



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 03:40 PM EST

PDB ID : 3W3D  
Title : Crystal structure of smooth muscle G actin DNase I complex  
Authors : Sakabe, N.; Sakabe, K.; Sasaki, K.; Kondo, H.; Shimomur, M.  
Deposited on : unknown  
Resolution : 1.80 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

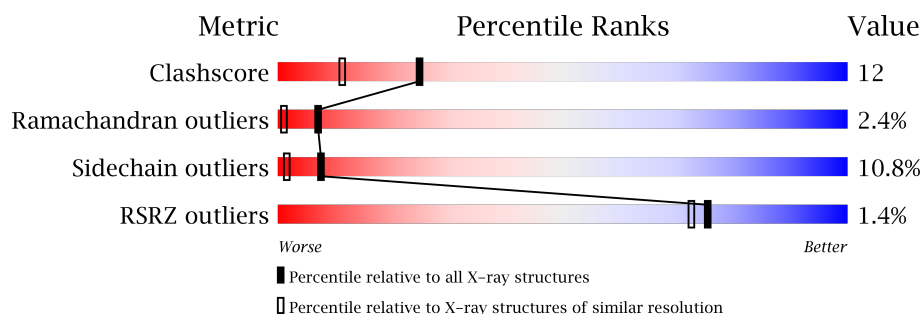
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	374	
2	B	260	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5472 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 Actin, gamma-enteric smooth muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2924	1849	492	562	21	0	0	0

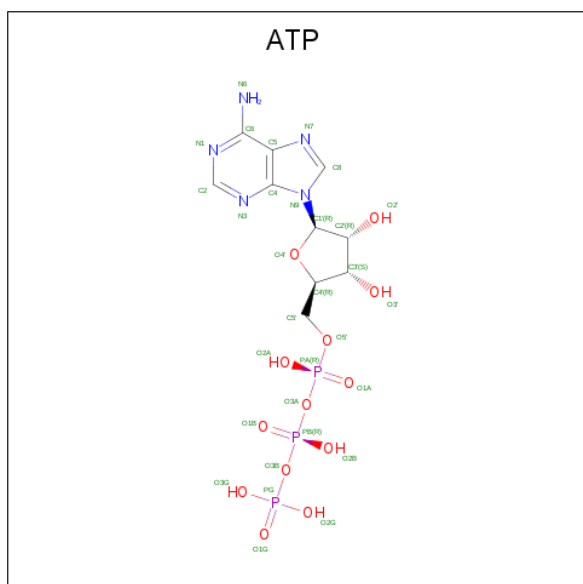
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	GLN	PRO	CONFLICT	UNP P63270

- Molecule 2 is a protein called Deoxyribonuclease-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	260	2049	1298	341	402	8	0	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

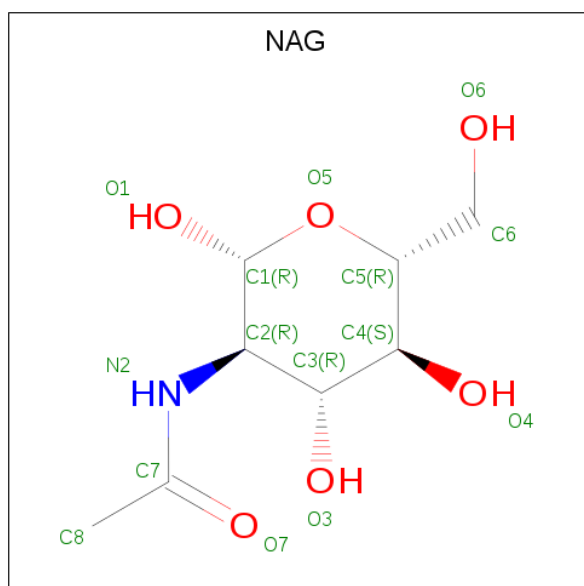


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

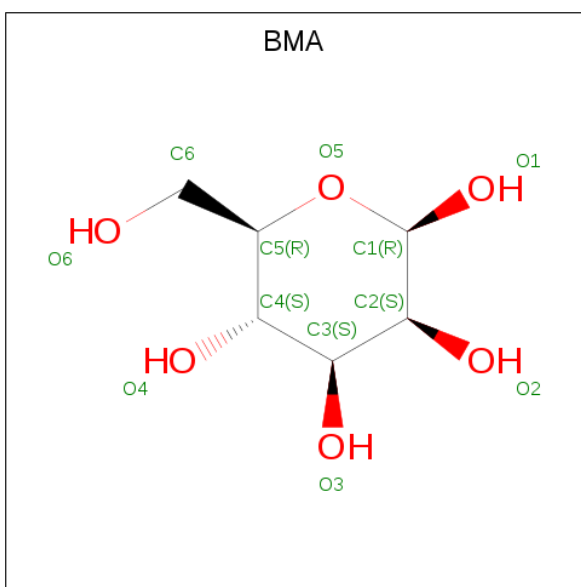
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



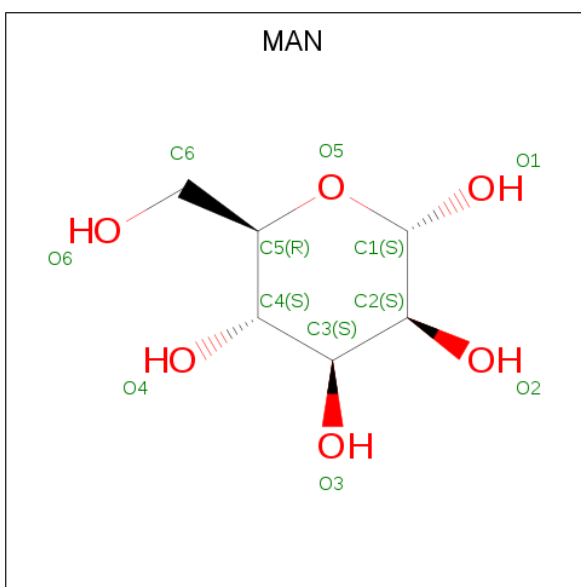
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		

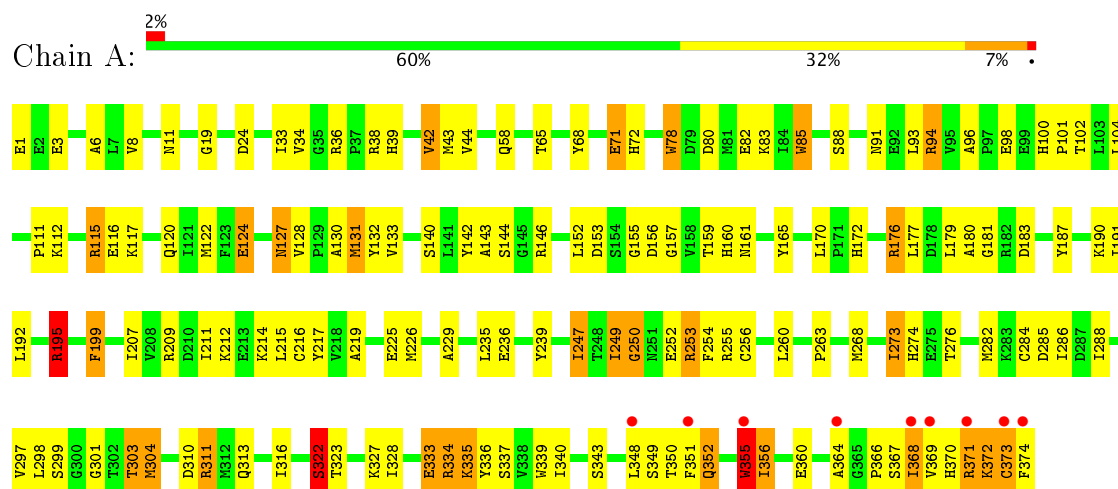
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	195	Total	O	0	0
			195	195		
8	B	188	Total	O	0	0
			188	188		

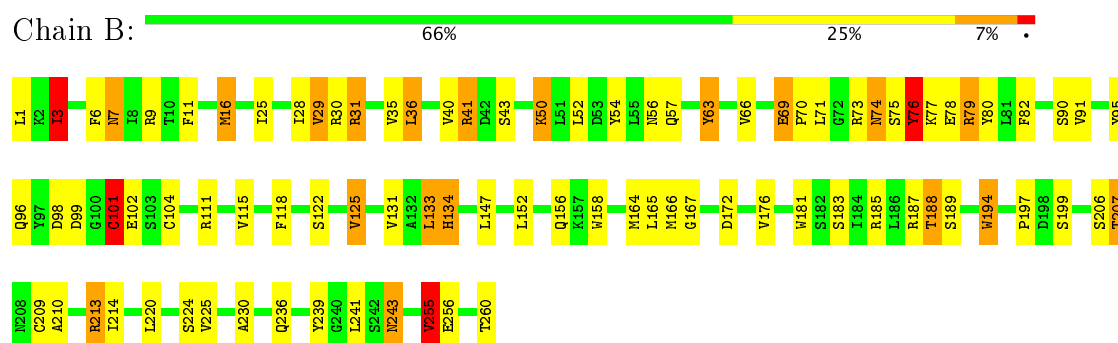
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Actin, gamma-enteric smooth muscle



- Molecule 2: Deoxyribonuclease-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.00 Å   225.30 Å   77.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 1.80 10.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 77.6 (10.00-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.196 , (Not available) 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.07 , 37.3	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.30$ , $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5472	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 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, HIC, ATP, MAN

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	0.85	0/2974	1.57	42/4025 (1.0%)
2	B	0.95	1/2095 (0.0%)	1.79	42/2853 (1.5%)
All	All	0.89	1/5069 (0.0%)	1.67	84/6878 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	158	TRP	CG-CD2	-5.25	1.34	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	ARG	NE-CZ-NH2	12.75	126.68	120.30
2	B	79	ARG	NE-CZ-NH2	11.57	126.08	120.30
2	B	95	TYR	CB-CG-CD1	-11.03	114.38	121.00
2	B	9	ARG	NE-CZ-NH1	-10.31	115.14	120.30
1	A	311	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	A	38	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	A	253	ARG	NE-CZ-NH2	9.44	125.02	120.30
2	B	213	ARG	NE-CZ-NH1	-9.24	115.68	120.30
1	A	78	TRP	CD1-CG-CD2	8.95	113.46	106.30
2	B	31	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	A	371	ARG	NE-CZ-NH2	8.70	124.65	120.30
2	B	194	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	339	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	311	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	A	364	ALA	N-CA-C	8.16	133.04	111.00
2	B	73	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	78	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	A	339	TRP	CE2-CD2-CG	-7.75	101.10	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	A	311	ARG	CA-CB-CG	-7.60	96.68	113.40
2	B	181	TRP	CD1-CG-CD2	7.32	112.16	106.30
2	B	181	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	B	76	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	A	85	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	355	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	44	VAL	CA-C-N	6.96	130.12	116.20
1	A	78	TRP	CG-CD2-CE3	6.85	140.07	133.90
1	A	334	ARG	NE-CZ-NH1	-6.77	116.91	120.30
2	B	79	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	372	LYS	N-CA-C	6.67	129.02	111.00
1	A	226	MET	CA-CB-CG	6.62	124.56	113.30
2	B	194	TRP	CE2-CD2-CG	-6.59	102.03	107.30
2	B	255	VAL	N-CA-CB	-6.52	97.16	111.50
2	B	255	VAL	CB-CA-C	6.43	123.62	111.40
1	A	78	TRP	CG-CD1-NE1	-6.43	103.67	110.10
2	B	30	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	B	91	VAL	CG1-CB-CG2	-6.38	100.69	110.90
1	A	371	ARG	N-CA-C	6.25	127.88	111.00
2	B	3	ILE	CG1-CB-CG2	-6.22	97.72	111.40
1	A	355	TRP	CD1-CG-CD2	6.20	111.26	106.30
2	B	82	PHE	CB-CG-CD1	-6.19	116.47	120.80
2	B	36	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	216	CYS	CA-CB-SG	-6.16	102.92	114.00
1	A	85	TRP	CE2-CD2-CG	-6.15	102.38	107.30
1	A	65	THR	N-CA-C	-6.12	94.47	111.00
1	A	43	MET	CG-SD-CE	-6.09	90.46	100.20
1	A	322	SER	N-CA-C	6.08	127.40	111.00
2	B	158	TRP	CE2-CD2-CG	-5.98	102.52	107.30
1	A	199	PHE	N-CA-C	-5.97	94.87	111.00
1	A	115	ARG	NE-CZ-NH2	5.94	123.27	120.30
2	B	9	ARG	NE-CZ-NH2	5.88	123.24	120.30
2	B	63	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	B	54	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	68	TYR	CA-CB-CG	5.84	124.50	113.40
1	A	78	TRP	CB-CG-CD1	-5.82	119.43	127.00
2	B	194	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	A	179	LEU	CA-CB-CG	5.74	128.51	115.30
2	B	6	PHE	CB-CG-CD2	-5.53	116.93	120.80
2	B	181	TRP	CG-CD2-CE3	5.53	138.88	133.90
2	B	188	THR	N-CA-CB	-5.45	99.95	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	MET	CA-CB-CG	5.41	122.50	113.30
2	B	16	MET	CG-SD-CE	-5.41	91.55	100.20
1	A	339	TRP	CG-CD1-NE1	-5.38	104.72	110.10
2	B	80	TYR	CB-CG-CD2	-5.36	117.78	121.00
2	B	213	ARG	NE-CZ-NH2	5.35	122.98	120.30
2	B	185	ARG	NE-CZ-NH2	5.33	122.97	120.30
2	B	189	SER	N-CA-CB	-5.23	102.65	110.50
1	A	322	SER	N-CA-CB	-5.19	102.71	110.50
2	B	176	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	176	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	371	ARG	N-CA-CB	-5.18	101.28	110.60
2	B	41	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	333	GLU	CA-CB-CG	5.16	124.76	113.40
2	B	133	LEU	CA-C-N	-5.15	105.87	117.20
1	A	368	ILE	N-CA-C	5.14	124.88	111.00
2	B	255	VAL	N-CA-C	-5.14	97.13	111.00
2	B	73	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	94	ARG	NE-CZ-NH1	-5.08	117.76	120.30
2	B	176	VAL	CA-CB-CG1	-5.07	103.29	110.90
2	B	29	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	A	255	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	B	172	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	226	MET	N-CA-CB	-5.02	101.57	110.60
1	A	44	VAL	CG1-CB-CG2	-5.02	102.87	110.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2924	0	2887	84	0
2	B	2049	0	1981	38	0
3	A	31	0	12	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	0	24	0	0
6	B	33	0	27	0	0
7	B	22	0	19	0	0
8	A	195	0	0	14	0
8	B	188	0	0	3	0
All	All	5472	0	4950	122	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 12.

All (122) 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)
2:B:99:ASP:HB3	2:B:104:CYS:HB3	1.59	0.83
2:B:207:THR:HG23	2:B:209:CYS:SG	2.19	0.82
2:B:56:ASN:HD21	2:B:63:TYR:H	1.34	0.74
1:A:219:ALA:HB1	1:A:225:GLU:HG3	1.73	0.70
1:A:239:TYR:HB3	1:A:247:ILE:HG22	1.75	0.69
1:A:191:ILE:HG21	1:A:252:GLU:HG3	1.75	0.67
2:B:74:ASN:HA	2:B:77:LYS:NZ	2.12	0.65
1:A:144:SER:HB2	1:A:146:ARG:HG2	1.78	0.64
1:A:152:LEU:HD11	1:A:273:ILE:HD12	1.79	0.64
2:B:11:PHE:HD2	2:B:40:VAL:HG13	1.64	0.63
2:B:239:TYR:HB2	2:B:241:LEU:HD13	1.82	0.61
1:A:122:MET:HB3	1:A:128:VAL:HG21	1.83	0.60
1:A:34:VAL:HG21	1:A:80:ASP:HB3	1.82	0.60
1:A:187:TYR:O	1:A:190:LYS:HB3	2.03	0.59
1:A:334:ARG:HA	1:A:337:SER:OG	2.02	0.59
2:B:3:ILE:HD11	2:B:164:MET:SD	2.44	0.58
1:A:219:ALA:CB	1:A:225:GLU:HG3	2.34	0.57
1:A:298:LEU:HB3	1:A:303:THR:HG23	1.85	0.57
1:A:195:ARG:NH1	1:A:249:ILE:HA	2.21	0.56
1:A:282:MET:SD	8:A:531:HOH:O	2.58	0.56
1:A:8:VAL:HG21	1:A:343:SER:HA	1.88	0.56
1:A:301:GLY:HA3	3:A:401:ATP:O4'	2.06	0.56
1:A:352:GLN:HA	1:A:355:TRP:HE3	1.71	0.55
1:A:153:ASP:HA	1:A:299:SER:O	2.06	0.55
1:A:161:ASN:HD22	1:A:276:THR:HG22	1.70	0.55
2:B:41:ARG:NE	2:B:76:TYR:HE1	2.05	0.55
2:B:70:PRO:HD3	2:B:79:ARG:NH2	2.22	0.55
1:A:301:GLY:O	1:A:304:MET:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:HIC:HD2	1:A:157:GLY:O	2.07	0.54
2:B:131:VAL:HG13	2:B:165:LEU:HG	1.88	0.54
1:A:209:ARG:O	1:A:212:LYS:HB3	2.07	0.54
2:B:101:CYS:O	2:B:104:CYS:HB2	2.08	0.53
1:A:316:ILE:HD12	1:A:328:ILE:HD11	1.90	0.53
1:A:217:TYR:O	1:A:254:PHE:HA	2.09	0.53
1:A:98:GLU:HA	1:A:127:ASN:O	2.09	0.52
1:A:88:SER:O	1:A:93:LEU:HB2	2.10	0.52
2:B:56:ASN:ND2	2:B:63:TYR:H	2.04	0.52
1:A:229:ALA:HB2	1:A:235:LEU:HD12	1.91	0.52
2:B:224:SER:O	2:B:260:THR:HG22	2.10	0.52
1:A:192:LEU:HD21	1:A:211:ILE:HD11	1.92	0.52
1:A:249:ILE:HB	1:A:252:GLU:HB2	1.92	0.51
1:A:152:LEU:HD21	1:A:273:ILE:HG23	1.92	0.51
1:A:42:VAL:HG12	2:B:66:VAL:HG13	1.92	0.51
2:B:133:LEU:O	2:B:167:GLY:HA3	2.11	0.51
1:A:122:MET:HB3	1:A:128:VAL:CG2	2.41	0.51
1:A:102:THR:O	1:A:131:MET:HA	2.11	0.50
1:A:24:ASP:HB2	8:A:516:HOH:O	2.11	0.50
1:A:33:ILE:HD11	1:A:58:GLN:HB2	1.94	0.49
1:A:160:HIS:CE1	1:A:176:ARG:HG3	2.47	0.49
2:B:28:ILE:O	2:B:31:ARG:HG3	2.12	0.49
1:A:112:LYS:HB3	8:A:659:HOH:O	2.13	0.49
1:A:142:TYR:HA	1:A:146:ARG:O	2.12	0.49
2:B:210:ALA:O	2:B:213:ARG:HD3	2.13	0.49
1:A:159:THR:HG21	1:A:273:ILE:HD11	1.93	0.49
1:A:170:LEU:HD12	1:A:284:CYS:SG	2.53	0.48
1:A:71:GLU:HB3	8:A:576:HOH:O	2.13	0.48
1:A:112:LYS:HZ3	1:A:369:VAL:H	1.61	0.48
2:B:11:PHE:HB3	2:B:40:VAL:HA	1.96	0.48
2:B:78:GLU:OE2	2:B:134:HIS:HD2	1.96	0.47
2:B:236:GLN:NE2	2:B:243:ASN:HA	2.29	0.47
1:A:120:GLN:O	1:A:124:GLU:HB2	2.14	0.47
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.96	0.47
1:A:239:TYR:HB3	1:A:247:ILE:CG2	2.44	0.47
1:A:249:ILE:H	1:A:249:ILE:HD13	1.78	0.47
2:B:96:GLN:HG2	8:B:532:HOH:O	2.15	0.47
1:A:263:PRO:HB3	1:A:268:MET:HB3	1.97	0.47
2:B:90:SER:O	2:B:118:PHE:HA	2.15	0.47
2:B:1:LEU:N	8:B:568:HOH:O	2.48	0.46
1:A:39:HIS:HA	8:A:672:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLY:HA3	8:A:626:HOH:O	2.16	0.46
2:B:197:PRO:HA	8:B:513:HOH:O	2.15	0.46
2:B:74:ASN:HA	2:B:77:LYS:HZ1	1.81	0.46
1:A:192:LEU:HB3	1:A:199:PHE:HE1	1.81	0.46
1:A:215:LEU:O	1:A:253:ARG:HD2	2.14	0.46
1:A:336:TYR:O	1:A:340:ILE:HG13	2.16	0.45
1:A:183:ASP:HB3	8:A:588:HOH:O	2.16	0.45
1:A:170:LEU:HB3	1:A:373:CYS:HB3	1.97	0.45
1:A:11:ASN:ND2	1:A:85:TRP:HE1	2.14	0.45
1:A:239:TYR:HA	8:A:618:HOH:O	2.16	0.45
1:A:152:LEU:CD2	1:A:273:ILE:HG23	2.47	0.45
1:A:115:ARG:HD3	1:A:368:ILE:HG12	1.99	0.45
1:A:101:PRO:HA	1:A:130:ALA:O	2.18	0.44
1:A:304:MET:HB3	3:A:401:ATP:C6	2.53	0.44
2:B:11:PHE:CD2	2:B:40:VAL:HG13	2.50	0.44
2:B:70:PRO:HB3	2:B:77:LYS:HB3	2.00	0.44
2:B:7:ASN:C	2:B:7:ASN:HD22	2.21	0.44
2:B:125:VAL:HG13	2:B:220:LEU:HB3	2.00	0.44
2:B:29:VAL:HG13	2:B:35:VAL:HG11	1.99	0.44
1:A:3:GLU:HB3	8:A:597:HOH:O	2.17	0.44
1:A:165:TYR:HB3	1:A:170:LEU:HD21	2.00	0.44
1:A:369:VAL:HG23	1:A:371:ARG:NH1	2.33	0.44
2:B:214:ILE:HG13	2:B:255:VAL:HG13	1.98	0.44
1:A:239:TYR:HE2	8:A:633:HOH:O	2.00	0.43
1:A:349:SER:HA	1:A:352:GLN:OE1	2.19	0.43
1:A:297:VAL:HG23	8:A:584:HOH:O	2.17	0.43
1:A:348:LEU:HB3	1:A:350:THR:OG1	2.19	0.43
1:A:236:GLU:HA	1:A:250:GLY:HA2	2.00	0.43
1:A:368:ILE:HG21	8:A:646:HOH:O	2.17	0.43
2:B:69:GLU:O	2:B:71:LEU:HG	2.19	0.42
1:A:78:TRP:CD2	1:A:117:LYS:HG2	2.55	0.42
1:A:91:ASN:O	1:A:94:ARG:HD3	2.19	0.42
2:B:16:MET:CE	2:B:25:ILE:HD12	2.49	0.42
1:A:335:LYS:HE3	1:A:335:LYS:HB2	1.86	0.42
1:A:132:TYR:CG	1:A:351:PHE:HZ	2.38	0.42
2:B:147:LEU:HA	2:B:147:LEU:HD12	1.89	0.42
1:A:303:THR:HG22	1:A:334:ARG:HE	1.85	0.42
2:B:230:ALA:HA	2:B:256:GLU:O	2.20	0.41
1:A:155:GLY:O	1:A:180:ALA:HB1	2.21	0.41
1:A:131:MET:O	1:A:356:ILE:HG23	2.20	0.41
2:B:3:ILE:HD11	2:B:166:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ALA:HA	1:A:101:PRO:HD2	2.02	0.41
1:A:115:ARG:HD2	1:A:368:ILE:HD11	2.02	0.41
1:A:153:ASP:O	1:A:159:THR:HA	2.20	0.41
1:A:96:ALA:O	1:A:100:HIS:HD2	2.04	0.41
1:A:156:ASP:HB2	3:A:401:ATP:H5'1	2.03	0.41
1:A:104:LEU:O	1:A:133:VAL:HA	2.20	0.41
1:A:172:HIS:HB2	1:A:373:CYS:O	2.21	0.41
1:A:140:SER:O	1:A:143:ALA:HB3	2.20	0.40
1:A:214:LYS:HE2	8:A:633:HOH:O	2.21	0.40
3:A:401:ATP:H1'	8:A:506:HOH:O	2.21	0.40
1:A:285:ASP:O	1:A:288:ILE:HG12	2.21	0.40
2:B:187:ARG:HD3	2:B:194:TRP:CE2	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	371/374 (99%)	339 (91%)	22 (6%)	10 (3%)	6	1
2	B	258/260 (99%)	244 (95%)	9 (4%)	5 (2%)	9	2
All	All	629/634 (99%)	583 (93%)	31 (5%)	15 (2%)	7	1

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	SER
1	A	367	SER
1	A	373	CYS
1	A	286	ILE
1	A	372	LYS
2	B	57	GLN

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Mol	Chain	Res	Type
1	A	195	ARG
2	B	43	SER
1	A	273	ILE
2	B	75	SER
2	B	74	ASN
2	B	101	CYS
1	A	250	GLY
1	A	366	PRO
1	A	181	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	316/316 (100%)	282 (89%)	34 (11%)	7	1
2	B	229/229 (100%)	204 (89%)	25 (11%)	7	1
All	All	545/545 (100%)	486 (89%)	59 (11%)	7	1

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	36	ARG
1	A	42	VAL
1	A	71	GLU
1	A	82	GLU
1	A	83	LYS
1	A	111	PRO
1	A	116	GLU
1	A	124	GLU
1	A	127	ASN
1	A	177	LEU
1	A	195	ARG
1	A	207	ILE
1	A	247	ILE

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Mol	Chain	Res	Type
1	A	249	ILE
1	A	256	CYS
1	A	260	LEU
1	A	274	HIS
1	A	303	THR
1	A	304	MET
1	A	310	ASP
1	A	311	ARG
1	A	313	GLN
1	A	322	SER
1	A	323	THR
1	A	327	LYS
1	A	333	GLU
1	A	335	LYS
1	A	352	GLN
1	A	355	TRP
1	A	356	ILE
1	A	360	GLU
1	A	370	HIS
1	A	374	PHE
2	B	3	ILE
2	B	7	ASN
2	B	36	LEU
2	B	50	LYS
2	B	52	LEU
2	B	69	GLU
2	B	76	TYR
2	B	98	ASP
2	B	101	CYS
2	B	102	GLU
2	B	111	ARG
2	B	115	VAL
2	B	122	SER
2	B	125	VAL
2	B	134	HIS
2	B	152	LEU
2	B	156	GLN
2	B	183	SER
2	B	188	THR
2	B	199	SER
2	B	206	SER
2	B	207	THR

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Mol	Chain	Res	Type
2	B	225	VAL
2	B	243	ASN
2	B	255	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	110	ASN
1	A	160	HIS
1	A	161	ASN
2	B	7	ASN
2	B	44	HIS
2	B	56	ASN
2	B	134	HIS
2	B	161	ASN
2	B	193	GLN
2	B	222	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	HIC	A	72	1	9,11,12	2.05	3 (33%)	7,14,16	4.03	3 (42%)

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
1	HIC	A	72	1	-	0/4/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	HIC	CD2-NE2	-4.51	1.31	1.38
1	A	72	HIC	CE1-ND1	-2.36	1.30	1.35
1	A	72	HIC	CA-C	2.41	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	HIC	CG-CD2-NE2	-7.95	99.38	107.78
1	A	72	HIC	CB-CA-C	-2.25	107.08	111.41
1	A	72	HIC	CD2-NE2-CE1	6.47	118.31	107.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	72	HIC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	ATP	A	401	4	27,33,33	1.39	5 (18%)	25,52,52	1.50	3 (12%)
5	NAG	B	301	2,5	14,14,15	1.22	1 (7%)	15,19,21	1.74	4 (26%)
5	NAG	B	302	5,6	14,14,15	1.33	1 (7%)	15,19,21	2.09	6 (40%)
6	BMA	B	303	5,7,6	11,11,12	2.06	3 (27%)	13,15,17	2.26	3 (23%)
7	MAN	B	304	6	11,11,12	1.78	3 (27%)	13,15,17	2.28	2 (15%)
6	BMA	B	305	7	11,11,12	1.34	2 (18%)	13,15,17	1.05	1 (7%)
6	BMA	B	306	7,6	11,11,12	1.72	1 (9%)	13,15,17	1.40	2 (15%)
7	MAN	B	307	6	11,11,12	1.31	2 (18%)	13,15,17	2.39	3 (23%)

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	ATP	A	401	4	-	0/18/38/38	0/3/3/3
5	NAG	B	301	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	302	5,6	-	0/6/23/26	0/1/1/1
6	BMA	B	303	5,7,6	-	0/2/19/22	0/1/1/1
7	MAN	B	304	6	-	0/2/19/22	1/1/1/1
6	BMA	B	305	7	-	0/2/19/22	0/1/1/1
6	BMA	B	306	7,6	-	0/2/19/22	0/1/1/1
7	MAN	B	307	6	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ATP	C2'-C1'	-3.82	1.47	1.53
3	A	401	ATP	C8-N7	-2.52	1.30	1.34
3	A	401	ATP	PG-O3G	-2.15	1.46	1.54
3	A	401	ATP	C5-C4	-2.02	1.35	1.40
7	B	307	MAN	C1-C2	2.05	1.57	1.52
7	B	304	MAN	O3-C3	2.18	1.48	1.43
6	B	303	BMA	C4-C3	2.24	1.58	1.52
7	B	304	MAN	C4-C3	2.36	1.58	1.52
6	B	305	BMA	C1-C2	2.39	1.57	1.52
7	B	307	MAN	C4-C5	2.43	1.58	1.53
6	B	305	BMA	C2-C3	2.46	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	NAG	O5-C5	2.63	1.49	1.43
3	A	401	ATP	PG-O3B	2.70	1.64	1.60
5	B	301	NAG	C4-C5	2.80	1.59	1.53
6	B	303	BMA	O3-C3	3.11	1.50	1.43
7	B	304	MAN	C4-C5	3.43	1.60	1.53
6	B	306	BMA	C2-C3	4.67	1.58	1.52
6	B	303	BMA	C2-C3	4.83	1.59	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ATP	C4'-O4'-C1'	-4.91	104.55	109.77
5	B	302	NAG	C3-C4-C5	-3.59	103.89	110.22
5	B	302	NAG	C4-C3-C2	-3.30	106.19	111.02
5	B	301	NAG	O5-C1-C2	-3.04	107.25	111.47
3	A	401	ATP	C1'-N9-C4	-2.31	122.64	126.64
5	B	302	NAG	C1-C2-N2	2.02	113.94	110.49
5	B	302	NAG	O4-C4-C3	2.02	114.76	110.36
7	B	304	MAN	C3-C4-C5	2.05	113.83	110.22
5	B	302	NAG	O4-C4-C5	2.08	114.52	109.28
7	B	307	MAN	O5-C1-C2	2.14	114.14	110.79
3	A	401	ATP	O4'-C4'-C3'	2.14	109.43	105.17
6	B	305	BMA	C1-O5-C5	2.52	115.64	112.17
6	B	306	BMA	C1-O5-C5	2.59	115.73	112.17
6	B	306	BMA	O3-C3-C2	2.65	114.84	110.02
5	B	301	NAG	C2-N2-C7	2.77	126.98	122.94
6	B	303	BMA	C1-C2-C3	2.81	113.21	109.65
6	B	303	BMA	C3-C4-C5	2.94	115.39	110.22
5	B	301	NAG	C1-C2-N2	3.53	116.51	110.49
7	B	307	MAN	C3-C4-C5	3.61	116.58	110.22
5	B	301	NAG	C1-O5-C5	3.63	117.17	112.17
5	B	302	NAG	C1-O5-C5	4.82	118.82	112.17
6	B	303	BMA	C1-O5-C5	6.33	120.89	112.17
7	B	307	MAN	C1-O5-C5	6.39	120.97	112.17
7	B	304	MAN	C1-O5-C5	7.15	122.02	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	304	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	373/374 (99%)	-0.16	9 (2%) 59 55	10, 34, 64, 72	0
2	B	260/260 (100%)	-0.79	0 100 100	4, 16, 42, 57	0
All	All	633/634 (99%)	-0.42	9 (1%) 75 72	4, 26, 61, 72	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	PHE	5.0
1	A	368	ILE	4.1
1	A	348	LEU	3.9
1	A	364	ALA	2.9
1	A	373	CYS	2.5
1	A	351	PHE	2.3
1	A	369	VAL	2.2
1	A	355	TRP	2.2
1	A	371	ARG	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HIC	A	72	11/12	0.97	0.06	-	14,18,23,26	0

### 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
3	ATP	A	401	31/31	0.99	0.05	-1.49	11,19,26,28	0
4	CA	B	308	1/1	1.00	0.04	-2.36	15,15,15,15	0
6	BMA	B	306	11/12	0.76	0.19	-	66,68,70,71	0
6	BMA	B	305	11/12	0.74	0.15	-	62,64,66,67	0
6	BMA	B	303	11/12	0.74	0.20	-	60,63,65,67	0
7	MAN	B	304	11/12	0.67	0.16	-	60,62,63,65	0
7	MAN	B	307	11/12	0.60	0.26	-	65,70,72,73	0
4	CA	A	402	1/1	0.99	0.03	-	29,29,29,29	0
5	NAG	B	302	14/15	0.81	0.14	-	53,58,60,61	0
5	NAG	B	301	14/15	0.93	0.07	-	36,40,45,49	0

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

There are no such residues in this entry.