



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2016 – 02:31 PM EDT

PDB ID : 5GMF  
Title : Crystal structure of monkey TLR7 in complex with guanosine and polyU  
Authors : Zhang, Z.; Ohto, U.; Shimizu, T.  
Deposited on : 2016-07-14  
Resolution : 2.50 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

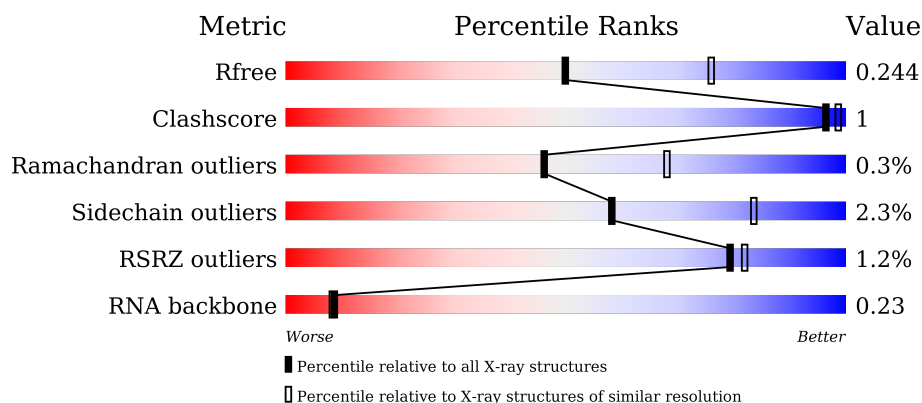
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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	817	<div> <div></div> <div>89% 5% • 5%</div> </div>
1	B	817	<div> <div>%</div> <div>89% 5% • 5%</div> </div>
1	C	817	<div> <div>2%</div> <div>89% 5% • 5%</div> </div>
1	D	817	<div> <div>%</div> <div>88% 6% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	4	 100%
2	F	4	 50%50%
2	G	4	 100%
2	H	4	 75%25%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26109 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	776	Total	C	N	O	S	0	0	0
			6298	4040	1073	1155	30			
1	B	776	Total	C	N	O	S	0	0	0
			6298	4040	1073	1155	30			
1	C	776	Total	C	N	O	S	0	0	0
			6298	4040	1073	1155	30			
1	D	776	Total	C	N	O	S	0	0	0
			6298	4040	1073	1155	30			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653
C	23	ARG	-	expression tag	UNP B3Y653
C	24	SER	-	expression tag	UNP B3Y653
C	25	PRO	-	expression tag	UNP B3Y653
C	26	TRP	-	expression tag	UNP B3Y653
C	167	GLN	ASN	engineered mutation	UNP B3Y653

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Chain	Residue	Modelled	Actual	Comment	Reference
C	389	GLN	ASN	engineered mutation	UNP B3Y653
C	488	GLN	ASN	engineered mutation	UNP B3Y653
C	799	GLN	ASN	engineered mutation	UNP B3Y653
D	23	ARG	-	expression tag	UNP B3Y653
D	24	SER	-	expression tag	UNP B3Y653
D	25	PRO	-	expression tag	UNP B3Y653
D	26	TRP	-	expression tag	UNP B3Y653
D	167	GLN	ASN	engineered mutation	UNP B3Y653
D	389	GLN	ASN	engineered mutation	UNP B3Y653
D	488	GLN	ASN	engineered mutation	UNP B3Y653
D	799	GLN	ASN	engineered mutation	UNP B3Y653

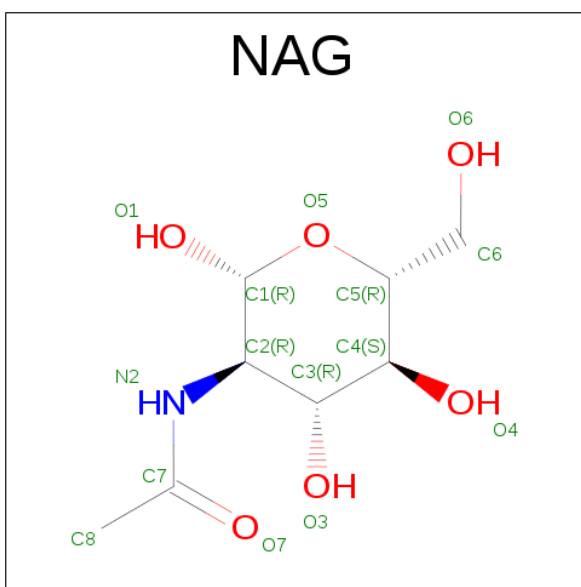
- Molecule 2 is a RNA chain called RNA (5'-R(P\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			64	27	6	27	4			
2	F	4	Total	C	N	O	P	0	0	0
			64	27	6	27	4			
2	G	4	Total	C	N	O	P	0	0	0
			64	27	6	27	4			
2	H	4	Total	C	N	O	P	0	0	0
			64	27	6	27	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



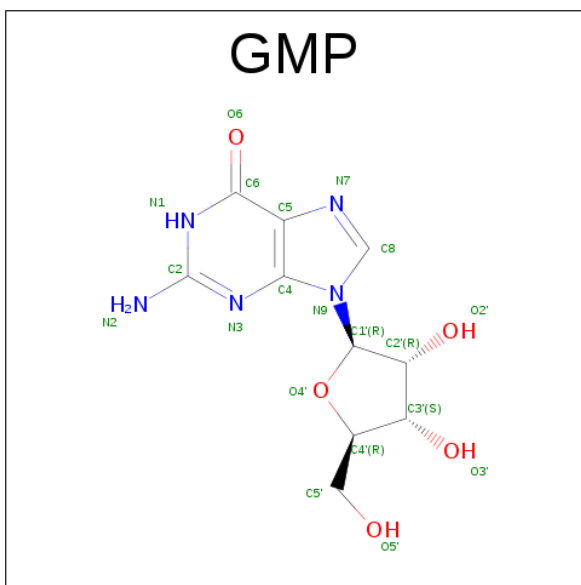
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GUANOSINE (three-letter code: GMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			20	10	5	5		
5	C	1	Total	C	N	O	0	0
			20	10	5	5		
5	C	1	Total	C	N	O	0	0
			20	10	5	5		
5	D	1	Total	C	N	O	0	0
			20	10	5	5		

- Molecule 6 is water.

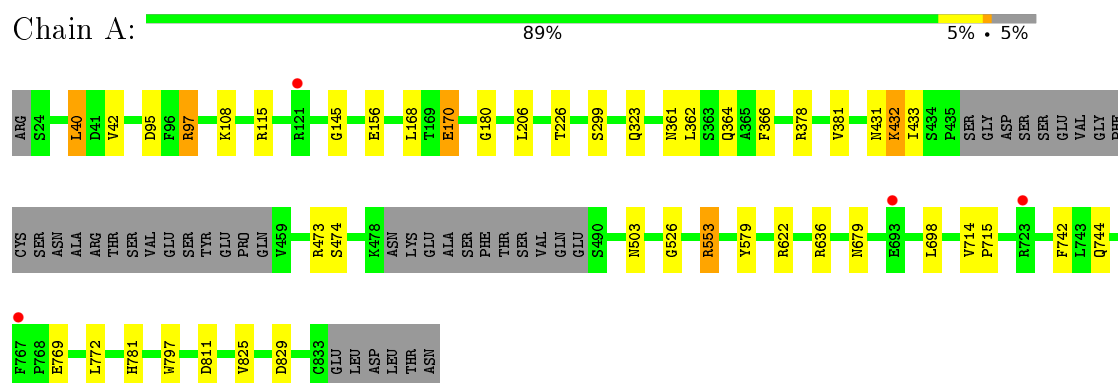
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	43	Total	O	0	0
			43	43		
6	C	41	Total	O	0	0
			41	41		
6	D	26	Total	O	0	0
			26	26		



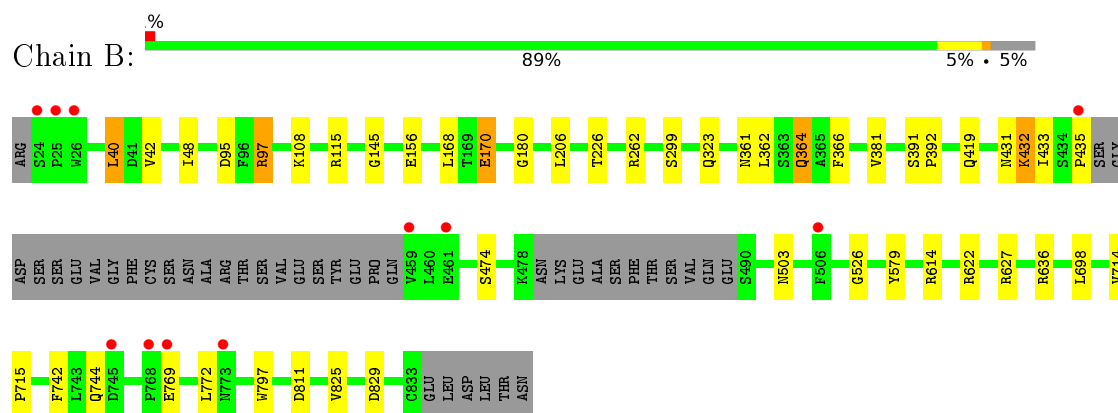
### 3 Residue-property plots

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.

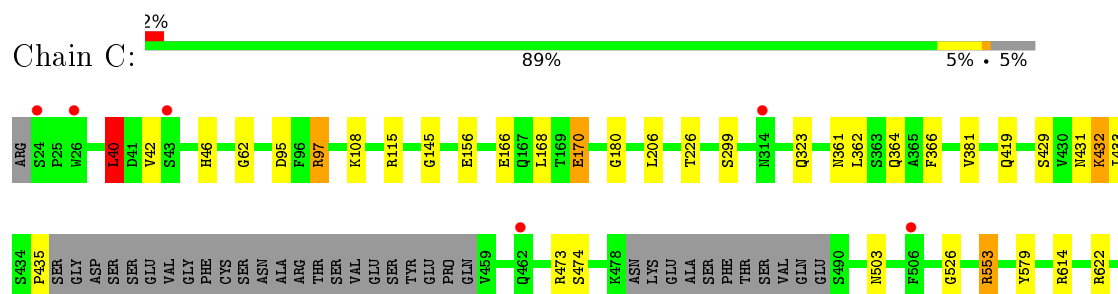
#### • Molecule 1: Toll-like receptor 7

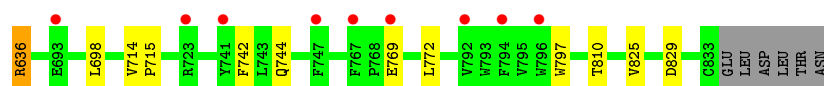


#### • Molecule 1: Toll-like receptor 7

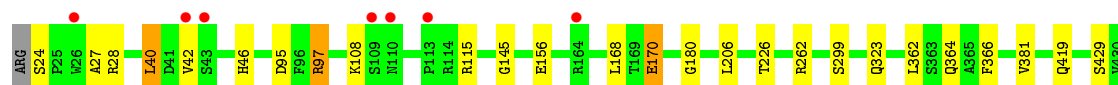
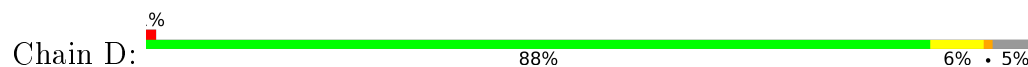


#### • Molecule 1: Toll-like receptor 7





- Molecule 1: Toll-like receptor 7



- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*U)-3')



There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*U)-3')

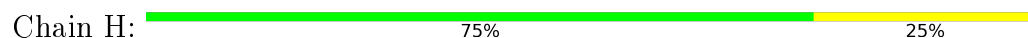


- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*U)-3')



There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*U)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.08 Å   111.33 Å   113.38 Å 93.83°   94.34°   91.48°	Depositor
Resolution (Å)	50.01 – 2.50 48.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.01-2.50) 95.4 (48.93-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.208 , 0.243 0.212 , 0.244	Depositor DCC
$R_{free}$ test set	7968 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: CA, GMP, NAG

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	0.66	0/6433	0.84	9/8717 (0.1%)
1	B	0.65	0/6433	0.85	7/8717 (0.1%)
1	C	0.65	1/6433 (0.0%)	0.85	10/8717 (0.1%)
1	D	0.66	1/6433 (0.0%)	0.87	15/8717 (0.2%)
2	E	0.59	0/69	1.06	0/105
2	F	0.51	0/69	1.06	1/105 (1.0%)
2	G	0.59	0/69	1.03	0/105
2	H	0.45	0/69	1.23	1/105 (1.0%)
All	All	0.65	2/26008 (0.0%)	0.86	43/35288 (0.1%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	429	SER	CB-OG	-5.24	1.35	1.42
1	C	429	SER	CB-OG	-5.02	1.35	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	476	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	H	1	U	O5'-P-OP1	-8.06	98.44	105.70
1	D	614	ARG	NE-CZ-NH2	-7.65	116.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	636	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	97	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	97	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	434	SER	CB-CA-C	6.79	123.01	110.10
1	A	97	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	D	614	ARG	CG-CD-NE	6.49	125.43	111.80
1	A	115	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	C	115	ARG	NE-CZ-NH2	6.35	123.48	120.30
1	B	115	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	B	614	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	476	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	614	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	D	614	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	262	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	97	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	115	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	B	829	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	28	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	829	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	97	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	97	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	473	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	97	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	829	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	473	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	F	1	U	O5'-P-OP1	-5.34	100.90	105.70
1	A	97	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	627	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	636	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	A	829	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	40	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	D	473	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	378	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	553	ARG	CB-CG-CD	-5.09	98.38	111.60
1	D	262	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	829	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	553	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	553	ARG	CB-CG-CD	-5.03	98.51	111.60
1	C	553	ARG	CB-CG-CD	-5.03	98.51	111.60
1	C	553	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	434	SER	Mainchain

## 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	6298	0	6351	18	0
1	B	6298	0	6350	19	0
1	C	6298	0	6348	19	0
1	D	6298	0	6350	21	0
2	E	64	0	30	0	0
2	F	64	0	30	0	0
2	G	64	0	30	0	0
2	H	64	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
4	A	98	0	89	1	0
4	B	112	0	102	1	0
4	C	112	0	103	0	0
4	D	98	0	90	0	0
5	B	20	0	13	0	0
5	C	40	0	26	0	0
5	D	20	0	13	0	0
6	A	47	0	0	0	0
6	B	43	0	0	0	0
6	C	41	0	0	1	0
6	D	26	0	0	0	0
All	All	26109	0	25955	70	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 1.

All (70) 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:723:ARG:O	1:D:748:GLN:HG3	1.59	1.02
1:B:431:ASN:HB2	1:B:503:ASN:HD21	1.54	0.72
1:D:431:ASN:HB2	1:D:503:ASN:HD21	1.55	0.71
1:C:431:ASN:HB2	1:C:503:ASN:HD21	1.56	0.70
1:A:431:ASN:HB2	1:A:503:ASN:HD21	1.56	0.69
1:C:95:ASP:OD1	1:C:97:ARG:HD3	1.99	0.63
1:D:95:ASP:OD1	1:D:97:ARG:HD3	1.99	0.62
1:C:62:GLY:O	6:C:1001:HOH:O	2.16	0.62
1:A:95:ASP:OD1	1:A:97:ARG:HD3	2.00	0.62
1:B:95:ASP:OD1	1:B:97:ARG:HD3	2.00	0.60
1:B:145:GLY:N	1:B:170:GLU:OE1	2.35	0.60
1:A:145:GLY:N	1:A:170:GLU:OE1	2.36	0.59
1:D:714:VAL:HB	1:D:715:PRO:HD2	1.85	0.59
1:B:48:ILE:HG12	4:B:904:NAG:H82	1.85	0.58
1:B:714:VAL:HB	1:B:715:PRO:HD2	1.86	0.58
1:D:145:GLY:N	1:D:170:GLU:OE1	2.36	0.58
1:C:145:GLY:N	1:C:170:GLU:OE1	2.37	0.57
1:C:714:VAL:HB	1:C:715:PRO:HD2	1.86	0.57
1:A:714:VAL:HB	1:A:715:PRO:HD2	1.89	0.54
1:A:206:LEU:O	1:A:226:THR:HG23	2.09	0.53
1:C:206:LEU:O	1:C:226:THR:HG23	2.09	0.52
1:B:206:LEU:O	1:B:226:THR:HG23	2.10	0.52
1:A:97:ARG:NH2	1:A:474:SER:O	2.43	0.52
1:D:810:THR:HG22	1:D:811:ASP:OD1	2.10	0.51
1:D:97:ARG:NH2	1:D:474:SER:O	2.43	0.51
1:D:206:LEU:O	1:D:226:THR:HG23	2.10	0.51
1:B:97:ARG:NH2	1:B:474:SER:O	2.44	0.50
1:C:97:ARG:NH2	1:C:474:SER:O	2.44	0.50
1:A:432:LYS:HE2	1:C:579:TYR:OH	2.12	0.49
1:B:433:ILE:H	1:B:503:ASN:HD22	1.60	0.49
1:A:40:LEU:HD23	1:A:42:VAL:HG22	1.95	0.48
1:B:40:LEU:HD23	1:B:42:VAL:HG22	1.96	0.48
1:A:433:ILE:H	1:A:503:ASN:HD22	1.62	0.48
1:D:299:SER:HA	1:D:323:GLN:O	2.14	0.48
1:A:299:SER:HA	1:A:323:GLN:O	2.13	0.47
1:B:299:SER:HA	1:B:323:GLN:O	2.13	0.47
1:D:40:LEU:HD23	1:D:42:VAL:HG22	1.96	0.47
1:B:431:ASN:HB2	1:B:503:ASN:ND2	2.28	0.47
1:C:362:LEU:HD22	1:C:366:PHE:CE1	2.50	0.47
1:C:299:SER:HA	1:C:323:GLN:O	2.14	0.47
1:C:433:ILE:H	1:C:503:ASN:HD22	1.63	0.47
1:C:40:LEU:HD23	1:C:46:HIS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD22	1:A:366:PHE:CE1	2.50	0.46
1:D:24:SER:N	1:D:27:ALA:HB3	2.31	0.45
1:D:433:ILE:H	1:D:503:ASN:HD22	1.63	0.45
1:B:579:TYR:OH	1:D:432:LYS:HE2	2.16	0.45
1:B:362:LEU:HD22	1:B:366:PHE:CE1	2.52	0.45
1:D:362:LEU:HD22	1:D:366:PHE:CE1	2.52	0.45
1:A:431:ASN:HB2	1:A:503:ASN:ND2	2.29	0.44
1:B:432:LYS:HE2	1:D:579:TYR:OH	2.16	0.44
1:C:772:LEU:HD13	1:C:797:TRP:CZ2	2.53	0.44
4:A:907:NAG:O6	1:B:364:GLN:HG2	2.18	0.44
1:C:156:GLU:HA	1:C:180:GLY:O	2.19	0.43
1:A:772:LEU:HD13	1:A:797:TRP:CZ2	2.54	0.42
1:D:614:ARG:HD3	1:D:641:ARG:HB3	2.01	0.42
1:A:781:HIS:H	1:A:781:HIS:CD2	2.36	0.42
1:A:156:GLU:HA	1:A:180:GLY:O	2.20	0.42
1:D:431:ASN:HB2	1:D:503:ASN:ND2	2.29	0.42
1:A:526:GLY:O	1:C:553:ARG:NH2	2.53	0.42
1:B:772:LEU:HD13	1:B:797:TRP:CZ2	2.55	0.42
1:A:579:TYR:OH	1:C:432:LYS:HE2	2.20	0.41
1:C:431:ASN:HB2	1:C:503:ASN:ND2	2.31	0.41
1:D:156:GLU:HA	1:D:180:GLY:O	2.21	0.41
1:D:772:LEU:HD13	1:D:797:TRP:CZ2	2.55	0.41
1:B:391:SER:N	1:B:392:PRO:CD	2.84	0.41
1:B:156:GLU:HA	1:B:180:GLY:O	2.20	0.41
1:C:40:LEU:HD13	1:C:42:VAL:HG22	2.03	0.40
1:B:526:GLY:O	1:D:553:ARG:NH2	2.54	0.40
1:A:553:ARG:NH2	1:C:526:GLY:O	2.55	0.40
1:D:820:HIS:CD2	1:D:828:LEU:HD11	2.56	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	770/817 (94%)	724 (94%)	44 (6%)	2 (0%)	46	68
1	B	770/817 (94%)	725 (94%)	43 (6%)	2 (0%)	46	68
1	C	770/817 (94%)	725 (94%)	43 (6%)	2 (0%)	46	68
1	D	770/817 (94%)	722 (94%)	45 (6%)	3 (0%)	39	61
All	All	3080/3268 (94%)	2896 (94%)	175 (6%)	9 (0%)	46	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	PHE
1	B	742	PHE
1	C	742	PHE
1	D	742	PHE
1	A	381	VAL
1	B	381	VAL
1	C	381	VAL
1	D	381	VAL
1	D	434	SER

### 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	731/768 (95%)	716 (98%)	15 (2%)	61	85
1	B	731/768 (95%)	715 (98%)	16 (2%)	60	84
1	C	731/768 (95%)	714 (98%)	17 (2%)	58	83
1	D	731/768 (95%)	713 (98%)	18 (2%)	55	82
All	All	2924/3072 (95%)	2858 (98%)	66 (2%)	58	83

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	108	LYS

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	170	GLU
1	A	361	ASN
1	A	364	GLN
1	A	432	LYS
1	A	622	ARG
1	A	636	ARG
1	A	679	ASN
1	A	698	LEU
1	A	744	GLN
1	A	769	GLU
1	A	811	ASP
1	A	825	VAL
1	B	40	LEU
1	B	108	LYS
1	B	168	LEU
1	B	170	GLU
1	B	361	ASN
1	B	364	GLN
1	B	419	GLN
1	B	432	LYS
1	B	435	PRO
1	B	622	ARG
1	B	636	ARG
1	B	698	LEU
1	B	744	GLN
1	B	769	GLU
1	B	811	ASP
1	B	825	VAL
1	C	40	LEU
1	C	108	LYS
1	C	166	GLU
1	C	168	LEU
1	C	170	GLU
1	C	361	ASN
1	C	364	GLN
1	C	419	GLN
1	C	432	LYS
1	C	435	PRO
1	C	622	ARG
1	C	636	ARG
1	C	698	LEU

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Mol	Chain	Res	Type
1	C	744	GLN
1	C	769	GLU
1	C	810	THR
1	C	825	VAL
1	D	40	LEU
1	D	46	HIS
1	D	108	LYS
1	D	168	LEU
1	D	170	GLU
1	D	364	GLN
1	D	419	GLN
1	D	432	LYS
1	D	435	PRO
1	D	476	ARG
1	D	622	ARG
1	D	636	ARG
1	D	647	LYS
1	D	679	ASN
1	D	698	LEU
1	D	744	GLN
1	D	769	GLU
1	D	825	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	276	ASN
1	A	503	ASN
1	A	781	HIS
1	A	782	HIS
1	A	799	GLN
1	A	820	HIS
1	B	241	GLN
1	B	276	ASN
1	B	503	ASN
1	B	648	ASN
1	B	763	GLN
1	B	799	GLN
1	C	167	GLN
1	C	276	ASN
1	C	419	GLN

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Mol	Chain	Res	Type
1	C	503	ASN
1	C	648	ASN
1	C	744	GLN
1	C	799	GLN
1	C	820	HIS
1	D	241	GLN
1	D	276	ASN
1	D	419	GLN
1	D	503	ASN
1	D	799	GLN
1	D	820	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	2/4 (50%)	0	0
2	F	2/4 (50%)	0	1 (50%)
2	G	2/4 (50%)	0	0
2	H	2/4 (50%)	0	0
All	All	8/16 (50%)	0	1 (12%)

There are no RNA backbone outliers to report.

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	F	3	U

## 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 38 ligands modelled in this entry, 4 are monoatomic - leaving 34 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	$\# Z  > 2$
4	NAG	A	902	1	14,14,15	0.92	1 (7%)	15,19,21	2.40	4 (26%)
4	NAG	A	903	1,4	14,14,15	0.69	1 (7%)	15,19,21	1.22	2 (13%)
4	NAG	A	904	4	14,14,15	0.62	0	15,19,21	1.29	3 (20%)
4	NAG	A	905	1,4	14,14,15	0.54	0	15,19,21	1.33	2 (13%)
4	NAG	A	906	4	14,14,15	0.54	0	15,19,21	2.07	2 (13%)
4	NAG	A	907	1	14,14,15	1.19	1 (7%)	15,19,21	1.32	1 (6%)
4	NAG	A	908	1	14,14,15	0.42	0	15,19,21	1.65	2 (13%)
5	GMP	B	901	-	18,22,22	1.51	4 (22%)	19,33,33	2.57	6 (31%)
4	NAG	B	903	1	14,14,15	0.83	0	15,19,21	2.63	7 (46%)
4	NAG	B	904	1,4	14,14,15	0.48	0	15,19,21	0.87	0
4	NAG	B	905	4	14,14,15	0.65	0	15,19,21	2.12	1 (6%)
4	NAG	B	906	1	14,14,15	1.12	1 (7%)	15,19,21	1.62	5 (33%)
4	NAG	B	907	1,4	14,14,15	0.65	0	15,19,21	1.50	3 (20%)
4	NAG	B	908	4	14,14,15	0.90	1 (7%)	15,19,21	2.55	5 (33%)
4	NAG	B	909	1	14,14,15	0.38	0	15,19,21	1.62	2 (13%)
4	NAG	B	910	1	14,14,15	0.44	0	15,19,21	1.02	1 (6%)
5	GMP	C	901	-	18,22,22	1.61	2 (11%)	19,33,33	2.30	4 (21%)
5	GMP	C	902	-	18,22,22	1.63	2 (11%)	19,33,33	2.58	5 (26%)
4	NAG	C	903	1	14,14,15	0.67	0	15,19,21	2.05	6 (40%)
4	NAG	C	904	1,4	14,14,15	0.56	0	15,19,21	1.34	3 (20%)
4	NAG	C	905	4	14,14,15	0.63	0	15,19,21	2.38	7 (46%)
4	NAG	C	906	1	14,14,15	0.57	0	15,19,21	1.42	1 (6%)
4	NAG	C	907	1	14,14,15	0.59	0	15,19,21	1.04	0
4	NAG	C	908	1	14,14,15	1.12	1 (7%)	15,19,21	1.27	1 (6%)
4	NAG	C	909	1	14,14,15	0.61	0	15,19,21	1.58	5 (33%)
4	NAG	C	910	1	14,14,15	0.89	1 (7%)	15,19,21	1.94	4 (26%)
5	GMP	D	901	-	18,22,22	1.39	2 (11%)	19,33,33	2.61	5 (26%)
4	NAG	D	904	1	14,14,15	0.79	0	15,19,21	1.85	5 (33%)
4	NAG	D	905	1,4	14,14,15	0.41	0	15,19,21	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	906	4	14,14,15	0.64	0	15,19,21	2.11	5 (33%)
4	NAG	D	907	1	14,14,15	0.62	0	15,19,21	0.89	0
4	NAG	D	908	1	14,14,15	1.05	1 (7%)	15,19,21	1.85	4 (26%)
4	NAG	D	909	1	14,14,15	0.47	0	15,19,21	1.51	2 (13%)
4	NAG	D	910	1	14,14,15	0.75	0	15,19,21	1.64	2 (13%)

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
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	904	4	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	906	4	-	0/6/23/26	0/1/1/1
4	NAG	A	907	1	-	0/6/23/26	0/1/1/1
4	NAG	A	908	1	-	0/6/23/26	0/1/1/1
5	GMP	B	901	-	-	0/2/22/22	0/3/3/3
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	904	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	905	4	-	0/6/23/26	0/1/1/1
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
4	NAG	B	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	908	4	-	0/6/23/26	0/1/1/1
4	NAG	B	909	1	-	0/6/23/26	0/1/1/1
4	NAG	B	910	1	-	0/6/23/26	0/1/1/1
5	GMP	C	901	-	-	0/2/22/22	0/3/3/3
5	GMP	C	902	-	-	0/2/22/22	0/3/3/3
4	NAG	C	903	1	-	0/6/23/26	0/1/1/1
4	NAG	C	904	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	905	4	-	0/6/23/26	0/1/1/1
4	NAG	C	906	1	-	0/6/23/26	0/1/1/1
4	NAG	C	907	1	-	0/6/23/26	0/1/1/1
4	NAG	C	908	1	-	0/6/23/26	0/1/1/1
4	NAG	C	909	1	-	0/6/23/26	0/1/1/1
4	NAG	C	910	1	-	0/6/23/26	0/1/1/1
5	GMP	D	901	-	-	0/2/22/22	0/3/3/3
4	NAG	D	904	1	-	0/6/23/26	0/1/1/1
4	NAG	D	905	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	906	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	907	1	-	0/6/23/26	0/1/1/1
4	NAG	D	908	1	-	0/6/23/26	0/1/1/1
4	NAG	D	909	1	-	0/6/23/26	0/1/1/1
4	NAG	D	910	1	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	GMP	C2'-C1'	-3.05	1.48	1.53
4	A	903	NAG	O5-C1	-2.20	1.40	1.43
4	A	902	NAG	O7-C7	-2.01	1.18	1.23
4	B	908	NAG	O5-C1	2.08	1.47	1.43
4	C	910	NAG	C1-C2	2.12	1.55	1.52
5	B	901	GMP	C8-N7	2.17	1.38	1.34
5	B	901	GMP	C6-C5	2.32	1.46	1.41
4	D	908	NAG	O4-C4	2.85	1.49	1.43
5	D	901	GMP	C6-C5	2.95	1.47	1.41
5	D	901	GMP	C5-C4	2.99	1.47	1.40
5	C	902	GMP	C5-C4	3.09	1.47	1.40
4	B	906	NAG	C1-C2	3.17	1.57	1.52
4	C	908	NAG	C1-C2	3.28	1.57	1.52
5	B	901	GMP	C5-C4	3.65	1.48	1.40
5	C	901	GMP	C5-C4	3.79	1.49	1.40
4	A	907	NAG	C1-C2	3.84	1.57	1.52
5	C	901	GMP	C6-C5	4.66	1.50	1.41
5	C	902	GMP	C6-C5	4.79	1.51	1.41

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	902	GMP	C5-C6-N1	-4.85	117.18	123.52
5	B	901	GMP	C5-C6-N1	-4.79	117.27	123.52
5	D	901	GMP	C5-C6-N1	-4.74	117.33	123.52
5	D	901	GMP	C6-C5-C4	-4.66	115.53	120.86
5	C	902	GMP	N3-C2-N1	-4.44	121.51	127.56
5	C	902	GMP	C6-C5-C4	-4.43	115.80	120.86
5	C	901	GMP	C5-C6-N1	-4.38	117.79	123.52
5	C	901	GMP	C6-C5-C4	-4.36	115.87	120.86
4	B	903	NAG	O3-C3-C2	-4.26	100.26	109.37
5	B	901	GMP	N3-C2-N1	-4.24	121.78	127.56
5	B	901	GMP	C6-C5-C4	-3.87	116.44	120.86
5	D	901	GMP	N3-C2-N1	-3.84	122.33	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	908	NAG	O3-C3-C4	-3.62	102.20	110.36
4	B	907	NAG	C3-C4-C5	-3.55	103.89	110.23
4	D	908	NAG	C3-C4-C5	-3.51	103.97	110.23
4	D	906	NAG	C4-C3-C2	-3.29	106.24	111.34
4	C	905	NAG	C8-C7-N2	-3.25	109.86	116.10
5	C	901	GMP	N3-C2-N1	-3.22	123.18	127.56
4	A	908	NAG	O4-C4-C3	-2.92	103.78	110.36
4	C	904	NAG	C3-C4-C5	-2.85	105.14	110.23
4	D	904	NAG	O7-C7-C8	-2.78	116.94	122.07
4	D	904	NAG	O3-C3-C2	-2.73	103.54	109.37
4	D	904	NAG	C6-C5-C4	-2.62	106.42	112.99
4	C	909	NAG	O4-C4-C3	-2.59	104.52	110.36
4	D	908	NAG	O7-C7-C8	-2.58	117.32	122.07
4	C	903	NAG	O6-C6-C5	-2.53	102.85	111.30
4	A	905	NAG	C3-C4-C5	-2.52	105.74	110.23
4	C	905	NAG	C3-C4-C5	-2.48	105.80	110.23
4	C	909	NAG	C8-C7-N2	-2.44	111.41	116.10
5	D	901	GMP	C4'-O4'-C1'	-2.44	107.05	109.64
4	C	910	NAG	C4-C3-C2	-2.42	107.59	111.34
4	B	910	NAG	C4-C3-C2	-2.35	107.69	111.34
4	A	904	NAG	O3-C3-C4	-2.33	105.11	110.36
4	C	904	NAG	C8-C7-N2	-2.31	111.66	116.10
4	C	903	NAG	O5-C5-C6	-2.31	102.40	107.34
4	B	908	NAG	C6-C5-C4	-2.26	107.32	112.99
4	A	902	NAG	C6-C5-C4	-2.24	107.37	112.99
4	B	903	NAG	C6-C5-C4	-2.19	107.50	112.99
5	B	901	GMP	C4'-O4'-C1'	-2.18	107.34	109.64
4	B	903	NAG	O3-C3-C4	-2.15	105.51	110.36
4	D	906	NAG	O7-C7-C8	-2.11	118.18	122.07
4	C	910	NAG	O5-C5-C4	-2.09	106.67	110.13
4	B	906	NAG	C6-C5-C4	-2.02	107.92	112.99
4	B	906	NAG	O3-C3-C2	2.02	113.70	109.37
4	A	903	NAG	O7-C7-N2	2.07	126.06	121.84
4	B	906	NAG	C1-O5-C5	2.08	115.19	112.14
4	C	905	NAG	O3-C3-C2	2.10	113.87	109.37
4	B	903	NAG	C2-N2-C7	2.12	125.86	123.11
4	A	906	NAG	C4-C3-C2	2.14	114.66	111.34
4	B	906	NAG	O7-C7-N2	2.15	126.22	121.84
4	C	905	NAG	C2-N2-C7	2.15	125.90	123.11
4	C	905	NAG	O7-C7-N2	2.16	126.26	121.84
4	C	905	NAG	O4-C4-C5	2.17	114.94	109.23
4	C	909	NAG	O7-C7-C8	2.20	126.12	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	909	NAG	O5-C5-C6	2.21	112.07	107.34
5	C	902	GMP	O4'-C4'-C3'	2.26	109.75	105.16
4	B	907	NAG	O4-C4-C5	2.26	115.19	109.23
4	A	904	NAG	C2-N2-C7	2.29	126.08	123.11
4	B	908	NAG	O4-C4-C5	2.30	115.28	109.23
4	A	905	NAG	O7-C7-N2	2.34	126.61	121.84
4	C	903	NAG	C4-C3-C2	2.34	114.97	111.34
4	B	907	NAG	C2-N2-C7	2.35	126.17	123.11
4	C	908	NAG	C2-N2-C7	2.38	126.20	123.11
4	D	906	NAG	O3-C3-C2	2.38	114.47	109.37
4	C	909	NAG	C4-C3-C2	2.39	115.05	111.34
4	C	904	NAG	O7-C7-N2	2.41	126.76	121.84
4	C	903	NAG	O5-C5-C4	2.42	114.14	110.13
5	B	901	GMP	N2-C2-N1	2.49	121.31	117.20
4	D	910	NAG	C2-N2-C7	2.59	126.48	123.11
4	A	903	NAG	C2-N2-C7	2.62	126.51	123.11
4	B	909	NAG	C3-C4-C5	2.62	114.91	110.23
4	D	904	NAG	C8-C7-N2	2.64	121.15	116.10
4	B	903	NAG	O5-C5-C4	2.66	114.54	110.13
4	A	904	NAG	O4-C4-C5	2.67	116.27	109.23
4	C	909	NAG	C3-C4-C5	2.72	115.08	110.23
4	D	908	NAG	C1-O5-C5	3.01	116.56	112.14
4	B	906	NAG	C2-N2-C7	3.05	127.07	123.11
4	A	907	NAG	C2-N2-C7	3.13	127.17	123.11
4	A	902	NAG	O5-C5-C4	3.16	115.37	110.13
4	C	903	NAG	C2-N2-C7	3.24	127.31	123.11
4	D	906	NAG	O5-C5-C4	3.28	115.57	110.13
4	D	908	NAG	O4-C4-C5	3.30	117.93	109.23
4	C	906	NAG	O5-C5-C6	3.39	114.60	107.34
4	D	904	NAG	C1-O5-C5	3.46	117.22	112.14
4	B	908	NAG	O5-C5-C4	3.75	116.34	110.13
4	D	909	NAG	C1-O5-C5	3.77	117.69	112.14
4	B	903	NAG	C4-C3-C2	3.89	117.37	111.34
4	C	903	NAG	C1-O5-C5	3.92	117.91	112.14
4	A	902	NAG	C2-N2-C7	4.12	128.47	123.11
4	A	908	NAG	C1-O5-C5	4.14	118.22	112.14
4	D	910	NAG	C1-O5-C5	4.24	118.37	112.14
4	C	910	NAG	C1-O5-C5	4.27	118.43	112.14
4	B	909	NAG	C1-O5-C5	4.40	118.61	112.14
4	C	910	NAG	O5-C5-C6	4.57	117.13	107.34
4	D	906	NAG	C1-O5-C5	4.76	119.14	112.14
5	C	901	GMP	C6-N1-C2	6.09	123.02	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	NAG	C1-O5-C5	6.20	121.25	112.14
4	B	903	NAG	C1-O5-C5	6.27	121.37	112.14
4	A	906	NAG	C1-O5-C5	6.34	121.47	112.14
4	C	905	NAG	C1-O5-C5	6.46	121.64	112.14
5	C	902	GMP	C6-N1-C2	7.04	124.12	115.88
4	B	908	NAG	C1-O5-C5	7.05	122.51	112.14
4	B	905	NAG	C1-O5-C5	7.14	122.64	112.14
5	D	901	GMP	C6-N1-C2	7.15	124.26	115.88
5	B	901	GMP	C6-N1-C2	7.18	124.29	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	907	NAG	1	0
4	B	904	NAG	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	776/817 (94%)	0.03	4 (0%) 91 92	28, 46, 76, 107	0
1	B	776/817 (94%)	-0.01	11 (1%) 78 80	28, 50, 81, 118	0
1	C	776/817 (94%)	-0.02	15 (1%) 70 73	30, 48, 76, 110	0
1	D	776/817 (94%)	0.01	9 (1%) 81 83	28, 52, 82, 107	0
2	E	4/4 (100%)	-0.61	0 100 100	51, 59, 74, 78	0
2	F	4/4 (100%)	-0.28	0 100 100	51, 60, 78, 83	0
2	G	4/4 (100%)	-0.16	0 100 100	49, 62, 77, 79	0
2	H	4/4 (100%)	-0.48	0 100 100	44, 61, 74, 81	0
All	All	3120/3284 (95%)	-0.00	39 (1%) 79 82	28, 49, 79, 118	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	TRP	4.5
1	B	25	PRO	4.2
1	C	26	TRP	4.1
1	A	121	ARG	3.6
1	C	723	ARG	3.5
1	B	461	GLU	3.0
1	C	792	VAL	2.9
1	C	767	PHE	2.9
1	B	24	SER	2.9
1	D	113	PRO	2.7
1	C	769	GLU	2.7
1	C	24	SER	2.7
1	D	435	PRO	2.6
1	C	747	PHE	2.6
1	C	462	GLN	2.6
1	C	794	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	594	ASN	2.5
1	D	164	ARG	2.5
1	A	693	GLU	2.5
1	D	42	VAL	2.4
1	B	768	PRO	2.4
1	B	506	PHE	2.4
1	C	314	ASN	2.4
1	B	459	VAL	2.3
1	B	773	ASN	2.3
1	B	769	GLU	2.3
1	B	745	ASP	2.3
1	A	767	PHE	2.2
1	D	43	SER	2.2
1	D	110	ASN	2.1
1	C	796	TRP	2.1
1	C	506	PHE	2.1
1	C	43	SER	2.1
1	D	109	SER	2.1
1	D	26	TRP	2.1
1	C	693	GLU	2.1
1	B	435	PRO	2.1
1	A	723	ARG	2.1
1	C	741	TYR	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( $\text{\AA}^2$ )	Q<0.9
4	NAG	D	910	14/15	0.92	0.18	1.27	51,58,62,69	0
4	NAG	D	909	14/15	0.95	0.17	0.61	55,69,75,75	0
4	NAG	B	903	14/15	0.95	0.15	0.52	34,38,46,48	0
4	NAG	C	908	14/15	0.94	0.17	0.38	55,62,67,67	0
4	NAG	B	909	14/15	0.94	0.14	0.34	59,70,81,84	0
3	CA	D	902	1/1	0.98	0.16	0.22	54,54,54,54	0
3	CA	B	902	1/1	0.96	0.15	0.21	53,53,53,53	0
4	NAG	C	903	14/15	0.96	0.15	0.14	36,41,48,55	0
4	NAG	A	902	14/15	0.97	0.15	0.11	37,38,47,49	0
4	NAG	B	907	14/15	0.97	0.14	0.07	55,60,72,79	0
5	GMP	B	901	20/20	0.97	0.17	0.05	30,36,41,45	0
4	NAG	A	908	14/15	0.95	0.15	0.03	57,64,76,78	0
4	NAG	D	905	14/15	0.97	0.14	0.01	51,62,69,70	0
4	NAG	D	907	14/15	0.95	0.14	0.00	58,64,79,87	0
4	NAG	D	904	14/15	0.95	0.14	-0.03	41,44,48,49	0
5	GMP	D	901	20/20	0.97	0.14	-0.12	30,37,43,44	0
4	NAG	B	910	14/15	0.91	0.17	-0.25	63,74,80,84	0
4	NAG	C	904	14/15	0.96	0.13	-0.43	39,50,56,57	0
5	GMP	C	902	20/20	0.98	0.14	-0.46	32,35,38,41	0
4	NAG	C	907	14/15	0.94	0.14	-0.58	52,62,66,67	0
4	NAG	C	906	14/15	0.96	0.14	-0.62	50,55,58,60	0
4	NAG	B	904	14/15	0.96	0.12	-0.68	51,55,67,67	0
3	CA	A	901	1/1	0.96	0.12	-0.71	57,57,57,57	0
4	NAG	A	903	14/15	0.93	0.14	-0.86	47,52,57,65	0
4	NAG	A	905	14/15	0.98	0.11	-1.07	43,49,57,60	0
4	NAG	D	908	14/15	0.91	0.15	-1.08	54,58,68,72	0
4	NAG	A	907	14/15	0.95	0.11	-1.31	50,56,60,63	0
4	NAG	B	906	14/15	0.96	0.14	-1.42	52,58,62,63	0
5	GMP	C	901	20/20	0.98	0.11	-1.87	30,39,41,42	0
4	NAG	D	906	14/15	0.91	0.24	-	68,78,87,97	0
3	CA	D	903	1/1	0.95	0.15	-	60,60,60,60	0
4	NAG	A	904	14/15	0.87	0.21	-	68,82,101,102	0
4	NAG	B	905	14/15	0.82	0.17	-	79,88,98,99	0
4	NAG	B	908	14/15	0.90	0.22	-	76,87,91,93	0
4	NAG	C	905	14/15	0.88	0.17	-	59,78,90,90	0
4	NAG	C	910	14/15	0.87	0.23	-	82,92,98,101	0
4	NAG	C	909	14/15	0.93	0.15	-	56,68,74,75	0
4	NAG	A	906	14/15	0.92	0.18	-	56,73,83,83	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.