



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:04 pm BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

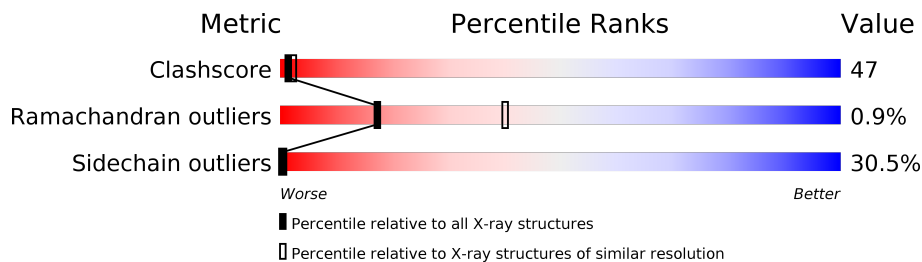
# 1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	17	6% 29% 65%
2	A	340	34% 39% 22%

## 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.

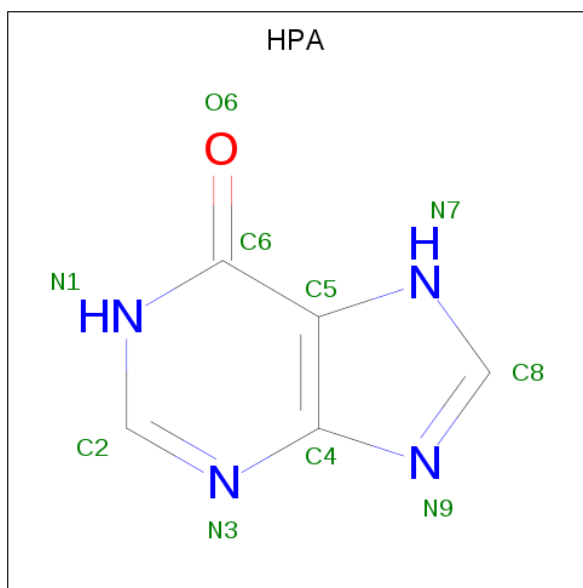
- Molecule 1 is a DNA chain called DNA (5'-D(\*AP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*GP\*T)-3').

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

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

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

- 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
			Total	C	N	O		
3	A	1	10	5	4	1	0	0

- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	2	Total 2	O 2	0	0
4	A	44	Total 44	O 44	0	0

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

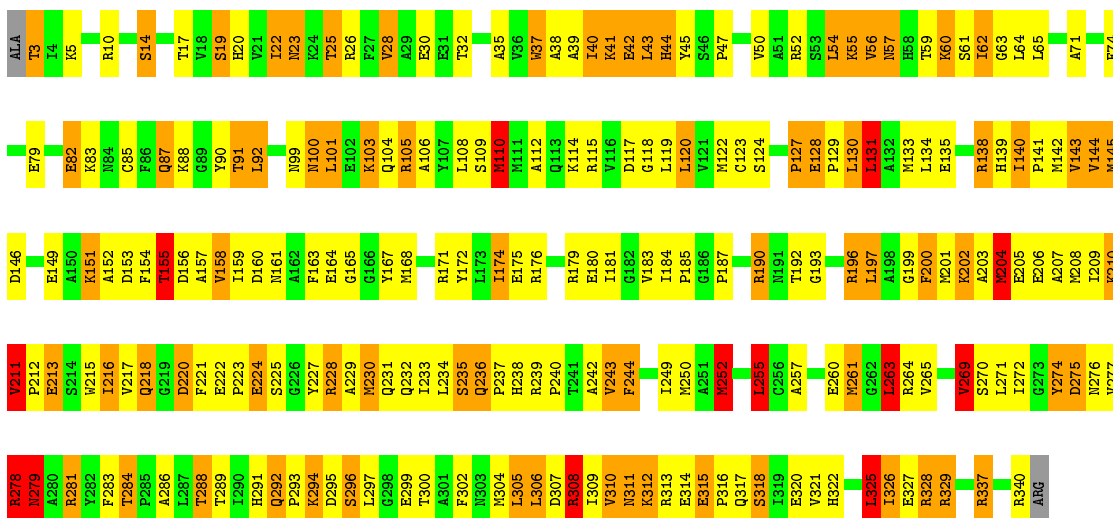
- Molecule 1: DNA (5'-D(\*AP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*GP\*T)-3')

Chain B: 



- Molecule 2: PROTEIN (PURINE REPRESSOR)

Chain A: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore 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.	Xtrriage
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 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: 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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



Continued from previous page...

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

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
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.61	0.83
1:B:712:DT:H2''	1:B:713:DC:H5''	1.58	0.83
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.61	0.81
2:A:61:SER:HB2	2:A:91:THR:CG2	2.07	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:181:ILE:HD13	2:A:204:MET:HE3	1.64	0.78
2:A:200:PHE:HD2	2:A:201:MET:CE	1.96	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

*Continued on next page...*

*Continued from previous page...*

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:286:ALA:HB1	2:A:328:ARG:HG2	1.70	0.71
2:A:337:ARG:HG2	2:A:337:ARG:NH1	2.03	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:237:PRO:HG2	2:A:238:HIS:H	1.61	0.65
2:A:309:ILE:HG22	2:A:310:VAL:N	2.12	0.65
2:A:140:ILE:HD12	2:A:141:PRO:N	2.11	0.65
2:A:130:LEU:O	2:A:130:LEU:HD22	1.96	0.65
1:B:714:DG:H5''	1:B:714:DG:H8	1.62	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

*Continued on next page...*

*Continued from previous page...*

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:105:ARG:HA	2:A:133:MET:HE1	1.83	0.61
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.01	0.61
2:A:183:VAL:HG13	2:A:216:ILE:HB	1.84	0.60
2:A:23:ASN:H	2:A:23:ASN:HD22	1.48	0.60
2:A:231:GLN:O	2:A:235:SER:HB2	2.02	0.60
2:A:237:PRO:CG	2:A:238:HIS:H	2.15	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:112:ALA:O	2:A:115:ARG:N	2.37	0.56
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: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

*Continued on next page...*

*Continued from previous page...*

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:702:DG:C8	1:B:702:DG:H5'	2.42	0.54
1:B:714:DG:C5'	1:B:714:DG:C8	2.90	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:222:GLU:HB3	2:A:223:PRO:HD2	1.90	0.53
2:A:274:TYR:HD1	2:A:275:ASP:N	2.07	0.53
2:A:179:ARG:HA	2:A:209:ILE:CD1	2.38	0.53
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.54	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:114:LYS:O	2:A:115:ARG:HB2	2.10	0.51
2:A:183:VAL:HA	2:A:244:PHE:O	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:105:ARG:HA	2:A:133:MET:HE3	1.91	0.51
2:A:279:ASN:HD22	2:A:279:ASN:C	2.13	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:184:ILE:HD13	2:A:229:ALA:HB3	1.93	0.51
2:A:236:GLN:HB2	2:A:237:PRO:HD3	1.93	0.51
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.75	0.51
2:A:3:THR:HG23	2:A:45:TYR:CD1	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

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:709:DT:H2''	1:B:710:DT:H5'	1.92	0.50
1:B:714:DG:H5''	1:B:714:DG:C8	2.45	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:179:ARG:HA	2:A:209:ILE:HD13	1.94	0.49
2:A:233:ILE:O	2:A:236:GLN:HG2	2.12	0.49
2:A:286:ALA:CB	2:A:328:ARG:HG2	2.41	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:112:ALA:O	2:A:115:ARG:HD3	2.14	0.48
2:A:144:VAL:HG23	2:A:146:ASP:H	1.79	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:120:LEU:CD1	2:A:143:VAL:HG13	2.45	0.46
2:A:202:LYS:HG3	2:A:203:ALA:N	2.28	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:184:ILE:HA	2:A:217:VAL:O	2.15	0.46
2:A:281:ARG:O	2:A:281:ARG:HG2	2.15	0.46
2:A:101:LEU:C	2:A:104:GLN:HG2	2.36	0.46
1:B:706:DA:N3	2:A:55:LYS:HE2	2.31	0.46
2:A:45:TYR:CZ	2:A:47:PRO:HA	2.50	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:237:PRO:CG	2:A:238:HIS:N	2.79	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
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
1:B:715:DT:H2'	1:B:715:DT:H6	1.30	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:192:THR:HG1	2:A:221:PHE:HZ	1.64	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:167:TYR:CE1	2:A:202:LYS:CG	3.00	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: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:106:ALA:O	2:A:110:MET:HG3	2.17	0.44
2:A:184:ILE:HD13	2:A:229:ALA:CB	2.48	0.44
2:A:128:GLU:N	2:A:129:PRO:CD	2.80	0.44
2:A:152:ALA:HB1	2:A:154:PHE:CD1	2.52	0.44
2:A:313:ARG:NH1	2:A:315:GLU:O	2.47	0.44
2:A:37:TRP:O	2:A:40:ILE:HB	2.17	0.44
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.99	0.44
2:A:64:LEU:HB2	2:A:92:LEU:HD21	2.00	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

*Continued on next page...*

*Continued from previous page...*

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
2:A:154:PHE:CD1	2:A:154:PHE:N	2.87	0.42
2:A:281:ARG:HH11	2:A:281:ARG:HG2	1.83	0.42
1:B:713:DC:C2'	1:B:714:DG:C8	2.97	0.42
2:A:143:VAL:HG23	2:A:144:VAL:N	2.35	0.41
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: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:212:PRO:CG	2:A:215:TRP:CE3	3.03	0.41
2:A:252:MET:CE	2:A:283:PHE:CZ	3.02	0.41
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.15	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:131:LEU:HD12	2:A:131:LEU:HA	1.58	0.41
2:A:161:ASN:HD21	2:A:320:GLU:HB3	1.85	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:310:VAL:C	2:A:312:LYS:H	2.24	0.41
2:A:337:ARG:O	2:A:337:ARG:NH1	2.53	0.41
2:A:149:GLU:CG	2:A:151:LYS:HD2	2.49	0.40
2:A:212:PRO:HG2	2:A:215:TRP:CE3	2.56	0.40
2:A:274:TYR:CD1	2:A:275:ASP:N	2.88	0.40
1:B:702:DG:H5'	1:B:702:DG:H2'	1.94	0.40
2:A:14:SER:O	2:A:17:THR:N	2.54	0.40
2:A:329:ARG:CZ	2:A:329:ARG:CB	2.98	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:236:GLN:HG3	2:A:237:PRO:HD2	2.04	0.40
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

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%)	<b>17</b> <b>40</b>

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>0</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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

*Continued on next page...*

*Continued from previous page...*

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	1.64	2 (25%)	5,15,15	2.79	2 (40%)

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	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	HPA	C6-N1	3.37	1.38	1.33
3	A	599	HPA	C2-N1	2.05	1.37	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	HPA	C2-N1-C6	5.34	124.82	115.88
3	A	599	HPA	N3-C2-N1	-2.80	124.31	128.68

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 [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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.