



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 AM GMT

PDB ID : 3FTQ  
Title : Crystal structure of Septin 2 in complex with GppNHp and Mg2+  
Authors : Sirajuddin, M.; Wittinghofer, A.  
Deposited on : 2009-01-13  
Resolution : 2.90 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.

---

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

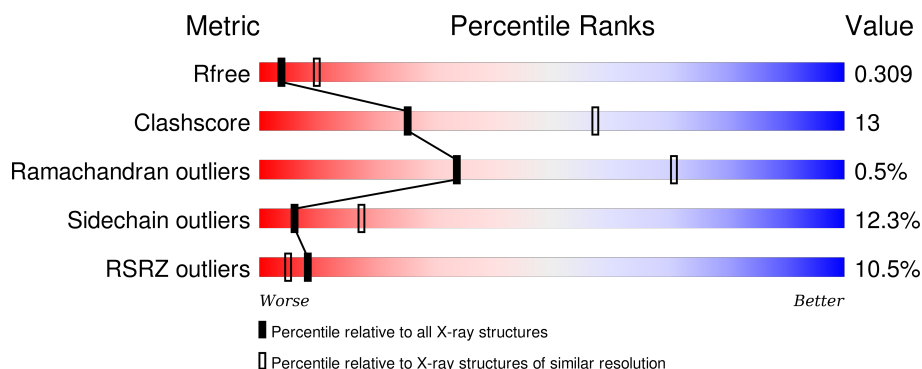
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	274	<div> <div>9%</div> <div>61% 25% 6% • 7%</div> </div>
1	B	274	<div> <div>8%</div> <div>62% 24% 5% • 8%</div> </div>
1	C	274	<div> <div>10%</div> <div>66% 21% 5% 9%</div> </div>
1	D	274	<div> <div>10%</div> <div>56% 26% 7% 11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8382 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 Septin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2070	1316	363	383	8			
1	B	252	Total	C	N	O	S	0	0	0
			2059	1314	358	379	8			
1	C	250	Total	C	N	O	S	0	0	0
			2045	1303	357	377	8			
1	D	243	Total	C	N	O	S	0	0	0
			1973	1261	342	362	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	D	1	Total 32	C 10	N 6	O 13	P 3	0	0

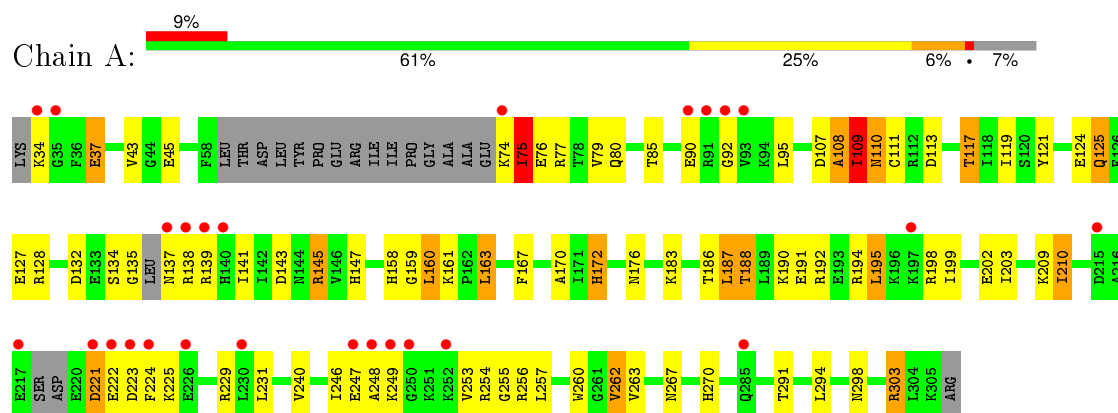
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	B	31	Total O 31 31	0	0
4	C	23	Total O 23 23	0	0
4	D	16	Total O 16 16	0	0

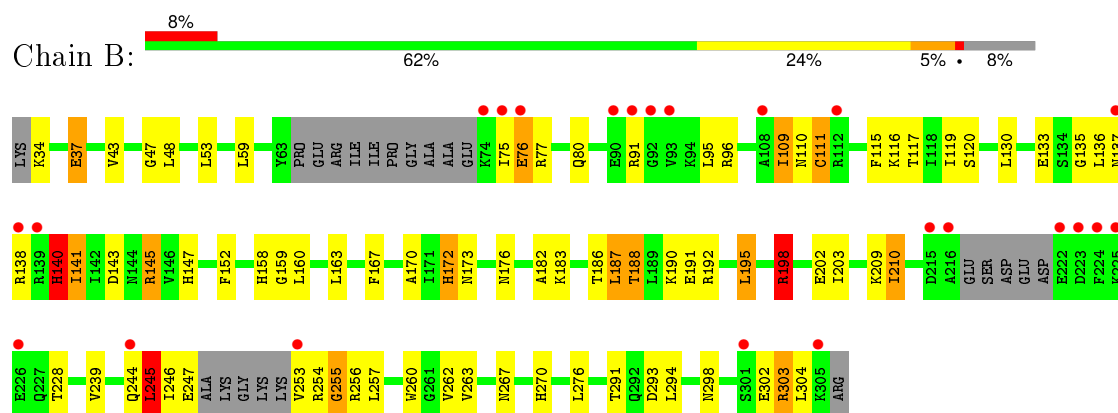
### 3 Residue-property plots [i](#)

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.

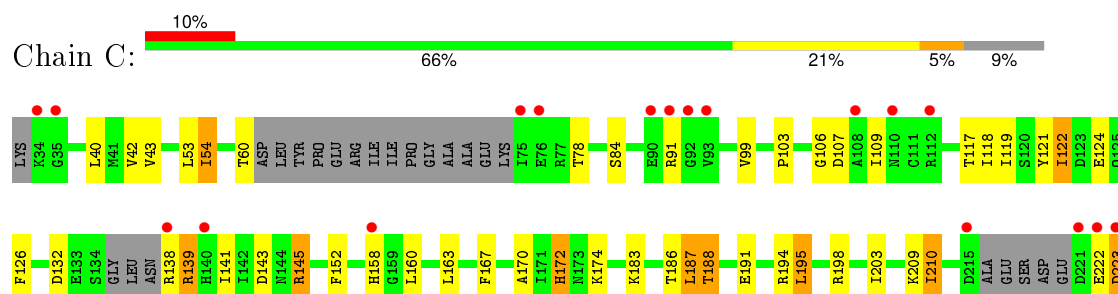
#### • Molecule 1: Septin-2

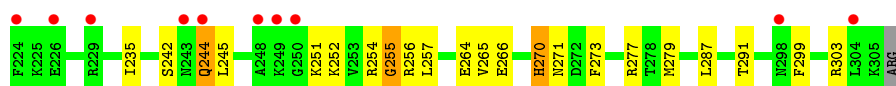


#### • Molecule 1: Septin-2

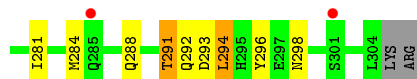
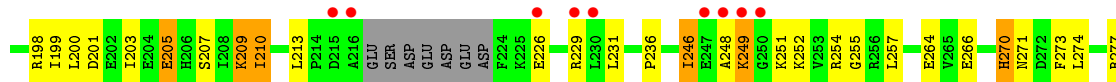
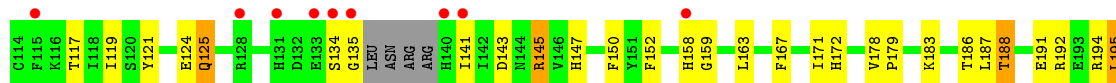
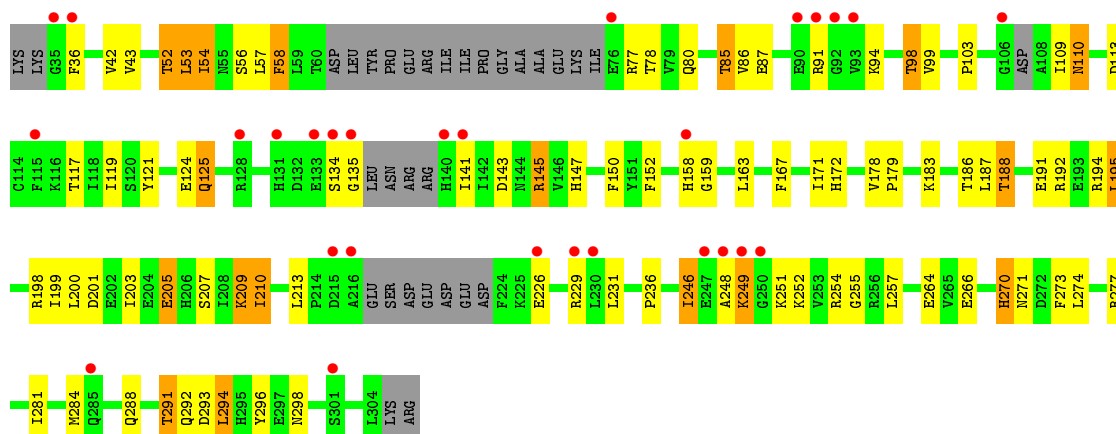


#### • Molecule 1: Septin-2





● Molecule 1: Septin-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.98Å 118.44Å 190.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.90 19.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.90) 99.7 (19.96-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.247 , 0.290 0.265 , 0.309	Depositor DCC
$R_{free}$ test set	1689 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33760 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, 0.375 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: GNP, MG

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	0/2106	0.78	13/2831 (0.5%)
1	B	0.46	1/2096 (0.0%)	0.84	11/2823 (0.4%)
1	C	0.44	0/2081	0.71	4/2799 (0.1%)
1	D	0.43	0/2008	0.70	8/2702 (0.3%)
All	All	0.44	1/8291 (0.0%)	0.76	36/11155 (0.3%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	ARG	CZ-NH2	5.01	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	ASN	N-CA-CB	12.04	132.28	110.60
1	B	109	ILE	CB-CA-C	10.39	132.38	111.60
1	C	106	GLY	N-CA-C	9.70	137.35	113.10
1	B	140	HIS	CB-CA-C	9.39	129.18	110.40
1	C	107	ASP	N-CA-CB	9.14	127.05	110.60
1	A	249	LYS	N-CA-C	8.94	135.14	111.00
1	B	140	HIS	N-CA-C	-8.78	87.29	111.00
1	B	198	ARG	NH1-CZ-NH2	-8.59	109.96	119.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLY	N-CA-C	-8.00	93.11	113.10
1	A	221	ASP	CB-CA-C	-7.22	95.96	110.40
1	B	141	ILE	N-CA-C	-7.07	91.91	111.00
1	D	159	GLY	N-CA-C	-6.90	95.84	113.10
1	B	141	ILE	N-CA-CB	6.71	126.22	110.80
1	D	251	LYS	N-CA-CB	6.59	122.47	110.60
1	D	158	HIS	CB-CA-C	-6.51	97.39	110.40
1	B	109	ILE	N-CA-C	-6.42	93.65	111.00
1	B	245	LEU	CB-CA-C	-6.39	98.05	110.20
1	D	294	LEU	N-CA-C	6.30	128.00	111.00
1	A	76	GLU	N-CA-C	6.26	127.89	111.00
1	A	109	ILE	N-CA-CB	5.96	124.50	110.80
1	D	291	THR	CB-CA-C	5.71	127.02	111.60
1	B	159	GLY	N-CA-C	-5.71	98.83	113.10
1	A	108	ALA	CB-CA-C	-5.70	101.56	110.10
1	A	222	GLU	N-CA-C	5.46	125.73	111.00
1	D	246	ILE	CB-CA-C	5.42	122.43	111.60
1	A	248	ALA	N-CA-CB	5.36	117.61	110.10
1	C	109	ILE	CB-CA-C	5.32	122.24	111.60
1	A	249	LYS	CB-CA-C	-5.30	99.79	110.40
1	A	253	VAL	CB-CA-C	-5.27	101.38	111.40
1	A	75	ILE	N-CA-C	5.27	125.23	111.00
1	D	209	LYS	CD-CE-NZ	5.24	123.76	111.70
1	A	223	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	223	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	293	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	293	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	247	GLU	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	ARG	Sidechain

## 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	2070	0	2079	60	0
1	B	2059	0	2069	50	0
1	C	2045	0	2062	46	0
1	D	1973	0	1988	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	13	0	0
3	B	32	0	13	0	0
3	C	32	0	13	1	0
3	D	32	0	13	3	0
4	A	33	0	0	1	0
4	B	31	0	0	0	0
4	C	23	0	0	1	0
4	D	16	0	0	0	0
All	All	8382	0	8250	208	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 13.

All (208) 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:D:110:ASN:C	1:D:110:ASN:HD22	1.66	0.99
1:A:110:ASN:C	1:A:110:ASN:HD22	1.63	0.99
1:C:54:ILE:HG13	1:C:99:VAL:HG11	1.44	0.98
1:C:172:HIS:HD2	1:C:209:LYS:H	1.11	0.97
1:B:75:ILE:O	1:B:75:ILE:HG22	1.65	0.96
1:A:303:ARG:HH11	1:A:303:ARG:HG2	1.31	0.94
1:A:270:HIS:CE1	1:B:260:TRP:HB3	2.03	0.94
1:A:270:HIS:HE1	1:B:260:TRP:HB3	1.33	0.90
1:C:122:ILE:HD11	1:C:174:LYS:HB3	1.53	0.89
1:A:260:TRP:HB3	1:B:270:HIS:CE1	2.08	0.89
1:B:172:HIS:HD2	1:B:209:LYS:H	1.20	0.88
1:A:172:HIS:HD2	1:A:209:LYS:H	1.15	0.88
1:A:260:TRP:HB3	1:B:270:HIS:HE1	1.38	0.88
1:C:264:GLU:H	1:C:270:HIS:HD2	1.25	0.85
1:A:75:ILE:HG23	1:A:75:ILE:O	1.75	0.83
1:D:194:ARG:O	1:D:198:ARG:HG2	1.80	0.82
1:D:172:HIS:CD2	1:D:209:LYS:HB2	2.16	0.81
1:D:172:HIS:HD2	1:D:209:LYS:HB2	1.44	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:HIS:O	1:B:198:ARG:HD2	1.82	0.80
1:D:42:VAL:HG21	1:D:54:ILE:HD13	1.62	0.78
1:B:267:ASN:CG	1:B:270:HIS:HD2	1.87	0.78
1:C:54:ILE:HG13	1:C:99:VAL:CG1	2.14	0.77
1:B:183:LYS:O	1:B:186:THR:HG23	1.85	0.76
1:B:256:ARG:HB2	1:B:263:VAL:HB	1.68	0.76
1:A:303:ARG:HG2	1:A:303:ARG:NH1	1.95	0.76
1:C:139:ARG:CG	1:C:139:ARG:HH11	1.97	0.75
1:A:256:ARG:HB2	1:A:263:VAL:HB	1.68	0.75
1:D:42:VAL:HG21	1:D:54:ILE:CD1	2.18	0.74
1:D:147:HIS:CD2	1:D:291:THR:HG21	2.22	0.74
1:D:110:ASN:ND2	1:D:110:ASN:C	2.40	0.74
1:D:147:HIS:HD2	1:D:291:THR:HG21	1.51	0.74
1:A:125:GLN:HE21	1:A:125:GLN:HA	1.53	0.73
3:C:372:GNP:O2A	4:C:318:HOH:O	2.05	0.73
1:C:122:ILE:HD11	1:C:174:LYS:CB	2.17	0.72
1:A:267:ASN:CG	1:A:270:HIS:HD2	1.93	0.72
1:A:135:GLY:O	1:A:137:ASN:N	2.23	0.72
1:A:158:HIS:O	1:A:198:ARG:HD3	1.89	0.72
1:A:110:ASN:C	1:A:110:ASN:ND2	2.39	0.71
1:B:75:ILE:O	1:B:75:ILE:CG2	2.39	0.69
1:A:221:ASP:O	1:A:225:LYS:HG3	1.93	0.68
1:A:303:ARG:HH11	1:A:303:ARG:CG	2.03	0.68
1:C:203:ILE:HD13	1:C:210:ILE:HD12	1.75	0.68
1:C:139:ARG:HG2	1:C:139:ARG:HH11	1.57	0.67
1:D:56:SER:HA	1:D:254:ARG:NH1	2.10	0.67
1:B:188:THR:HG22	1:B:191:GLU:H	1.59	0.67
1:A:194:ARG:O	1:A:198:ARG:HG3	1.94	0.66
1:A:294:LEU:O	1:A:298:ASN:ND2	2.29	0.66
1:D:54:ILE:HG13	1:D:99:VAL:HG11	1.76	0.65
1:D:183:LYS:O	1:D:186:THR:HG23	1.96	0.65
1:B:111:CYS:SG	1:B:115:PHE:CE1	2.89	0.65
1:D:53:LEU:HD22	1:D:152:PHE:HZ	1.60	0.65
1:A:188:THR:HG22	1:A:191:GLU:H	1.61	0.65
1:B:203:ILE:HD13	1:B:210:ILE:HD12	1.79	0.65
1:A:183:LYS:O	1:A:186:THR:HG23	1.96	0.65
1:A:203:ILE:HD13	1:A:210:ILE:HD12	1.79	0.64
1:A:125:GLN:HE21	1:A:125:GLN:CA	2.11	0.64
1:A:172:HIS:CD2	1:A:209:LYS:H	2.07	0.64
1:D:264:GLU:H	1:D:270:HIS:HD2	1.46	0.64
1:C:53:LEU:HD22	1:C:152:PHE:HZ	1.63	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:HIS:O	1:C:198:ARG:HD3	1.98	0.63
1:C:194:ARG:O	1:C:198:ARG:HG3	1.98	0.63
1:C:172:HIS:CD2	1:C:209:LYS:H	2.03	0.63
1:D:125:GLN:HE21	1:D:125:GLN:HA	1.62	0.62
1:A:45:GLU:OE1	1:A:161:LYS:NZ	2.33	0.62
1:C:60:THR:HG22	1:C:254:ARG:HH22	1.65	0.62
1:A:147:HIS:HA	1:A:291:THR:HG21	1.81	0.61
1:C:244:GLN:H	1:C:244:GLN:HE21	1.47	0.61
1:C:139:ARG:NH1	1:C:139:ARG:HG2	2.12	0.61
1:B:303:ARG:HG3	1:B:304:LEU:N	2.16	0.61
1:B:147:HIS:HA	1:B:291:THR:HG21	1.81	0.61
1:C:42:VAL:HG21	1:C:54:ILE:HD13	1.83	0.60
1:D:85:THR:HG23	1:D:98:THR:HB	1.82	0.60
1:B:172:HIS:CD2	1:B:209:LYS:H	2.11	0.60
1:A:34:LYS:HB3	1:A:92:GLY:O	2.02	0.60
1:D:56:SER:HA	1:D:254:ARG:HH12	1.66	0.59
1:C:188:THR:HG22	1:C:191:GLU:H	1.67	0.59
1:D:52:THR:HG23	3:D:372:GNP:O1A	2.02	0.59
1:B:244:GLN:O	1:B:255:GLY:HA3	2.03	0.58
1:D:203:ILE:HD13	1:D:210:ILE:HD12	1.84	0.58
1:C:242:SER:OG	1:C:256:ARG:HG3	2.03	0.58
1:D:125:GLN:HE21	1:D:125:GLN:CA	2.17	0.57
1:C:78:THR:O	1:C:103:PRO:HB3	2.04	0.57
1:A:107:ASP:O	1:A:108:ALA:HB3	2.05	0.56
1:B:37:GLU:HG3	1:B:143:ASP:HB3	1.88	0.56
1:D:172:HIS:CD2	1:D:209:LYS:H	2.24	0.55
1:A:74:LYS:O	1:A:75:ILE:HG22	2.07	0.55
1:C:42:VAL:HG21	1:C:54:ILE:CD1	2.36	0.55
1:C:244:GLN:H	1:C:244:GLN:NE2	2.03	0.55
1:C:183:LYS:O	1:C:186:THR:HG23	2.06	0.55
1:A:37:GLU:HG3	1:A:143:ASP:HB3	1.89	0.54
1:A:267:ASN:CB	1:A:270:HIS:HD2	2.20	0.54
1:B:173:ASN:HD21	1:B:209:LYS:NZ	2.06	0.54
1:A:125:GLN:NE2	1:A:125:GLN:HA	2.22	0.54
1:D:54:ILE:HG13	1:D:99:VAL:CG1	2.36	0.53
1:C:132:ASP:HB3	1:C:141:ILE:HG21	1.91	0.53
1:C:264:GLU:HG3	1:C:270:HIS:CD2	2.44	0.52
1:D:188:THR:HG22	1:D:191:GLU:H	1.74	0.52
1:B:116:LYS:O	1:B:120:SER:HB2	2.09	0.52
1:C:287:LEU:O	1:C:291:THR:OG1	2.26	0.52
1:B:111:CYS:SG	1:B:163:LEU:HD22	2.50	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:HG2	1:B:77:ARG:N	2.25	0.52
1:D:179:PRO:HG2	1:D:236:PRO:HB3	1.92	0.52
1:A:132:ASP:O	1:A:138:ARG:HB2	2.10	0.51
1:C:254:ARG:O	1:C:265:VAL:N	2.43	0.51
1:D:87:GLU:OE2	1:D:94:LYS:HE2	2.11	0.51
1:A:172:HIS:CD2	1:A:209:LYS:HB2	2.46	0.51
1:B:119:ILE:HD11	1:B:170:ALA:HB1	1.92	0.51
1:D:172:HIS:HD2	1:D:209:LYS:H	1.58	0.51
1:D:246:ILE:O	1:D:252:LYS:HA	2.11	0.50
1:A:246:ILE:HD11	1:A:262:VAL:HG23	1.93	0.50
1:D:294:LEU:O	1:D:294:LEU:HD12	2.12	0.50
1:A:267:ASN:ND2	1:A:270:HIS:HD2	2.10	0.49
1:C:251:LYS:HG2	1:C:252:LYS:H	1.76	0.49
1:A:158:HIS:CD2	1:A:202:GLU:OE2	2.65	0.49
1:C:251:LYS:HG2	1:C:252:LYS:N	2.27	0.49
1:B:190:LYS:HD2	1:B:190:LYS:H	1.77	0.49
1:B:143:ASP:OD2	1:B:145:ARG:HD3	2.12	0.49
1:B:267:ASN:ND2	1:B:270:HIS:HD2	2.09	0.49
1:B:187:LEU:HD21	1:B:195:LEU:HD12	1.93	0.49
1:D:125:GLN:NE2	1:D:125:GLN:HA	2.28	0.49
1:C:256:ARG:NH2	1:D:191:GLU:OE2	2.46	0.49
1:D:248:ALA:O	1:D:249:LYS:HG3	2.13	0.48
1:A:113:ASP:O	1:A:117:THR:HG22	2.13	0.48
1:B:158:HIS:HE1	1:B:160:LEU:O	1.95	0.48
1:A:270:HIS:HD1	1:B:260:TRP:HE3	1.61	0.48
1:D:54:ILE:HD12	1:D:54:ILE:HA	1.65	0.48
1:A:77:ARG:NH2	1:A:107:ASP:O	2.46	0.48
1:D:271:ASN:ND2	1:D:273:PHE:HB2	2.29	0.48
1:C:186:THR:HG22	1:D:186:THR:HB	1.95	0.48
1:D:57:LEU:HA	1:D:273:PHE:HZ	1.78	0.48
1:B:133:GLU:HA	1:B:138:ARG:HG2	1.96	0.47
1:D:294:LEU:O	1:D:298:ASN:HB2	2.14	0.47
1:D:121:TYR:O	1:D:125:GLN:HG2	2.15	0.47
1:A:125:GLN:NE2	1:A:128:ARG:HD3	2.30	0.47
1:B:135:GLY:HA3	1:B:136:LEU:HA	1.56	0.47
1:D:78:THR:O	1:D:103:PRO:HB3	2.14	0.47
1:D:119:ILE:HG12	1:D:171:ILE:HG22	1.97	0.47
1:B:267:ASN:ND2	1:B:270:HIS:CD2	2.82	0.47
1:A:160:LEU:HD11	1:A:199:ILE:HG23	1.97	0.47
1:C:271:ASN:HD21	1:C:273:PHE:HB2	1.80	0.47
1:B:267:ASN:CG	1:B:270:HIS:CD2	2.78	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HB3	1:A:270:HIS:CD2	2.50	0.46
1:A:187:LEU:HD21	1:A:195:LEU:HD12	1.96	0.46
1:B:192:ARG:NH2	1:B:270:HIS:O	2.39	0.46
1:A:119:ILE:HD11	1:A:170:ALA:HB1	1.96	0.46
1:A:191:GLU:OE2	1:B:256:ARG:NH2	2.48	0.46
1:D:77:ARG:HD2	3:D:372:GNP:O3G	2.16	0.46
1:D:143:ASP:OD2	1:D:145:ARG:HD3	2.15	0.46
1:D:150:PHE:HD1	1:D:178:VAL:HB	1.81	0.45
1:D:226:GLU:HG2	1:D:229:ARG:HH12	1.81	0.45
1:C:264:GLU:H	1:C:270:HIS:CD2	2.17	0.44
1:B:143:ASP:OD1	1:B:145:ARG:NH2	2.50	0.44
1:A:190:LYS:H	1:A:190:LYS:HD2	1.81	0.44
1:B:160:LEU:HD23	1:B:202:GLU:HB2	1.98	0.44
1:A:267:ASN:ND2	1:A:270:HIS:CD2	2.85	0.44
1:A:192:ARG:NH2	1:A:270:HIS:O	2.37	0.44
1:B:47:GLY:HA2	1:B:77:ARG:HH12	1.82	0.44
1:B:245:LEU:HA	1:B:254:ARG:HA	2.00	0.44
1:A:121:TYR:O	1:A:125:GLN:HG2	2.18	0.44
1:C:54:ILE:HA	1:C:54:ILE:HD12	1.68	0.44
1:C:118:ILE:O	1:C:122:ILE:HG23	2.17	0.43
1:B:34:LYS:HB2	1:B:140:HIS:CE1	2.53	0.43
1:D:266:GLU:HG2	1:D:274:LEU:HD21	2.00	0.43
1:C:222:GLU:HG3	1:C:223:ASP:H	1.84	0.43
1:B:294:LEU:O	1:B:298:ASN:ND2	2.52	0.43
1:D:201:ASP:O	1:D:205:GLU:HB2	2.18	0.43
1:C:187:LEU:HD21	1:C:195:LEU:HD12	1.99	0.43
1:B:176:ASN:ND2	1:B:291:THR:HG23	2.34	0.43
1:A:267:ASN:HB3	1:A:270:HIS:HD2	1.84	0.42
1:D:195:LEU:HD22	1:D:199:ILE:HG13	2.00	0.42
1:B:53:LEU:HD22	1:B:152:PHE:HZ	1.84	0.42
1:D:213:LEU:HD21	1:D:231:LEU:HD23	2.01	0.42
1:C:139:ARG:HG3	1:C:139:ARG:HH11	1.80	0.42
1:D:147:HIS:HD2	1:D:291:THR:CG2	2.25	0.42
1:A:176:ASN:ND2	1:A:291:THR:HG23	2.33	0.42
1:A:143:ASP:OD2	1:A:145:ARG:HD3	2.18	0.42
1:A:240:VAL:HG11	1:A:263:VAL:HG11	2.01	0.42
1:C:191:GLU:OE2	3:D:372:GNP:O2'	2.28	0.42
1:B:143:ASP:CG	1:B:145:ARG:HH21	2.22	0.42
1:C:143:ASP:OD2	1:C:145:ARG:HD3	2.18	0.42
1:D:264:GLU:HG3	1:D:270:HIS:CD2	2.55	0.42
1:A:108:ALA:O	1:A:109:ILE:HG12	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ASP:O	1:D:117:THR:HG22	2.19	0.42
1:D:192:ARG:NH2	1:D:270:HIS:O	2.33	0.42
1:D:125:GLN:NE2	1:D:125:GLN:CA	2.83	0.42
1:D:58:PHE:CE2	1:D:86:VAL:HG23	2.54	0.42
1:D:284:MET:O	1:D:288:GLN:HB2	2.20	0.42
1:C:254:ARG:HA	1:C:255:GLY:HA3	1.78	0.42
1:B:138:ARG:NE	1:B:141:ILE:HD11	2.35	0.42
1:B:137:ASN:HD22	1:B:137:ASN:HA	1.66	0.42
1:C:119:ILE:HD11	1:C:170:ALA:HB1	2.02	0.42
1:A:111:CYS:HB2	1:A:163:LEU:HD12	2.02	0.42
1:A:127:GLU:OE1	1:A:303:ARG:HD2	2.21	0.41
1:D:134:SER:HA	1:D:135:GLY:HA2	1.60	0.41
1:B:239:VAL:HG11	1:B:276:LEU:HD22	2.01	0.41
1:C:121:TYR:O	1:C:124:GLU:HB3	2.20	0.41
1:C:126:PHE:HB3	1:C:299:PHE:CD2	2.55	0.41
1:C:264:GLU:CG	1:C:270:HIS:CD2	3.02	0.41
1:A:160:LEU:CD1	1:A:199:ILE:HG23	2.50	0.41
1:D:277:ARG:O	1:D:281:ILE:HG12	2.20	0.41
1:D:292:GLN:HA	1:D:296:TYR:HB3	2.02	0.41
1:C:172:HIS:CD2	1:C:209:LYS:HB2	2.56	0.41
1:A:138:ARG:O	1:A:141:ILE:HG13	2.20	0.41
1:D:36:PHE:CZ	1:D:288:GLN:NE2	2.77	0.41
1:B:48:LEU:O	1:B:182:ALA:HB1	2.21	0.40
1:A:77:ARG:HG3	4:A:310:HOH:O	2.21	0.40
1:B:80:GLN:HE21	1:B:80:GLN:HB2	1.53	0.40
1:D:172:HIS:CD2	1:D:209:LYS:HD3	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	246/274 (90%)	240 (98%)	5 (2%)	1 (0%)	39	74
1	B	244/274 (89%)	238 (98%)	4 (2%)	2 (1%)	24	60
1	C	242/274 (88%)	238 (98%)	3 (1%)	1 (0%)	39	74
1	D	233/274 (85%)	225 (97%)	7 (3%)	1 (0%)	39	74
All	All	965/1096 (88%)	941 (98%)	19 (2%)	5 (0%)	34	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	ILE
1	A	255	GLY
1	C	255	GLY
1	B	255	GLY
1	D	255	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	230/248 (93%)	199 (86%)	31 (14%)	5	13
1	B	230/248 (93%)	203 (88%)	27 (12%)	7	19
1	C	229/248 (92%)	202 (88%)	27 (12%)	6	19
1	D	220/248 (89%)	193 (88%)	27 (12%)	6	17
All	All	909/992 (92%)	797 (88%)	112 (12%)	6	17

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	43	VAL
1	A	75	ILE
1	A	79	VAL
1	A	80	GLN
1	A	85	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	90	GLU
1	A	95	LEU
1	A	109	ILE
1	A	110	ASN
1	A	117	THR
1	A	124	GLU
1	A	125	GLN
1	A	134	SER
1	A	139	ARG
1	A	145	ARG
1	A	160	LEU
1	A	163	LEU
1	A	167	PHE
1	A	172	HIS
1	A	187	LEU
1	A	188	THR
1	A	195	LEU
1	A	210	ILE
1	A	224	PHE
1	A	229	ARG
1	A	231	LEU
1	A	254	ARG
1	A	257	LEU
1	A	262	VAL
1	A	303	ARG
1	B	37	GLU
1	B	43	VAL
1	B	59	LEU
1	B	76	GLU
1	B	91	ARG
1	B	95	LEU
1	B	96	ARG
1	B	111	CYS
1	B	117	THR
1	B	130	LEU
1	B	140	HIS
1	B	145	ARG
1	B	167	PHE
1	B	172	HIS
1	B	187	LEU
1	B	188	THR
1	B	195	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	210	ILE
1	B	228	THR
1	B	245	LEU
1	B	246	ILE
1	B	247	GLU
1	B	253	VAL
1	B	257	LEU
1	B	262	VAL
1	B	302	GLU
1	B	303	ARG
1	C	40	LEU
1	C	43	VAL
1	C	54	ILE
1	C	84	SER
1	C	91	ARG
1	C	117	THR
1	C	122	ILE
1	C	138	ARG
1	C	139	ARG
1	C	145	ARG
1	C	160	LEU
1	C	163	LEU
1	C	167	PHE
1	C	172	HIS
1	C	187	LEU
1	C	188	THR
1	C	195	LEU
1	C	210	ILE
1	C	235	ILE
1	C	244	GLN
1	C	245	LEU
1	C	257	LEU
1	C	266	GLU
1	C	270	HIS
1	C	277	ARG
1	C	279	MET
1	C	303	ARG
1	D	43	VAL
1	D	52	THR
1	D	53	LEU
1	D	54	ILE
1	D	58	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	80	GLN
1	D	85	THR
1	D	91	ARG
1	D	98	THR
1	D	109	ILE
1	D	110	ASN
1	D	124	GLU
1	D	125	GLN
1	D	141	ILE
1	D	145	ARG
1	D	163	LEU
1	D	167	PHE
1	D	187	LEU
1	D	188	THR
1	D	195	LEU
1	D	200	LEU
1	D	205	GLU
1	D	207	SER
1	D	210	ILE
1	D	249	LYS
1	D	257	LEU
1	D	270	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	125	GLN
1	A	131	HIS
1	A	172	HIS
1	A	270	HIS
1	A	283	HIS
1	A	298	ASN
1	B	80	GLN
1	B	137	ASN
1	B	158	HIS
1	B	172	HIS
1	B	173	ASN
1	B	270	HIS
1	C	172	HIS
1	C	244	GLN
1	C	270	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	271	ASN
1	C	292	GLN
1	D	80	GLN
1	D	110	ASN
1	D	125	GLN
1	D	172	HIS
1	D	270	HIS
1	D	271	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](#)

Of 8 ligands modelled in this entry, 4 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	GNP	A	372	2	28,34,34	1.73	5 (17%)	33,54,54	2.42	10 (30%)
3	GNP	B	372	2	28,34,34	1.76	6 (21%)	33,54,54	2.35	10 (30%)
3	GNP	C	372	2	28,34,34	1.73	5 (17%)	33,54,54	2.25	8 (24%)
3	GNP	D	372	2	28,34,34	1.81	6 (21%)	33,54,54	2.41	9 (27%)

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	GNP	A	372	2	-	0/12/38/38	0/3/3/3
3	GNP	B	372	2	-	0/12/38/38	0/3/3/3
3	GNP	C	372	2	-	1/12/38/38	0/3/3/3
3	GNP	D	372	2	-	0/12/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	372	GNP	PB-O3A	-3.91	1.54	1.59
3	C	372	GNP	PB-O3A	-3.90	1.54	1.59
3	B	372	GNP	PB-O3A	-3.49	1.54	1.59
3	A	372	GNP	PB-O3A	-3.38	1.54	1.59
3	C	372	GNP	PB-O2B	-2.96	1.48	1.56
3	A	372	GNP	PB-O2B	-2.90	1.48	1.56
3	B	372	GNP	PB-O2B	-2.87	1.48	1.56
3	D	372	GNP	PB-O2B	-2.87	1.48	1.56
3	B	372	GNP	C8-N7	-2.14	1.30	1.34
3	D	372	GNP	PG-O3G	-2.08	1.50	1.56
3	C	372	GNP	PG-O2G	-2.06	1.50	1.56
3	B	372	GNP	PB-O1B	2.14	1.48	1.46
3	D	372	GNP	PB-O1B	2.61	1.49	1.46
3	A	372	GNP	PB-O1B	2.95	1.49	1.46
3	A	372	GNP	C6-N1	3.19	1.39	1.33
3	C	372	GNP	C6-N1	3.44	1.39	1.33
3	B	372	GNP	C6-N1	3.56	1.39	1.33
3	D	372	GNP	C6-N1	3.66	1.39	1.33
3	D	372	GNP	PG-O1G	4.23	1.51	1.46
3	B	372	GNP	PG-O1G	4.67	1.51	1.46
3	A	372	GNP	PG-O1G	4.68	1.51	1.46
3	C	372	GNP	PG-O1G	4.79	1.51	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	372	GNP	C5-C6-N1	-8.40	112.11	123.59
3	D	372	GNP	C5-C6-N1	-8.05	112.58	123.59
3	B	372	GNP	C5-C6-N1	-7.94	112.73	123.59
3	C	372	GNP	C5-C6-N1	-7.43	113.43	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	372	GNP	O3G-PG-O1G	-3.55	104.05	113.49
3	D	372	GNP	O3G-PG-O1G	-3.50	104.20	113.49
3	A	372	GNP	O3G-PG-O1G	-3.34	104.61	113.49
3	C	372	GNP	O3G-PG-O1G	-3.04	105.42	113.49
3	D	372	GNP	N3-C2-N1	-3.03	122.83	127.44
3	A	372	GNP	O1G-PG-N3B	-2.66	107.82	111.90
3	C	372	GNP	N3-C2-N1	-2.51	123.63	127.44
3	B	372	GNP	PA-O3A-PB	-2.50	124.30	132.67
3	D	372	GNP	C6-C5-C4	-2.40	118.03	120.90
3	A	372	GNP	N3-C2-N1	-2.32	123.91	127.44
3	B	372	GNP	N3-C2-N1	-2.30	123.94	127.44
3	D	372	GNP	O1G-PG-N3B	-2.21	108.50	111.90
3	A	372	GNP	PA-O3A-PB	-2.13	125.51	132.67
3	A	372	GNP	N2-C2-N3	2.08	121.79	117.80
3	A	372	GNP	O3G-PG-O2G	2.10	113.80	107.58
3	D	372	GNP	O3G-PG-O2G	2.17	114.00	107.58
3	B	372	GNP	N2-C2-N3	2.20	122.02	117.80
3	C	372	GNP	N2-C2-N3	2.31	122.24	117.80
3	B	372	GNP	C4-C5-N7	2.46	111.75	109.48
3	C	372	GNP	C4-C5-N7	2.52	111.80	109.48
3	B	372	GNP	O2B-PB-O1B	2.69	115.61	110.00
3	C	372	GNP	O3G-PG-O2G	2.80	115.89	107.58
3	A	372	GNP	O2B-PB-O1B	2.82	115.88	110.00
3	D	372	GNP	C4-C5-N7	3.03	112.27	109.48
3	B	372	GNP	O3A-PA-O5'	3.03	110.98	102.94
3	B	372	GNP	O3G-PG-O2G	3.14	116.89	107.58
3	A	372	GNP	C4-C5-N7	3.27	112.48	109.48
3	D	372	GNP	O2B-PB-O1B	3.33	116.94	110.00
3	C	372	GNP	O2B-PB-O1B	3.40	117.10	110.00
3	C	372	GNP	C6-N1-C2	5.74	123.91	115.94
3	B	372	GNP	C6-N1-C2	5.98	124.24	115.94
3	A	372	GNP	C6-N1-C2	6.56	125.05	115.94
3	D	372	GNP	C6-N1-C2	6.71	125.26	115.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	372	GNP	O1B-PB-N3B-PG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	372	GNP	1	0
3	D	372	GNP	3	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	254/274 (92%)	0.47	26 (10%) 9 5	15, 29, 46, 60	0
1	B	252/274 (91%)	0.52	23 (9%) 11 7	13, 28, 46, 58	0
1	C	250/274 (91%)	0.56	28 (11%) 7 4	15, 30, 51, 60	0
1	D	243/274 (88%)	0.57	28 (11%) 6 4	13, 32, 51, 57	0
All	All	999/1096 (91%)	0.53	105 (10%) 8 5	13, 30, 49, 60	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	GLY	6.6
1	C	249	LYS	6.4
1	D	140	HIS	6.3
1	C	223	ASP	5.4
1	A	249	LYS	5.0
1	B	226	GLU	4.9
1	C	222	GLU	4.8
1	C	250	GLY	4.7
1	B	223	ASP	4.7
1	C	75	ILE	4.6
1	B	93	VAL	4.4
1	B	305	LYS	4.3
1	C	92	GLY	4.3
1	D	226	GLU	4.2
1	D	249	LYS	4.1
1	B	91	ARG	4.1
1	D	91	ARG	3.9
1	D	247	GLU	3.9
1	B	253	VAL	3.8
1	C	34	LYS	3.7
1	A	250	GLY	3.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	3.6
1	D	134	SER	3.6
1	D	215	ASP	3.5
1	A	215	ASP	3.5
1	C	243	ASN	3.5
1	B	75	ILE	3.4
1	D	35	GLY	3.4
1	A	221	ASP	3.4
1	D	216	ALA	3.4
1	A	91	ARG	3.3
1	A	34	LYS	3.3
1	C	35	GLY	3.3
1	A	223	ASP	3.2
1	A	252	LYS	3.2
1	D	92	GLY	3.2
1	C	221	ASP	3.1
1	D	131	HIS	3.1
1	C	93	VAL	3.1
1	C	226	GLU	3.1
1	C	91	ARG	3.0
1	B	112	ARG	3.0
1	D	285	GLN	3.0
1	B	90	GLU	3.0
1	B	138	ARG	2.9
1	B	139	ARG	2.9
1	D	128	ARG	2.9
1	B	216	ALA	2.9
1	B	222	GLU	2.9
1	C	298	ASN	2.9
1	D	141	ILE	2.8
1	D	76	GLU	2.8
1	C	158	HIS	2.8
1	A	217	GLU	2.8
1	A	138	ARG	2.8
1	A	35	GLY	2.7
1	A	92	GLY	2.7
1	B	76	GLU	2.7
1	D	93	VAL	2.7
1	A	224	PHE	2.7
1	D	133	GLU	2.7
1	C	248	ALA	2.7
1	D	158	HIS	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	74	LYS	2.6
1	C	229	ARG	2.6
1	D	135	GLY	2.6
1	C	76	GLU	2.6
1	C	244	GLN	2.6
1	A	197	LYS	2.5
1	D	250	GLY	2.5
1	D	115	PHE	2.5
1	C	215	ASP	2.5
1	A	139	ARG	2.4
1	D	106	GLY	2.4
1	B	215	ASP	2.4
1	C	108	ALA	2.4
1	A	140	HIS	2.4
1	A	248	ALA	2.3
1	D	36	PHE	2.3
1	D	230	LEU	2.3
1	B	108	ALA	2.3
1	A	230	LEU	2.3
1	C	112	ARG	2.3
1	A	247	GLU	2.3
1	B	244	GLN	2.3
1	C	304	LEU	2.3
1	B	137	ASN	2.3
1	D	301	SER	2.2
1	C	90	GLU	2.2
1	D	229	ARG	2.2
1	C	140	HIS	2.2
1	A	90	GLU	2.2
1	A	226	GLU	2.2
1	A	93	VAL	2.2
1	A	285	GLN	2.2
1	A	74	LYS	2.2
1	C	110	ASN	2.2
1	A	137	ASN	2.1
1	D	248	ALA	2.1
1	C	138	ARG	2.1
1	D	90	GLU	2.1
1	C	224	PHE	2.1
1	B	301	SER	2.0
1	B	224	PHE	2.0
1	B	225	LYS	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, 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(Å <sup>2</sup> )	Q<0.9
2	MG	B	371	1/1	0.94	0.24	-0.02	29,29,29,29	0
3	GNP	B	372	32/32	0.97	0.22	-0.18	28,32,36,37	0
3	GNP	D	372	32/32	0.97	0.20	-0.21	29,32,33,34	0
3	GNP	A	372	32/32	0.97	0.20	-0.32	27,28,29,29	0
3	GNP	C	372	32/32	0.96	0.20	-0.33	37,38,40,40	0
2	MG	D	371	1/1	0.93	0.14	-0.88	36,36,36,36	0
2	MG	C	371	1/1	0.86	0.13	-1.03	42,42,42,42	0
2	MG	A	371	1/1	0.91	0.13	-1.91	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.