



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1PNR  
Title : PURINE REPRESSOR-HYPOXANTHINE-PURF-OPERATOR COMPLEX  
Authors : Schumacher, M.A.; Choi, K.Y.; Zalkin, H.; Brennan, R.G.  
Deposited on : 1995-03-29  
Resolution : 2.70 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

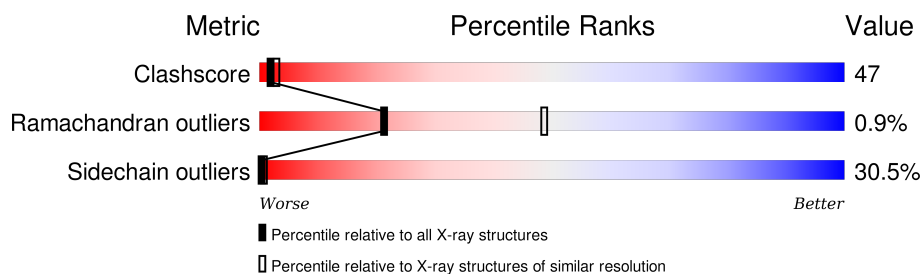
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.


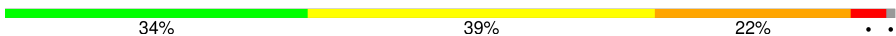
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	17	
2	A	340	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3054 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.

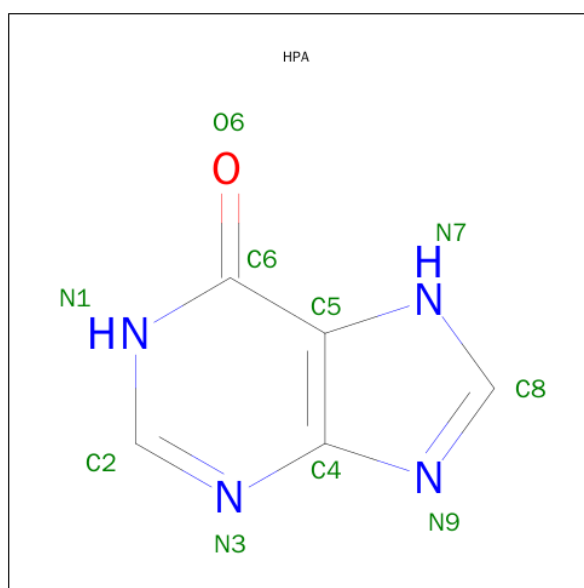
- Molecule 1 is a DNA chain called DNA (5'-D(\*AP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	17	Total	C	N	O	P	0	0	0
			346	167	64	99	16			

- Molecule 2 is a protein called PROTEIN (PURINE REPRESSOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	338	Total	C	N	O	S	0	0	0
			2652	1671	469	493	19			

- Molecule 3 is HYPOXANTHINE (three-letter code: HPA) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	2	Total 2	O 2	0	0

### 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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(\*AP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*GP\*T)-3')

Chain B: 

A699  
A700  
G701  
G702  
A703  
A704  
A705  
A706  
C707  
G708  
T709  
T710  
T711  
T712  
C713  
G714  
T715

- Molecule 2: PROTEIN (PURINE REPRESSOR)

Chain A: 

ALA  
T3  
I4  
K5  
R10  
S14  
T17  
V18  
S19  
H20  
T21  
V21  
I22  
N23  
K24  
T25  
R26  
F27  
K103  
Y107  
L108  
S109  
A35  
V36  
M111  
W37  
A38  
A39  
I40  
K41  
E42  
L43  
H44  
Y45  
S46  
P47  
V50  
A51  
R52  
S53  
L54  
K55  
V56  
N57  
H58  
T59  
K60  
S61  
I62  
G63  
L64  
L65  
A71  
F74

E79  
E82  
K83  
R84  
C85  
F86  
Q87  
K88  
Y90  
T91  
L92  
N99  
M100  
L101  
E102  
K103  
Y107  
L108  
S109  
M110  
A112  
Q113  
K114  
R115  
V116  
D117  
G118  
L119  
Y120  
V121  
M122  
C123  
S124  
P127  
E128  
L129  
K130  
V131  
M132  
H133  
T134  
E135  
R138  
H139  
I140  
P141  
M142  
V143  
I144  
M145

D146  
E149  
A150  
K151  
A152  
D153  
F154  
T155  
D156  
V158  
I159  
D160  
N161  
A162  
F163  
E164  
G165  
G166  
R171  
Y172  
L173  
I174  
R176  
R179  
E180  
I181  
G182  
V183  
I184  
P185  
G186  
P187  
R190  
N191  
T192  
G193  
R196  
L197  
A198  
G199  
F200  
M201  
R202  
A203  
M204  
E205  
E206  
A207  
M208  
I209  
K210

V211  
F212  
S213  
S214  
W215  
I216  
V217  
Q218  
G219  
D220  
F221  
E222  
P223  
E224  
S225  
G226  
Y227  
R228  
A229  
M230  
Q231  
Q232  
T233  
L234  
S235  
Q236  
P237  
H238  
R239  
D240  
T241  
A242  
V243  
F244  
I249  
M250  
A251  
R252  
L255  
C256  
A257  
E260  
M261  
G262  
L263  
R264  
V265  
Y269  
S270  
L271  
I272  
G273  
Y274  
D275  
I276  
V277

R278  
M279  
A280  
R281  
F282  
Y283  
T284  
F285  
A286  
L287  
L288  
T289  
I290  
H291  
Q292  
P293  
K294  
D295  
S296  
L297  
G298  
E299  
T300  
T301  
A302  
R303  
M304  
L305  
L306  
D307  
R308  
I309  
V310  
N311  
K312  
R313  
R314  
E315  
P316  
Q317  
S318  
I319  
E320  
V321  
H322  
L325  
I326  
E327  
R328  
R329  
R337  
R340  
ARG

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.85Å 94.79Å 81.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HPA

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	B	0.87	0/388	2.80	33/597 (5.5%)
2	A	1.31	5/2706 (0.2%)	1.64	43/3660 (1.2%)
All	All	1.26	5/3094 (0.2%)	1.85	76/4257 (1.8%)

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
2	A	2	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	37	TRP	CB-CG	-6.38	1.38	1.50
2	A	213	GLU	CG-CD	6.07	1.61	1.51
2	A	244	PHE	CE2-CZ	5.76	1.48	1.37
2	A	243	VAL	CB-CG1	-5.62	1.41	1.52
2	A	243	VAL	CA-CB	-5.16	1.44	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	DA	C4-N9-C1'	-18.56	92.89	126.30
1	B	703	DA	C8-N9-C1'	18.32	160.68	127.70
1	B	705	DA	C8-N9-C1'	13.55	152.08	127.70
1	B	705	DA	C4-N9-C1'	-13.51	101.98	126.30
1	B	706	DA	C8-N9-C1'	12.45	150.11	127.70
1	B	706	DA	C4-N9-C1'	-12.13	104.47	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	713	DC	C2-N1-C1'	-11.85	105.76	118.80
1	B	711	DT	C6-N1-C1'	11.52	137.68	120.40
1	B	715	DT	C6-N1-C1'	-11.51	103.14	120.40
2	A	139	HIS	CA-CB-CG	11.31	132.83	113.60
1	B	699	DA	C8-N9-C1'	-11.24	107.46	127.70
1	B	699	DA	C4-N9-C1'	11.22	146.49	126.30
1	B	711	DT	C2-N1-C1'	-11.21	100.26	118.20
1	B	709	DT	C6-N1-C1'	-10.87	104.10	120.40
1	B	701	DC	C2-N1-C1'	-10.79	106.94	118.80
1	B	715	DT	C2-N1-C1'	10.65	135.24	118.20
1	B	709	DT	C2-N1-C1'	10.23	134.56	118.20
1	B	700	DA	C4-N9-C1'	-10.16	108.01	126.30
1	B	700	DA	C8-N9-C1'	9.89	145.50	127.70
1	B	701	DC	C6-N1-C1'	9.20	131.84	120.80
1	B	713	DC	C6-N1-C1'	9.19	131.83	120.80
2	A	236	GLN	C-N-CD	-9.08	100.62	120.60
1	B	712	DT	C6-N1-C1'	8.85	133.68	120.40
2	A	263	LEU	CB-CG-CD1	-8.50	96.56	111.00
2	A	131	LEU	CB-CG-CD2	-8.40	96.71	111.00
1	B	704	DA	C4-N9-C1'	-8.28	111.41	126.30
1	B	704	DA	C8-N9-C1'	8.25	142.56	127.70
2	A	155	THR	CB-CA-C	-8.06	89.84	111.60
1	B	703	DA	O4'-C4'-C3'	-7.92	101.25	106.00
1	B	707	DC	C2-N1-C1'	-7.82	110.19	118.80
2	A	294	LYS	CB-CA-C	7.74	125.88	110.40
2	A	340	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	B	712	DT	C2-N1-C1'	-7.61	106.02	118.20
2	A	228	ARG	NE-CZ-NH2	7.54	124.07	120.30
2	A	269	VAL	CB-CA-C	-7.45	97.25	111.40
1	B	707	DC	C6-N1-C1'	7.13	129.36	120.80
2	A	54	LEU	N-CA-CB	7.07	124.55	110.40
2	A	255	LEU	CB-CG-CD2	-6.97	99.15	111.00
1	B	703	DA	C5-C6-N6	-6.93	118.15	123.70
2	A	325	LEU	CA-CB-CG	6.80	130.93	115.30
1	B	710	DT	O4'-C1'-N1	-6.73	103.29	108.00
1	B	715	DT	O4'-C1'-N1	6.70	112.69	108.00
2	A	220	ASP	CB-CG-OD1	6.65	124.29	118.30
1	B	703	DA	N1-C6-N6	6.61	122.57	118.60
2	A	306	LEU	CA-CB-CG	-6.61	100.11	115.30
2	A	56	VAL	CA-CB-CG2	-6.46	101.22	110.90
2	A	230	MET	CG-SD-CE	-6.39	89.98	100.20
2	A	200	PHE	CB-CA-C	-6.29	97.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	139	HIS	N-CA-CB	-6.17	99.50	110.60
2	A	122	MET	CG-SD-CE	6.12	109.99	100.20
2	A	204	MET	CG-SD-CE	6.08	109.93	100.20
2	A	208	MET	CG-SD-CE	5.95	109.72	100.20
2	A	250	MET	CG-SD-CE	5.91	109.65	100.20
2	A	190	ARG	NE-CZ-NH2	5.86	123.23	120.30
2	A	197	LEU	CB-CA-C	-5.80	99.18	110.20
1	B	702	DG	C4-N9-C1'	5.68	133.88	126.50
2	A	306	LEU	CB-CG-CD1	-5.66	101.38	111.00
2	A	308	ARG	NE-CZ-NH1	-5.55	117.53	120.30
2	A	28	VAL	CB-CA-C	-5.54	100.88	111.40
2	A	322	HIS	N-CA-C	5.54	125.94	111.00
2	A	110	MET	CG-SD-CE	5.52	109.04	100.20
1	B	707	DC	O4'-C1'-N1	-5.46	104.18	108.00
2	A	158	VAL	CA-CB-CG2	-5.46	102.71	110.90
2	A	252	MET	CG-SD-CE	5.43	108.89	100.20
2	A	171	ARG	NE-CZ-NH1	-5.36	117.62	120.30
2	A	158	VAL	N-CA-C	-5.33	96.61	111.00
2	A	326	ILE	CB-CA-C	-5.33	100.95	111.60
2	A	211	VAL	CB-CA-C	5.25	121.38	111.40
2	A	279	ASN	CB-CA-C	5.24	120.88	110.40
2	A	249	ILE	CG1-CB-CG2	5.15	122.74	111.40
2	A	325	LEU	CB-CG-CD2	-5.14	102.25	111.00
2	A	196	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	A	305	LEU	CA-CB-CG	5.10	127.04	115.30
2	A	165	GLY	N-CA-C	-5.09	100.38	113.10
2	A	25	THR	N-CA-CB	-5.06	100.69	110.30
2	A	57	ASN	N-CA-C	5.00	124.50	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	211	VAL	CA
2	A	294	LYS	CA

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	B	346	0	194	25	2
2	A	2652	0	2636	254	0
3	A	10	0	4	0	0
4	A	44	0	0	0	1
4	B	2	0	0	0	0
All	All	3054	0	2834	275	3

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 47.

All (275) 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:B:713:DC:H2''	1:B:714:DG:H5''	1.25	1.16
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.16	1.08
2:A:61:SER:HB2	2:A:91:THR:HG22	1.16	1.08
2:A:337:ARG:HG2	2:A:337:ARG:HH11	1.26	1.01
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.81	0.95
2:A:210:LYS:H	2:A:210:LYS:HD3	1.31	0.94
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.85	0.91
2:A:292:GLN:HG3	2:A:293:PRO:HD2	1.51	0.91
2:A:292:GLN:HG3	2:A:293:PRO:CD	2.02	0.89
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.01	0.89
2:A:140:ILE:HD12	2:A:141:PRO:CD	2.05	0.86
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.57	0.85
1:B:713:DC:C2'	1:B:714:DG:H5''	2.05	0.83
2:A:135:GLU:O	2:A:138:ARG:HG2	1.78	0.83
2:A:61:SER:CB	2:A:91:THR:HG22	2.07	0.83
1:B:712:DT:H2''	1:B:713:DC:H5''	1.58	0.83
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.61	0.83
2:A:61:SER:HB2	2:A:91:THR:CG2	2.07	0.81
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.61	0.81
2:A:181:ILE:CD1	2:A:204:MET:HE3	2.12	0.80
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.64	0.78
1:B:713:DC:H2''	1:B:714:DG:H8	1.49	0.78
2:A:200:PHE:HD2	2:A:201:MET:CE	1.96	0.78
2:A:181:ILE:HD13	2:A:204:MET:HE3	1.64	0.78
2:A:167:TYR:CD1	2:A:202:LYS:HG2	2.19	0.78
1:B:713:DC:H2''	1:B:714:DG:C8	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.67	0.77
2:A:20:HIS:HA	2:A:25:THR:CG2	2.15	0.77
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.66	0.76
1:B:706:DA:C2	2:A:55:LYS:HE2	2.20	0.76
2:A:23:ASN:N	2:A:23:ASN:HD22	1.82	0.76
2:A:159:ILE:O	2:A:159:ILE:HD12	1.85	0.76
2:A:3:THR:HG23	2:A:45:TYR:CE1	2.22	0.75
1:B:714:DG:C2'	1:B:715:DT:H5'	2.17	0.75
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.50	0.74
2:A:277:VAL:HG12	2:A:279:ASN:H	1.51	0.74
2:A:164:GLU:O	2:A:168:MET:HG3	1.89	0.73
2:A:167:TYR:HD1	2:A:202:LYS:HG2	1.54	0.73
1:B:700:DA:H2''	1:B:701:DC:O5'	1.88	0.72
2:A:325:LEU:HD11	2:A:327:GLU:HG3	1.72	0.72
2:A:101:LEU:HA	2:A:104:GLN:HG2	1.70	0.71
2:A:337:ARG:HG2	2:A:337:ARG:NH1	2.03	0.71
2:A:286:ALA:HB1	2:A:328:ARG:HG2	1.70	0.71
2:A:23:ASN:ND2	2:A:23:ASN:N	2.38	0.71
2:A:257:ALA:O	2:A:261:MET:HG3	1.91	0.70
2:A:101:LEU:HA	2:A:104:GLN:CG	2.21	0.70
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.23	0.69
2:A:105:ARG:HA	2:A:133:MET:CE	2.22	0.69
1:B:706:DA:H2	2:A:55:LYS:HE2	1.57	0.69
2:A:224:GLU:O	2:A:224:GLU:HG3	1.93	0.68
2:A:40:ILE:HG22	2:A:41:LYS:HD3	1.74	0.68
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.29	0.68
2:A:210:LYS:N	2:A:210:LYS:HD3	2.07	0.67
2:A:210:LYS:H	2:A:210:LYS:CD	2.06	0.66
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.13	0.66
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.61	0.66
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.09	0.66
2:A:155:THR:HG22	2:A:156:ASP:N	2.11	0.65
2:A:306:LEU:O	2:A:310:VAL:N	2.29	0.65
2:A:309:ILE:HG22	2:A:310:VAL:N	2.12	0.65
2:A:237:PRO:HG2	2:A:238:HIS:H	1.61	0.65
2:A:140:ILE:HD12	2:A:141:PRO:N	2.11	0.65
1:B:714:DG:H5''	1:B:714:DG:H8	1.62	0.65
2:A:130:LEU:O	2:A:130:LEU:HD22	1.96	0.65
2:A:174:ILE:HG22	2:A:175:GLU:N	2.12	0.64
2:A:159:ILE:C	2:A:159:ILE:HD12	2.17	0.64
1:B:702:DG:H5'	1:B:702:DG:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:DG:H2''	1:B:715:DT:H5'	1.80	0.63
2:A:10:ARG:NE	2:A:42:GLU:OE1	2.30	0.63
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.28	0.63
2:A:62:ILE:HD12	2:A:63:GLY:N	2.14	0.63
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.33	0.63
2:A:281:ARG:O	2:A:281:ARG:NH1	2.27	0.62
2:A:149:GLU:HG2	2:A:151:LYS:HD2	1.82	0.62
2:A:200:PHE:CZ	2:A:204:MET:HE2	2.34	0.62
1:B:714:DG:C5'	1:B:714:DG:H8	2.13	0.61
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.29	0.61
2:A:252:MET:HE2	2:A:283:PHE:CE1	2.36	0.61
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.83	0.61
2:A:100:ASN:O	2:A:104:GLN:HG2	2.01	0.61
2:A:265:VAL:HG13	2:A:269:VAL:O	2.00	0.61
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.01	0.61
2:A:105:ARG:HA	2:A:133:MET:HE1	1.83	0.61
2:A:23:ASN:H	2:A:23:ASN:HD22	1.48	0.60
2:A:183:VAL:HG13	2:A:216:ILE:HB	1.84	0.60
2:A:237:PRO:CG	2:A:238:HIS:H	2.15	0.60
2:A:231:GLN:O	2:A:235:SER:HB2	2.02	0.60
2:A:19:SER:O	2:A:23:ASN:ND2	2.34	0.60
2:A:39:ALA:O	2:A:43:LEU:HB2	2.02	0.59
2:A:325:LEU:HD13	2:A:326:ILE:N	2.17	0.59
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.67	0.59
2:A:200:PHE:CZ	2:A:204:MET:CE	2.86	0.58
2:A:63:GLY:O	2:A:119:LEU:HD12	2.03	0.58
1:B:703:DA:H5'	1:B:703:DA:N9	2.19	0.58
2:A:157:ALA:O	2:A:318:SER:HA	2.04	0.58
2:A:155:THR:HG22	2:A:156:ASP:H	1.68	0.58
2:A:163:PHE:O	2:A:199:GLY:HA3	2.04	0.58
2:A:286:ALA:HB3	2:A:329:ARG:CG	2.34	0.58
2:A:243:VAL:HG12	2:A:244:PHE:N	2.18	0.57
2:A:28:VAL:HG12	2:A:32:THR:HB	1.85	0.57
2:A:101:LEU:HD13	2:A:104:GLN:HE21	1.69	0.57
2:A:82:GLU:HG3	2:A:83:LYS:N	2.20	0.57
2:A:196:ARG:HD3	2:A:274:TYR:CD2	2.40	0.57
2:A:310:VAL:HG22	2:A:311:ASN:OD1	2.04	0.56
2:A:35:ALA:O	2:A:38:ALA:HB3	2.06	0.56
2:A:112:ALA:O	2:A:115:ARG:N	2.37	0.56
2:A:181:ILE:HD12	2:A:204:MET:HE3	1.88	0.56
2:A:234:LEU:HD23	2:A:234:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.33	0.55
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.87	0.55
2:A:284:THR:O	2:A:284:THR:HG22	2.07	0.55
2:A:135:GLU:HG2	2:A:135:GLU:O	2.07	0.55
2:A:278:ARG:NH1	2:A:278:ARG:HG3	2.22	0.55
1:B:714:DG:C5'	1:B:714:DG:C8	2.90	0.54
1:B:702:DG:C8	1:B:702:DG:H5'	2.42	0.54
2:A:22:ILE:HG22	2:A:23:ASN:HD21	1.69	0.54
2:A:90:TYR:CD1	2:A:90:TYR:N	2.74	0.54
2:A:310:VAL:HG22	2:A:311:ASN:N	2.22	0.54
2:A:105:ARG:CA	2:A:133:MET:HE1	2.37	0.54
2:A:313:ARG:HG3	2:A:314:GLU:N	2.23	0.54
2:A:197:LEU:O	2:A:200:PHE:HB3	2.09	0.53
2:A:286:ALA:HB3	2:A:329:ARG:HG3	1.90	0.53
2:A:274:TYR:HD1	2:A:275:ASP:N	2.07	0.53
2:A:222:GLU:HB3	2:A:223:PRO:HD2	1.90	0.53
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.54	0.53
2:A:179:ARG:HA	2:A:209:ILE:CD1	2.38	0.53
2:A:152:ALA:HB1	2:A:154:PHE:CE1	2.44	0.53
2:A:337:ARG:HH11	2:A:337:ARG:CG	2.10	0.53
2:A:10:ARG:HG3	2:A:10:ARG:NH1	2.24	0.53
2:A:239:ARG:HB2	2:A:240:PRO:CD	2.38	0.53
2:A:201:MET:HE2	2:A:201:MET:HA	1.91	0.52
2:A:41:LYS:O	2:A:44:HIS:N	2.39	0.52
2:A:142:MET:CG	2:A:155:THR:HG23	2.39	0.52
2:A:130:LEU:HD22	2:A:134:LEU:HG	1.90	0.52
2:A:276:ASN:ND2	2:A:291:HIS:HD2	2.08	0.52
2:A:62:ILE:HD12	2:A:62:ILE:C	2.31	0.52
2:A:183:VAL:HA	2:A:244:PHE:O	2.10	0.51
2:A:114:LYS:O	2:A:115:ARG:HB2	2.10	0.51
2:A:236:GLN:CB	2:A:237:PRO:CD	2.88	0.51
2:A:296:SER:O	2:A:300:THR:HB	2.10	0.51
2:A:279:ASN:HD22	2:A:279:ASN:C	2.13	0.51
2:A:105:ARG:HA	2:A:133:MET:HE3	1.91	0.51
2:A:14:SER:O	2:A:17:THR:HB	2.10	0.51
2:A:236:GLN:HB2	2:A:237:PRO:CD	2.40	0.51
2:A:252:MET:HB2	2:A:283:PHE:CE2	2.45	0.51
2:A:3:THR:HG23	2:A:45:TYR:CD1	2.46	0.51
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.75	0.51
2:A:236:GLN:HB2	2:A:237:PRO:HD3	1.93	0.51
2:A:184:ILE:HD13	2:A:229:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:145:MET:HA	2:A:158:VAL:CG1	2.41	0.51
2:A:28:VAL:CG1	2:A:32:THR:HB	2.41	0.50
2:A:160:ASP:O	2:A:161:ASN:HB2	2.11	0.50
2:A:201:MET:CA	2:A:201:MET:HE2	2.41	0.50
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.94	0.50
2:A:308:ARG:HH21	2:A:316:PRO:HA	1.76	0.50
2:A:56:VAL:HG23	2:A:57:ASN:N	2.26	0.50
1:B:714:DG:H5"	1:B:714:DG:C8	2.45	0.50
1:B:709:DT:H2"	1:B:710:DT:H5'	1.92	0.50
2:A:64:LEU:C	2:A:64:LEU:HD12	2.31	0.49
2:A:101:LEU:HD12	2:A:104:GLN:HG3	1.94	0.49
2:A:179:ARG:NH2	2:A:207:ALA:O	2.45	0.49
1:B:701:DC:H2"	1:B:702:DG:H5"	1.95	0.49
2:A:156:ASP:HB3	2:A:304:MET:HE1	1.94	0.49
2:A:286:ALA:CB	2:A:328:ARG:HG2	2.41	0.49
2:A:233:ILE:O	2:A:236:GLN:HG2	2.12	0.49
2:A:179:ARG:HA	2:A:209:ILE:HD13	1.94	0.49
2:A:210:LYS:O	2:A:210:LYS:HG2	2.13	0.48
2:A:120:LEU:HD13	2:A:305:LEU:HD22	1.95	0.48
1:B:707:DC:H2"	2:A:54:LEU:HD11	1.95	0.48
2:A:144:VAL:HG23	2:A:146:ASP:H	1.79	0.48
2:A:112:ALA:O	2:A:115:ARG:HD3	2.14	0.48
2:A:140:ILE:CD1	2:A:141:PRO:HD2	2.40	0.48
2:A:60:LYS:N	2:A:117:ASP:OD2	2.39	0.47
2:A:304:MET:O	2:A:307:ASP:HB3	2.13	0.47
2:A:304:MET:HE3	2:A:317:GLN:HG2	1.95	0.47
2:A:304:MET:CE	2:A:317:GLN:HG2	2.44	0.47
1:B:703:DA:H5'	1:B:703:DA:C8	2.49	0.47
2:A:54:LEU:O	2:A:54:LEU:HD12	2.13	0.47
2:A:211:VAL:HG23	2:A:212:PRO:HD2	1.97	0.47
2:A:211:VAL:CB	2:A:212:PRO:HD2	2.44	0.47
2:A:64:LEU:HD12	2:A:65:LEU:N	2.30	0.47
2:A:200:PHE:HD2	2:A:201:MET:HE1	1.75	0.47
2:A:252:MET:CE	2:A:283:PHE:CE1	2.97	0.47
2:A:123:CYS:O	2:A:124:SER:HB2	2.13	0.46
2:A:140:ILE:HD12	2:A:140:ILE:C	2.35	0.46
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.45	0.46
2:A:243:VAL:CG1	2:A:244:PHE:N	2.77	0.46
2:A:274:TYR:N	2:A:289:THR:OG1	2.48	0.46
2:A:202:LYS:HG3	2:A:203:ALA:N	2.28	0.46
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:281:ARG:O	2:A:281:ARG:HG2	2.15	0.46
2:A:184:ILE:HA	2:A:217:VAL:O	2.15	0.46
1:B:706:DA:N3	2:A:55:LYS:HE2	2.31	0.46
2:A:101:LEU:C	2:A:104:GLN:HG2	2.36	0.46
2:A:45:TYR:CZ	2:A:47:PRO:HA	2.50	0.46
2:A:237:PRO:CG	2:A:238:HIS:N	2.79	0.46
2:A:131:LEU:O	2:A:134:LEU:HB2	2.15	0.46
2:A:222:GLU:O	2:A:225:SER:N	2.47	0.46
2:A:152:ALA:CB	2:A:154:PHE:CE1	2.99	0.46
2:A:272:ILE:HG21	2:A:272:ILE:HD13	1.64	0.46
2:A:310:VAL:CG2	2:A:311:ASN:N	2.79	0.45
2:A:142:MET:HG3	2:A:155:THR:HG23	1.97	0.45
2:A:185:PRO:HD2	2:A:218:GLN:HA	1.98	0.45
1:B:715:DT:H2'	1:B:715:DT:H6	1.30	0.45
2:A:201:MET:CA	2:A:201:MET:CE	2.94	0.45
2:A:277:VAL:CG1	2:A:278:ARG:N	2.78	0.45
2:A:201:MET:HE3	2:A:201:MET:HB2	1.60	0.45
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.78	0.45
2:A:167:TYR:OH	2:A:206:GLU:OE1	2.29	0.45
2:A:43:LEU:HA	2:A:43:LEU:HD22	1.18	0.45
2:A:183:VAL:O	2:A:216:ILE:HA	2.17	0.45
2:A:180:GLU:HB3	2:A:240:PRO:HA	1.98	0.45
2:A:227:TYR:OH	2:A:260:GLU:OE1	2.29	0.45
2:A:192:THR:HG1	2:A:221:PHE:HZ	1.64	0.45
2:A:167:TYR:CE1	2:A:202:LYS:CG	3.00	0.44
2:A:20:HIS:CE1	2:A:26:ARG:HB3	2.52	0.44
2:A:291:HIS:CE1	2:A:293:PRO:HA	2.52	0.44
2:A:117:ASP:O	2:A:141:PRO:HG2	2.17	0.44
2:A:142:MET:HG2	2:A:155:THR:HG23	1.98	0.44
2:A:187:PRO:O	2:A:193:GLY:HA3	2.17	0.44
2:A:184:ILE:HD13	2:A:229:ALA:CB	2.48	0.44
2:A:106:ALA:O	2:A:110:MET:HG3	2.17	0.44
2:A:128:GLU:N	2:A:129:PRO:CD	2.80	0.44
2:A:37:TRP:O	2:A:40:ILE:HB	2.17	0.44
2:A:313:ARG:NH1	2:A:315:GLU:O	2.47	0.44
2:A:152:ALA:HB1	2:A:154:PHE:CD1	2.52	0.44
2:A:64:LEU:HB2	2:A:92:LEU:HD21	2.00	0.44
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.99	0.44
2:A:105:ARG:N	2:A:133:MET:HE1	2.32	0.43
2:A:142:MET:O	2:A:155:THR:HG22	2.18	0.43
2:A:212:PRO:HG2	2:A:215:TRP:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:ILE:HD13	2:A:204:MET:CE	2.42	0.43
2:A:261:MET:HB3	2:A:261:MET:HE3	1.62	0.43
2:A:87:GLN:OE1	2:A:88:LYS:HD3	2.18	0.43
2:A:59:THR:HG21	2:A:115:ARG:O	2.18	0.43
2:A:134:LEU:HD23	2:A:134:LEU:HA	1.70	0.43
2:A:181:ILE:HA	2:A:242:ALA:O	2.19	0.43
2:A:210:LYS:CD	2:A:210:LYS:N	2.75	0.43
2:A:263:LEU:HD13	2:A:263:LEU:N	2.32	0.43
2:A:313:ARG:CG	2:A:314:GLU:N	2.81	0.42
2:A:71:ALA:O	2:A:74:PHE:HB2	2.19	0.42
2:A:85:CYS:HA	2:A:302:PHE:CZ	2.55	0.42
2:A:20:HIS:HA	2:A:25:THR:HG22	1.97	0.42
2:A:200:PHE:CZ	2:A:204:MET:HE1	2.54	0.42
2:A:252:MET:HE3	2:A:283:PHE:CZ	2.55	0.42
1:B:713:DC:C2'	1:B:714:DG:C8	2.97	0.42
2:A:281:ARG:HH11	2:A:281:ARG:HG2	1.83	0.42
2:A:154:PHE:CD1	2:A:154:PHE:N	2.87	0.42
2:A:202:LYS:CG	2:A:203:ALA:N	2.83	0.41
2:A:325:LEU:HD13	2:A:326:ILE:C	2.40	0.41
2:A:143:VAL:HG23	2:A:144:VAL:N	2.35	0.41
2:A:161:ASN:HB3	2:A:164:GLU:HG2	2.03	0.41
2:A:202:LYS:HE3	2:A:206:GLU:HG3	2.02	0.41
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.15	0.41
2:A:252:MET:CE	2:A:283:PHE:CZ	3.02	0.41
2:A:212:PRO:CG	2:A:215:TRP:CE3	3.03	0.41
2:A:143:VAL:HA	2:A:155:THR:HG22	2.01	0.41
2:A:297:LEU:HD23	2:A:297:LEU:O	2.21	0.41
2:A:315:GLU:HB3	2:A:316:PRO:HD2	2.01	0.41
2:A:161:ASN:HD21	2:A:320:GLU:HB3	1.85	0.41
2:A:131:LEU:HD12	2:A:131:LEU:HA	1.58	0.41
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.01	0.41
2:A:277:VAL:O	2:A:279:ASN:N	2.54	0.41
2:A:288:THR:OG1	2:A:328:ARG:N	2.30	0.41
2:A:337:ARG:O	2:A:337:ARG:NH1	2.53	0.41
2:A:310:VAL:C	2:A:312:LYS:H	2.24	0.41
1:B:702:DG:H5'	1:B:702:DG:H2'	1.94	0.40
2:A:149:GLU:CG	2:A:151:LYS:HD2	2.49	0.40
2:A:274:TYR:CD1	2:A:275:ASP:N	2.88	0.40
2:A:212:PRO:HG2	2:A:215:TRP:CE3	2.56	0.40
2:A:329:ARG:CZ	2:A:329:ARG:CB	2.98	0.40
2:A:14:SER:O	2:A:17:THR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:278:ARG:CG	2:A:278:ARG:HH11	2.34	0.40
2:A:42:GLU:C	2:A:44:HIS:N	2.74	0.40
2:A:236:GLN:HG3	2:A:237:PRO:HD2	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:718:HOH:O	4:A:718:HOH:O[4_555]	1.83	0.37
1:B:703:DA:N6	1:B:712:DT:O4[4_555]	2.07	0.13
1:B:702:DG:O6	1:B:713:DC:N4[4_555]	2.19	0.01

## 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	
2	A	336/340 (99%)	302 (90%)	31 (9%)	3 (1%)	21	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	278	ARG
2	A	311	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	279/280 (100%)	194 (70%)	85 (30%)	<b>0</b> <b>1</b>

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR
2	A	5	LYS
2	A	14	SER
2	A	19	SER
2	A	22	ILE
2	A	23	ASN
2	A	30	GLU
2	A	40	ILE
2	A	41	LYS
2	A	42	GLU
2	A	43	LEU
2	A	44	HIS
2	A	50	VAL
2	A	52	ARG
2	A	55	LYS
2	A	60	LYS
2	A	62	ILE
2	A	79	GLU
2	A	82	GLU
2	A	87	GLN
2	A	91	THR
2	A	92	LEU
2	A	99	ASN
2	A	100	ASN
2	A	101	LEU
2	A	103	LYS
2	A	105	ARG
2	A	109	SER
2	A	110	MET
2	A	120	LEU
2	A	127	PRO
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	138	ARG
2	A	140	ILE

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Mol	Chain	Res	Type
2	A	143	VAL
2	A	144	VAL
2	A	145	MET
2	A	151	LYS
2	A	153	ASP
2	A	155	THR
2	A	174	ILE
2	A	176	ARG
2	A	190	ARG
2	A	202	LYS
2	A	204	MET
2	A	205	GLU
2	A	210	LYS
2	A	211	VAL
2	A	213	GLU
2	A	216	ILE
2	A	218	GLN
2	A	224	GLU
2	A	228	ARG
2	A	230	MET
2	A	232	GLN
2	A	235	SER
2	A	252	MET
2	A	255	LEU
2	A	261	MET
2	A	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	270	SER
2	A	274	TYR
2	A	278	ARG
2	A	279	ASN
2	A	281	ARG
2	A	284	THR
2	A	288	THR
2	A	292	GLN
2	A	294	LYS
2	A	295	ASP
2	A	296	SER
2	A	299	GLU
2	A	308	ARG
2	A	310	VAL

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Mol	Chain	Res	Type
2	A	312	LYS
2	A	315	GLU
2	A	318	SER
2	A	325	LEU
2	A	328	ARG
2	A	329	ARG
2	A	337	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	ASN
2	A	34	ASN
2	A	58	HIS
2	A	96	ASN
2	A	99	ASN
2	A	218	GLN
2	A	279	ASN
2	A	291	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	HPA	A	599	-	8,11,11	1.55	2 (25%)	4,15,15	4.21	2 (50%)

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	HPA	A	599	-	-	0/0/0/0	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	HPA	C2-N1	2.01	1.37	1.33
3	A	599	HPA	C6-N1	3.12	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	HPA	N3-C2-N1	-5.99	124.31	128.89
3	A	599	HPA	C2-N1-C6	5.79	124.82	116.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.