



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:14 PM GMT

PDB ID : 1JFS  
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 : 2.90 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

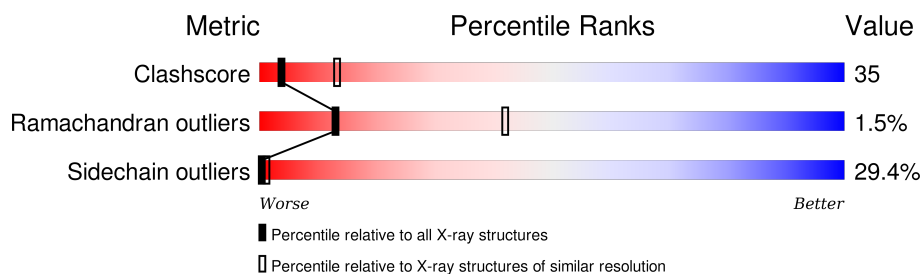
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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 3040 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			

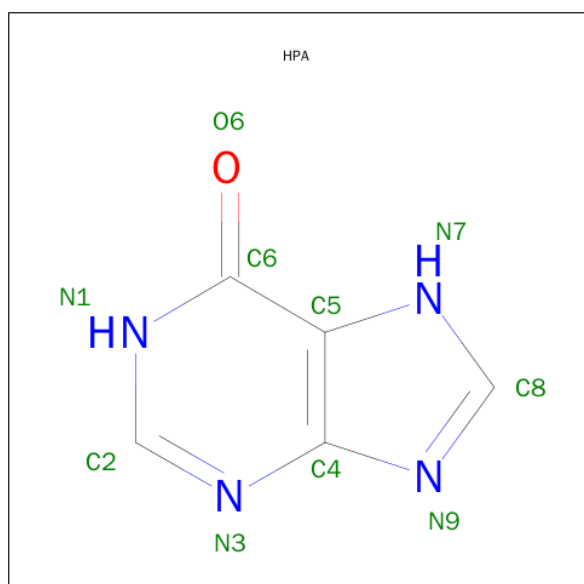
- Molecule 2 is a protein called PURINE NUCLEOTIDE SYNTHESIS REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	339	Total	C	N	O	S	0	0	0
			2654	1672	469	494	19			

There is a discrepancy between the modelled and reference sequences:

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

- 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	28	Total	O	0	0
			28	28		
4	B	3	Total	O	0	0
			3	3		

### 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  
C701  
G702  
C703  
A704  
A705  
A706  
C707  
G708  
T709  
T710  
T711  
G712  
C713  
G714  
T715

- Molecule 2: PURINE NUCLEOTIDE SYNTHESIS REPRESSOR

Chain A: 

A2  
T3  
I4  
K5  
D6  
V7  
A8  
K9  
R10  
A11  
M12  
V13  
S14  
T15  
T16  
T17  
V18  
S19  
R20  
V21  
I22  
M23  
K24  
T25  
R26  
F27  
V28  
A29  
E30  
E31  
K37  
T40  
K41  
E42  
L43  
H44  
Y45  
S46  
P47  
R52  
S53  
L54  
K55  
V56  
K60  
S61  
R62  
G63  
L64  
L65  
S69  
I77  
I78  
E79

A80  
R83  
N84  
Q87  
K88  
G89  
Y90  
T91  
L92  
A97  
R98  
N99  
M100  
L101  
E102  
K103  
Q104  
R105  
A106  
Y107  
L108  
S109  
M110  
M111  
D117  
G118  
E180  
L119  
Y121  
M122  
C123  
S124  
E125  
Y126  
P127  
E128  
P129  
L130  
L131  
A132  
M133  
E135  
E136  
Y137  
R138  
H139  
I140  
P141  
M142  
V143  
V144  
M145  
D146  
F147  
G148

E149  
A150  
K151  
A152  
D153  
F154  
T155  
D156  
A157  
V158  
I159  
D160  
N161  
A162  
F163  
G166  
Y167  
R171  
Y172  
L173  
I174  
E175  
R176  
G177  
H178  
R179  
E180  
I181  
G182  
Y183  
I184  
P185  
G186  
P187  
L188  
E189  
R190  
N191  
T192  
R196  
G199  
F200  
M201  
D202  
A203  
M204  
A207  
M208  
I209  
K210  
V211  
P212  
E213  
W215

I216  
V217  
Q218  
G219  
D220  
F221  
E222  
P223  
R228  
A229  
M230  
Q231  
Q232  
I233  
L234  
Q235  
Q236  
P237  
R238  
R239  
P240  
T241  
A242  
C245  
G246  
G247  
D248  
I249  
M250  
A251  
M252  
L255  
R252  
C256  
A257  
E260  
M261  
G262  
L263  
R264  
V265  
P266  
Q267  
D268  
V269  
S270  
L271  
I272  
G273  
Y274  
D275  
N276  
Y277  
R278  
R281  
Y282

F283  
T284  
P285  
A286  
L287  
I290  
H291  
Q292  
P293  
S296  
E299  
T300  
A301  
F302  
N303  
K304  
L305  
L306  
D307  
R308  
I309  
V310  
N311  
R312  
R313  
Q317  
S318  
I319  
E320  
V321  
R322  
P323  
G324  
L325  
I326  
E327  
R328  
P335  
F336  
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, $\alpha$ , $\beta$ , $\gamma$	176.05Å 95.04Å 81.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	97.9 (10.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	7.54	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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	1.82	9/386 (2.3%)	4.11	81/594 (13.6%)
2	A	0.91	0/2707	1.01	5/3660 (0.1%)
All	All	1.06	9/3093 (0.3%)	1.80	86/4254 (2.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	706	DA	N3-C4	-7.24	1.30	1.34
1	B	705	DA	C3'-O3'	-6.58	1.35	1.44
1	B	702	DG	C3'-O3'	6.27	1.52	1.44
1	B	701	DC	C1'-N1	-5.98	1.38	1.47
1	B	701	DC	C4-C5	5.53	1.47	1.43
1	B	699	DT	N1-C2	5.46	1.42	1.38
1	B	706	DA	C6-N1	-5.35	1.31	1.35
1	B	702	DG	C5-C6	-5.29	1.37	1.42
1	B	712	DG	C3'-O3'	5.09	1.50	1.44

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	715	DT	C6-N1-C1'	-22.95	85.97	120.40
1	B	700	DA	C8-N9-C1'	-19.94	91.81	127.70
1	B	714	DG	C4-N9-C1'	-19.46	101.20	126.50
1	B	715	DT	C2-N1-C1'	19.23	148.96	118.20
1	B	714	DG	C8-N9-C1'	18.41	150.93	127.00
1	B	700	DA	C4-N9-C1'	18.06	158.80	126.30
1	B	712	DG	C4-N9-C1'	-16.16	105.48	126.50
1	B	712	DG	C8-N9-C1'	16.11	147.95	127.00
1	B	701	DC	C6-N1-C1'	-15.44	102.27	120.80
1	B	701	DC	C2-N1-C1'	13.88	134.06	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	706	DA	C8-N9-C1'	13.86	152.64	127.70
1	B	706	DA	C4-N9-C1'	-13.27	102.42	126.30
1	B	702	DG	C4-N9-C1'	12.61	142.90	126.50
1	B	700	DA	C1'-O4'-C4'	-12.60	97.50	110.10
1	B	702	DG	C8-N9-C1'	-12.51	110.74	127.00
1	B	702	DG	O4'-C1'-C2'	-11.22	96.92	105.90
1	B	711	DT	C2-N1-C1'	-10.87	100.80	118.20
1	B	707	DC	C2-N1-C1'	-10.77	106.96	118.80
1	B	711	DT	C6-N1-C1'	10.55	136.22	120.40
1	B	715	DT	O4'-C1'-N1	10.35	115.24	108.00
1	B	707	DC	C6-N1-C1'	10.11	132.93	120.80
1	B	700	DA	O4'-C4'-C3'	-9.97	100.02	106.00
1	B	702	DG	C5-C6-O6	-9.94	122.64	128.60
1	B	704	DA	C4-N9-C1'	-9.88	108.52	126.30
1	B	713	DC	C2-N1-C1'	-9.84	107.98	118.80
1	B	702	DG	C4-C5-N7	9.78	114.71	110.80
1	B	706	DA	P-O3'-C3'	9.76	131.41	119.70
1	B	701	DC	C1'-O4'-C4'	-9.56	100.54	110.10
1	B	705	DA	C4-N9-C1'	-9.21	109.72	126.30
1	B	713	DC	P-O5'-C5'	-9.14	106.27	120.90
1	B	704	DA	C8-N9-C1'	9.01	143.91	127.70
1	B	703	DC	C4'-C3'-C2'	-8.98	95.02	103.10
1	B	705	DA	C8-N9-C1'	8.90	143.73	127.70
1	B	699	DT	N3-C2-O2	-8.79	117.03	122.30
1	B	700	DA	C8-N9-C4	8.63	109.25	105.80
1	B	702	DG	C4'-C3'-C2'	-8.37	95.57	103.10
1	B	712	DG	P-O3'-C3'	8.04	129.35	119.70
1	B	701	DC	C6-N1-C2	8.03	123.51	120.30
1	B	703	DC	P-O3'-C3'	7.91	129.19	119.70
2	A	269	VAL	CB-CA-C	-7.87	96.45	111.40
1	B	712	DG	C2-N3-C4	-7.68	108.06	111.90
1	B	713	DC	C6-N1-C2	7.61	123.34	120.30
2	A	340	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	699	DT	C5-C6-N1	-7.32	119.31	123.70
1	B	700	DA	N7-C8-N9	-7.11	110.25	113.80
1	B	702	DG	C6-C5-N7	-7.04	126.18	130.40
1	B	712	DG	C5-C6-N1	-6.91	108.04	111.50
1	B	710	DT	P-O5'-C5'	-6.83	109.97	120.90
1	B	709	DT	C6-N1-C1'	-6.77	110.25	120.40
1	B	699	DT	C2-N3-C4	-6.60	123.24	127.20
1	B	699	DT	C6-C5-C7	-6.52	118.99	122.90
1	B	702	DG	C5-N7-C8	-6.49	101.05	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	711	DT	C6-C5-C7	-6.43	119.04	122.90
1	B	699	DT	C4-C5-C6	6.36	121.81	118.00
1	B	702	DG	P-O3'-C3'	6.33	127.30	119.70
1	B	712	DG	O4'-C1'-N9	-5.99	103.81	108.00
1	B	704	DA	P-O5'-C5'	-5.99	111.32	120.90
1	B	714	DG	C4'-C3'-C2'	5.98	108.48	103.10
1	B	705	DA	C2-N3-C4	-5.94	107.63	110.60
1	B	701	DC	P-O5'-C5'	5.82	130.21	120.90
1	B	708	DG	O4'-C1'-C2'	5.80	110.54	105.90
1	B	699	DT	O3'-P-O5'	-5.77	93.04	104.00
1	B	715	DT	C1'-O4'-C4'	-5.76	104.34	110.10
1	B	703	DC	C2-N1-C1'	5.73	125.10	118.80
1	B	700	DA	O3'-P-O5'	-5.72	93.13	104.00
2	A	290	ILE	CB-CA-C	-5.68	100.24	111.60
1	B	699	DT	N1-C2-N3	5.68	118.01	114.60
1	B	699	DT	N3-C4-O4	-5.65	116.51	119.90
1	B	713	DC	C5-C6-N1	-5.60	118.20	121.00
2	A	158	VAL	N-CA-C	-5.48	96.20	111.00
1	B	701	DC	C2-N3-C4	-5.46	117.17	119.90
1	B	701	DC	N3-C4-C5	5.44	124.08	121.90
1	B	710	DT	C3'-C2'-C1'	-5.33	96.11	102.50
1	B	713	DC	C6-N1-C1'	5.33	127.19	120.80
2	A	306	LEU	CA-CB-CG	-5.33	103.05	115.30
1	B	708	DG	C5-C6-O6	-5.32	125.41	128.60
1	B	702	DG	C5-C6-N1	5.30	114.15	111.50
1	B	702	DG	N1-C6-O6	5.29	123.08	119.90
1	B	709	DT	C2-N1-C1'	5.29	126.66	118.20
1	B	708	DG	O3'-P-O5'	-5.26	94.01	104.00
1	B	707	DC	O4'-C1'-N1	-5.26	104.32	108.00
1	B	708	DG	C8-N9-C1'	-5.21	120.23	127.00
1	B	701	DC	C5-C6-N1	-5.18	118.41	121.00
1	B	705	DA	P-O5'-C5'	-5.09	112.76	120.90
1	B	708	DG	C5-C6-N1	5.07	114.03	111.50
1	B	703	DC	O4'-C1'-C2'	-5.01	101.89	105.90

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	B	345	0	194	14	0
2	A	2654	0	2640	193	0
3	A	10	0	4	0	0
4	A	28	0	0	1	0
4	B	3	0	0	0	0
All	All	3040	0	2838	206	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 35.

All (206) 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''	1.41	0.99
2:A:236:GLN:HB2	2:A:237:PRO:HD2	1.50	0.94
1:B:712:DG:H2''	1:B:713:DC:H5''	1.52	0.90
2:A:100:ASN:HD22	2:A:103:LYS:H	1.13	0.89
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.87	0.88
2:A:142:MET:HG3	2:A:155:THR:HG22	1.58	0.83
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.92	0.83
2:A:292:GLN:HG3	2:A:293:PRO:HD2	1.60	0.83
2:A:97:ALA:HB1	2:A:104:GLN:HG3	1.62	0.82
2:A:192:THR:O	2:A:196:ARG:HD2	1.81	0.81
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.47	0.80
2:A:135:GLU:O	2:A:138:ARG:HG2	1.84	0.77
2:A:107:TYR:O	2:A:111:MET:HG3	1.84	0.76
2:A:137:TYR:HB3	2:A:140:ILE:CD1	2.15	0.76
2:A:100:ASN:ND2	2:A:103:LYS:H	1.83	0.76
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.68	0.75
2:A:247:GLY:HA2	2:A:274:TYR:O	1.88	0.74
2:A:234:LEU:HD22	2:A:263:LEU:HD23	1.70	0.74
2:A:196:ARG:HG2	2:A:274:TYR:CE1	2.24	0.73
2:A:160:ASP:HA	2:A:321:VAL:HG23	1.71	0.72
2:A:145:MET:HA	2:A:158:VAL:CG1	2.20	0.72
2:A:62:ILE:HD12	2:A:90:TYR:CD1	2.25	0.71
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.71	0.71
2:A:97:ALA:CB	2:A:104:GLN:HG3	2.21	0.69
2:A:61:SER:HB2	2:A:91:THR:HG22	1.74	0.69
1:B:714:DG:H4'	1:B:714:DG:OP1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:LEU:O	2:A:328:ARG:HD2	1.92	0.69
2:A:137:TYR:HB3	2:A:140:ILE:HD13	1.74	0.69
2:A:236:GLN:HB2	2:A:237:PRO:CD	2.23	0.68
2:A:20:HIS:HA	2:A:25:THR:CG2	2.23	0.67
2:A:40:ILE:HD13	2:A:45:TYR:HD1	1.57	0.67
2:A:266:PRO:HA	2:A:269:VAL:O	1.94	0.67
2:A:207:ALA:HB3	2:A:209:ILE:HG13	1.77	0.66
2:A:21:VAL:HG12	2:A:28:VAL:HG21	1.76	0.66
1:B:712:DG:H2''	1:B:713:DC:C5'	2.26	0.66
2:A:61:SER:CB	2:A:91:THR:HG22	2.25	0.66
2:A:156:ASP:HB3	2:A:304:MET:CE	2.26	0.65
2:A:257:ALA:O	2:A:261:MET:HG3	1.96	0.65
2:A:292:GLN:HG3	2:A:293:PRO:CD	2.26	0.65
2:A:174:ILE:HG22	2:A:175:GLU:N	2.11	0.64
2:A:20:HIS:HA	2:A:25:THR:HG22	1.79	0.64
2:A:290:ILE:HD13	2:A:325:LEU:HD23	1.80	0.64
2:A:135:GLU:HA	2:A:154:PHE:CE1	2.32	0.64
1:B:709:DT:H2''	1:B:710:DT:H5'	1.78	0.64
2:A:87:GLN:OE1	2:A:88:LYS:HD2	1.99	0.62
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.63	0.62
2:A:304:MET:CE	2:A:317:GLN:HB3	2.29	0.62
2:A:264:ARG:HB2	2:A:268:ASP:OD2	1.99	0.61
1:B:700:DA:H2''	1:B:701:DC:O5'	2.00	0.61
2:A:221:PHE:HA	2:A:250:MET:HG3	1.83	0.61
2:A:256:CYS:O	2:A:260:GLU:HG2	2.01	0.61
2:A:52:ARG:NH1	2:A:56:VAL:HG11	2.15	0.61
2:A:252:MET:HB2	2:A:283:PHE:CE2	2.35	0.61
2:A:152:ALA:HB1	2:A:154:PHE:CE2	2.36	0.60
2:A:101:LEU:HA	2:A:104:GLN:NE2	2.16	0.60
2:A:184:ILE:HA	2:A:217:VAL:O	2.01	0.60
2:A:156:ASP:HB3	2:A:304:MET:HE1	1.83	0.59
2:A:230:MET:O	2:A:234:LEU:HD12	2.03	0.59
2:A:78:ILE:HG22	2:A:79:GLU:N	2.16	0.59
2:A:43:LEU:HD23	2:A:43:LEU:N	2.17	0.58
2:A:308:ARG:O	2:A:312:LYS:HA	2.04	0.58
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.33	0.58
2:A:8:ALA:HB1	2:A:13:VAL:O	2.04	0.57
2:A:286:ALA:HB1	2:A:328:ARG:HD3	1.85	0.57
2:A:245:CYS:HB2	2:A:271:LEU:HD11	1.85	0.57
2:A:142:MET:CG	2:A:155:THR:HG22	2.33	0.57
2:A:325:LEU:HD22	2:A:326:ILE:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:166:GLY:HA3	2:A:196:ARG:O	2.06	0.56
2:A:3:THR:HG23	2:A:5:LYS:H	1.70	0.56
2:A:167:TYR:CD2	2:A:202:LYS:HG3	2.41	0.56
2:A:117:ASP:O	2:A:141:PRO:HG2	2.05	0.56
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.41	0.56
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.87	0.56
2:A:101:LEU:HA	2:A:104:GLN:HE21	1.70	0.56
2:A:304:MET:HE3	2:A:317:GLN:HB3	1.88	0.55
2:A:105:ARG:NH1	2:A:133:MET:HE2	2.22	0.55
2:A:3:THR:HG22	2:A:6:ASP:OD2	2.06	0.55
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.89	0.54
2:A:207:ALA:O	2:A:208:MET:HB2	2.07	0.54
2:A:63:GLY:O	2:A:119:LEU:HD22	2.08	0.54
2:A:304:MET:O	2:A:307:ASP:HB3	2.08	0.54
2:A:215:TRP:CE2	2:A:240:PRO:HD3	2.43	0.54
2:A:10:ARG:CG	2:A:10:ARG:HH11	2.21	0.53
2:A:3:THR:HG22	2:A:6:ASP:H	1.73	0.53
2:A:159:ILE:HD11	2:A:320:GLU:CD	2.28	0.53
2:A:7:VAL:HG12	2:A:18:VAL:HG21	1.91	0.53
2:A:40:ILE:HD13	2:A:45:TYR:CD1	2.42	0.53
2:A:336:PHE:CD1	2:A:336:PHE:N	2.77	0.53
2:A:163:PHE:O	2:A:199:GLY:HA3	2.09	0.52
2:A:23:ASN:N	2:A:23:ASN:HD22	2.08	0.52
2:A:239:ARG:HB2	2:A:240:PRO:HD2	1.91	0.52
2:A:304:MET:SD	2:A:319:ILE:HD12	2.49	0.52
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.91	0.52
2:A:90:TYR:CD2	2:A:90:TYR:N	2.78	0.52
2:A:245:CYS:SG	2:A:251:ALA:HA	2.51	0.51
2:A:158:VAL:O	2:A:158:VAL:HG13	2.11	0.51
2:A:16:THR:HG22	2:A:20:HIS:HD2	1.76	0.51
2:A:11:ALA:HB3	2:A:13:VAL:HG22	1.93	0.51
2:A:101:LEU:HD11	2:A:133:MET:HE3	1.92	0.51
2:A:122:MET:HA	2:A:146:ASP:OD1	2.10	0.51
2:A:222:GLU:HB3	2:A:223:PRO:HD2	1.93	0.51
2:A:308:ARG:HA	2:A:313:ARG:HB3	1.92	0.50
2:A:231:GLN:O	2:A:235:SER:HB2	2.11	0.50
1:B:711:DT:H2"	1:B:712:DG:N7	2.26	0.50
2:A:11:ALA:O	2:A:12:ASN:HB2	2.10	0.50
2:A:62:ILE:HD12	2:A:90:TYR:HD1	1.72	0.50
2:A:220:ASP:O	2:A:221:PHE:HB2	2.11	0.50
2:A:187:PRO:HA	2:A:218:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:41:LYS:HD2	2:A:41:LYS:N	2.25	0.50
2:A:296:SER:O	2:A:300:THR:HB	2.12	0.50
2:A:158:VAL:HA	2:A:319:ILE:O	2.12	0.49
2:A:179:ARG:HA	2:A:209:ILE:CD1	2.41	0.49
2:A:126:TYR:CG	2:A:147:PHE:HE2	2.30	0.49
1:B:702:DG:H2'	1:B:702:DG:O5'	2.11	0.49
2:A:180:GLU:HB2	2:A:241:THR:HG23	1.93	0.49
2:A:135:GLU:HA	2:A:154:PHE:CZ	2.48	0.49
2:A:160:ASP:O	2:A:161:ASN:HB2	2.12	0.49
2:A:10:ARG:HG3	2:A:10:ARG:NH1	2.21	0.49
2:A:118:GLY:HA2	2:A:141:PRO:HD2	1.93	0.49
2:A:100:ASN:HD22	2:A:103:LYS:N	1.95	0.49
2:A:233:ILE:HG22	2:A:234:LEU:HG	1.95	0.49
2:A:159:ILE:HG13	2:A:159:ILE:O	2.13	0.48
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.95	0.48
1:B:714:DG:C2'	1:B:715:DT:H5'	2.43	0.48
1:B:709:DT:H2''	1:B:710:DT:C5'	2.44	0.48
2:A:16:THR:HG22	2:A:20:HIS:CD2	2.49	0.48
2:A:185:PRO:HD2	2:A:218:GLN:HA	1.96	0.48
2:A:179:ARG:HA	2:A:209:ILE:HD13	1.96	0.47
2:A:200:PHE:CZ	2:A:204:MET:HE3	2.50	0.47
2:A:123:CYS:HB2	2:A:126:TYR:CE2	2.48	0.47
2:A:147:PHE:CD1	2:A:151:LYS:HB2	2.50	0.47
2:A:135:GLU:OE2	2:A:138:ARG:HD2	2.14	0.46
2:A:140:ILE:H	2:A:140:ILE:HD12	1.79	0.46
2:A:77:ILE:HG21	2:A:122:MET:CE	2.45	0.46
2:A:187:PRO:HD2	2:A:221:PHE:CE2	2.50	0.46
2:A:171:ARG:O	2:A:174:ILE:HB	2.16	0.46
1:B:702:DG:OP2	2:A:14:SER:HB3	2.16	0.46
2:A:167:TYR:HD2	2:A:202:LYS:HG3	1.80	0.46
2:A:310:VAL:CG2	2:A:311:ASN:N	2.78	0.46
2:A:181:ILE:HG22	2:A:182:GLY:N	2.31	0.46
1:B:714:DG:H2''	1:B:715:DT:H5'	1.98	0.45
2:A:271:LEU:HD12	2:A:272:ILE:N	2.30	0.45
2:A:126:TYR:CD1	2:A:147:PHE:HE2	2.35	0.45
2:A:325:LEU:HD22	2:A:326:ILE:H	1.81	0.45
2:A:52:ARG:O	2:A:56:VAL:HG22	2.16	0.45
2:A:131:LEU:HD12	2:A:131:LEU:HA	1.72	0.45
2:A:322:HIS:HA	2:A:323:PRO:HD3	1.71	0.45
2:A:335:PRO:HB2	2:A:336:PHE:CD1	2.52	0.45
2:A:157:ALA:O	2:A:318:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:335:PRO:HB2	2:A:336:PHE:CE1	2.52	0.45
2:A:173:LEU:HD13	2:A:181:ILE:HD13	1.98	0.45
1:B:710:DT:O5'	1:B:710:DT:H2'	2.16	0.44
2:A:100:ASN:HB3	2:A:103:LYS:CB	2.47	0.44
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.57	0.44
2:A:17:THR:O	2:A:21:VAL:HG13	2.17	0.44
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.10	0.44
2:A:310:VAL:HG23	2:A:311:ASN:OD1	2.18	0.44
2:A:100:ASN:ND2	2:A:103:LYS:HB2	2.33	0.44
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.75	0.44
2:A:126:TYR:CD2	2:A:130:LEU:HD12	2.53	0.44
2:A:207:ALA:CB	2:A:209:ILE:HG13	2.45	0.44
2:A:177:GLY:O	2:A:336:PHE:HD1	2.01	0.44
2:A:120:LEU:HD12	2:A:120:LEU:HA	1.55	0.43
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.48	0.43
2:A:126:TYR:CD1	2:A:147:PHE:CE2	3.06	0.43
2:A:265:VAL:HA	2:A:266:PRO:HA	1.54	0.43
2:A:84:ASN:HB3	2:A:302:PHE:CD2	2.54	0.43
2:A:249:ILE:HG23	2:A:249:ILE:HD12	1.75	0.43
2:A:162:ALA:HB1	2:A:196:ARG:HG3	2.00	0.43
2:A:284:THR:HA	2:A:285:PRO:HA	1.81	0.43
2:A:43:LEU:HA	2:A:43:LEU:HD22	1.67	0.43
2:A:183:VAL:HG13	2:A:216:ILE:HG12	2.00	0.43
2:A:174:ILE:C	2:A:176:ARG:H	2.21	0.43
2:A:64:LEU:HD12	2:A:65:LEU:N	2.34	0.43
2:A:3:THR:HG22	2:A:6:ASP:CG	2.39	0.43
2:A:284:THR:O	2:A:284:THR:HG22	2.18	0.43
2:A:187:PRO:HG2	2:A:190:ARG:HD3	2.01	0.42
2:A:181:ILE:HA	2:A:242:ALA:O	2.19	0.42
2:A:188:LEU:HA	2:A:188:LEU:HD23	1.69	0.42
1:B:715:DT:H6	1:B:715:DT:H2'	0.83	0.42
2:A:200:PHE:HD2	2:A:201:MET:CE	2.28	0.42
2:A:201:MET:CA	2:A:201:MET:HE2	2.49	0.42
2:A:233:ILE:O	2:A:236:GLN:HG2	2.19	0.42
2:A:106:ALA:O	2:A:110:MET:HG3	2.20	0.42
2:A:249:ILE:HA	2:A:249:ILE:HD13	1.75	0.42
2:A:11:ALA:CB	2:A:13:VAL:HG22	2.49	0.42
2:A:123:CYS:O	2:A:124:SER:HB2	2.20	0.42
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.37	0.42
2:A:107:TYR:HA	2:A:110:MET:HG3	2.01	0.42
2:A:101:LEU:O	2:A:104:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:10:ARG:CG	2:A:10:ARG:NH1	2.79	0.41
2:A:90:TYR:N	2:A:90:TYR:HD2	2.19	0.41
2:A:125:GLU:HG2	2:A:190:ARG:HD2	2.00	0.41
2:A:144:VAL:HG21	2:A:147:PHE:CD2	2.55	0.41
2:A:264:ARG:HD2	2:A:264:ARG:HA	1.64	0.41
2:A:3:THR:HG23	2:A:5:LYS:N	2.33	0.41
2:A:211:VAL:HA	2:A:212:PRO:HD3	1.86	0.41
2:A:126:TYR:HD2	2:A:130:LEU:HD12	1.86	0.41
2:A:23:ASN:ND2	2:A:23:ASN:N	2.68	0.41
2:A:105:ARG:HB2	2:A:133:MET:SD	2.61	0.41
2:A:45:TYR:CE1	2:A:47:PRO:HG3	2.56	0.41
2:A:167:TYR:CE2	2:A:202:LYS:HG3	2.56	0.41
2:A:80:ALA:O	2:A:83:LYS:HB2	2.21	0.41
2:A:21:VAL:CG2	2:A:22:ILE:N	2.82	0.40
2:A:45:TYR:HA	4:A:810:HOH:O	2.22	0.40
2:A:61:SER:CB	2:A:91:THR:CG2	2.98	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	
2	A	337/340 (99%)	297 (88%)	35 (10%)	5 (2%)	13	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	309	ILE
2	A	312	LYS
2	A	124	SER
2	A	246	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
2	A	279/280 (100%)	197 (71%)	82 (29%)	<b>0</b> <b>1</b>

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR
2	A	5	LYS
2	A	7	VAL
2	A	9	LYS
2	A	10	ARG
2	A	14	SER
2	A	21	VAL
2	A	22	ILE
2	A	23	ASN
2	A	26	ARG
2	A	30	GLU
2	A	31	GLU
2	A	40	ILE
2	A	41	LYS
2	A	43	LEU
2	A	44	HIS
2	A	54	LEU
2	A	55	LYS
2	A	60	LYS
2	A	62	ILE
2	A	64	LEU
2	A	69	SER
2	A	87	GLN
2	A	88	LYS
2	A	90	TYR
2	A	91	THR
2	A	92	LEU
2	A	99	ASN
2	A	103	LYS
2	A	105	ARG

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Mol	Chain	Res	Type
2	A	107	TYR
2	A	109	SER
2	A	119	LEU
2	A	120	LEU
2	A	122	MET
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	133	MET
2	A	135	GLU
2	A	136	GLU
2	A	138	ARG
2	A	143	VAL
2	A	145	MET
2	A	147	PHE
2	A	149	GLU
2	A	151	LYS
2	A	158	VAL
2	A	183	VAL
2	A	202	LYS
2	A	208	MET
2	A	209	ILE
2	A	210	LYS
2	A	213	GLU
2	A	228	ARG
2	A	232	GLN
2	A	233	ILE
2	A	234	LEU
2	A	235	SER
2	A	241	THR
2	A	255	LEU
2	A	260	GLU
2	A	261	MET
2	A	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	270	SER
2	A	271	LEU
2	A	274	TYR
2	A	278	ARG
2	A	281	ARG
2	A	292	GLN

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Mol	Chain	Res	Type
2	A	296	SER
2	A	299	GLU
2	A	306	LEU
2	A	309	ILE
2	A	310	VAL
2	A	317	GLN
2	A	318	SER
2	A	321	VAL
2	A	336	PHE
2	A	337	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	ASN
2	A	34	ASN
2	A	58	HIS
2	A	84	ASN
2	A	100	ASN
2	A	104	GLN
2	A	218	GLN
2	A	291	HIS
2	A	292	GLN

### 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	1.67	2 (25%)	4,15,15	3.88	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	2.20	1.38	1.33
3	A	599	HPA	C6-N1	3.42	1.39	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	-5.47	124.70	128.89
3	A	599	HPA	C2-N1-C6	5.32	124.11	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.