



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2017 – 07:08 PM EST

PDB ID : 5GNR  
Title : the structure of mini-MFN1 K88A in complex with GDP  
Authors : Yan, L.; Yu, C.; Ming, Z.; Lou, Z.; Rao, Z.; Hu, J.  
Deposited on : unknown  
Resolution : 2.65 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

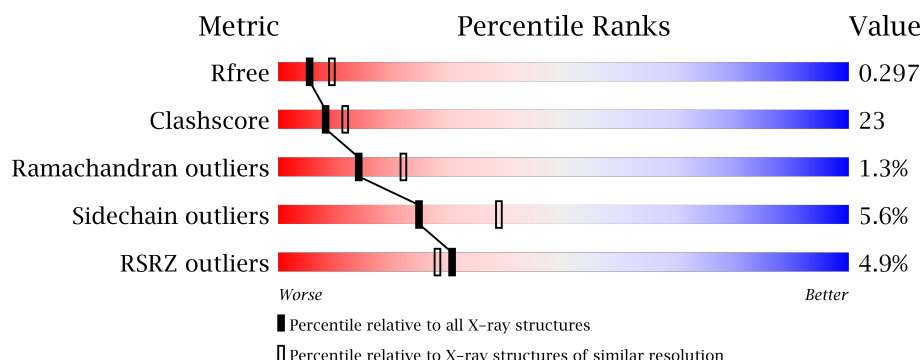
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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  $\geq 3$ , 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	421	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3116 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 Mitofusin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	3069	1944	527	584	14	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ALA	LYS	engineered mutation	UNP Q8IWA4
A	365	GLY	-	expression tag	UNP Q8IWA4
A	366	SER	-	expression tag	UNP Q8IWA4
A	367	GLY	-	expression tag	UNP Q8IWA4
A	368	SER	-	expression tag	UNP Q8IWA4
A	369	GLY	-	expression tag	UNP Q8IWA4
A	370	SER	-	expression tag	UNP Q8IWA4
A	371	GLY	-	expression tag	UNP Q8IWA4
A	372	GLY	-	expression tag	UNP Q8IWA4
A	373	SER	-	expression tag	UNP Q8IWA4
A	374	GLU	-	expression tag	UNP Q8IWA4
A	375	ILE	-	expression tag	UNP Q8IWA4
A	376	ALA	-	expression tag	UNP Q8IWA4
A	377	ARG	-	expression tag	UNP Q8IWA4
A	378	LEU	-	expression tag	UNP Q8IWA4
A	379	PRO	-	expression tag	UNP Q8IWA4
A	380	LYS	-	expression tag	UNP Q8IWA4
A	381	GLU	-	expression tag	UNP Q8IWA4
A	382	ILE	-	expression tag	UNP Q8IWA4
A	383	ASP	-	expression tag	UNP Q8IWA4
A	384	GLN	-	expression tag	UNP Q8IWA4
A	385	LEU	-	expression tag	UNP Q8IWA4
A	386	GLU	-	expression tag	UNP Q8IWA4
A	387	LYS	-	expression tag	UNP Q8IWA4
A	388	ILE	-	expression tag	UNP Q8IWA4
A	389	GLN	-	expression tag	UNP Q8IWA4
A	390	ASN	-	expression tag	UNP Q8IWA4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	391	ASN	-	expression tag	UNP Q8IWA4
A	392	SER	-	expression tag	UNP Q8IWA4
A	393	LYS	-	expression tag	UNP Q8IWA4
A	394	LEU	-	expression tag	UNP Q8IWA4
A	395	LEU	-	expression tag	UNP Q8IWA4
A	396	ARG	-	expression tag	UNP Q8IWA4
A	397	ASN	-	expression tag	UNP Q8IWA4
A	398	LYS	-	expression tag	UNP Q8IWA4
A	399	ALA	-	expression tag	UNP Q8IWA4
A	400	VAL	-	expression tag	UNP Q8IWA4
A	401	GLN	-	expression tag	UNP Q8IWA4
A	402	LEU	-	expression tag	UNP Q8IWA4
A	403	GLU	-	expression tag	UNP Q8IWA4
A	404	ASN	-	expression tag	UNP Q8IWA4
A	405	GLU	-	expression tag	UNP Q8IWA4
A	406	LEU	-	expression tag	UNP Q8IWA4
A	407	GLU	-	expression tag	UNP Q8IWA4
A	408	ASN	-	expression tag	UNP Q8IWA4
A	409	PHE	-	expression tag	UNP Q8IWA4
A	410	THR	-	expression tag	UNP Q8IWA4
A	411	LYS	-	expression tag	UNP Q8IWA4
A	412	GLN	-	expression tag	UNP Q8IWA4
A	413	PHE	-	expression tag	UNP Q8IWA4
A	414	LEU	-	expression tag	UNP Q8IWA4
A	415	PRO	-	expression tag	UNP Q8IWA4
A	416	SER	-	expression tag	UNP Q8IWA4
A	417	SER	-	expression tag	UNP Q8IWA4
A	418	ASN	-	expression tag	UNP Q8IWA4
A	419	GLU	-	expression tag	UNP Q8IWA4
A	420	GLU	-	expression tag	UNP Q8IWA4
A	421	SER	-	expression tag	UNP Q8IWA4

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

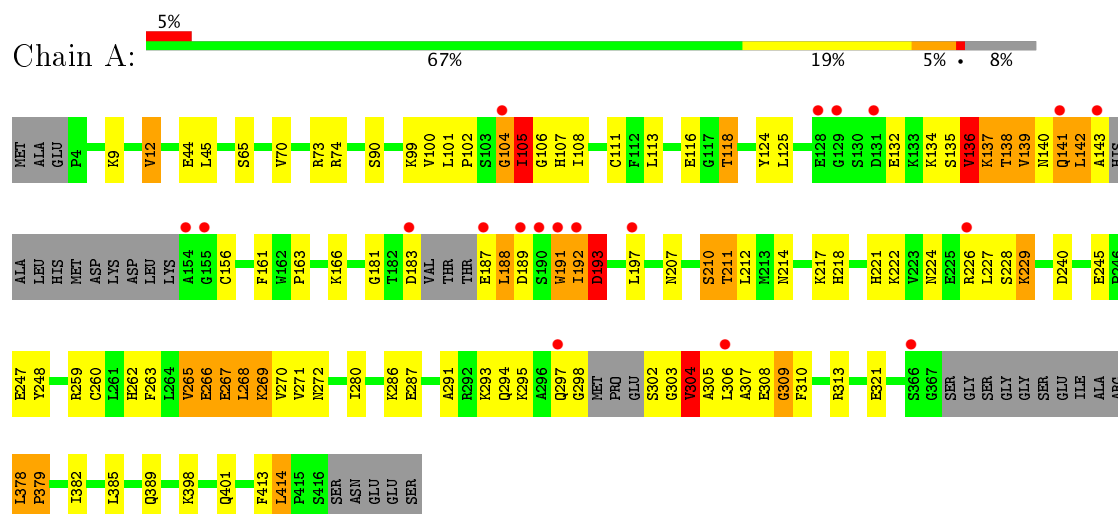
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	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 the various outlier classes 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: Mitofusin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.34Å 74.97Å 94.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.96 – 2.65 39.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	51.4 (39.96-2.65) 89.9 (39.96-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, $R_{free}$	0.216 , 0.302 0.222 , 0.297	Depositor DCC
$R_{free}$ test set	1389 reflections (10.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GDP

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	0.57	0/3119	0.88	18/4198 (0.4%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	268	LEU	CB-CA-C	-11.42	88.51	110.20
1	A	191	TRP	CB-CA-C	-9.88	90.65	110.40
1	A	104	GLY	N-CA-C	9.50	136.86	113.10
1	A	210	SER	CB-CA-C	-8.76	93.45	110.10
1	A	193	ASP	CB-CA-C	8.11	126.62	110.40
1	A	265	VAL	CB-CA-C	8.00	126.60	111.40
1	A	224	ASN	CB-CA-C	-7.72	94.95	110.40
1	A	192	ILE	N-CA-CB	-7.50	93.56	110.80
1	A	266	GLU	N-CA-CB	-7.19	97.66	110.60
1	A	211	THR	N-CA-CB	-6.82	97.35	110.30
1	A	298	GLY	N-CA-C	-6.50	96.86	113.10
1	A	309	GLY	N-CA-C	6.15	128.47	113.10
1	A	297	GLN	CB-CA-C	6.04	122.48	110.40
1	A	266	GLU	N-CA-C	5.83	126.75	111.00
1	A	105	ILE	N-CA-CB	-5.65	97.80	110.80
1	A	307	ALA	N-CA-C	-5.38	96.48	111.00
1	A	378	LEU	C-N-CD	-5.32	108.89	120.60
1	A	137	LYS	CB-CA-C	-5.30	99.81	110.40

There are no chirality outliers.

There are no planarity outliers.



## 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	3069	0	3066	144	0
2	A	28	0	12	1	0
3	A	19	0	0	5	0
All	All	3116	0	3078	144	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 23.

All (144) 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:102:PRO:HG2	1:A:105:ILE:CD1	1.41	1.49
1:A:136:VAL:HG13	1:A:137:LYS:N	1.54	1.15
1:A:142:LEU:HD12	1:A:143:ALA:N	1.62	1.15
1:A:136:VAL:CG1	1:A:137:LYS:H	1.58	1.12
1:A:102:PRO:HG2	1:A:105:ILE:HD11	1.24	1.08
1:A:102:PRO:CG	1:A:105:ILE:CD1	2.31	1.08
1:A:139:VAL:HG23	1:A:139:VAL:O	1.56	1.04
1:A:102:PRO:CG	1:A:105:ILE:HD11	1.86	1.04
1:A:102:PRO:HG2	1:A:105:ILE:HD13	1.40	0.99
1:A:187:GLU:OE2	1:A:187:GLU:HA	1.63	0.97
1:A:142:LEU:HD12	1:A:142:LEU:C	1.88	0.93
1:A:102:PRO:O	1:A:105:ILE:HD11	1.73	0.88
1:A:304:VAL:HG13	1:A:305:ALA:N	1.85	0.88
1:A:270:VAL:HG13	1:A:271:VAL:HG23	1.56	0.88
1:A:142:LEU:CD1	1:A:143:ALA:N	2.36	0.87
1:A:136:VAL:HG13	1:A:137:LYS:H	0.72	0.85
1:A:192:ILE:H	1:A:192:ILE:HD12	1.39	0.85
1:A:140:ASN:C	1:A:142:LEU:H	1.81	0.83
1:A:262:HIS:O	1:A:267:GLU:HG3	1.79	0.83
1:A:189:ASP:HB2	1:A:222:LYS:HZ2	1.45	0.80
1:A:187:GLU:OE2	1:A:188:LEU:HA	1.82	0.79
1:A:102:PRO:O	1:A:105:ILE:CG1	2.31	0.78
1:A:140:ASN:OD1	1:A:140:ASN:O	2.02	0.78
1:A:102:PRO:O	1:A:105:ILE:CD1	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:HA	1:A:192:ILE:HD13	1.67	0.75
1:A:192:ILE:H	1:A:192:ILE:CD1	1.96	0.72
1:A:142:LEU:CG	1:A:143:ALA:N	2.53	0.71
1:A:142:LEU:C	1:A:142:LEU:CD1	2.58	0.70
1:A:102:PRO:HG2	1:A:105:ILE:HD12	1.62	0.70
1:A:321:GLU:OE2	3:A:1101:HOH:O	2.10	0.69
1:A:136:VAL:CG1	1:A:137:LYS:N	2.28	0.69
1:A:140:ASN:C	1:A:142:LEU:N	2.44	0.69
1:A:142:LEU:CG	1:A:143:ALA:H	2.06	0.69
1:A:104:GLY:HA3	1:A:108:ILE:CD1	2.23	0.68
1:A:142:LEU:O	1:A:143:ALA:C	2.30	0.68
1:A:102:PRO:O	1:A:105:ILE:HG12	1.93	0.68
1:A:139:VAL:CG2	1:A:139:VAL:O	2.30	0.67
1:A:141:GLN:CG	1:A:141:GLN:O	2.43	0.67
1:A:309:GLY:HA3	1:A:313:ARG:HH21	1.59	0.67
1:A:141:GLN:O	1:A:141:GLN:HG2	1.95	0.67
1:A:142:LEU:HG	1:A:143:ALA:H	1.58	0.66
1:A:73:ARG:NH2	3:A:1104:HOH:O	2.28	0.65
1:A:187:GLU:HB3	1:A:188:LEU:HG	1.80	0.64
1:A:197:LEU:HD21	1:A:226:ARG:NH1	2.12	0.64
1:A:100:VAL:O	1:A:137:LYS:HE2	1.97	0.64
1:A:125:LEU:HD13	1:A:136:VAL:HA	1.80	0.64
1:A:268:LEU:O	1:A:270:VAL:N	2.31	0.64
1:A:142:LEU:HD12	1:A:143:ALA:CA	2.29	0.63
1:A:266:GLU:HA	1:A:269:LYS:HG2	1.80	0.62
1:A:304:VAL:CG1	1:A:305:ALA:N	2.58	0.61
1:A:268:LEU:O	1:A:269:LYS:C	2.39	0.61
1:A:99:LYS:HE3	1:A:102:PRO:HA	1.83	0.61
1:A:398:LYS:O	1:A:401:GLN:HG3	2.01	0.60
1:A:378:LEU:HB3	1:A:382:ILE:HG13	1.82	0.60
1:A:266:GLU:HA	1:A:269:LYS:CG	2.30	0.60
1:A:102:PRO:C	1:A:105:ILE:HD11	2.22	0.59
1:A:197:LEU:HD21	1:A:226:ARG:CZ	2.32	0.59
1:A:102:PRO:CD	1:A:105:ILE:HD11	2.32	0.59
1:A:218:HIS:CE1	1:A:222:LYS:NZ	2.71	0.59
1:A:286:LYS:HD3	1:A:306:LEU:HD11	1.85	0.59
1:A:188:LEU:O	1:A:192:ILE:CD1	2.51	0.59
1:A:218:HIS:CE1	1:A:222:LYS:HZ3	2.21	0.58
1:A:135:SER:O	1:A:136:VAL:O	2.21	0.58
1:A:104:GLY:HA3	1:A:108:ILE:HG13	1.85	0.58
1:A:191:TRP:HB2	1:A:192:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:HB2	1:A:222:LYS:NZ	2.19	0.56
1:A:102:PRO:CA	1:A:105:ILE:HD11	2.35	0.56
1:A:118:THR:OG1	1:A:161:PHE:HB3	2.05	0.56
1:A:245:GLU:HB3	1:A:248:TYR:HB3	1.88	0.56
1:A:270:VAL:C	1:A:271:VAL:HG23	2.25	0.56
1:A:197:LEU:CD2	1:A:226:ARG:NH1	2.69	0.56
1:A:270:VAL:O	1:A:270:VAL:HG22	2.06	0.56
1:A:304:VAL:HG13	1:A:305:ALA:O	2.06	0.55
1:A:134:LYS:HB3	1:A:139:VAL:HG21	1.89	0.55
1:A:193:ASP:HB2	1:A:197:LEU:HD11	1.88	0.55
1:A:207:ASN:O	1:A:210:SER:O	2.25	0.55
1:A:188:LEU:O	1:A:192:ILE:HD11	2.07	0.55
1:A:309:GLY:HA3	1:A:313:ARG:NH2	2.20	0.54
1:A:136:VAL:HG13	1:A:137:LYS:HG3	1.89	0.54
1:A:74:ARG:HG2	1:A:74:ARG:HH11	1.72	0.54
1:A:226:ARG:HG3	1:A:227:LEU:HD12	1.89	0.54
1:A:263:PHE:HA	1:A:267:GLU:HG3	1.90	0.53
1:A:270:VAL:C	1:A:271:VAL:CG2	2.75	0.53
1:A:385:LEU:O	1:A:389:GLN:HG3	2.09	0.52
1:A:70:VAL:O	1:A:74:ARG:HG2	2.09	0.52
1:A:137:LYS:O	1:A:138:THR:C	2.48	0.52
1:A:104:GLY:C	1:A:108:ILE:HG13	2.31	0.51
1:A:107:HIS:ND1	3:A:1107:HOH:O	2.34	0.51
1:A:137:LYS:HA	1:A:140:ASN:HB2	1.93	0.51
1:A:111:CYS:HB2	1:A:156:CYS:O	2.11	0.51
1:A:104:GLY:HA3	1:A:108:ILE:CG1	2.41	0.51
1:A:229:LYS:HG2	1:A:270:VAL:HG23	1.93	0.50
1:A:163:PRO:HB2	1:A:166:LYS:HG3	1.93	0.50
1:A:102:PRO:CD	1:A:105:ILE:CD1	2.87	0.50
1:A:214:ASN:HA	1:A:217:LYS:HB2	1.94	0.50
1:A:188:LEU:CD1	1:A:191:TRP:CZ2	2.94	0.49
1:A:266:GLU:CA	1:A:269:LYS:HG2	2.39	0.49
1:A:287:GLU:OE1	1:A:313:ARG:HD2	2.12	0.49
1:A:270:VAL:O	1:A:271:VAL:HG22	2.13	0.49
1:A:118:THR:HG21	1:A:124:TYR:HE1	1.76	0.49
1:A:398:LYS:HA	1:A:401:GLN:HG2	1.93	0.49
1:A:137:LYS:O	1:A:140:ASN:N	2.35	0.49
1:A:102:PRO:N	1:A:105:ILE:HD11	2.29	0.48
1:A:102:PRO:CB	1:A:105:ILE:HD11	2.41	0.48
1:A:212:LEU:HB3	1:A:259:ARG:HD3	1.96	0.48
1:A:44:GLU:O	1:A:45:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:OE2	1:A:313:ARG:NH1	2.47	0.47
1:A:308:GLU:HB3	1:A:310:PHE:HB3	1.95	0.47
1:A:188:LEU:CD1	1:A:191:TRP:CH2	2.97	0.47
1:A:181:GLY:C	1:A:183:ASP:H	2.17	0.47
1:A:188:LEU:O	1:A:192:ILE:HD13	2.14	0.47
1:A:221:HIS:NE2	1:A:267:GLU:O	2.40	0.47
1:A:90:SER:OG	2:A:1000:GDP:O2A	2.26	0.46
1:A:193:ASP:HB2	1:A:197:LEU:CD1	2.44	0.46
1:A:210:SER:OG	1:A:211:THR:N	2.49	0.46
1:A:140:ASN:C	1:A:140:ASN:OD1	2.54	0.46
1:A:181:GLY:C	1:A:183:ASP:N	2.70	0.46
1:A:44:GLU:C	1:A:45:LEU:HD23	2.36	0.45
1:A:9:LYS:HA	1:A:12:VAL:HG13	1.98	0.45
1:A:132:GLU:HG3	1:A:134:LYS:HE3	1.99	0.45
1:A:262:HIS:O	1:A:267:GLU:CG	2.59	0.45
1:A:101:LEU:HA	1:A:102:PRO:HD2	1.85	0.44
1:A:262:HIS:ND1	1:A:267:GLU:OE2	2.45	0.44
1:A:262:HIS:HA	3:A:1102:HOH:O	2.17	0.44
1:A:270:VAL:O	1:A:271:VAL:CG2	2.65	0.44
1:A:240:ASP:N	1:A:240:ASP:OD1	2.51	0.43
1:A:188:LEU:HD13	1:A:191:TRP:CZ2	2.53	0.43
1:A:104:GLY:CA	1:A:108:ILE:HG13	2.48	0.43
1:A:70:VAL:O	1:A:74:ARG:NH1	2.52	0.43
1:A:294:GLN:OE1	1:A:302:SER:HA	2.19	0.42
1:A:105:ILE:HA	1:A:106:GLY:HA2	1.56	0.42
1:A:247:GLU:H	1:A:247:GLU:CD	2.22	0.42
1:A:104:GLY:HA3	1:A:108:ILE:HD11	1.98	0.42
1:A:265:VAL:HG13	1:A:272:ASN:HA	2.01	0.42
1:A:378:LEU:HA	1:A:379:PRO:HD2	1.80	0.42
1:A:197:LEU:N	1:A:197:LEU:HD12	2.34	0.41
1:A:197:LEU:HG	1:A:227:LEU:HD11	2.02	0.41
1:A:302:SER:O	1:A:302:SER:OG	2.30	0.41
1:A:266:GLU:N	3:A:1102:HOH:O	2.13	0.41
1:A:266:GLU:HA	1:A:269:LYS:HG3	2.00	0.41
1:A:291:ALA:O	1:A:294:GLN:HG2	2.21	0.41
1:A:413:PHE:O	1:A:414:LEU:HD23	2.21	0.41
1:A:260:CYS:HB3	1:A:280:ILE:HD13	2.04	0.40
1:A:303:GLY:HA2	1:A:304:VAL:HA	1.71	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	377/421 (90%)	344 (91%)	28 (7%)	5 (1%)	14 22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	379	PRO
1	A	193	ASP
1	A	304	VAL
1	A	414	LEU

### 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	339/367 (92%)	320 (94%)	19 (6%)	25 39

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	65	SER
1	A	105	ILE
1	A	113	LEU
1	A	116	GLU
1	A	118	THR

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	136	VAL
1	A	138	THR
1	A	139	VAL
1	A	141	GLN
1	A	142	LEU
1	A	188	LEU
1	A	228	SER
1	A	229	LYS
1	A	267	GLU
1	A	269	LYS
1	A	293	LYS
1	A	295	LYS
1	A	304	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	218	HIS
1	A	256	HIS

### 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	GDP	A	1000	-	25,30,30	1.23	2 (8%)	26,47,47	2.16	7 (26%)

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	GDP	A	1000	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	GDP	C5-C4	3.10	1.47	1.40
2	A	1000	GDP	C6-C5	3.83	1.48	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	GDP	C6-C5-C4	-4.51	116.36	120.84
2	A	1000	GDP	C5-C6-N1	-3.88	117.96	123.48
2	A	1000	GDP	N3-C2-N1	-3.64	122.14	127.46
2	A	1000	GDP	C4-C5-N7	-3.27	106.25	109.41
2	A	1000	GDP	C1'-N9-C4	-2.40	122.48	126.64
2	A	1000	GDP	C6-N1-C2	4.79	122.95	116.06
2	A	1000	GDP	C2-N3-C4	5.00	121.00	115.16

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	1000	GDP	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	387/421 (91%)	0.10	19 (4%) 30 28	17, 36, 72, 128	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	TRP	8.9
1	A	154	ALA	7.9
1	A	155	GLY	6.7
1	A	297	GLN	4.3
1	A	190	SER	4.2
1	A	189	ASP	3.8
1	A	306	LEU	3.7
1	A	129	GLY	3.1
1	A	192	ILE	3.1
1	A	197	LEU	2.9
1	A	183	ASP	2.6
1	A	141	GLN	2.5
1	A	143	ALA	2.5
1	A	128	GLU	2.2
1	A	226	ARG	2.1
1	A	366	SER	2.1
1	A	104	GLY	2.1
1	A	131	ASP	2.1
1	A	187	GLU	2.0

### 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 [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	GDP	A	1000	28/28	0.97	0.13	-0.86	20,35,41,43	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.