



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:33 PM GMT

PDB ID : 1BDI  
Title : PURINE REPRESSOR MUTANT-HYPOXANTHINE-PALINDROMIC  
OPERATOR COMPLEX  
Authors : Glasfeld, A.; Schumacher, M.A.; Choi, K.Y.; Zalkin, H.; Brennan, R.G.  
Deposited on : 1996-07-25  
Resolution : 3.00 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

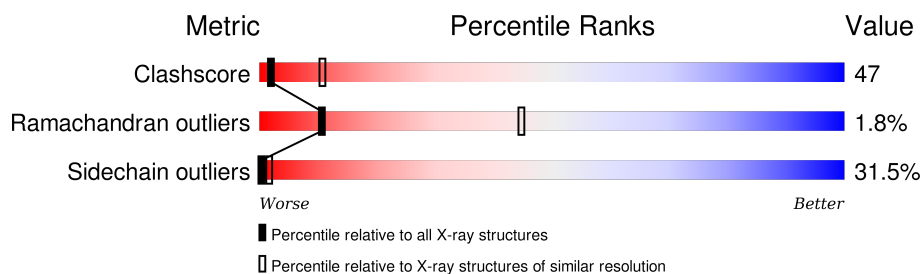
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 3009 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.

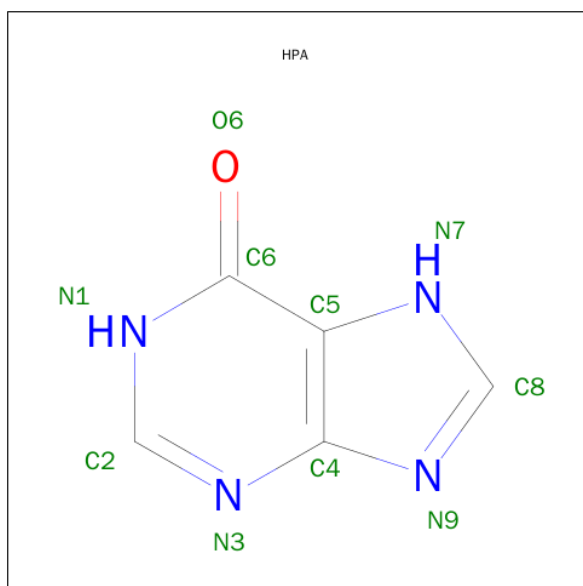
- Molecule 1 is a DNA chain called DNA (5'-D(\*TP\*AP\*CP\*GP\*CP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*GP\*CP\*GP\*T)-3').

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 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	2	Total	O	0	0
			2	2		

### 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.

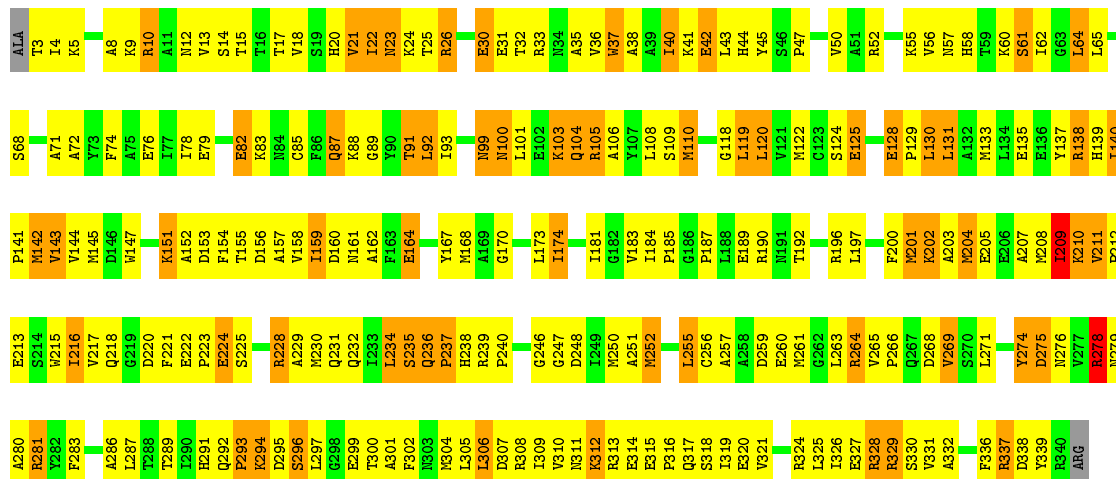
- Molecule 1: DNA (5'-D(\*TP\*AP\*CP\*GP\*CP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*GP\*CP\*GP\*T)-3')

Chain B: 



- Molecule 2: PROTEIN (PURINE REPRESSOR)

Chain A: 



## 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, $\alpha$ , $\beta$ , $\gamma$	176.16 Å 94.99 Å 81.57 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	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	3009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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	0.55	0/386	1.06	3/594 (0.5%)
2	A	0.93	1/2706 (0.0%)	1.11	4/3660 (0.1%)
All	All	0.89	1/3092 (0.0%)	1.11	7/4254 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	37	TRP	CB-CG	-6.03	1.39	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	236	GLN	C-N-CD	-13.05	91.89	120.60
1	B	702	DG	O4'-C4'-C3'	-7.65	101.41	106.00
2	A	269	VAL	CB-CA-C	-7.05	98.01	111.40
1	B	703	DC	O4'-C4'-C3'	-5.88	102.15	104.50
2	A	306	LEU	CA-CB-CG	-5.51	102.62	115.30
2	A	209	ILE	N-CA-C	-5.36	96.53	111.00
1	B	713	DC	O5'-P-OP2	-5.23	101.00	105.70

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	2652	0	2636	258	0
3	A	10	0	4	1	0
4	A	2	0	0	0	0
All	All	3009	0	2834	272	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 47.

All (272) 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:230:MET:HG3	2:A:234:LEU:HD11	1.33	1.09
2:A:181:ILE:HD12	2:A:204:MET:HE1	1.20	1.07
1:B:713:DC:H2''	1:B:714:DG:C5'	1.94	0.98
1:B:713:DC:C2'	1:B:714:DG:H5''	1.92	0.98
1:B:713:DC:H2''	1:B:714:DG:H5''	0.99	0.95
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.48	0.95
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.83	0.92
2:A:181:ILE:HD12	2:A:204:MET:CE	2.01	0.90
2:A:140:ILE:HD12	2:A:141:PRO:CD	2.02	0.89
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.36	0.89
2:A:156:ASP:HB3	2:A:304:MET:HE1	1.55	0.87
2:A:20:HIS:CE1	2:A:26:ARG:HD3	2.11	0.85
2:A:92:LEU:HD22	2:A:93:ILE:N	1.92	0.85
2:A:292:GLN:HG3	2:A:293:PRO:HD2	1.59	0.84
1:B:703:DC:H5'	1:B:703:DC:C6	2.13	0.83
2:A:156:ASP:HB3	2:A:304:MET:CE	2.08	0.83
2:A:61:SER:HB2	2:A:91:THR:CG2	2.09	0.83
2:A:135:GLU:HB2	2:A:154:PHE:CZ	2.14	0.81
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.62	0.80
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.63	0.80
2:A:212:PRO:HG2	2:A:215:TRP:HB2	1.65	0.79
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.01	0.79
2:A:61:SER:HB2	2:A:91:THR:HG22	1.64	0.79
2:A:236:GLN:HG3	2:A:237:PRO:HD2	1.65	0.78
2:A:231:GLN:O	2:A:235:SER:HB2	1.83	0.77
2:A:145:MET:HA	2:A:158:VAL:HG12	1.66	0.77
2:A:82:GLU:HG3	2:A:83:LYS:N	1.99	0.76
2:A:230:MET:HG3	2:A:234:LEU:CD1	2.16	0.75
2:A:92:LEU:HD22	2:A:93:ILE:H	1.54	0.72
2:A:210:LYS:N	2:A:210:LYS:HD3	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:286:ALA:HB1	2:A:328:ARG:HG2	1.71	0.72
2:A:100:ASN:HD22	2:A:103:LYS:H	1.37	0.72
2:A:167:TYR:CD2	2:A:202:LYS:HG2	2.26	0.71
2:A:181:ILE:CD1	2:A:204:MET:HE1	2.10	0.70
2:A:230:MET:CG	2:A:234:LEU:HD11	2.17	0.70
2:A:210:LYS:H	2:A:210:LYS:HD3	1.56	0.70
2:A:252:MET:HE3	2:A:283:PHE:CZ	2.26	0.70
1:B:703:DC:H1'	1:B:704:DA:H5'	1.73	0.69
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.74	0.69
1:B:700:DA:H2''	1:B:701:DC:O5'	1.90	0.69
2:A:137:TYR:HA	2:A:139:HIS:CD2	2.28	0.69
2:A:197:LEU:HD11	2:A:201:MET:HE1	1.74	0.68
2:A:185:PRO:HD2	2:A:217:VAL:O	1.94	0.68
2:A:118:GLY:HA2	2:A:141:PRO:HG2	1.76	0.68
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.75	0.67
2:A:204:MET:HG3	2:A:209:ILE:CG2	2.25	0.67
2:A:184:ILE:HG12	2:A:229:ALA:HB1	1.77	0.67
2:A:256:CYS:O	2:A:259:ASP:HB3	1.95	0.67
2:A:309:ILE:HG22	2:A:310:VAL:N	2.08	0.66
2:A:30:GLU:HG2	2:A:33:ARG:NH1	2.10	0.66
2:A:192:THR:O	2:A:196:ARG:HD2	1.96	0.66
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.43	0.65
2:A:99:ASN:HD21	2:A:125:GLU:HB2	1.61	0.65
2:A:153:ASP:O	2:A:316:PRO:HG3	1.96	0.65
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.25	0.65
2:A:130:LEU:O	2:A:130:LEU:HD22	1.97	0.65
2:A:22:ILE:HG22	2:A:23:ASN:ND2	2.11	0.65
2:A:292:GLN:HG3	2:A:293:PRO:CD	2.26	0.65
2:A:280:ALA:HA	2:A:283:PHE:CD1	2.33	0.64
2:A:184:ILE:HA	2:A:217:VAL:O	1.96	0.64
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.28	0.64
2:A:201:MET:HE2	2:A:201:MET:N	2.13	0.64
2:A:200:PHE:HD2	2:A:201:MET:CE	2.10	0.64
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.79	0.63
2:A:145:MET:HA	2:A:158:VAL:CG1	2.29	0.63
2:A:201:MET:CA	2:A:201:MET:HE2	2.27	0.63
2:A:13:VAL:HG23	2:A:14:SER:O	1.99	0.63
2:A:184:ILE:HG23	2:A:217:VAL:O	1.97	0.63
2:A:247:GLY:HA2	2:A:274:TYR:O	1.97	0.63
1:B:702:DG:H5'	1:B:702:DG:H8	1.64	0.63
2:A:157:ALA:O	2:A:318:SER:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3:THR:HG23	2:A:45:TYR:CE1	2.33	0.62
2:A:276:ASN:HA	2:A:289:THR:HG21	1.82	0.61
2:A:281:ARG:O	2:A:281:ARG:HD3	2.00	0.61
2:A:100:ASN:ND2	2:A:103:LYS:H	1.98	0.61
2:A:105:ARG:HA	2:A:133:MET:CE	2.31	0.61
2:A:325:LEU:HD11	2:A:327:GLU:HG3	1.82	0.60
2:A:155:THR:HG22	2:A:156:ASP:N	2.17	0.60
2:A:152:ALA:HB1	2:A:154:PHE:CE1	2.36	0.60
2:A:167:TYR:HD2	2:A:202:LYS:HG2	1.66	0.60
2:A:200:PHE:HD2	2:A:201:MET:HE1	1.67	0.59
2:A:237:PRO:CG	2:A:238:HIS:H	2.14	0.59
1:B:702:DG:C8	1:B:702:DG:H5'	2.36	0.59
2:A:71:ALA:HB3	2:A:74:PHE:HD2	1.66	0.59
2:A:329:ARG:HH11	2:A:329:ARG:HG3	1.68	0.59
2:A:210:LYS:H	2:A:210:LYS:CD	2.15	0.59
2:A:64:LEU:HD13	2:A:120:LEU:HB3	1.85	0.59
2:A:61:SER:CB	2:A:91:THR:HG22	2.32	0.58
2:A:147:TRP:CZ3	2:A:151:LYS:HB2	2.38	0.58
2:A:71:ALA:HB3	2:A:74:PHE:CD2	2.39	0.58
2:A:35:ALA:O	2:A:38:ALA:HB3	2.04	0.57
1:B:701:DC:H2''	1:B:702:DG:H5''	1.86	0.57
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.33	0.57
2:A:64:LEU:HD12	2:A:65:LEU:N	2.19	0.57
2:A:8:ALA:HB1	2:A:13:VAL:O	2.05	0.57
2:A:197:LEU:HD11	2:A:201:MET:CE	2.34	0.57
2:A:101:LEU:HA	2:A:104:GLN:CG	2.35	0.57
2:A:38:ALA:O	2:A:42:GLU:HG2	2.05	0.57
2:A:101:LEU:HA	2:A:104:GLN:HG2	1.87	0.56
1:B:712:DG:H2''	1:B:713:DC:H5''	1.88	0.56
2:A:276:ASN:ND2	2:A:291:HIS:HD2	2.03	0.56
2:A:143:VAL:HA	2:A:155:THR:HG22	1.87	0.56
2:A:20:HIS:HA	2:A:25:THR:CG2	2.37	0.55
2:A:236:GLN:HB2	2:A:237:PRO:HD3	1.88	0.55
2:A:162:ALA:O	2:A:196:ARG:HA	2.06	0.55
2:A:162:ALA:HB1	2:A:196:ARG:HG3	1.87	0.55
2:A:224:GLU:HG3	2:A:228:ARG:HD2	1.88	0.55
2:A:145:MET:HE3	2:A:301:ALA:HB2	1.89	0.55
2:A:187:PRO:HB2	2:A:190:ARG:HD3	1.89	0.55
2:A:257:ALA:O	2:A:261:MET:HG3	2.07	0.55
2:A:125:GLU:OE1	2:A:190:ARG:HD2	2.07	0.54
2:A:10:ARG:HG3	2:A:10:ARG:NH1	2.12	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.38	0.54
2:A:281:ARG:C	2:A:281:ARG:HD3	2.28	0.54
2:A:144:VAL:HG21	2:A:147:TRP:CE2	2.43	0.54
2:A:142:MET:HG2	2:A:155:THR:HG23	1.90	0.54
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.72	0.54
2:A:337:ARG:NH1	2:A:338:ASP:HA	2.23	0.53
2:A:155:THR:HG22	2:A:156:ASP:H	1.71	0.53
2:A:20:HIS:NE2	2:A:26:ARG:HD3	2.23	0.53
2:A:105:ARG:HB2	2:A:133:MET:SD	2.49	0.53
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.39	0.53
2:A:147:TRP:CE3	2:A:151:LYS:HB2	2.44	0.53
2:A:236:GLN:CB	2:A:237:PRO:HD3	2.40	0.52
2:A:40:ILE:HG22	2:A:41:LYS:HD3	1.92	0.52
2:A:118:GLY:C	2:A:140:ILE:HD11	2.30	0.52
2:A:106:ALA:O	2:A:110:MET:HG3	2.10	0.52
2:A:278:ARG:NH1	2:A:278:ARG:HG3	2.24	0.51
2:A:212:PRO:HG2	2:A:215:TRP:CB	2.36	0.51
2:A:8:ALA:HB2	2:A:15:THR:HA	1.91	0.51
2:A:160:ASP:O	2:A:161:ASN:HB2	2.10	0.51
2:A:204:MET:CE	2:A:209:ILE:HG21	2.41	0.51
2:A:237:PRO:HG2	2:A:238:HIS:H	1.74	0.51
2:A:210:LYS:O	2:A:210:LYS:HG2	2.11	0.51
2:A:135:GLU:HG2	2:A:138:ARG:HD2	1.93	0.50
2:A:304:MET:O	2:A:307:ASP:HB3	2.11	0.50
2:A:236:GLN:CB	2:A:237:PRO:CD	2.89	0.50
2:A:105:ARG:HA	2:A:133:MET:HE1	1.93	0.50
2:A:325:LEU:CD1	2:A:327:GLU:HG3	2.41	0.50
2:A:224:GLU:O	2:A:224:GLU:HG3	2.12	0.50
2:A:120:LEU:HD13	2:A:305:LEU:HD22	1.92	0.50
1:B:714:DG:H2''	1:B:715:DT:H5'	1.94	0.50
2:A:87:GLN:OE1	2:A:88:LYS:HE2	2.12	0.50
2:A:222:GLU:HB3	2:A:223:PRO:HD2	1.93	0.50
2:A:212:PRO:HG2	2:A:215:TRP:CG	2.47	0.49
2:A:135:GLU:HG2	2:A:138:ARG:HG2	1.94	0.49
2:A:192:THR:HG1	2:A:221:PHE:HZ	1.55	0.49
2:A:310:VAL:CG2	2:A:311:ASN:N	2.75	0.49
2:A:105:ARG:CA	2:A:133:MET:HE1	2.41	0.49
2:A:265:VAL:HG13	2:A:266:PRO:HA	1.94	0.49
2:A:336:PHE:CD1	2:A:336:PHE:N	2.80	0.49
2:A:197:LEU:O	2:A:200:PHE:HB3	2.12	0.49
2:A:128:GLU:N	2:A:129:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:304:MET:CE	2:A:317:GLN:HB3	2.43	0.49
2:A:296:SER:O	2:A:300:THR:HB	2.13	0.49
1:B:714:DG:H5''	1:B:714:DG:H8	1.78	0.48
2:A:287:LEU:O	2:A:328:ARG:HB2	2.12	0.48
2:A:64:LEU:C	2:A:64:LEU:HD12	2.33	0.48
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.95	0.48
2:A:280:ALA:HA	2:A:283:PHE:CE1	2.47	0.48
2:A:184:ILE:HG12	2:A:229:ALA:CB	2.43	0.48
2:A:325:LEU:HD13	2:A:326:ILE:N	2.29	0.48
2:A:119:LEU:HB3	2:A:142:MET:HB2	1.96	0.48
2:A:252:MET:HB2	2:A:283:PHE:CE2	2.49	0.48
2:A:293:PRO:HG2	2:A:321:VAL:HG22	1.96	0.48
2:A:286:ALA:HB3	2:A:329:ARG:HG2	1.94	0.48
2:A:100:ASN:HB3	2:A:103:LYS:CB	2.43	0.48
2:A:294:LYS:HG2	2:A:294:LYS:H	1.22	0.47
2:A:140:ILE:HD12	2:A:141:PRO:N	2.28	0.47
2:A:125:GLU:HG3	2:A:189:GLU:HB3	1.96	0.47
1:B:714:DG:C5'	1:B:714:DG:H8	2.27	0.47
2:A:239:ARG:HB2	2:A:240:PRO:HD2	1.97	0.47
2:A:204:MET:HG3	2:A:209:ILE:HG22	1.96	0.47
2:A:137:TYR:O	2:A:140:ILE:HG23	2.15	0.47
2:A:224:GLU:HG3	2:A:228:ARG:CD	2.44	0.47
2:A:337:ARG:HH12	2:A:338:ASP:HA	1.79	0.47
2:A:101:LEU:O	2:A:104:GLN:HG2	2.14	0.47
2:A:40:ILE:CG2	2:A:41:LYS:HD3	2.45	0.47
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.79	0.47
2:A:308:ARG:O	2:A:312:LYS:HA	2.15	0.47
2:A:152:ALA:CB	2:A:154:PHE:CE1	2.98	0.47
2:A:30:GLU:HG2	2:A:33:ARG:HH12	1.77	0.46
2:A:3:THR:HG23	2:A:45:TYR:CD1	2.51	0.46
2:A:17:THR:HG22	2:A:18:VAL:N	2.29	0.46
2:A:85:CYS:HA	2:A:302:PHE:CZ	2.50	0.46
2:A:201:MET:HE3	2:A:201:MET:HB2	1.64	0.46
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.46	0.46
2:A:265:VAL:CG1	2:A:266:PRO:HA	2.45	0.46
2:A:331:VAL:CG1	2:A:332:ALA:N	2.78	0.46
2:A:237:PRO:CG	2:A:238:HIS:N	2.79	0.46
2:A:57:ASN:O	2:A:58:HIS:HB3	2.16	0.46
2:A:145:MET:HE3	2:A:301:ALA:CB	2.46	0.45
2:A:140:ILE:O	2:A:140:ILE:HG13	2.10	0.45
2:A:158:VAL:O	2:A:158:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:216:ILE:HG12	2:A:216:ILE:O	2.16	0.45
2:A:252:MET:CB	2:A:283:PHE:CE2	2.99	0.45
2:A:32:THR:O	2:A:35:ALA:HB3	2.16	0.45
2:A:144:VAL:HG12	2:A:155:THR:HG21	1.99	0.45
2:A:212:PRO:O	2:A:215:TRP:HB2	2.17	0.45
2:A:287:LEU:HA	2:A:287:LEU:HD12	1.71	0.45
2:A:167:TYR:CE2	2:A:202:LYS:HG2	2.51	0.45
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.22	0.45
2:A:237:PRO:CD	2:A:238:HIS:H	2.30	0.45
2:A:10:ARG:CG	2:A:10:ARG:HH11	2.16	0.44
2:A:152:ALA:HB1	2:A:154:PHE:CD1	2.52	0.44
2:A:156:ASP:HB3	2:A:304:MET:HE2	1.92	0.44
2:A:297:LEU:C	2:A:297:LEU:HD23	2.37	0.44
2:A:263:LEU:N	2:A:263:LEU:CD1	2.79	0.44
2:A:105:ARG:N	2:A:133:MET:HE1	2.32	0.44
2:A:313:ARG:HG3	2:A:314:GLU:N	2.33	0.44
2:A:120:LEU:HD12	2:A:120:LEU:HA	1.43	0.44
2:A:325:LEU:HD13	2:A:325:LEU:C	2.38	0.44
2:A:128:GLU:N	2:A:129:PRO:HD2	2.33	0.44
2:A:104:GLN:O	2:A:108:LEU:HB2	2.18	0.44
2:A:304:MET:HE3	2:A:317:GLN:HB3	2.00	0.44
2:A:292:GLN:O	2:A:294:LYS:HG2	2.18	0.44
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.82	0.44
2:A:164:GLU:O	2:A:168:MET:HG3	2.17	0.44
2:A:30:GLU:CG	2:A:33:ARG:HH12	2.31	0.43
2:A:220:ASP:O	2:A:221:PHE:HB2	2.18	0.43
2:A:204:MET:HE2	2:A:209:ILE:HG21	2.00	0.43
2:A:248:ASP:O	2:A:251:ALA:HB3	2.18	0.43
2:A:135:GLU:HG3	2:A:154:PHE:CD1	2.53	0.43
2:A:125:GLU:HG3	2:A:189:GLU:CB	2.49	0.43
2:A:286:ALA:HB1	2:A:328:ARG:CG	2.46	0.43
2:A:276:ASN:HB2	2:A:291:HIS:HA	1.99	0.43
2:A:145:MET:H	2:A:145:MET:HG2	1.64	0.43
1:B:706:DA:H2"	1:B:707:DC:C6	2.54	0.43
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.53	0.43
2:A:215:TRP:CZ2	2:A:239:ARG:HA	2.54	0.43
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.54	0.43
2:A:286:ALA:HB3	2:A:329:ARG:CG	2.49	0.43
2:A:220:ASP:OD1	2:A:225:SER:HB3	2.19	0.42
2:A:23:ASN:ND2	2:A:23:ASN:N	2.66	0.42
2:A:266:PRO:HB3	2:A:330:SER:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.67	0.42
2:A:20:HIS:HA	2:A:25:THR:HG22	2.01	0.42
2:A:135:GLU:O	2:A:135:GLU:HG2	2.18	0.42
2:A:331:VAL:HG12	2:A:332:ALA:N	2.34	0.42
2:A:315:GLU:HA	2:A:316:PRO:HD2	1.71	0.42
2:A:87:GLN:HB2	2:A:87:GLN:HE21	1.61	0.42
2:A:45:TYR:CE2	2:A:47:PRO:HG3	2.55	0.42
2:A:215:TRP:CZ2	2:A:240:PRO:N	2.88	0.42
2:A:23:ASN:N	2:A:23:ASN:HD22	2.17	0.42
2:A:207:ALA:O	2:A:208:MET:HB2	2.20	0.42
2:A:276:ASN:ND2	2:A:291:HIS:CD2	2.77	0.42
2:A:202:LYS:CG	2:A:203:ALA:N	2.80	0.42
2:A:264:ARG:H	2:A:268:ASP:HB2	1.85	0.42
2:A:329:ARG:HG3	2:A:329:ARG:NH1	2.34	0.41
2:A:120:LEU:HD12	2:A:143:VAL:HG13	2.01	0.41
2:A:61:SER:HA	2:A:91:THR:H	1.85	0.41
2:A:197:LEU:HA	2:A:197:LEU:HD12	1.72	0.41
2:A:32:THR:O	2:A:36:VAL:HG23	2.21	0.41
2:A:275:ASP:O	2:A:294:LYS:HE3	2.21	0.41
2:A:292:GLN:HA	2:A:293:PRO:HD3	1.58	0.41
2:A:211:VAL:CG2	2:A:216:ILE:HG22	2.50	0.41
2:A:170:GLY:O	2:A:173:LEU:HB2	2.20	0.41
2:A:52:ARG:O	2:A:56:VAL:HG22	2.21	0.41
2:A:101:LEU:HD12	2:A:104:GLN:HG3	2.03	0.41
2:A:252:MET:CE	2:A:283:PHE:CZ	3.01	0.41
2:A:239:ARG:HB2	2:A:240:PRO:CD	2.51	0.41
2:A:236:GLN:CG	2:A:237:PRO:HD2	2.43	0.41
2:A:286:ALA:CB	2:A:328:ARG:HG2	2.46	0.41
2:A:131:LEU:HD13	2:A:131:LEU:HA	1.59	0.41
2:A:64:LEU:HD23	2:A:78:ILE:HG12	2.02	0.41
2:A:204:MET:HG3	2:A:209:ILE:HG21	2.00	0.40
2:A:196:ARG:NH2	3:A:599:HPA:H8	2.36	0.40
2:A:21:VAL:HG11	2:A:36:VAL:HG21	2.03	0.40
2:A:174:ILE:HD11	2:A:209:ILE:HD13	2.03	0.40
2:A:119:LEU:O	2:A:142:MET:HB2	2.21	0.40
2:A:45:TYR:CZ	2:A:47:PRO:HA	2.57	0.40
2:A:72:ALA:O	2:A:76:GLU:HG3	2.20	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	336/340 (99%)	296 (88%)	34 (10%)	6 (2%)	11	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	278	ARG
2	A	246	GLY
2	A	124	SER
2	A	89	GLY
2	A	237	PRO

### 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%)	191 (68%)	88 (32%)	0	2

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	ILE
2	A	5	LYS
2	A	9	LYS
2	A	10	ARG
2	A	12	ASN

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Mol	Chain	Res	Type
2	A	21	VAL
2	A	22	ILE
2	A	23	ASN
2	A	24	LYS
2	A	26	ARG
2	A	30	GLU
2	A	31	GLU
2	A	40	ILE
2	A	42	GLU
2	A	43	LEU
2	A	44	HIS
2	A	50	VAL
2	A	55	LYS
2	A	60	LYS
2	A	61	SER
2	A	62	ILE
2	A	64	LEU
2	A	68	SER
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	103	LYS
2	A	104	GLN
2	A	105	ARG
2	A	109	SER
2	A	110	MET
2	A	119	LEU
2	A	120	LEU
2	A	122	MET
2	A	125	GLU
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	138	ARG
2	A	140	ILE
2	A	142	MET
2	A	143	VAL
2	A	151	LYS

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Mol	Chain	Res	Type
2	A	159	ILE
2	A	164	GLU
2	A	174	ILE
2	A	183	VAL
2	A	201	MET
2	A	202	LYS
2	A	204	MET
2	A	205	GLU
2	A	209	ILE
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	232	GLN
2	A	234	LEU
2	A	235	SER
2	A	250	MET
2	A	252	MET
2	A	255	LEU
2	A	260	GLU
2	A	264	ARG
2	A	269	VAL
2	A	274	TYR
2	A	278	ARG
2	A	279	ASN
2	A	281	ARG
2	A	293	PRO
2	A	294	LYS
2	A	295	ASP
2	A	296	SER
2	A	299	GLU
2	A	312	LYS
2	A	319	ILE
2	A	324	ARG
2	A	328	ARG
2	A	329	ARG
2	A	337	ARG
2	A	339	TYR

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	99	ASN
2	A	100	ASN
2	A	139	HIS
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	1.67	1 (12%)	4,15,15	4.41	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	HPA	C6-N1	3.48	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	-6.73	123.74	128.89
3	A	599	HPA	C2-N1-C6	5.42	124.25	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	599	HPA	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.