:A:214:ILE:HG21	1:A:229:VAL:HG11	1.99	0.45
1:A:105:ASP:OD1	1:A:108:ARG:NH2	2.49	0.45
1:A:56:GLY:O	1:A:57:ILE:O	2.34	0.44
1:A:284:TYR:O	1:A:288:THR:HG23	2.18	0.44
1:A:79:THR:HB	1:A:81:GLU:HB2	2.00	0.44
1:A:58:VAL:HG23	1:A:59:THR:HG22	2.00	0.44
1:A:228:ASP:HB3	1:A:234:VAL:CG1	2.48	0.44
1:A:226:ALA:CB	1:A:229:VAL:HB	2.47	0.43
1:A:58:VAL:C	1:A:59:THR:CG2	2.86	0.43
1:A:81:GLU:OE1	1:A:83:ASN:ND2	2.52	0.43
1:A:33:THR:HG23	1:A:34:GLN:O	2.19	0.42
1:A:75:LYS:HB2	1:A:86:GLU:HG2	2.00	0.42
1:A:160:LYS:C	1:A:160:LYS:HD2	2.37	0.42
1:A:731:ARG:O	1:A:731:ARG:HG3	2.20	0.42
1:A:126:SER:HA	1:A:127:PRO:HD3	1.85	0.42
1:A:77:LYS:HD2	1:A:84:GLY:HA2	2.01	0.42
1:A:315:TYR:CZ	1:A:716:MET:HG2	2.55	0.42
1:A:731:ARG:O	1:A:731:ARG:CD	2.68	0.41
1:A:39:SER:HA	1:A:42:LEU:HD12	2.03	0.41
1:A:216:LYS:HD3	1:A:219:LEU:HD12	2.03	0.41
1:A:731:ARG:O	1:A:732:GLU:C	2.57	0.41
1:A:210:THR:O	1:A:237:VAL:HG13	2.20	0.41
1:A:122:ASN:O	1:A:123:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD12	1:A:717:LEU:HD12	2.02	0.41
1:A:57:ILE:C	1:A:58:VAL:CG1	2.80	0.41
1:A:325:PRO:HD2	1:A:706:SER:HA	2.04	0.40
1:A:160:LYS:HG3	1:A:162:ILE:HG22	2.03	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	356/369 (96%)	335 (94%)	19 (5%)	2 (1%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	VAL
1	A	56	GLY

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	312/323 (97%)	281 (90%)	31 (10%)	10	11

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	18	VAL
1	A	35	SER
1	A	49	ASP
1	A	53	ARG
1	A	57	ILE
1	A	60	ARG
1	A	78	THR
1	A	79	THR
1	A	86	GLU
1	A	118	ILE
1	A	119	SER
1	A	121	ASN
1	A	153	VAL
1	A	160	LYS
1	A	165	GLN
1	A	185	THR
1	A	206	ASP
1	A	227	MET
1	A	230	LEU
1	A	231	MET
1	A	234	VAL
1	A	259	THR
1	A	288	THR
1	A	298	ARG
1	A	301	LEU
1	A	306	THR
1	A	311	LEU
1	A	319	LEU
1	A	324	GLU
1	A	733	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	246	ASN

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)

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	$\#|Z| > 2$
2	GNP	A	801	-	28,34,34	1.89	5 (17%)	33,54,54	2.41	8 (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	GNP	A	801	-	-	0/12/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GNP	PB-O3A	-5.44	1.52	1.59
2	A	801	GNP	PB-O2B	-2.95	1.48	1.56
2	A	801	GNP	PB-O1B	2.06	1.48	1.46
2	A	801	GNP	C6-N1	3.58	1.39	1.33
2	A	801	GNP	PG-O1G	4.58	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	GNP	C5-C6-N1	-8.73	111.65	123.59
2	A	801	GNP	O3G-PG-O1G	-3.66	103.75	113.49
2	A	801	GNP	PA-O3A-PB	-3.61	120.55	132.67
2	A	801	GNP	O1G-PG-N3B	-2.83	107.56	111.90
2	A	801	GNP	N3-C2-N1	-2.25	124.02	127.44
2	A	801	GNP	O3G-PG-O2G	2.62	115.33	107.58
2	A	801	GNP	O2B-PB-O1B	3.41	117.12	110.00
2	A	801	GNP	C6-N1-C2	6.44	124.88	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GNP	1	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	358/369 (97%)	0.87	51 (14%)	4	6	22, 40, 87, 113	15 (4%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	GLY	17.1
1	A	703	GLY	15.0
1	A	327	ASP	12.6
1	A	57	ILE	10.1
1	A	704	SER	9.5
1	A	119	SER	8.9
1	A	229	VAL	8.4
1	A	84	GLY	8.3
1	A	230	LEU	7.2
1	A	325	PRO	7.2
1	A	83	ASN	7.1
1	A	733	THR	6.9
1	A	59	THR	6.6
1	A	705	GLY	6.6
1	A	323	GLY	5.9
1	A	121	ASN	5.9
1	A	118	ILE	5.6
1	A	80	GLY	5.1
1	A	117	ARG	5.0
1	A	326	VAL	5.0
1	A	231	MET	5.0
1	A	122	ASN	4.8
1	A	79	THR	4.7
1	A	706	SER	4.5
1	A	707	GLY	4.5
1	A	225	ASP	4.5
1	A	116	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	55	THR	4.3
1	A	123	LYS	4.2
1	A	82	GLU	4.2
1	A	732	GLU	4.1
1	A	58	VAL	3.9
1	A	81	GLU	3.7
1	A	232	GLY	3.6
1	A	53	ARG	3.6
1	A	324	GLU	3.6
1	A	60	ARG	3.3
1	A	266	TYR	3.2
1	A	1	MET	3.1
1	A	226	ALA	3.0
1	A	233	ARG	3.0
1	A	54	GLY	2.8
1	A	56	GLY	2.8
1	A	259	THR	2.8
1	A	263	ARG	2.7
1	A	115	THR	2.4
1	A	731	ARG	2.4
1	A	78	THR	2.2
1	A	124	GLY	2.1
1	A	257	SER	2.1
1	A	287	ARG	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
2	GNP	A	801	32/32	0.90	0.18	-0.09	31,47,75,86	0

6.5 Other polymers (i)

There are no such residues in this entry.