



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TL7  
Title : Complex Of Gs- With The Catalytic Domains Of Mammalian Adenylyl Cyclase: Complex With 2'(3')-O-(N-methylanthraniloyl)-guanosine 5'-triphosphate and Mn  
Authors : Mou, T.C.; Gille, A.; Seifert, R.J.; Sprang, S.R.  
Deposited on : 2004-06-09  
Resolution : 2.80 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 (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

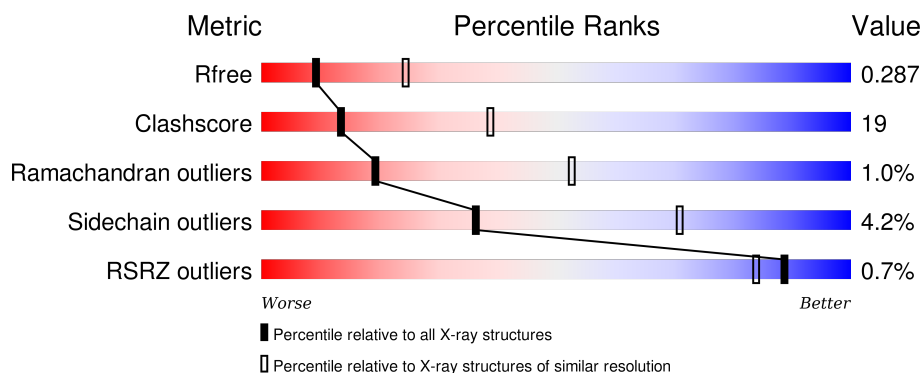
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	217	<div> <div></div> <div>47%</div> <div>36%</div> <div>•</div> <div>13%</div> </div>
2	B	212	<div> <div>54%</div> <div>32%</div> <div>•</div> <div>11%</div> </div>
3	C	402	<div> <div>54%</div> <div>28%</div> <div>18%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	C	403	-	-	-	X
8	FOK	A	101	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5770 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 Adenylate cyclase, type V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1476	929	259	271	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	476	MET	VAL	CONFLICT	UNP P30803

- Molecule 2 is a protein called Adenylate cyclase, type II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	0	0
			1467	936	242	279	10			

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s), alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	330	Total	C	N	O	S	0	0	0
			2702	1714	470	505	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	71	GLY	-	CONFLICT	UNP P04896
C	?	-	GLN	DELETION	UNP P04896
C	79	ASN	ALA	CONFLICT	UNP P04896
C	81	LYS	ARG	CONFLICT	UNP P04896
C	395	GLY	-	EXPRESSION TAG	UNP P04896
C	396	GLY	-	EXPRESSION TAG	UNP P04896
C	397	HIS	-	EXPRESSION TAG	UNP P04896
C	398	HIS	-	EXPRESSION TAG	UNP P04896
C	399	HIS	-	EXPRESSION TAG	UNP P04896

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Chain	Residue	Modelled	Actual	Comment	Reference
C	400	HIS	-	EXPRESSION TAG	UNP P04896
C	401	HIS	-	EXPRESSION TAG	UNP P04896
C	402	HIS	-	EXPRESSION TAG	UNP P04896

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

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

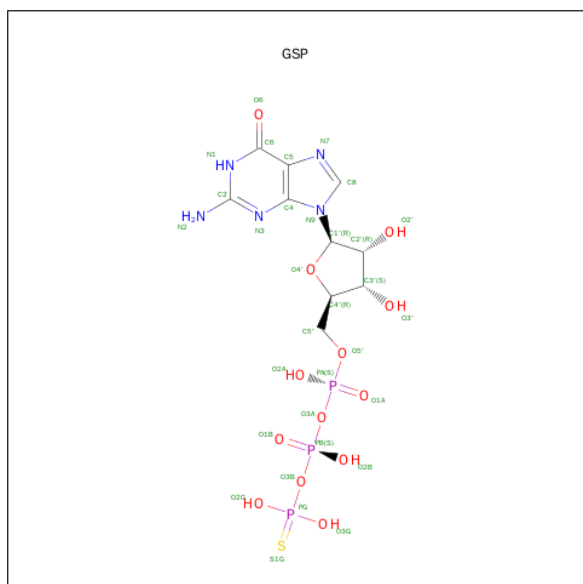
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

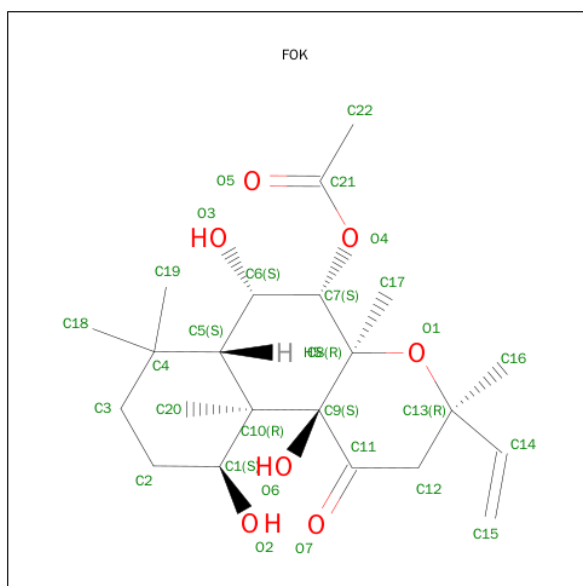
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mn 2 2	0	0

- Molecule 7 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



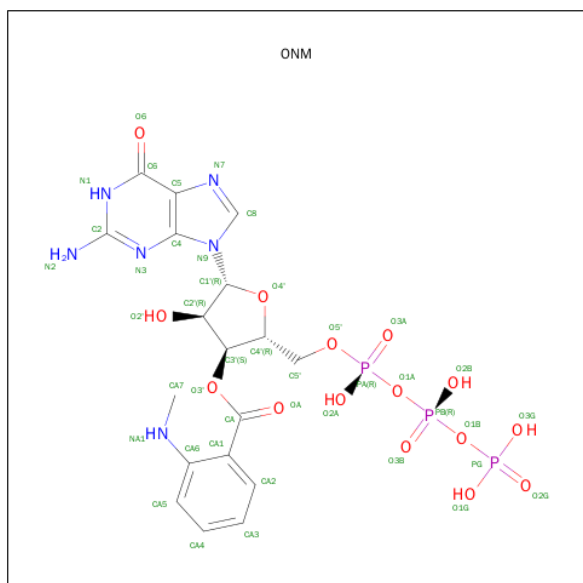
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	S	
			32	10	5	13	3	1	
								0	0

- Molecule 8 is FORSKOLIN (three-letter code: FOK) (formula:  $C_{22}H_{34}O_7$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C O		
			29	22 7	0	0

- Molecule 9 is 3'-O-(N-METHYLANTHRANILOYL)-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: ONM) (formula:  $C_{18}H_{23}N_6O_{15}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			42	18	6	15	3		

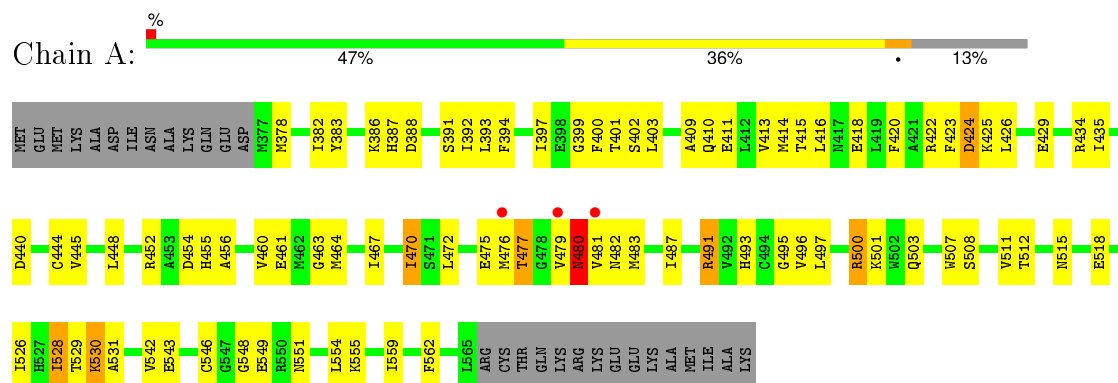
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		
10	B	9	Total	O	0	0
			9	9		
10	C	8	Total	O	0	0
			8	8		

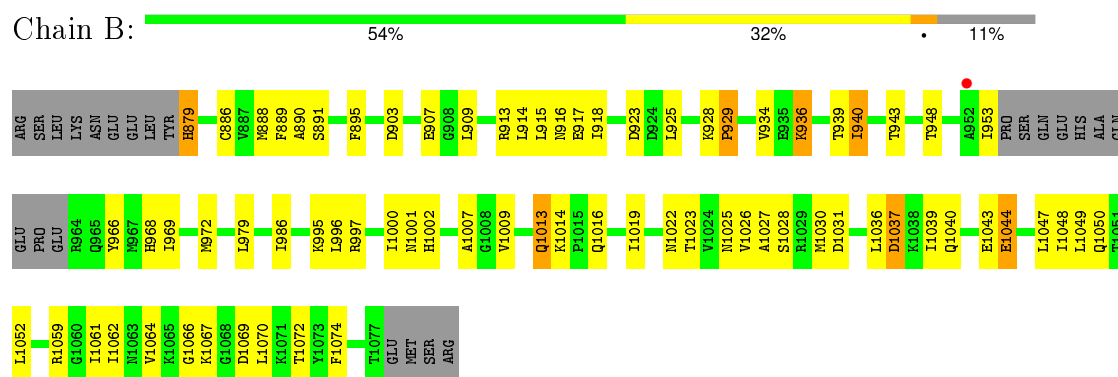
### 3 Residue-property plots

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.

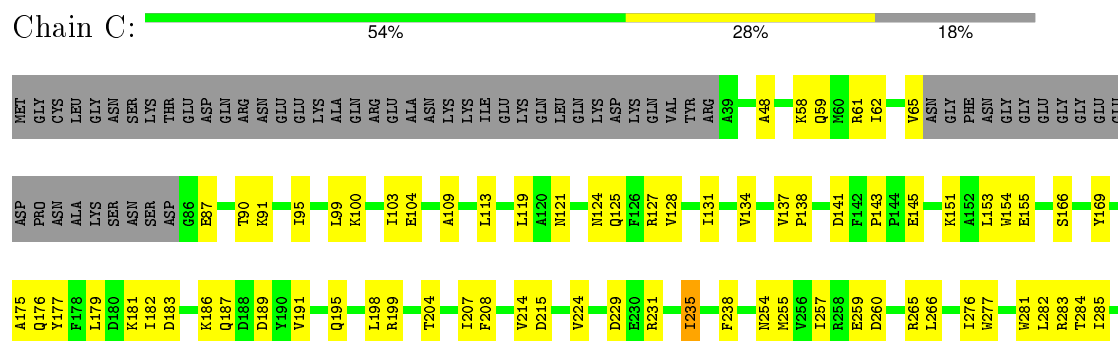
- Molecule 1: Adenylate cyclase, type V



- Molecule 2: Adenylate cyclase, type II



- Molecule 3: Guanine nucleotide-binding protein G(s), alpha subunit







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.23 Å   133.60 Å   70.35 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	14.99 – 2.80 48.44 – 2.69	Depositor EDS
% Data completeness (in resolution range)	81.2 (14.99-2.80) 76.5 (48.44-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.69 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.254   ,   0.298 0.253   ,   0.287	Depositor DCC
$R_{free}$ test set	1104 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	1.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	1 of 24256 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	5770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, MG, ONM, CL, MN, FOK

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	0.33	0/1504	0.61	0/2027
2	B	0.38	0/1492	0.58	0/2014
3	C	0.36	0/2759	0.58	0/3733
All	All	0.35	0/5755	0.59	0/7774

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1476	0	1450	82	0
2	B	1467	0	1470	64	0
3	C	2702	0	2652	78	0
4	C	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	0	0
7	C	32	0	12	1	0
8	A	29	0	34	2	0
9	A	42	0	19	1	0
10	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	9	0	0	0	0
10	C	8	0	0	2	0
All	All	5770	0	5637	213	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 19.

All (213) 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:477:THR:HB	1:A:479:VAL:HG12	1.43	0.97
1:A:554:LEU:HA	1:A:559:ILE:HD12	1.58	0.84
3:C:321:PRO:HG2	3:C:324:ALA:HB2	1.60	0.83
3:C:207:ILE:HG12	3:C:224:VAL:HG12	1.61	0.83
1:A:420:PHE:HA	1:A:423:PHE:HB2	1.63	0.81
1:A:500:ARG:HH11	1:A:500:ARG:HB3	1.46	0.80
2:B:886:CYS:HB2	2:B:969:ILE:HD13	1.66	0.77
2:B:1030:MET:HE3	2:B:1040:GLN:HG2	1.66	0.76
1:A:542:VAL:HB	1:A:562:PHE:HB3	1.68	0.75
2:B:953:ILE:HD12	2:B:953:ILE:H	1.51	0.75
1:A:378:MET:HE1	3:C:283:ARG:N	2.02	0.75
3:C:121:ASN:HB2	3:C:124:ASN:ND2	2.06	0.71
1:A:530:LYS:HD2	1:A:531:ALA:N	2.06	0.71
1:A:470:ILE:HG13	1:A:483:MET:HG2	1.73	0.70
3:C:257:ILE:HD13	3:C:259:GLU:HB2	1.74	0.69
1:A:546:CYS:O	1:A:549:GLU:HG2	1.93	0.68
2:B:918:ILE:HG12	2:B:986:ILE:HD13	1.75	0.68
1:A:477:THR:HB	1:A:479:VAL:CG1	2.23	0.68
1:A:463:GLY:O	1:A:467:ILE:HG12	1.94	0.68
2:B:1026:VAL:O	2:B:1030:MET:HG2	1.95	0.66
2:B:936:LYS:HE3	2:B:939:THR:HG23	1.77	0.66
8:A:101:FOK:H201	8:A:101:FOK:H173	1.78	0.66
3:C:121:ASN:HB2	3:C:124:ASN:HD22	1.59	0.65
9:A:100:ONM:HA72	2:B:1022:ASN:HB2	1.79	0.65
1:A:452:ARG:HD3	1:A:454:ASP:HB3	1.79	0.65
3:C:151:LYS:O	3:C:155:GLU:HG2	1.98	0.64
2:B:888:MET:HG3	2:B:1000:ILE:HG12	1.79	0.64
1:A:528:ILE:HD13	1:A:528:ILE:H	1.62	0.63
1:A:508:SER:OG	1:A:511:VAL:HG23	1.98	0.63
3:C:195:GLN:HA	3:C:198:LEU:HD12	1.80	0.63
3:C:255:MET:HB2	3:C:265:ARG:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:THR:HG21	1:A:481:VAL:HG11	1.81	0.63
1:A:529:THR:HG22	1:A:530:LYS:H	1.64	0.62
3:C:119:LEU:HD11	3:C:128:VAL:HG21	1.81	0.62
1:A:452:ARG:HG2	1:A:454:ASP:H	1.64	0.62
2:B:1009:VAL:HG13	2:B:1016:GLN:O	2.00	0.61
2:B:940:ILE:H	2:B:940:ILE:HD12	1.66	0.61
3:C:166:SER:HA	3:C:169:TYR:CE2	2.35	0.61
1:A:529:THR:HG22	1:A:530:LYS:N	2.16	0.60
3:C:179:LEU:O	3:C:182:ILE:HG12	2.00	0.60
2:B:1049:LEU:HA	2:B:1052:LEU:HD12	1.83	0.60
8:A:101:FOK:H202	8:A:101:FOK:H193	1.83	0.60
3:C:87:GLU:O	3:C:90:THR:HG22	2.02	0.59
3:C:326:PRO:HG3	3:C:335:THR:HG21	1.84	0.59
2:B:1001:ASN:HB3	2:B:1027:ALA:HB2	1.83	0.59
2:B:1043:GLU:O	2:B:1047:LEU:HG	2.03	0.59
2:B:1048:ILE:O	2:B:1052:LEU:HG	2.03	0.57
3:C:365:CYS:H	3:C:371:ASN:ND2	2.02	0.57
2:B:934:VAL:HA	2:B:948:THR:HG22	1.87	0.57
2:B:891:SER:HB3	2:B:943:THR:HG23	1.86	0.56
1:A:392:ILE:HD13	1:A:511:VAL:HG22	1.87	0.56
1:A:434:ARG:HD2	1:A:435:ILE:N	2.20	0.56
1:A:456:ALA:O	1:A:460:VAL:HG23	2.07	0.55
2:B:1064:VAL:HG21	2:B:1070:LEU:HD12	1.88	0.55
3:C:331:ASP:HB3	3:C:334:VAL:HG23	1.88	0.55
2:B:1067:LYS:HD3	2:B:1070:LEU:HD11	1.87	0.55
1:A:470:ILE:O	1:A:470:ILE:HD13	2.06	0.55
3:C:100:LYS:O	3:C:104:GLU:HG2	2.06	0.54
3:C:255:MET:CB	3:C:265:ARG:HD2	2.38	0.54
3:C:103:ILE:HG23	3:C:104:GLU:N	2.23	0.54
3:C:307:LYS:HB2	3:C:310:ASP:OD2	2.08	0.54
1:A:548:GLY:O	1:A:555:LYS:HB2	2.07	0.54
1:A:416:LEU:HG	1:A:420:PHE:HE2	1.73	0.53
3:C:364:THR:HA	3:C:371:ASN:HD21	1.74	0.53
3:C:235:ILE:HD13	3:C:235:ILE:O	2.09	0.53
2:B:1047:LEU:HA	2:B:1050:GLN:NE2	2.23	0.53
2:B:890:ALA:HB1	2:B:996:LEU:HD21	1.90	0.52
1:A:378:MET:CE	3:C:284:THR:H	2.21	0.52
3:C:59:GLN:OE1	3:C:59:GLN:HA	2.10	0.52
1:A:501:LYS:HB2	2:B:936:LYS:HD2	1.91	0.52
1:A:425:LYS:O	1:A:429:GLU:HG3	2.10	0.52
3:C:131:ILE:HG13	3:C:153:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:ASP:HA	3:C:186:LYS:HE2	1.91	0.51
2:B:891:SER:HB3	2:B:943:THR:OG1	2.10	0.51
3:C:297:LEU:HD21	3:C:341:ILE:HD12	1.92	0.51
2:B:891:SER:O	2:B:996:LEU:HD12	2.10	0.51
1:A:383:TYR:O	1:A:495:GLY:HA3	2.11	0.51
1:A:526:ILE:HD12	1:A:526:ILE:N	2.26	0.50
3:C:127:ARG:O	3:C:131:ILE:HG12	2.11	0.50
3:C:124:ASN:HA	3:C:127:ARG:HD2	1.93	0.50
1:A:551:ASN:HB3	1:A:554:LEU:HD12	1.94	0.50
1:A:391:SER:O	1:A:445:VAL:HG23	2.12	0.50
1:A:512:THR:O	1:A:515:ASN:HB3	2.11	0.50
2:B:1059:ARG:NH2	2:B:1062:ILE:HD11	2.27	0.49
3:C:386:MET:HB2	3:C:388:LEU:HG	1.94	0.49
1:A:410:GLN:O	1:A:414:MET:HG3	2.12	0.49
1:A:382:ILE:HG12	2:B:913:ARG:NH1	2.27	0.49
2:B:1025:ASN:HA	2:B:1028:SER:HB3	1.94	0.49
1:A:393:LEU:HD12	1:A:487:ILE:HD11	1.95	0.49
2:B:1059:ARG:CZ	2:B:1062:ILE:HD11	2.43	0.49
1:A:472:LEU:O	1:A:475:GLU:HG2	2.12	0.49
3:C:199:ARG:HA	7:C:405:GSP:O2'	2.13	0.49
3:C:281:TRP:O	3:C:282:LEU:HD23	2.13	0.49
2:B:995:LYS:HD2	2:B:1037:ASP:OD1	2.13	0.49
1:A:397:ILE:HA	1:A:482:ASN:O	2.13	0.48
1:A:422:ARG:O	1:A:426:LEU:HG	2.12	0.48
3:C:109:ALA:O	3:C:113:LEU:HG	2.14	0.48
1:A:470:ILE:HD12	1:A:482:ASN:HA	1.96	0.48
3:C:176:GLN:N	10:C:411:HOH:O	2.47	0.48
2:B:928:LYS:HB3	2:B:929:PRO:CD	2.44	0.48
1:A:400:PHE:O	1:A:403:LEU:HB3	2.14	0.47
1:A:400:PHE:CD1	1:A:403:LEU:HD23	2.48	0.47
3:C:99:LEU:HD11	3:C:182:ILE:HD13	1.96	0.47
1:A:409:ALA:O	1:A:413:VAL:HG23	2.14	0.47
3:C:368:ASP:O	3:C:372:ILE:HG12	2.13	0.47
1:A:415:THR:O	1:A:418:GLU:HB3	2.15	0.47
1:A:497:LEU:HD22	2:B:916:ASN:HB2	1.95	0.47
1:A:386:LYS:HE3	1:A:491:ARG:HD3	1.97	0.47
1:A:507:TRP:O	1:A:508:SER:HB3	2.15	0.47
1:A:434:ARG:C	1:A:434:ARG:HD2	2.35	0.47
3:C:176:GLN:HB3	10:C:411:HOH:O	2.15	0.47
3:C:366:ALA:HA	3:C:372:ILE:HD11	1.96	0.47
2:B:925:LEU:HD12	2:B:979:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:895:PHE:CZ	2:B:915:LEU:HB2	2.50	0.47
2:B:915:LEU:HA	2:B:918:ILE:HD12	1.97	0.46
2:B:1009:VAL:HG13	2:B:1016:GLN:C	2.36	0.46
1:A:401:THR:HG21	2:B:1066:GLY:HA3	1.95	0.46
3:C:254:ASN:OD1	3:C:255:MET:HG3	2.16	0.46
3:C:99:LEU:HD11	3:C:182:ILE:CD1	2.44	0.46
2:B:879:HIS:HB2	2:B:1007:ALA:O	2.16	0.46
1:A:393:LEU:HD12	1:A:487:ILE:CD1	2.45	0.46
3:C:266:LEU:HD23	3:C:312:PHE:CZ	2.50	0.46
1:A:378:MET:HE1	3:C:283:ARG:H	1.79	0.46
2:B:948:THR:HG23	2:B:972:MET:SD	2.55	0.46
1:A:530:LYS:C	1:A:530:LYS:HD2	2.36	0.46
2:B:1059:ARG:HB2	2:B:1074:PHE:CE2	2.51	0.46
3:C:380:ARG:O	3:C:384:GLN:HG2	2.16	0.46
2:B:903:ASP:HA	2:B:907:GLU:OE2	2.15	0.46
3:C:204:THR:HG23	3:C:208:PHE:CE1	2.51	0.46
3:C:143:PRO:HB2	3:C:145:GLU:OE2	2.16	0.46
1:A:382:ILE:HD12	1:A:382:ILE:O	2.16	0.46
3:C:284:THR:C	3:C:357:HIS:HB3	2.36	0.46
2:B:891:SER:HB3	2:B:943:THR:CG2	2.45	0.46
1:A:424:ASP:OD2	2:B:1013:GLN:HB2	2.15	0.45
1:A:403:LEU:HD22	1:A:481:VAL:HG12	1.98	0.45
1:A:500:ARG:NH1	1:A:500:ARG:HB3	2.24	0.45
1:A:528:ILE:HD11	1:A:562:PHE:HB2	1.98	0.45
3:C:353:GLY:O	3:C:356:ARG:HB2	2.17	0.45
1:A:452:ARG:HG2	1:A:454:ASP:N	2.31	0.45
1:A:435:ILE:HG13	1:A:444:CYS:HA	1.98	0.45
2:B:995:LYS:HB2	2:B:1036:LEU:HD22	1.97	0.45
2:B:966:TYR:HA	2:B:968:HIS:CE1	2.51	0.45
3:C:282:LEU:HD22	3:C:285:ILE:HD12	1.98	0.45
3:C:177:TYR:CE2	3:C:199:ARG:HG3	2.52	0.44
3:C:276:ILE:O	3:C:282:LEU:HD12	2.18	0.44
3:C:375:VAL:O	3:C:378:ASP:HB2	2.17	0.44
3:C:125:GLN:O	3:C:128:VAL:HB	2.18	0.44
3:C:103:ILE:HG23	3:C:104:GLU:H	1.80	0.44
3:C:58:LYS:O	3:C:62:ILE:HG12	2.17	0.44
1:A:378:MET:HE1	3:C:284:THR:H	1.83	0.44
3:C:291:LEU:HD11	3:C:342:ARG:HG3	2.00	0.44
2:B:1039:ILE:N	2:B:1039:ILE:HD12	2.33	0.44
3:C:238:PHE:CD2	3:C:282:LEU:HD21	2.53	0.43
3:C:91:LYS:O	3:C:95:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1061:ILE:CG2	2:B:1069:ASP:HB3	2.47	0.43
2:B:913:ARG:O	2:B:917:GLU:HG2	2.18	0.43
3:C:277:TRP:NE1	3:C:349:SER:HA	2.33	0.43
1:A:496:VAL:HG12	1:A:503:GLN:O	2.18	0.43
2:B:966:TYR:HB3	2:B:969:ILE:HG13	2.01	0.43
1:A:467:ILE:O	1:A:470:ILE:HG22	2.19	0.43
1:A:497:LEU:HD13	2:B:915:LEU:HG	1.99	0.43
2:B:997:ARG:HB3	2:B:1031:ASP:OD1	2.17	0.43
2:B:1030:MET:HB3	2:B:1040:GLN:O	2.19	0.42
2:B:888:MET:HG3	2:B:1000:ILE:CG1	2.49	0.42
3:C:145:GLU:CD	3:C:145:GLU:H	2.22	0.42
3:C:376:PHE:O	3:C:380:ARG:HG3	2.19	0.42
2:B:1007:ALA:HA	2:B:1019:ILE:HG22	2.00	0.42
3:C:293:LYS:HD3	3:C:296:LEU:HD12	2.01	0.42
1:A:416:LEU:HG	1:A:420:PHE:CE2	2.54	0.42
1:A:493:HIS:CE1	2:B:909:LEU:HD13	2.54	0.42
3:C:134:VAL:HA	3:C:137:VAL:HG23	2.02	0.42
3:C:124:ASN:O	3:C:128:VAL:HG23	2.19	0.42
1:A:434:ARG:HH11	1:A:434:ARG:HG3	1.84	0.42
1:A:394:PHE:CB	1:A:518:GLU:HB2	2.50	0.42
1:A:397:ILE:HG12	1:A:440:ASP:HB2	2.01	0.42
1:A:394:PHE:HB2	1:A:518:GLU:HB2	2.01	0.42
3:C:61:ARG:HA	3:C:65:VAL:CG2	2.49	0.42
2:B:928:LYS:CB	2:B:929:PRO:CD	2.98	0.42
3:C:292:ASN:CG	3:C:293:LYS:H	2.23	0.42
3:C:191:VAL:O	3:C:191:VAL:HG13	2.20	0.42
3:C:276:ILE:HG23	3:C:282:LEU:CD1	2.49	0.42
2:B:1002:HIS:C	2:B:1023:THR:HG23	2.40	0.41
2:B:914:LEU:O	2:B:918:ILE:HG13	2.21	0.41
1:A:435:ILE:HD11	1:A:445:VAL:HG12	2.01	0.41
1:A:461:GLU:O	1:A:464:MET:HB2	2.20	0.41
1:A:378:MET:HE2	3:C:284:THR:H	1.84	0.41
1:A:397:ILE:CG1	1:A:440:ASP:HB2	2.50	0.41
1:A:382:ILE:H	1:A:382:ILE:HG13	1.55	0.41
2:B:1030:MET:HE3	2:B:1072:THR:HB	2.02	0.41
3:C:257:ILE:HD11	3:C:260:ASP:CG	2.41	0.41
3:C:254:ASN:HA	3:C:311:TYR:CE2	2.55	0.41
2:B:1044:GLU:HA	2:B:1047:LEU:HD12	2.03	0.41
3:C:317:ARG:HD3	3:C:317:ARG:HA	1.95	0.41
1:A:479:VAL:HG22	1:A:480:ASN:N	2.36	0.41
2:B:1050:GLN:HB2	2:B:1050:GLN:HE21	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:NH2	2:B:1014:LYS:O	2.54	0.41
1:A:391:SER:OG	1:A:456:ALA:HA	2.21	0.41
3:C:297:LEU:O	3:C:301:VAL:HG23	2.21	0.41
1:A:387:HIS:CD2	1:A:448:LEU:HD21	2.56	0.41
3:C:307:LYS:HB3	3:C:309:GLU:CD	2.41	0.41
2:B:1025:ASN:O	2:B:1028:SER:HB3	2.21	0.41
3:C:187:GLN:HB3	3:C:189:ASP:OD1	2.21	0.41
1:A:543:GLU:O	1:A:562:PHE:HA	2.21	0.40
2:B:890:ALA:HA	2:B:997:ARG:O	2.21	0.40
2:B:888:MET:HG2	2:B:889:PHE:N	2.36	0.40
3:C:214:VAL:O	3:C:215:ASP:HB2	2.22	0.40
3:C:362:HIS:HE1	3:C:378:ASP:HB3	1.85	0.40
1:A:452:ARG:O	1:A:455:HIS:HB3	2.21	0.40
2:B:1036:LEU:O	2:B:1037:ASP:HB2	2.21	0.40
1:A:397:ILE:HD13	1:A:483:MET:SD	2.61	0.40
1:A:411:GLU:HA	1:A:414:MET:CE	2.51	0.40
3:C:282:LEU:CD2	3:C:285:ILE:HD12	2.52	0.40
1:A:386:LYS:HB2	1:A:493:HIS:CE1	2.56	0.40

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	187/217 (86%)	161 (86%)	24 (13%)	2 (1%)	17	50
2	B	185/212 (87%)	169 (91%)	15 (8%)	1 (0%)	34	69
3	C	326/402 (81%)	303 (93%)	19 (6%)	4 (1%)	16	47
All	All	698/831 (84%)	633 (91%)	58 (8%)	7 (1%)	19	52

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ASN
3	C	48	ALA
3	C	175	ALA
2	B	929	PRO
3	C	138	PRO
3	C	231	ARG
1	A	399	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	158/182 (87%)	147 (93%)	11 (7%)	19	47
2	B	162/184 (88%)	155 (96%)	7 (4%)	35	70
3	C	297/357 (83%)	289 (97%)	8 (3%)	52	85
All	All	617/723 (85%)	591 (96%)	26 (4%)	36	71

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	ASP
1	A	402	SER
1	A	424	ASP
1	A	470	ILE
1	A	476	MET
1	A	477	THR
1	A	480	ASN
1	A	491	ARG
1	A	500	ARG
1	A	528	ILE
1	A	530	LYS
2	B	879	HIS
2	B	923	ASP
2	B	936	LYS
2	B	940	ILE
2	B	1013	GLN

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Mol	Chain	Res	Type
2	B	1037	ASP
2	B	1044	GLU
3	C	141	ASP
3	C	154	TRP
3	C	181	LYS
3	C	229	ASP
3	C	235	ILE
3	C	354	ASP
3	C	357	HIS
3	C	370	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	387	HIS
1	A	430	ASN
1	A	482	ASN
1	A	493	HIS
1	A	509	ASN
1	A	515	ASN
1	A	537	ASN
2	B	879	HIS
2	B	1001	ASN
2	B	1013	GLN
2	B	1050	GLN
2	B	1063	ASN
2	B	1076	ASN
3	C	93	GLN
3	C	97	ASN
3	C	195	GLN
3	C	362	HIS
3	C	371	ASN
3	C	377	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z  > 2$
9	ONM	A	100	6	36,45,45	3.54	14 (38%)	50,69,69	3.06	28 (56%)
8	FOK	A	101	-	26,31,31	3.10	6 (23%)	35,54,54	1.62	5 (14%)
7	GSP	C	405	4	25,34,34	1.76	5 (20%)	31,54,54	2.74	8 (25%)

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
9	ONM	A	100	6	-	0/28/48/48	0/4/4/4
8	FOK	A	101	-	-	0/7/80/80	0/3/3/3
7	GSP	C	405	4	-	0/15/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	101	FOK	C4-C5	-3.92	1.50	1.56
7	C	405	GSP	C8-N7	-2.30	1.30	1.34
9	A	100	ONM	CA7-NA1	2.05	1.48	1.45
8	A	101	FOK	C12-C11	2.12	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	405	GSP	C2'-C3'	2.14	1.59	1.53
8	A	101	FOK	C6-C7	2.30	1.58	1.53
9	A	100	ONM	CA3-CA4	2.36	1.44	1.38
9	A	100	ONM	O3'-C3'	2.50	1.48	1.44
9	A	100	ONM	CA1-CA	2.72	1.56	1.50
9	A	100	ONM	PG-O2G	2.80	1.60	1.51
7	C	405	GSP	O4'-C1'	2.92	1.44	1.41
9	A	100	ONM	PA-O3A	3.10	1.62	1.51
9	A	100	ONM	PB-O3B	3.21	1.62	1.51
8	A	101	FOK	C17-C8	3.36	1.57	1.51
7	C	405	GSP	C2-N1	3.39	1.41	1.35
9	A	100	ONM	O4'-C1'	3.58	1.45	1.41
9	A	100	ONM	C2-N1	3.79	1.42	1.35
7	C	405	GSP	C6-N1	3.97	1.40	1.33
9	A	100	ONM	C6-N1	5.29	1.42	1.33
8	A	101	FOK	C10-C5	5.62	1.67	1.56
9	A	100	ONM	CA5-CA6	7.39	1.52	1.39
9	A	100	ONM	OA-CA	8.69	1.46	1.22
9	A	100	ONM	CA3-CA2	8.99	1.57	1.38
9	A	100	ONM	CA4-CA5	10.31	1.60	1.38
8	A	101	FOK	O7-C11	12.39	1.43	1.21

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	405	GSP	C5-C6-N1	-9.87	110.09	123.59
9	A	100	ONM	O1G-PG-O3G	-8.51	74.97	107.38
9	A	100	ONM	PB-O1B-PG	-8.29	104.88	132.67
9	A	100	ONM	N3-C2-N1	-5.82	118.57	127.44
9	A	100	ONM	PB-O1A-PA	-4.85	119.10	132.73
8	A	101	FOK	C20-C10-C1	-4.27	101.27	107.56
9	A	100	ONM	CA3-CA4-CA5	-4.23	113.99	120.19
9	A	100	ONM	O1G-PG-O1B	-3.96	87.11	105.09
9	A	100	ONM	C1'-N9-C4	-3.89	121.07	126.94
7	C	405	GSP	N3-C2-N1	-3.60	121.96	127.44
9	A	100	ONM	C6-C5-C4	-3.32	116.93	120.90
7	C	405	GSP	PA-O3A-PB	-3.19	123.78	132.73
7	C	405	GSP	C1'-N9-C4	-2.86	122.63	126.94
7	C	405	GSP	PB-O3B-PG	-2.75	123.43	132.67
9	A	100	ONM	O5'-PA-O3A	-2.49	99.94	109.62
9	A	100	ONM	O3'-CA-OA	-2.38	119.55	123.53
9	A	100	ONM	C4-C5-N7	-2.32	107.35	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	100	ONM	O2B-PB-O3B	-2.25	100.33	112.53
9	A	100	ONM	C4'-O4'-C1'	-2.24	107.26	109.72
9	A	100	ONM	C5-C6-N1	-2.13	120.67	123.59
9	A	100	ONM	CA4-CA5-CA6	2.01	122.77	118.53
9	A	100	ONM	O3G-PG-O2G	2.11	117.37	110.58
9	A	100	ONM	O4'-C1'-N9	2.11	112.52	108.10
7	C	405	GSP	C4'-O4'-C1'	2.29	112.24	109.72
9	A	100	ONM	N2-C2-N1	2.42	121.20	117.20
9	A	100	ONM	C6-N1-C2	2.48	119.37	115.94
8	A	101	FOK	C9-C10-C1	2.55	113.28	110.90
8	A	101	FOK	C19-C4-C5	2.56	121.03	111.85
9	A	100	ONM	C5'-C4'-C3'	2.90	124.75	114.31
9	A	100	ONM	O2B-PB-O1B	3.02	118.80	105.09
9	A	100	ONM	O5'-C5'-C4'	3.03	120.29	109.12
7	C	405	GSP	O2B-PB-O3B	3.15	119.36	105.09
8	A	101	FOK	C2-C3-C4	3.17	119.49	113.42
9	A	100	ONM	CA7-NA1-CA6	3.34	128.03	122.52
9	A	100	ONM	O3'-C3'-C4'	3.36	118.02	109.54
9	A	100	ONM	O2A-PA-O1A	3.98	123.13	105.09
9	A	100	ONM	O3G-PG-O1B	4.04	123.44	105.09
8	A	101	FOK	C13-O1-C8	5.05	125.33	120.02
9	A	100	ONM	C3'-O3'-CA	5.06	125.69	117.24
9	A	100	ONM	O3'-CA-CA1	5.20	120.38	111.77
7	C	405	GSP	C6-N1-C2	7.95	126.97	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	100	ONM	1	0
8	A	101	FOK	2	0
7	C	405	GSP	1	0

## 5.7 Other polymers [i](#)

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 [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, 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	189/217 (87%)	-0.12	3 (1%) 74 66	22, 54, 83, 99	0
2	B	189/212 (89%)	-0.26	1 (0%) 91 88	12, 38, 73, 94	0
3	C	330/402 (82%)	-0.36	1 (0%) 94 92	18, 40, 68, 92	0
All	All	708/831 (85%)	-0.27	5 (0%) 89 84	12, 43, 74, 99	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	VAL	4.3
2	B	952	ALA	3.6
1	A	476	MET	2.7
1	A	481	VAL	2.5
3	C	385	ARG	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
4	MG	C	403	1/1	0.92	0.20	3.06	0,0,0,0	0
8	FOK	A	101	29/29	0.91	0.23	2.15	26,30,36,40	0
7	GSP	C	405	32/32	0.95	0.17	0.95	23,28,58,66	0
9	ONM	A	100	42/42	0.91	0.22	0.82	44,54,62,64	0
5	CL	C	404	1/1	0.94	0.12	-0.77	49,49,49,49	0
6	MN	A	582	1/1	0.95	0.14	-1.79	37,37,37,37	0
6	MN	A	581	1/1	0.96	0.14	-	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.