



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:14 PM GMT

PDB ID : 1JFT  
Title : PURINE REPRESSOR MUTANT-HYPOXANTHINE-PURF OPERATOR  
COMPLEX  
Authors : Huffman, J.L.; Lu, F.; Zalkin, H.; Brennan, R.G.  
Deposited on : 2001-06-21  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

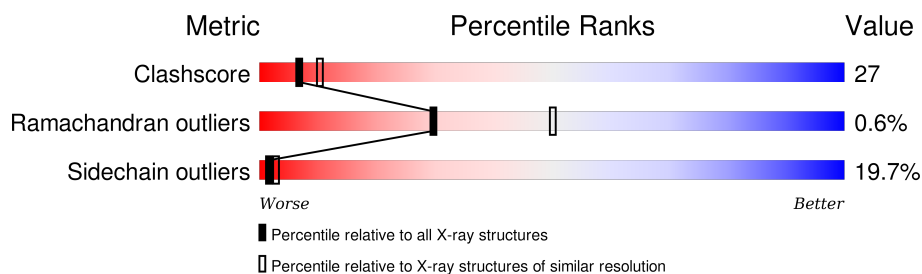
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 5 unique types of molecules in this entry. The entry contains 3085 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 5'-D(\*TP\*AP\*CP\*GP\*CP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*GP\*CP\*GP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	17	Total	C	N	O	P	0	0	0
			345	166	62	101	16			

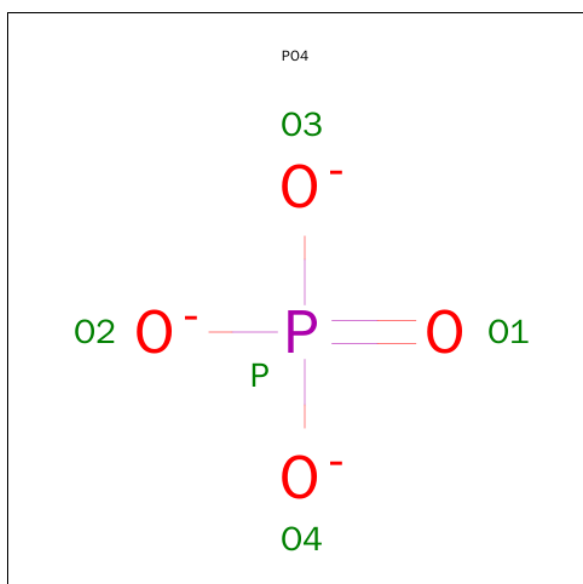
- Molecule 2 is a protein called PURINE NUCLEOTIDE SYNTHESIS REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	340	Total	C	N	O	S	0	0	0
			2660	1672	473	496	19			

There is a discrepancy between the modelled and reference sequences:

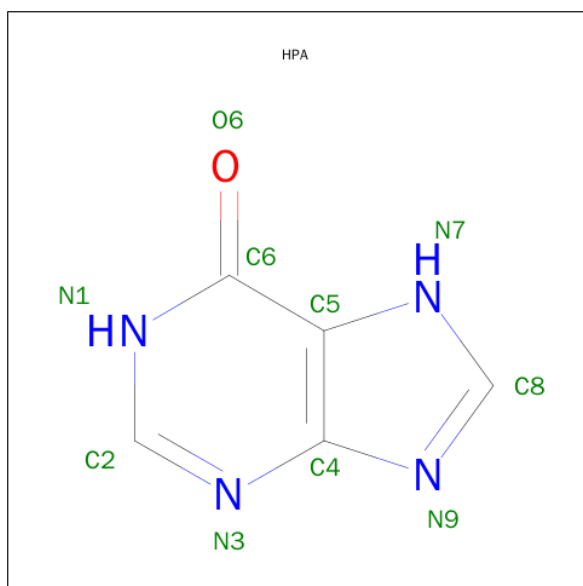
Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	TRP	ENGINEERED	UNP P0ACP7

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is HYPOXANTHINE (three-letter code: HPA) (formula:  $C_5H_4N_4O$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	5	Total	O	0	0
			5	5		

### 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: 5'-D(\*TP\*AP\*CP\*GP\*CP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*GP\*CP\*GP\*T)-3',

Chain B: 

T699  
A700  
G701  
G702  
G703  
A704  
A705  
A706  
G707  
G708  
G709  
T710  
T711  
G712  
G713  
G714  
T715

- Molecule 2: PURINE NUCLEOTIDE SYNTHESIS REPRESSOR

Chain A: 

A2  
T3  
D6  
R9  
R10  
A11  
R12  
S14  
T15  
T16  
S19  
E20  
V21  
T22  
T23  
T24  
T25  
K37  
L40  
K41  
R44  
Y45  
S46  
P47  
L54  
K55  
D153  
K60  
S61  
L62  
G63  
L64  
L65  
S68  
Q67  
Y90  
T91  
L92  
A97  
R98  
N99  
N100  
L101  
P102  
K103  
Q104  
R105  
A106

Y107  
L108  
S109  
M110  
D117  
L120  
G123  
S124  
E125  
Y126  
P127  
E128  
P129  
L130  
L131  
A132  
M133  
L134  
E135  
Y137  
R138  
H139  
I140  
P141  
M142  
V143  
V144  
M145  
A152  
D153  
F154  
A157  
V158  
I159  
D160  
N161  
A162  
F163  
E164  
Y167  
R176  
E180  
I181  
T184  
P185  
G186  
P187  
R190  
N191

T192  
G193  
R196  
G199  
F200  
K201  
K202  
A203  
K210  
V211  
P212  
E213  
S214  
W215  
T216  
V217  
Q218  
G219  
D220  
F221  
E222  
P223  
E224  
R228  
A229  
M230  
Q231  
L234  
S235  
Q236  
P237  
H238  
R239  
P240  
T241  
A242  
G247  
D248  
L249  
M250  
A251  
M252  
L255  
L263  
R264  
V265  
D268  
V269  
S270  
L271

Y274  
D275  
M276  
A280  
R281  
Y282  
F283  
T284  
L287  
T288  
T289  
L290  
Q291  
Q292  
P293  
F302  
R303  
R304  
L305  
L306  
R307  
R308  
I309  
V310  
K311  
K312  
E315  
F316  
Q317  
S318  
I319  
E320  
V321  
L325  
I326  
E327  
R328  
R329  
R337  
D338  
Y339  
R340  
R341

## 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, $\alpha$ , $\beta$ , $\gamma$	175.92Å 95.25Å 81.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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, PO4

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	2.05	12/386 (3.1%)	3.55	79/594 (13.3%)
2	A	2.44	1/2712 (0.0%)	1.00	5/3665 (0.1%)
All	All	2.39	13/3098 (0.4%)	1.62	84/4259 (2.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	341	ARG	C-OXT	117.21	3.46	1.23
1	B	709	DT	N1-C2	-6.67	1.32	1.38
1	B	702	DG	C5-C6	-6.26	1.36	1.42
1	B	701	DC	C1'-N1	-6.18	1.38	1.47
1	B	713	DC	C1'-N1	-5.78	1.39	1.47
1	B	699	DT	N1-C2	5.73	1.42	1.38
1	B	705	DA	C3'-O3'	-5.60	1.36	1.44
1	B	708	DG	C5-C6	-5.47	1.36	1.42
1	B	711	DT	N1-C6	-5.47	1.34	1.38
1	B	706	DA	N3-C4	-5.29	1.31	1.34
1	B	713	DC	C3'-O3'	5.13	1.50	1.44
1	B	709	DT	C2-N3	-5.10	1.33	1.37
1	B	710	DT	N1-C2	5.01	1.42	1.38

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	715	DT	C6-N1-C1'	-17.71	93.84	120.40
1	B	702	DG	C8-N9-C1'	-17.59	104.13	127.00
1	B	702	DG	C4-N9-C1'	17.10	148.72	126.50
1	B	715	DT	C2-N1-C1'	15.18	142.48	118.20
1	B	714	DG	C4-N9-C1'	-11.38	111.71	126.50
1	B	715	DT	O4'-C1'-N1	11.19	115.83	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	714	DG	C8-N9-C1'	10.98	141.28	127.00
1	B	712	DG	C4-N9-C1'	-10.69	112.61	126.50
1	B	701	DC	C6-N1-C2	10.29	124.42	120.30
1	B	701	DC	N3-C4-C5	10.28	126.01	121.90
1	B	713	DC	C3'-C2'-C1'	-10.25	90.20	102.50
1	B	700	DA	C8-N9-C1'	-9.82	110.03	127.70
1	B	705	DA	C8-N9-C1'	9.75	145.25	127.70
1	B	705	DA	C4-N9-C1'	-9.74	108.77	126.30
1	B	712	DG	C8-N9-C1'	9.57	139.44	127.00
1	B	701	DC	C1'-O4'-C4'	-9.07	101.03	110.10
1	B	711	DT	C2-N1-C1'	-8.98	103.82	118.20
1	B	713	DC	O4'-C1'-N1	8.97	114.28	108.00
1	B	712	DG	C2-N3-C4	-8.93	107.44	111.90
1	B	701	DC	C2-N3-C4	-8.81	115.49	119.90
1	B	708	DG	C5-C6-O6	-8.78	123.33	128.60
1	B	708	DG	N9-C4-C5	-8.71	101.92	105.40
1	B	701	DC	O4'-C4'-C3'	-8.63	100.82	106.00
1	B	713	DC	C6-N1-C2	8.60	123.74	120.30
1	B	702	DG	C5-C6-O6	-8.42	123.55	128.60
1	B	700	DA	C4-N9-C1'	8.26	141.16	126.30
1	B	699	DT	C5-C6-N1	-8.25	118.75	123.70
1	B	712	DG	P-O3'-C3'	8.10	129.41	119.70
1	B	711	DT	C6-N1-C1'	7.76	132.05	120.40
1	B	713	DC	C4'-C3'-C2'	-7.67	96.19	103.10
1	B	700	DA	O4'-C4'-C3'	-7.57	101.46	106.00
2	A	340	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	B	699	DT	N3-C2-O2	-7.46	117.82	122.30
1	B	708	DG	C8-N9-C4	7.19	109.28	106.40
1	B	708	DG	O3'-P-O5'	-7.14	90.44	104.00
1	B	713	DC	C1'-O4'-C4'	-7.05	103.05	110.10
1	B	699	DT	C2-N3-C4	-7.03	122.98	127.20
1	B	710	DT	O4'-C1'-N1	-6.94	103.14	108.00
1	B	700	DA	O4'-C1'-N9	-6.89	103.17	108.00
1	B	713	DC	P-O3'-C3'	6.88	127.95	119.70
1	B	708	DG	C4-C5-N7	6.87	113.55	110.80
2	A	328	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	B	704	DA	O4'-C4'-C3'	-6.80	101.78	104.50
1	B	708	DG	C5-C6-N1	6.74	114.87	111.50
2	A	340	ARG	CB-CA-C	-6.53	97.34	110.40
1	B	705	DA	C2-N3-C4	-6.44	107.38	110.60
1	B	714	DG	N1-C6-O6	-6.28	116.13	119.90
1	B	710	DT	P-O5'-C5'	-6.12	111.11	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	714	DG	C4'-C3'-C2'	6.06	108.55	103.10
1	B	714	DG	C5-C6-N1	6.05	114.53	111.50
1	B	700	DA	C8-N9-C4	6.03	108.21	105.80
1	B	712	DG	N3-C4-C5	6.01	131.60	128.60
1	B	703	DC	C5-C6-N1	-5.95	118.03	121.00
1	B	712	DG	N1-C6-O6	5.88	123.42	119.90
1	B	704	DA	C4-N9-C1'	-5.87	115.74	126.30
1	B	708	DG	C8-N9-C1'	-5.81	119.44	127.00
1	B	699	DT	N3-C4-O4	-5.79	116.42	119.90
1	B	701	DC	P-O3'-C3'	5.70	126.54	119.70
1	B	700	DA	C1'-O4'-C4'	-5.69	104.41	110.10
1	B	702	DG	C5-C6-N1	5.68	114.34	111.50
1	B	703	DC	C2-N3-C4	-5.65	117.08	119.90
1	B	701	DC	O4'-C1'-N1	-5.61	104.07	108.00
1	B	702	DG	C4-C5-N7	5.56	113.03	110.80
1	B	704	DA	C3'-C2'-C1'	-5.54	95.85	102.50
1	B	705	DA	C5-C6-N1	-5.52	114.94	117.70
1	B	708	DG	O4'-C1'-N9	-5.51	104.14	108.00
1	B	702	DG	P-O5'-C5'	-5.40	112.27	120.90
2	A	269	VAL	CB-CA-C	-5.39	101.15	111.40
2	A	92	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	705	DA	N1-C2-N3	5.32	131.96	129.30
1	B	708	DG	P-O5'-C5'	-5.31	112.40	120.90
1	B	702	DG	O4'-C1'-C2'	-5.29	101.66	105.90
1	B	703	DC	P-O3'-C3'	5.29	126.04	119.70
1	B	711	DT	C6-N1-C2	5.27	123.93	121.30
1	B	705	DA	P-O5'-C5'	-5.19	112.60	120.90
1	B	707	DC	C2-N1-C1'	-5.14	113.14	118.80
1	B	703	DC	P-O5'-C5'	-5.14	112.68	120.90
1	B	704	DA	N9-C4-C5	-5.12	103.75	105.80
1	B	708	DG	C6-C5-N7	-5.10	127.34	130.40
1	B	703	DC	C2-N1-C1'	5.08	124.39	118.80
1	B	708	DG	N7-C8-N9	-5.03	110.58	113.10
1	B	715	DT	C1'-O4'-C4'	-5.03	105.08	110.10
1	B	702	DG	C3'-C2'-C1'	-5.02	96.47	102.50
1	B	712	DG	N9-C1'-C2'	-5.02	103.06	112.60

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	B	345	0	193	8	1
2	A	2660	0	2649	150	1
3	A	5	0	0	1	0
4	A	10	0	4	0	0
5	A	60	0	0	2	0
5	B	5	0	0	1	0
All	All	3085	0	2846	158	1

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 27.

All (158) 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:A:40:ILE:HG22	2:A:41:LYS:HD3	1.46	0.96
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.82	0.93
2:A:100:ASN:ND2	2:A:103:LYS:HB2	1.83	0.92
2:A:341:ARG:HH11	2:A:341:ARG:HG3	1.36	0.90
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.54	0.89
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.90	0.87
2:A:22:ILE:HD11	2:A:40:ILE:HD11	1.57	0.85
2:A:237:PRO:HG2	2:A:238:HIS:H	1.43	0.84
2:A:105:ARG:HB2	2:A:105:ARG:HH11	1.43	0.83
2:A:239:ARG:HB3	2:A:239:ARG:HH11	1.42	0.82
2:A:341:ARG:OXT	2:A:341:ARG:HA	1.82	0.78
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.01	0.78
2:A:101:LEU:HA	2:A:104:GLN:HE21	1.49	0.77
2:A:187:PRO:HB2	2:A:190:ARG:HD3	1.68	0.75
2:A:292:GLN:HE21	2:A:293:PRO:HD3	1.53	0.74
2:A:135:GLU:O	2:A:138:ARG:HG2	1.88	0.74
2:A:101:LEU:HA	2:A:104:GLN:NE2	2.03	0.73
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.35	0.73
2:A:152:ALA:HB1	2:A:154:PHE:CE2	2.23	0.73
2:A:325:LEU:HD22	2:A:326:ILE:N	2.04	0.73
2:A:265:VAL:HG13	2:A:269:VAL:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:292:GLN:HE21	2:A:293:PRO:CD	2.03	0.72
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.73	0.71
2:A:341:ARG:HG3	2:A:341:ARG:NH1	2.06	0.71
2:A:239:ARG:CB	2:A:239:ARG:HH11	2.05	0.69
2:A:214:SER:HB2	2:A:236:GLN:OE1	1.93	0.69
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.76	0.68
2:A:100:ASN:HD22	2:A:103:LYS:HB2	1.56	0.68
2:A:264:ARG:HD2	2:A:265:VAL:N	2.09	0.68
2:A:304:MET:CE	2:A:317:GLN:HB3	2.24	0.68
2:A:309:ILE:HG22	2:A:310:VAL:N	2.09	0.67
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.25	0.66
2:A:159:ILE:HG12	2:A:320:GLU:HG2	1.77	0.66
2:A:230:MET:HG3	2:A:234:LEU:HD11	1.77	0.66
2:A:135:GLU:HA	2:A:154:PHE:CE1	2.30	0.66
2:A:180:GLU:HB2	2:A:241:THR:HG23	1.78	0.65
2:A:202:LYS:HG3	2:A:203:ALA:N	2.11	0.65
2:A:100:ASN:HD22	2:A:103:LYS:HD3	1.62	0.64
2:A:236:GLN:HB3	2:A:237:PRO:HD2	1.77	0.64
2:A:280:ALA:HA	2:A:283:PHE:CE1	2.33	0.64
2:A:22:ILE:HG22	2:A:23:ASN:HD21	1.60	0.63
2:A:105:ARG:NH1	2:A:105:ARG:HB2	2.13	0.63
2:A:180:GLU:HG2	5:A:801:HOH:O	1.99	0.63
1:B:709:DT:H2''	1:B:710:DT:H5'	1.82	0.61
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.30	0.61
2:A:20:HIS:HA	2:A:25:THR:CG2	2.31	0.60
2:A:293:PRO:HG2	2:A:321:VAL:HG22	1.84	0.60
2:A:160:ASP:HA	2:A:321:VAL:CG1	2.32	0.60
2:A:105:ARG:HG3	2:A:106:ALA:N	2.15	0.60
1:B:700:DA:H2''	1:B:701:DC:O5'	2.00	0.60
2:A:106:ALA:O	2:A:110:MET:HG3	2.01	0.59
1:B:707:DC:C2'	1:B:708:DG:H5'	2.33	0.59
2:A:310:VAL:HG23	2:A:311:ASN:OD1	2.02	0.58
2:A:97:ALA:HB1	2:A:104:GLN:HG3	1.85	0.58
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.34	0.57
2:A:125:GLU:HG2	2:A:190:ARG:HG3	1.85	0.57
2:A:237:PRO:CG	2:A:238:HIS:H	2.15	0.57
2:A:325:LEU:HD22	2:A:326:ILE:H	1.69	0.57
2:A:230:MET:HG3	2:A:234:LEU:CD1	2.35	0.57
2:A:157:ALA:O	2:A:318:SER:HA	2.05	0.56
2:A:281:ARG:O	2:A:281:ARG:HD3	2.06	0.55
2:A:302:PHE:CE2	2:A:306:LEU:HD22	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ILE:HG22	2:A:41:LYS:CD	2.30	0.55
2:A:145:MET:HA	2:A:158:VAL:HG13	1.89	0.55
2:A:117:ASP:O	2:A:141:PRO:HG2	2.07	0.55
2:A:239:ARG:HH11	2:A:239:ARG:CG	2.20	0.54
2:A:292:GLN:HE21	2:A:292:GLN:HA	1.73	0.54
2:A:163:PHE:O	2:A:199:GLY:HA3	2.08	0.54
2:A:264:ARG:HD2	2:A:265:VAL:H	1.71	0.54
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.43	0.53
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.39	0.53
2:A:159:ILE:HD11	2:A:320:GLU:HB3	1.91	0.52
2:A:287:LEU:HG	2:A:288:THR:N	2.24	0.52
2:A:159:ILE:O	2:A:321:VAL:HG12	2.10	0.51
2:A:287:LEU:O	2:A:328:ARG:HD2	2.11	0.51
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.92	0.51
2:A:159:ILE:HD11	2:A:320:GLU:CB	2.41	0.51
2:A:290:ILE:HD13	2:A:325:LEU:HD23	1.93	0.50
2:A:325:LEU:CD1	2:A:327:GLU:HG3	2.42	0.50
2:A:317:GLN:HA	5:A:769:HOH:O	2.10	0.50
2:A:22:ILE:CD1	2:A:40:ILE:HD11	2.35	0.50
2:A:62:ILE:HD13	2:A:302:PHE:CE1	2.47	0.50
2:A:284:THR:O	2:A:284:THR:HG22	2.10	0.50
2:A:90:TYR:CD2	2:A:90:TYR:N	2.79	0.50
2:A:62:ILE:HD13	2:A:302:PHE:HE1	1.77	0.49
2:A:22:ILE:C	2:A:23:ASN:HD22	2.15	0.49
2:A:14:SER:OG	2:A:16:THR:HB	2.12	0.49
2:A:231:GLN:O	2:A:235:SER:HB2	2.13	0.49
2:A:187:PRO:HD2	2:A:221:PHE:CE2	2.47	0.49
2:A:192:THR:O	2:A:196:ARG:HD2	2.13	0.48
2:A:292:GLN:NE2	2:A:292:GLN:HA	2.29	0.48
2:A:123:CYS:O	2:A:124:SER:HB2	2.14	0.47
2:A:3:THR:HG22	2:A:6:ASP:OD2	2.14	0.47
2:A:130:LEU:HD22	2:A:130:LEU:O	2.15	0.47
2:A:160:ASP:O	2:A:161:ASN:HB2	2.13	0.47
2:A:264:ARG:H	2:A:268:ASP:HB2	1.79	0.47
2:A:202:LYS:HB2	2:A:202:LYS:HE3	1.67	0.47
2:A:337:ARG:NH1	2:A:338:ASP:HA	2.30	0.47
2:A:184:ILE:HA	2:A:217:VAL:O	2.15	0.47
2:A:98:TRP:O	2:A:99:ASN:HB2	2.15	0.46
2:A:223:PRO:HG3	2:A:249:ILE:HG22	1.97	0.46
1:B:713:DC:H5"	5:B:800:HOH:O	2.14	0.46
2:A:234:LEU:HD22	2:A:263:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:DG:C2'	1:B:715:DT:H5'	2.44	0.46
2:A:201:MET:HA	2:A:201:MET:HE2	1.96	0.46
1:B:703:DC:H2''	1:B:704:DA:C8	2.51	0.46
2:A:105:ARG:NH1	2:A:105:ARG:CB	2.78	0.45
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.98	0.45
2:A:201:MET:CA	2:A:201:MET:HE2	2.47	0.45
2:A:140:ILE:HG22	2:A:141:PRO:HD2	1.99	0.45
2:A:126:TYR:HB3	2:A:131:LEU:CD1	2.47	0.45
2:A:239:ARG:NH1	2:A:239:ARG:CG	2.79	0.45
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.45	0.45
2:A:304:MET:HE3	2:A:317:GLN:HB3	1.99	0.44
2:A:161:ASN:HB3	2:A:164:GLU:HG2	1.99	0.44
2:A:16:THR:HG22	2:A:20:HIS:HD2	1.82	0.44
2:A:293:PRO:HA	3:A:717:PO4:O4	2.18	0.44
2:A:325:LEU:HD11	2:A:327:GLU:HG3	2.00	0.44
2:A:308:ARG:O	2:A:312:LYS:HA	2.18	0.43
2:A:137:TYR:HB3	2:A:140:ILE:HD13	2.01	0.43
2:A:64:LEU:HB2	2:A:92:LEU:HD21	2.01	0.43
2:A:105:ARG:HA	2:A:133:MET:HE3	2.00	0.43
2:A:276:ASN:ND2	2:A:291:HIS:HD2	2.07	0.43
2:A:101:LEU:HD12	2:A:101:LEU:HA	1.47	0.43
2:A:222:GLU:HA	2:A:223:PRO:HD3	1.80	0.43
2:A:9:LYS:HE3	2:A:9:LYS:HB2	1.35	0.43
2:A:290:ILE:HD13	2:A:325:LEU:HA	2.01	0.43
2:A:224:GLU:HG3	2:A:228:ARG:CD	2.49	0.43
2:A:181:ILE:HA	2:A:242:ALA:O	2.18	0.43
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.81	0.42
2:A:200:PHE:HD2	2:A:201:MET:CE	2.31	0.42
2:A:212:PRO:O	2:A:215:TRP:HB2	2.19	0.42
2:A:185:PRO:HD2	2:A:218:GLN:HA	2.00	0.42
2:A:187:PRO:O	2:A:193:GLY:HA3	2.20	0.42
2:A:20:HIS:ND1	2:A:25:THR:CG2	2.73	0.42
2:A:159:ILE:HD11	2:A:320:GLU:HG2	2.02	0.42
2:A:152:ALA:HB1	2:A:154:PHE:CD2	2.55	0.42
2:A:167:TYR:CD2	2:A:202:LYS:HG3	2.55	0.42
1:B:714:DG:H2''	1:B:715:DT:H5'	2.01	0.42
2:A:154:PHE:CD2	2:A:154:PHE:N	2.87	0.42
2:A:223:PRO:HG3	2:A:249:ILE:CG2	2.50	0.42
2:A:46:SER:HA	2:A:47:PRO:HD2	1.87	0.42
2:A:23:ASN:N	2:A:23:ASN:HD22	2.18	0.42
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.85	0.41
2:A:20:HIS:HA	2:A:25:THR:HG22	2.00	0.41
2:A:140:ILE:CG2	2:A:141:PRO:HD2	2.49	0.41
2:A:237:PRO:CG	2:A:238:HIS:N	2.80	0.41
2:A:11:ALA:HB3	2:A:13:VAL:CG2	2.51	0.41
1:B:707:DC:H2''	1:B:708:DG:H5'	2.02	0.41
2:A:140:ILE:HD12	2:A:140:ILE:H	1.85	0.41
2:A:87:GLN:HB2	2:A:87:GLN:HE21	1.74	0.41
2:A:247:GLY:HA2	2:A:274:TYR:O	2.21	0.41
2:A:255:LEU:HA	2:A:255:LEU:HD12	1.70	0.41
2:A:224:GLU:HG3	2:A:228:ARG:HD3	2.04	0.40
2:A:37:TRP:CZ3	2:A:40:ILE:HD12	2.56	0.40
2:A:22:ILE:HD11	2:A:40:ILE:CD1	2.39	0.40
2:A:190:ARG:HD2	2:A:190:ARG:HH11	1.71	0.40

All (1) 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)
1:B:715:DT:OP2	2:A:337:ARG:NH2[5_445]	2.06	0.14

## 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	338/340 (99%)	305 (90%)	31 (9%)	2 (1%)	30 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	309	ILE

### 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
2	A	279/279 (100%)	224 (80%)	55 (20%)	<b>1</b> <b>3</b>

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR
2	A	9	LYS
2	A	13	VAL
2	A	14	SER
2	A	19	SER
2	A	21	VAL
2	A	40	ILE
2	A	41	LYS
2	A	44	HIS
2	A	54	LEU
2	A	55	LYS
2	A	60	LYS
2	A	61	SER
2	A	68	SER
2	A	87	GLN
2	A	91	THR
2	A	92	LEU
2	A	103	LYS
2	A	105	ARG
2	A	108	LEU
2	A	109	SER
2	A	120	LEU
2	A	128	GLU
2	A	130	LEU
2	A	143	VAL
2	A	145	MET
2	A	153	ASP
2	A	158	VAL
2	A	176	ARG
2	A	201	MET

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Mol	Chain	Res	Type
2	A	202	LYS
2	A	210	LYS
2	A	213	GLU
2	A	214	SER
2	A	228	ARG
2	A	230	MET
2	A	234	LEU
2	A	235	SER
2	A	236	GLN
2	A	239	ARG
2	A	250	MET
2	A	252	MET
2	A	255	LEU
2	A	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	270	SER
2	A	274	TYR
2	A	281	ARG
2	A	293	PRO
2	A	310	VAL
2	A	315	GLU
2	A	329	ARG
2	A	337	ARG
2	A	341	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	ASN
2	A	34	ASN
2	A	58	HIS
2	A	99	ASN
2	A	100	ASN
2	A	104	GLN
2	A	161	ASN
2	A	291	HIS
2	A	292	GLN
2	A	322	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](#)

2 ligands are 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	$\# Z  > 2$
4	HPA	A	599	-	8,11,11	1.65	2 (25%)	4,15,15	4.48	2 (50%)
3	PO4	A	717	-	4,4,4	1.77	1 (25%)	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HPA	A	599	-	-	0/0/0/0	0/2/2/2
3	PO4	A	717	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	717	PO4	P-O4	-3.12	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	599	HPA	C2-N1	2.33	1.38	1.33
4	A	599	HPA	C6-N1	3.47	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	599	HPA	N3-C2-N1	-6.10	124.22	128.89
4	A	599	HPA	C2-N1-C6	6.29	125.57	116.04

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
3	A	717	PO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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