



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:53 am GMT

PDB ID : 1JH9  
Title : PURINE REPRESSOR MUTANT-HYPOXANTHINE-PURF OPERATOR  
COMPLEX  
Authors : Huffman, J.L.; Lu, F.; Zalkin, H.; Brennan, R.G.  
Deposited on : 2001-06-27  
Resolution : 2.55 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

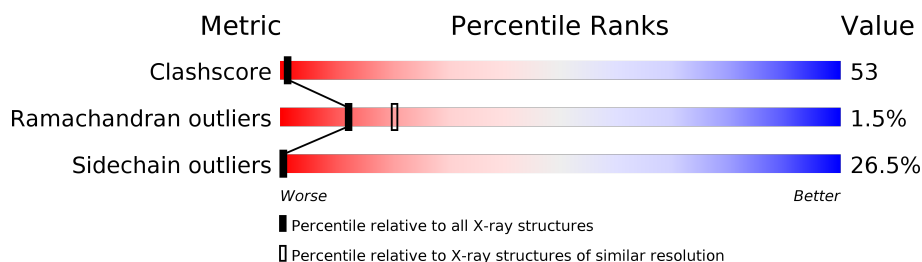
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	799	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3136 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(\*AP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*GP\*T)-3'.

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

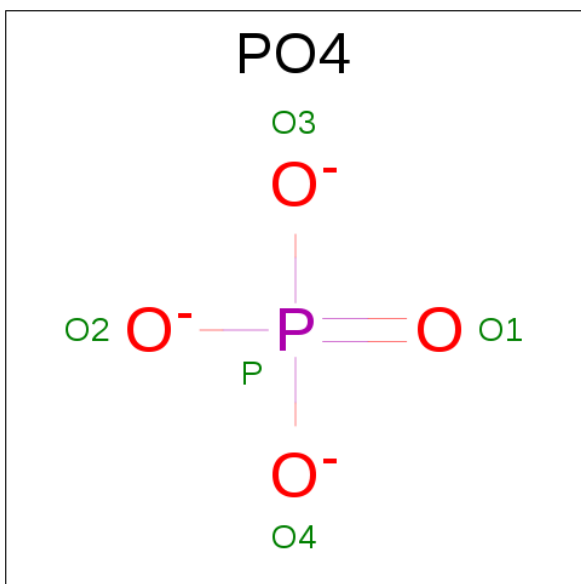
- Molecule 2 is a protein called PURINE NUCLEOTIDE SYNTHESIS REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	339	Total	C	N	O	S	0	0	0
			2654	1669	472	494	19			

There is a discrepancy between the modelled and reference sequences:

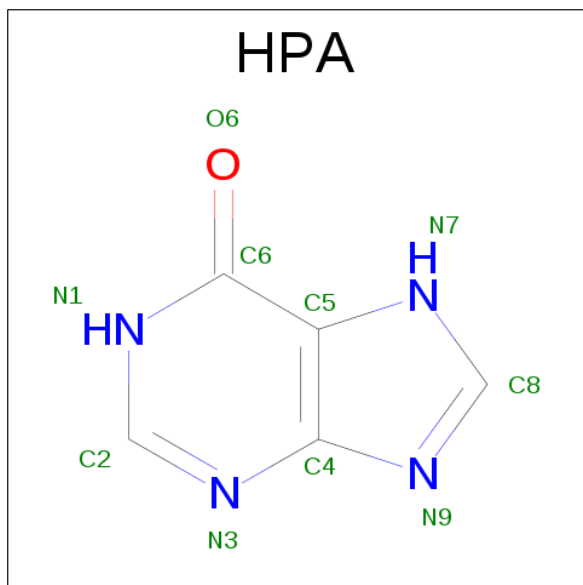
Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ARG	TRP	ENGINEERED	UNP P0ACP7

- 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		
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.

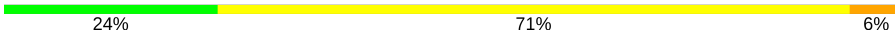
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total	O	0	0
			107	107		
5	B	9	Total	O	0	0
			9	9		

### 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 the various outlier classes 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.

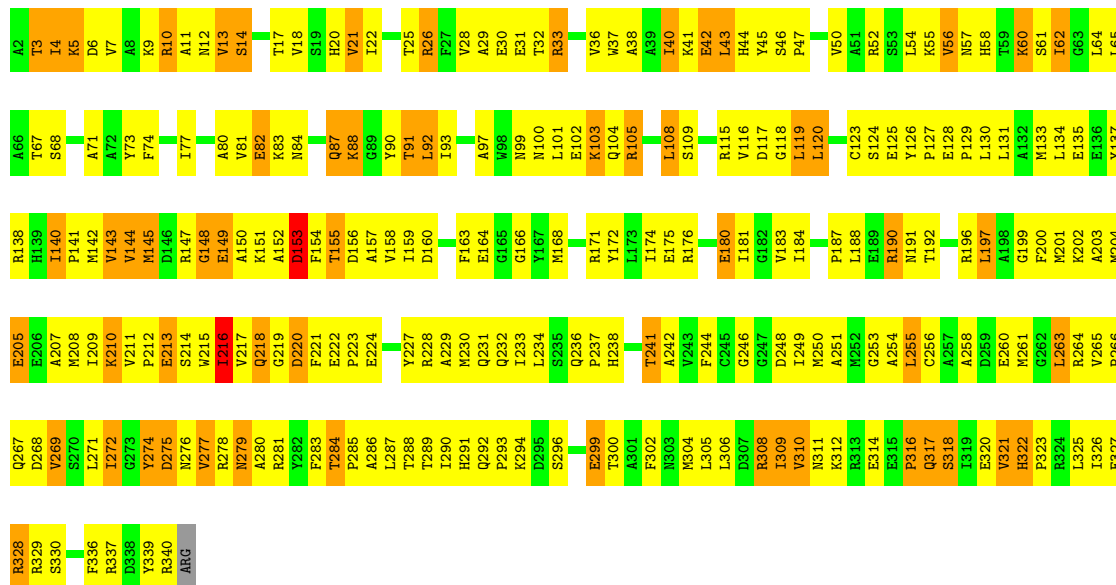
- Molecule 1: 5'-D(\*AP\*AP\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*GP\*T)-3',

Chain B: 



- Molecule 2: PURINE NUCLEOTIDE SYNTHESIS REPRESSOR

Chain A: 



## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	175.38Å 92.61Å 80.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.55	Depositor
% Data completeness (in resolution range)	96.0 (10.00-2.55)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	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	0.71	0/388	0.98	1/597 (0.2%)
2	A	1.02	0/2706	1.09	8/3658 (0.2%)
All	All	0.99	0/3094	1.08	9/4255 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	216	ILE	CG1-CB-CG2	-8.54	92.61	111.40
2	A	340	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	A	220	ASP	CB-CG-OD1	6.42	124.08	118.30
2	A	180	GLU	N-CA-C	-5.83	95.25	111.00
2	A	322	HIS	N-CA-C	5.62	126.19	111.00
2	A	197	LEU	CB-CG-CD1	-5.17	102.22	111.00
2	A	204	MET	CG-SD-CE	5.16	108.46	100.20
1	B	704	DA	O4'-C1'-N9	5.08	111.56	108.00
2	A	56	VAL	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	346	0	194	13	0
2	A	2654	0	2644	299	0
3	A	10	0	0	2	0
4	A	10	0	4	0	0
5	A	107	0	0	9	1
5	B	9	0	0	0	0
All	All	3136	0	2842	310	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 53.

All (310) 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:210:LYS:H	2:A:210:LYS:HD3	1.18	1.04
2:A:223:PRO:HD3	2:A:249:ILE:HG22	1.38	1.03
2:A:126:TYR:HB3	2:A:131:LEU:HD21	1.44	0.98
2:A:183:VAL:CG1	2:A:216:ILE:HG22	2.03	0.89
2:A:101:LEU:HA	2:A:104:GLN:NE2	1.88	0.88
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.90	0.86
2:A:3:THR:HG22	2:A:5:LYS:H	1.44	0.83
2:A:264:ARG:HH21	2:A:267:GLN:HE22	1.23	0.83
2:A:10:ARG:HH11	2:A:10:ARG:HG3	1.45	0.82
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.61	0.82
2:A:10:ARG:HD3	2:A:43:LEU:HD21	1.61	0.81
2:A:102:GLU:HG2	2:A:105:ARG:NH1	1.94	0.80
2:A:88:LYS:HG3	2:A:302:PHE:HE2	1.46	0.79
2:A:21:VAL:HG21	2:A:36:VAL:HG11	1.64	0.79
2:A:205:GLU:HG2	5:A:888:HOH:O	1.83	0.79
2:A:33:ARG:HG2	2:A:33:ARG:HH11	1.47	0.78
2:A:3:THR:O	2:A:7:VAL:HG23	1.84	0.78
1:B:702:DG:OP2	2:A:14:SER:HB3	1.84	0.78
2:A:87:GLN:HG3	2:A:88:LYS:N	1.98	0.77
2:A:152:ALA:HA	2:A:154:PHE:CE1	2.19	0.76
2:A:308:ARG:HH11	2:A:308:ARG:HG3	1.50	0.76
2:A:192:THR:O	2:A:196:ARG:HD2	1.86	0.76
2:A:157:ALA:O	2:A:318:SER:HA	1.86	0.75
2:A:272:ILE:HD12	2:A:288:THR:HG22	1.69	0.74
2:A:214:SER:HB2	2:A:236:GLN:OE1	1.87	0.74
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.18	0.73
2:A:306:LEU:O	2:A:310:VAL:HG13	1.88	0.73
2:A:84:ASN:HA	2:A:87:GLN:HG2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:LYS:N	2:A:210:LYS:HD3	1.99	0.72
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.71	0.72
2:A:97:ALA:HB1	2:A:104:GLN:HG3	1.72	0.71
2:A:87:GLN:HG3	2:A:88:LYS:HG2	1.71	0.71
2:A:286:ALA:HB1	2:A:328:ARG:HG2	1.70	0.71
2:A:83:LYS:HG3	5:A:896:HOH:O	1.88	0.71
2:A:147:ARG:HH12	2:A:151:LYS:HB2	1.55	0.71
1:B:709:DT:H2''	1:B:710:DT:H5'	1.70	0.71
1:B:712:DT:H2''	1:B:713:DC:H5''	1.73	0.70
2:A:157:ALA:N	2:A:304:MET:HE1	2.06	0.70
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.74	0.70
2:A:183:VAL:HG12	2:A:216:ILE:HG22	1.73	0.70
2:A:325:LEU:HD11	2:A:327:GLU:HG3	1.73	0.70
2:A:141:PRO:O	2:A:305:LEU:HD11	1.91	0.70
2:A:308:ARG:O	2:A:312:LYS:HA	1.90	0.70
2:A:101:LEU:HA	2:A:104:GLN:HE21	1.53	0.70
2:A:183:VAL:HG13	2:A:216:ILE:HG22	1.72	0.69
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.54	0.69
1:B:700:DA:H2''	1:B:701:DC:O5'	1.92	0.69
2:A:325:LEU:CD1	2:A:327:GLU:HG3	2.22	0.69
2:A:21:VAL:CG2	2:A:36:VAL:HG11	2.22	0.69
2:A:300:THR:O	2:A:304:MET:HB2	1.93	0.69
2:A:308:ARG:NH1	2:A:308:ARG:HG3	2.07	0.69
2:A:223:PRO:HD3	2:A:249:ILE:CG2	2.21	0.69
2:A:180:GLU:HB2	2:A:241:THR:HG22	1.75	0.69
2:A:264:ARG:NH2	2:A:267:GLN:HE22	1.92	0.68
2:A:64:LEU:HB2	2:A:92:LEU:HD21	1.76	0.68
2:A:187:PRO:HD2	2:A:221:PHE:CE2	2.29	0.67
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.29	0.67
2:A:126:TYR:HB3	2:A:131:LEU:CD2	2.22	0.66
2:A:168:MET:HE2	2:A:325:LEU:H	1.60	0.66
2:A:3:THR:HG22	2:A:5:LYS:N	2.10	0.66
2:A:264:ARG:HH21	2:A:267:GLN:NE2	1.92	0.66
2:A:61:SER:HB2	2:A:91:THR:HG22	1.77	0.66
2:A:168:MET:CE	2:A:325:LEU:H	2.09	0.65
2:A:168:MET:HE2	2:A:325:LEU:N	2.12	0.65
2:A:256:CYS:O	2:A:260:GLU:HG3	1.96	0.65
2:A:266:PRO:HA	2:A:269:VAL:O	1.96	0.65
2:A:29:ALA:O	2:A:32:THR:HB	1.96	0.65
2:A:3:THR:CG2	2:A:5:LYS:H	2.09	0.64
2:A:157:ALA:H	2:A:304:MET:HE1	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:152:ALA:HB1	2:A:155:THR:OG1	1.98	0.64
2:A:309:ILE:HG22	2:A:310:VAL:N	2.11	0.64
2:A:159:ILE:HG12	2:A:320:GLU:HG2	1.80	0.64
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.27	0.63
2:A:62:ILE:HD11	2:A:120:LEU:HB2	1.80	0.63
2:A:325:LEU:HD13	2:A:326:ILE:N	2.13	0.63
2:A:138:ARG:NH2	2:A:154:PHE:HB3	2.13	0.63
2:A:77:ILE:O	2:A:80:ALA:HB3	1.99	0.62
2:A:100:ASN:OD1	2:A:103:LYS:HB2	1.98	0.62
2:A:278:ARG:NH1	2:A:278:ARG:HG3	2.13	0.62
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.34	0.62
2:A:237:PRO:CD	2:A:238:HIS:H	2.12	0.62
2:A:233:ILE:O	2:A:236:GLN:HG2	1.99	0.62
2:A:142:MET:O	2:A:155:THR:HG22	2.00	0.62
2:A:88:LYS:HG3	2:A:302:PHE:CE2	2.33	0.62
2:A:149:GLU:H	2:A:149:GLU:CD	2.04	0.61
2:A:43:LEU:HD23	2:A:43:LEU:N	2.14	0.61
2:A:125:GLU:HG3	2:A:190:ARG:HD2	1.83	0.60
2:A:234:LEU:HD21	2:A:269:VAL:HG11	1.82	0.60
2:A:125:GLU:CG	2:A:190:ARG:HD2	2.31	0.60
2:A:280:ALA:HA	2:A:283:PHE:CD1	2.34	0.60
2:A:163:PHE:O	2:A:199:GLY:HA3	2.00	0.60
2:A:149:GLU:HG2	2:A:150:ALA:H	1.66	0.60
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.19	0.60
2:A:149:GLU:HG2	2:A:150:ALA:N	2.17	0.60
2:A:152:ALA:HA	2:A:154:PHE:HE1	1.63	0.60
2:A:220:ASP:OD1	2:A:222:GLU:HB2	2.02	0.60
1:B:714:DG:H2'	1:B:715:DT:C6	2.37	0.60
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.32	0.59
2:A:64:LEU:CD1	2:A:120:LEU:HB3	2.32	0.59
1:B:708:DG:H2''	1:B:709:DT:OP2	2.02	0.59
2:A:279:ASN:H	2:A:279:ASN:HD22	1.48	0.59
2:A:45:TYR:CE2	2:A:47:PRO:HD3	2.38	0.58
2:A:5:LYS:CG	2:A:9:LYS:HE2	2.33	0.58
2:A:37:TRP:HA	2:A:40:ILE:HG13	1.86	0.58
2:A:5:LYS:O	2:A:9:LYS:HG3	2.02	0.58
2:A:10:ARG:CD	2:A:43:LEU:HD21	2.33	0.58
2:A:166:GLY:HA3	2:A:196:ARG:O	2.03	0.58
2:A:125:GLU:OE2	2:A:190:ARG:HD2	2.03	0.58
2:A:293:PRO:HG2	2:A:321:VAL:HG22	1.86	0.58
2:A:105:ARG:HA	2:A:133:MET:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:120:LEU:HD12	2:A:143:VAL:HG13	1.86	0.58
2:A:153:ASP:OD2	2:A:154:PHE:HD1	1.87	0.57
2:A:138:ARG:CZ	2:A:154:PHE:HB3	2.35	0.57
2:A:286:ALA:CB	2:A:329:ARG:HH11	2.18	0.57
2:A:21:VAL:HG21	2:A:36:VAL:CG1	2.32	0.57
2:A:62:ILE:HD13	2:A:305:LEU:CD2	2.35	0.56
2:A:38:ALA:O	2:A:42:GLU:HG2	2.05	0.56
2:A:147:ARG:HH22	2:A:151:LYS:HD2	1.70	0.56
2:A:159:ILE:HG13	2:A:159:ILE:O	2.06	0.56
2:A:236:GLN:HB3	2:A:237:PRO:HD2	1.87	0.56
1:B:707:DC:H2''	1:B:708:DG:H5'	1.87	0.56
2:A:276:ASN:HA	2:A:289:THR:HG21	1.87	0.56
2:A:40:ILE:HG23	2:A:45:TYR:HB3	1.86	0.56
2:A:286:ALA:HB2	2:A:329:ARG:HH11	1.71	0.55
2:A:71:ALA:HB3	2:A:74:PHE:CD2	2.41	0.55
2:A:221:PHE:HA	2:A:250:MET:HG3	1.88	0.55
2:A:212:PRO:HG2	2:A:215:TRP:CE3	2.42	0.55
2:A:147:ARG:HD3	5:A:905:HOH:O	2.07	0.55
2:A:119:LEU:O	2:A:142:MET:HB2	2.06	0.55
2:A:184:ILE:HG23	2:A:217:VAL:O	2.06	0.55
2:A:265:VAL:HG13	2:A:269:VAL:O	2.07	0.54
2:A:116:VAL:HG23	2:A:140:ILE:CD1	2.37	0.54
2:A:60:LYS:HD2	2:A:90:TYR:CE1	2.42	0.54
2:A:67:THR:HA	5:A:823:HOH:O	2.08	0.54
2:A:20:HIS:HA	2:A:25:THR:HG22	1.89	0.54
2:A:308:ARG:HH11	2:A:308:ARG:CG	2.21	0.54
2:A:64:LEU:HD13	2:A:120:LEU:HB3	1.89	0.54
2:A:10:ARG:HG3	2:A:10:ARG:NH1	2.20	0.54
2:A:274:TYR:HD1	2:A:275:ASP:N	2.05	0.53
2:A:37:TRP:HB3	2:A:41:LYS:HE2	1.90	0.53
2:A:171:ARG:O	2:A:175:GLU:HG3	2.09	0.53
2:A:87:GLN:HG3	2:A:88:LYS:CG	2.38	0.53
2:A:90:TYR:CD1	2:A:90:TYR:N	2.75	0.53
2:A:219:GLY:HA3	2:A:250:MET:SD	2.48	0.53
2:A:290:ILE:HD13	2:A:325:LEU:HA	1.91	0.53
2:A:84:ASN:CA	2:A:87:GLN:HG2	2.39	0.53
2:A:174:ILE:HD13	2:A:207:ALA:HB2	1.90	0.53
2:A:207:ALA:CB	2:A:209:ILE:HD12	2.39	0.52
2:A:293:PRO:HA	3:A:799:PO4:P	2.49	0.52
2:A:117:ASP:O	2:A:141:PRO:HG2	2.09	0.52
2:A:227:TYR:HA	2:A:253:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:276:ASN:HD22	2:A:291:HIS:HB2	1.74	0.52
2:A:102:GLU:HG2	2:A:105:ARG:HH12	1.72	0.52
2:A:291:HIS:O	2:A:323:PRO:HA	2.09	0.52
2:A:148:GLY:HA3	5:A:878:HOH:O	2.09	0.52
2:A:154:PHE:CD1	2:A:154:PHE:N	2.78	0.52
2:A:88:LYS:O	2:A:90:TYR:HD1	1.93	0.52
2:A:187:PRO:HD2	2:A:221:PHE:CD2	2.45	0.51
2:A:337:ARG:O	2:A:337:ARG:HD2	2.10	0.51
2:A:101:LEU:O	2:A:104:GLN:HB2	2.10	0.51
2:A:92:LEU:HD22	2:A:93:ILE:N	2.25	0.51
2:A:339:TYR:CD1	2:A:339:TYR:N	2.79	0.51
2:A:187:PRO:HB2	2:A:190:ARG:HD3	1.93	0.51
2:A:263:LEU:N	2:A:263:LEU:CD1	2.73	0.51
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.93	0.51
2:A:207:ALA:HB3	2:A:209:ILE:HD12	1.93	0.50
2:A:286:ALA:HB2	2:A:329:ARG:NH1	2.26	0.50
2:A:84:ASN:O	2:A:87:GLN:HG2	2.11	0.50
2:A:37:TRP:CE3	2:A:41:LYS:NZ	2.79	0.50
2:A:280:ALA:HA	2:A:283:PHE:CE1	2.46	0.50
2:A:3:THR:CG2	2:A:5:LYS:HB2	2.41	0.50
2:A:60:LYS:HD2	2:A:90:TYR:CZ	2.47	0.50
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.72	0.50
2:A:279:ASN:N	2:A:279:ASN:HD22	2.09	0.50
2:A:188:LEU:HG	2:A:218:GLN:OE1	2.12	0.49
2:A:292:GLN:O	2:A:294:LYS:HE3	2.12	0.49
2:A:200:PHE:CD2	2:A:201:MET:CE	2.96	0.49
2:A:264:ARG:O	2:A:268:ASP:HB2	2.11	0.49
2:A:287:LEU:O	2:A:328:ARG:HB2	2.12	0.49
2:A:11:ALA:HB3	2:A:13:VAL:HG22	1.93	0.49
2:A:264:ARG:HB2	2:A:268:ASP:OD2	2.12	0.49
2:A:3:THR:HB	2:A:6:ASP:OD2	2.12	0.49
2:A:41:LYS:HD3	2:A:41:LYS:N	2.28	0.48
2:A:237:PRO:CG	2:A:238:HIS:H	2.26	0.48
2:A:21:VAL:HG11	2:A:36:VAL:HG21	1.95	0.48
2:A:255:LEU:HD13	2:A:271:LEU:CD2	2.44	0.48
2:A:33:ARG:NH1	2:A:33:ARG:HG2	2.23	0.48
2:A:137:TYR:N	2:A:137:TYR:CD1	2.82	0.48
2:A:171:ARG:NH2	2:A:175:GLU:HG2	2.28	0.48
2:A:184:ILE:HD13	2:A:229:ALA:HB3	1.95	0.48
2:A:248:ASP:O	2:A:251:ALA:HB3	2.14	0.47
2:A:314:GLU:O	2:A:316:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:TYR:H	2:A:90:TYR:HD1	1.61	0.47
2:A:97:ALA:CB	2:A:104:GLN:HG3	2.42	0.47
2:A:123:CYS:O	2:A:124:SER:HB2	2.14	0.47
2:A:11:ALA:O	2:A:12:ASN:HB2	2.15	0.47
1:B:699:DA:H5'	1:B:699:DA:C8	2.50	0.47
2:A:140:ILE:HG13	2:A:141:PRO:HD2	1.97	0.47
2:A:21:VAL:CG2	2:A:22:ILE:N	2.77	0.47
2:A:223:PRO:CD	2:A:249:ILE:HG22	2.27	0.47
2:A:33:ARG:CG	2:A:33:ARG:HH11	2.18	0.47
2:A:127:PRO:O	2:A:131:LEU:HD23	2.15	0.47
2:A:3:THR:HG22	2:A:5:LYS:CB	2.45	0.47
2:A:265:VAL:HG22	2:A:269:VAL:HG23	1.97	0.46
2:A:120:LEU:HD13	2:A:305:LEU:HD22	1.96	0.46
2:A:244:PHE:HA	2:A:272:ILE:HG23	1.97	0.46
2:A:275:ASP:O	2:A:276:ASN:HB3	2.14	0.46
2:A:88:LYS:HD2	2:A:306:LEU:HD22	1.96	0.46
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.46	0.46
2:A:310:VAL:CG2	2:A:311:ASN:N	2.79	0.46
2:A:135:GLU:O	2:A:138:ARG:HG2	2.16	0.46
2:A:60:LYS:HD3	2:A:60:LYS:HA	1.63	0.46
1:B:707:DC:C2'	1:B:708:DG:H5'	2.45	0.46
2:A:118:GLY:HA2	2:A:141:PRO:HD2	1.97	0.46
2:A:237:PRO:HD2	2:A:238:HIS:H	1.80	0.46
2:A:57:ASN:O	2:A:58:HIS:HB3	2.16	0.46
2:A:149:GLU:CG	2:A:150:ALA:N	2.77	0.45
2:A:277:VAL:HG12	2:A:279:ASN:H	1.81	0.45
2:A:11:ALA:HB3	2:A:13:VAL:CG2	2.46	0.45
2:A:155:THR:HG22	2:A:156:ASP:H	1.82	0.45
2:A:20:HIS:CG	2:A:26:ARG:HG2	2.52	0.45
2:A:279:ASN:N	2:A:279:ASN:ND2	2.64	0.45
2:A:286:ALA:CB	2:A:329:ARG:NH1	2.79	0.45
2:A:45:TYR:OH	2:A:47:PRO:HA	2.17	0.45
2:A:62:ILE:HG22	2:A:90:TYR:HD2	1.81	0.45
2:A:116:VAL:HG23	2:A:140:ILE:HD13	1.99	0.45
2:A:88:LYS:HD2	2:A:306:LEU:CD2	2.47	0.45
2:A:200:PHE:HD2	2:A:201:MET:CE	2.30	0.45
2:A:277:VAL:CG1	2:A:278:ARG:N	2.80	0.45
2:A:84:ASN:OD1	2:A:299:GLU:HB2	2.17	0.45
2:A:52:ARG:O	2:A:56:VAL:HG13	2.17	0.45
2:A:10:ARG:CG	2:A:10:ARG:NH1	2.79	0.45
2:A:3:THR:HG22	2:A:5:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:PHE:O	2:A:203:ALA:HB3	2.17	0.44
2:A:237:PRO:CG	2:A:238:HIS:N	2.79	0.44
2:A:236:GLN:HB2	2:A:238:HIS:O	2.17	0.44
2:A:277:VAL:HG13	2:A:278:ARG:N	2.33	0.44
2:A:293:PRO:HA	3:A:799:PO4:O3	2.18	0.44
2:A:310:VAL:C	2:A:312:LYS:H	2.21	0.44
2:A:101:LEU:O	2:A:101:LEU:HD12	2.17	0.44
2:A:211:VAL:HA	2:A:212:PRO:HD3	1.60	0.44
2:A:131:LEU:HD13	2:A:131:LEU:HA	1.88	0.44
2:A:279:ASN:ND2	2:A:279:ASN:H	2.14	0.44
2:A:62:ILE:HD13	2:A:305:LEU:HD21	1.99	0.44
2:A:213:GLU:HA	2:A:216:ILE:HG12	2.00	0.44
2:A:237:PRO:CD	2:A:238:HIS:N	2.79	0.44
2:A:304:MET:HE2	2:A:317:GLN:HB3	2.00	0.44
2:A:62:ILE:HG22	2:A:90:TYR:CD2	2.53	0.44
2:A:144:VAL:CG2	2:A:147:ARG:HG3	2.48	0.44
2:A:181:ILE:HA	2:A:242:ALA:O	2.18	0.44
2:A:284:THR:O	2:A:284:THR:HG22	2.18	0.44
2:A:304:MET:CE	2:A:317:GLN:HB3	2.47	0.44
2:A:199:GLY:O	2:A:202:LYS:HB3	2.18	0.43
1:B:704:DA:H2'	1:B:704:DA:O5'	2.19	0.43
2:A:255:LEU:HD12	2:A:255:LEU:HA	1.75	0.43
2:A:264:ARG:HG3	5:A:812:HOH:O	2.18	0.43
2:A:73:TYR:HB2	5:A:832:HOH:O	2.17	0.43
2:A:120:LEU:HD12	2:A:120:LEU:HA	1.80	0.43
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.18	0.43
2:A:261:MET:HB3	2:A:261:MET:HE3	1.62	0.43
2:A:217:VAL:HG11	2:A:229:ALA:HA	2.00	0.43
2:A:37:TRP:HA	2:A:37:TRP:HE3	1.82	0.43
2:A:26:ARG:O	2:A:28:VAL:HG23	2.19	0.43
2:A:283:PHE:CD2	2:A:287:LEU:HD22	2.54	0.42
2:A:119:LEU:HB3	2:A:142:MET:HB2	2.00	0.42
2:A:254:ALA:HB3	2:A:271:LEU:HD21	2.00	0.42
2:A:33:ARG:CG	2:A:33:ARG:NH1	2.79	0.42
2:A:140:ILE:HG13	2:A:141:PRO:CD	2.49	0.42
2:A:224:GLU:HG3	2:A:228:ARG:HD3	2.02	0.42
2:A:264:ARG:N	2:A:268:ASP:HB2	2.34	0.42
2:A:45:TYR:CD2	2:A:47:PRO:HD3	2.55	0.42
2:A:265:VAL:HA	2:A:269:VAL:O	2.20	0.42
2:A:46:SER:HA	2:A:47:PRO:HD2	1.93	0.42
2:A:71:ALA:HB3	2:A:74:PHE:HD2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:191:ASN:HB3	5:A:897:HOH:O	2.20	0.42
2:A:284:THR:HA	2:A:285:PRO:HA	1.80	0.42
2:A:130:LEU:O	2:A:134:LEU:HG	2.20	0.41
2:A:322:HIS:HA	2:A:323:PRO:HD3	1.82	0.41
1:B:713:DC:H2''	1:B:714:DG:O5'	2.19	0.41
2:A:105:ARG:HG3	2:A:133:MET:SD	2.60	0.41
2:A:201:MET:HG3	5:A:888:HOH:O	2.18	0.41
1:B:699:DA:H2''	1:B:700:DA:OP2	2.18	0.41
2:A:288:THR:HG23	2:A:327:GLU:HA	2.02	0.41
2:A:126:TYR:CE1	2:A:147:ARG:HG2	2.56	0.41
2:A:272:ILE:O	2:A:272:ILE:HG23	2.21	0.41
2:A:216:ILE:HD12	2:A:216:ILE:HG21	1.45	0.41
2:A:276:ASN:ND2	2:A:291:HIS:HD2	2.17	0.41
2:A:237:PRO:HG2	2:A:238:HIS:H	1.85	0.41
2:A:81:VAL:HG12	2:A:82:GLU:N	2.32	0.41
2:A:216:ILE:HG23	2:A:216:ILE:HD13	1.29	0.41
2:A:37:TRP:O	2:A:41:LYS:HD3	2.21	0.41
2:A:87:GLN:CG	2:A:88:LYS:HG2	2.46	0.41
2:A:4:ILE:HG13	2:A:18:VAL:HG11	2.01	0.41
1:B:708:DG:O4'	2:A:54:LEU:HD11	2.21	0.41
2:A:82:GLU:HG3	2:A:83:LYS:N	2.34	0.41
2:A:104:GLN:HE21	2:A:104:GLN:HB2	1.58	0.41
2:A:30:GLU:O	2:A:33:ARG:HB3	2.21	0.40
2:A:145:MET:HE3	2:A:145:MET:HB3	1.57	0.40
2:A:197:LEU:HA	2:A:197:LEU:HD12	1.83	0.40
2:A:274:TYR:CD1	2:A:275:ASP:N	2.89	0.40
2:A:276:ASN:ND2	2:A:291:HIS:CD2	2.89	0.40
2:A:336:PHE:CD1	2:A:336:PHE:N	2.89	0.40
2:A:71:ALA:O	2:A:74:PHE:HB2	2.22	0.40
2:A:105:ARG:N	2:A:133:MET:HE1	2.37	0.40
2:A:255:LEU:O	2:A:258:ALA:HB3	2.20	0.40
2:A:266:PRO:HB3	2:A:330:SER:C	2.41	0.40
2:A:171:ARG:NH2	2:A:175:GLU:CG	2.85	0.40
2:A:221:PHE:CA	2:A:250:MET:HG3	2.49	0.40
2:A:87:GLN:HG3	2:A:88:LYS:H	1.79	0.40
2:A:88:LYS:HB2	2:A:302:PHE:CZ	2.57	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)
5:A:847:HOH:O	5:A:847:HOH:O[4_555]	2.12	0.08

## 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%)	296 (88%)	36 (11%)	5 (2%)	12 20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	246	GLY
2	A	275	ASP
2	A	153	ASP
2	A	148	GLY
2	A	309	ILE

### 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%)	205 (74%)	74 (26%)	0 0

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR

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Mol	Chain	Res	Type
2	A	4	ILE
2	A	5	LYS
2	A	10	ARG
2	A	13	VAL
2	A	14	SER
2	A	17	THR
2	A	21	VAL
2	A	26	ARG
2	A	31	GLU
2	A	33	ARG
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	62	ILE
2	A	68	SER
2	A	82	GLU
2	A	87	GLN
2	A	88	LYS
2	A	91	THR
2	A	92	LEU
2	A	99	ASN
2	A	103	LYS
2	A	105	ARG
2	A	108	LEU
2	A	109	SER
2	A	115	ARG
2	A	119	LEU
2	A	120	LEU
2	A	128	GLU
2	A	129	PRO
2	A	140	ILE
2	A	143	VAL
2	A	144	VAL
2	A	145	MET
2	A	149	GLU
2	A	153	ASP
2	A	155	THR
2	A	158	VAL

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Mol	Chain	Res	Type
2	A	164	GLU
2	A	176	ARG
2	A	190	ARG
2	A	205	GLU
2	A	208	MET
2	A	210	LYS
2	A	213	GLU
2	A	216	ILE
2	A	218	GLN
2	A	230	MET
2	A	231	GLN
2	A	232	GLN
2	A	241	THR
2	A	255	LEU
2	A	263	LEU
2	A	269	VAL
2	A	272	ILE
2	A	274	TYR
2	A	277	VAL
2	A	279	ASN
2	A	281	ARG
2	A	284	THR
2	A	296	SER
2	A	299	GLU
2	A	308	ARG
2	A	310	VAL
2	A	316	PRO
2	A	317	GLN
2	A	318	SER
2	A	321	VAL
2	A	328	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	96	ASN
2	A	104	GLN
2	A	276	ASN
2	A	279	ASN
2	A	291	HIS
2	A	322	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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	1.78	2 (25%)	5,15,15	3.71	2 (40%)
3	PO4	A	799	-	4,4,4	1.95	2 (50%)	6,6,6	1.35	1 (16%)
3	PO4	A	800	-	4,4,4	2.42	3 (75%)	6,6,6	0.64	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	799	-	-	0/0/0/0	0/0/0/0
3	PO4	A	800	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	799	PO4	P-O2	-2.97	1.43	1.54
3	A	799	PO4	P-O3	-2.51	1.45	1.54
3	A	800	PO4	P-O2	-2.47	1.45	1.54
3	A	800	PO4	P-O4	-2.14	1.46	1.54
4	A	599	HPA	C2-N1	2.26	1.38	1.33
3	A	800	PO4	P-O1	3.11	1.57	1.50
4	A	599	HPA	C6-N1	3.78	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	599	HPA	N3-C2-N1	-5.96	123.67	128.86
3	A	799	PO4	O4-P-O3	2.26	116.21	107.90
4	A	599	HPA	C2-N1-C6	5.47	125.04	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	799	PO4	2	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 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.