



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:48 PM UTC

PDB ID : 1BDI / pdb_00001bdi
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

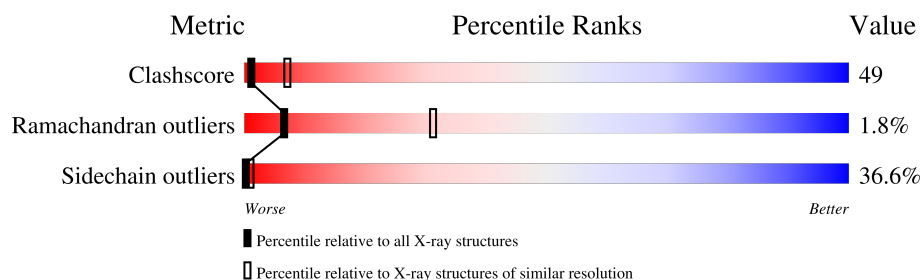
1 Overall quality at a glance

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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	17	35% 65%
2	A	340	26% 46% 23% 5% •

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.

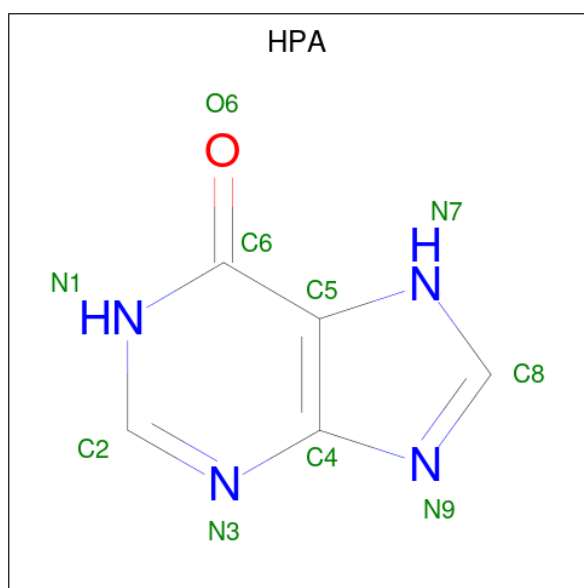
- Molecule 1 is a DNA chain called DNA (5'-D(*TP*AP*CP*GP*CP*AP*AP*AP*CP*GP*TP*TP*TP*GP*CP*GP*T)-3').

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 (CCD ID: HPA) (formula: C₅H₄N₄O).



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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

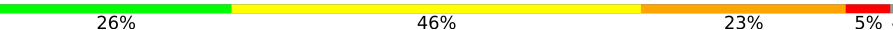
Note EDS was not executed.

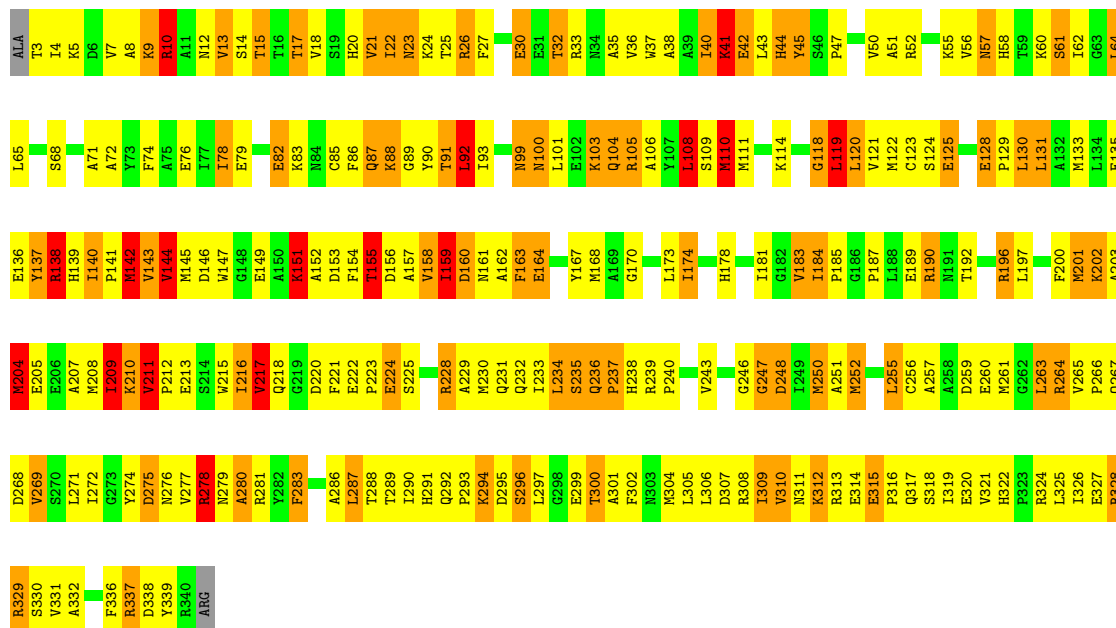
- Molecule 1: DNA (5'-D(*TP*AP*CP*GP*CP*AP*AP*AP*CP*GP*TP*TP*TP*GP*CP*GP*T)-3')

Chain B: 



- Molecule 2: PROTEIN (PURINE REPRESSOR)

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	176.16Å 94.99Å 81.57Å 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 ²)	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	0.38	0/386	0.89	0/594
2	A	1.25	11/2706 (0.4%)	1.57	52/3660 (1.4%)
All	All	1.18	11/3092 (0.4%)	1.49	52/4254 (1.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	184	ILE	CA-CB	-8.31	1.47	1.54
2	A	13	VAL	CA-CB	-6.78	1.44	1.54
2	A	243	VAL	CA-CB	-6.59	1.46	1.54
2	A	158	VAL	CA-CB	-6.41	1.46	1.54
2	A	290	ILE	CA-CB	-6.40	1.46	1.54
2	A	137	TYR	CA-C	-5.64	1.46	1.52
2	A	247	GLY	CA-C	5.46	1.56	1.51
2	A	204	MET	SD-CE	-5.45	1.66	1.79
2	A	32	THR	CA-CB	-5.39	1.45	1.53
2	A	118	GLY	CA-C	5.08	1.57	1.51
2	A	309	ILE	CA-CB	-5.08	1.47	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	267	GLN	N-CA-C	9.90	122.99	111.11
2	A	160	ASP	N-CA-C	8.40	123.53	113.28
2	A	322	HIS	N-CA-C	8.34	122.74	109.40
2	A	248	ASP	N-CA-C	8.16	121.21	111.33
2	A	136	GLU	N-CA-C	-8.13	101.47	112.94
2	A	209	ILE	N-CA-C	-8.12	96.53	108.87
2	A	236	GLN	C-N-CD	-8.08	91.89	125.00
2	A	15	THR	N-CA-C	-8.02	102.52	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	283	PHE	N-CA-C	-7.92	100.31	110.53
2	A	269	VAL	CB-CA-C	-7.77	98.01	110.28
2	A	146	ASP	N-CA-C	7.35	121.56	111.71
2	A	123	CYS	N-CA-C	7.35	122.27	113.16
2	A	51	ALA	N-CA-C	-7.33	102.98	110.97
2	A	121	VAL	N-CA-C	6.87	117.78	107.75
2	A	280	ALA	N-CA-C	-6.86	104.88	113.18
2	A	183	VAL	N-CA-C	6.71	117.21	108.35
2	A	90	TYR	N-CA-C	6.62	119.35	110.35
2	A	92	LEU	N-CA-C	6.62	120.02	109.24
2	A	10	ARG	N-CA-C	-6.61	104.11	111.71
2	A	196	ARG	N-CA-C	-6.46	104.16	111.14
2	A	57	ASN	N-CA-C	6.38	119.89	111.28
2	A	250	MET	N-CA-C	-6.38	104.33	111.28
2	A	236	GLN	CA-C-N	6.21	127.60	119.84
2	A	236	GLN	C-N-CA	6.21	127.60	119.84
2	A	9	LYS	N-CA-C	6.17	119.27	111.69
2	A	119	LEU	N-CA-C	6.09	118.87	108.02
2	A	211	VAL	CB-CA-C	6.08	116.59	110.94
2	A	158	VAL	N-CA-C	-6.01	99.76	108.17
2	A	184	ILE	N-CA-C	-5.98	102.23	108.15
2	A	138	ARG	N-CA-C	-5.93	105.14	112.38
2	A	78	ILE	N-CA-C	5.88	116.00	110.30
2	A	159	ILE	N-CA-C	5.86	116.56	108.12
2	A	151	LYS	N-CA-C	5.84	118.11	111.11
2	A	149	GLU	N-CA-C	-5.75	100.67	109.41
2	A	287	LEU	N-CA-C	5.68	118.48	109.96
2	A	144	VAL	N-CA-CB	5.64	117.81	111.21
2	A	142	MET	N-CA-C	5.61	117.63	108.76
2	A	45	TYR	N-CA-C	5.57	118.71	109.46
2	A	236	GLN	CB-CA-C	5.54	117.78	109.63
2	A	108	LEU	N-CA-C	-5.51	105.17	111.07
2	A	110	MET	N-CA-C	-5.42	104.61	111.11
2	A	41	LYS	N-CA-C	5.40	117.98	111.40
2	A	155	THR	CB-CA-C	-5.39	98.86	110.45
2	A	137	TYR	N-CA-C	-5.39	104.97	112.30
2	A	178	HIS	N-CA-C	5.26	118.52	110.20
2	A	9	LYS	CB-CA-C	5.26	120.33	110.70
2	A	217	VAL	N-CA-C	5.19	115.59	108.12
2	A	243	VAL	N-CA-C	5.18	115.58	108.12
2	A	290	ILE	CB-CA-C	-5.13	103.87	110.84
2	A	86	PHE	N-CA-C	5.11	117.25	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	111	MET	N-CA-C	5.01	116.43	111.07
2	A	163	PHE	N-CA-C	-5.00	104.83	112.04

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	273	0
3	A	10	0	4	1	0
4	A	2	0	0	0	0
All	All	3009	0	2834	287	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 49.

All (287) 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:181:ILE:HD12	2:A:204:MET:HE1	1.20	1.12
2:A:230:MET:HG3	2:A:234:LEU:HD11	1.33	1.09
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
2:A:20:HIS:HD1	2:A:25:THR:HG23	1.28	0.97
2:A:156:ASP:HB3	2:A:304:MET:HE2	1.46	0.96
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:105:ARG:HA	2:A:133:MET:HE1	1.69	0.74
2:A:197:LEU:HD11	2:A:201:MET:HE1	1.68	0.73
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
2:A:286:ALA:HB1	2:A:328:ARG:HG2	1.71	0.72
2:A:181:ILE:CD1	2:A:204:MET:HE1	2.12	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:230:MET:CG	2:A:234:LEU:HD11	2.17	0.70
2:A:210:LYS:HD3	2:A:210:LYS:H	1.56	0.70
1:B:703:DC:H1'	1:B:704:DA:H5'	1.73	0.69
2:A:252:MET:HE3	2:A:283:PHE:CZ	2.27	0.69
1:B:700:DA:H2''	1:B:701:DC:O5'	1.90	0.69
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.74	0.69
2:A:105:ARG:CA	2:A:133:MET:HE1	2.22	0.69
2:A:137:TYR:HA	2:A:139:HIS:CD2	2.28	0.69
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:184:ILE:HG12	2:A:229:ALA:HB1	1.77	0.67
2:A:204:MET:HG3	2:A:209:ILE:CG2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:304:MET:HE3	2:A:317:GLN:HB3	1.78	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:130:LEU:HD22	2:A:130:LEU:O	1.97	0.65
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.25	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:184:ILE:HA	2:A:217:VAL:O	1.96	0.64
2:A:280:ALA:HA	2:A:283:PHE:CD1	2.33	0.64
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.28	0.64
2:A:200:PHE:HD2	2:A:201:MET:CE	2.10	0.64
2:A:156:ASP:CB	2:A:304:MET:HE2	2.24	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: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
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:325:LEU:HD11	2:A:327:GLU:HG3	1.82	0.60
2:A:145:MET:HE3	2:A:301:ALA:HB2	1.83	0.60
2:A:152:ALA:HB1	2:A:154:PHE:CE1	2.36	0.60
2:A:155:THR:HG22	2:A:156:ASP:N	2.17	0.60
2:A:167:TYR:HD2	2:A:202:LYS:HG2	1.66	0.60
1:B:702:DG:H5'	1:B:702:DG:C8	2.36	0.59
2:A:71:ALA:HB3	2:A:74:PHE:HD2	1.66	0.59
2:A:237:PRO:CG	2:A:238:HIS:H	2.14	0.59
2:A:329:ARG:HG3	2:A:329:ARG:HH11	1.68	0.59
2:A:105:ARG:HA	2:A:133:MET:CE	2.31	0.59
2:A:201:MET:N	2:A:201:MET:HE2	2.17	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:281:ARG:HD3	2:A:281:ARG:C	2.28	0.58
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:201:MET:HE2	2:A:201:MET:CA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:ALA:HB1	2:A:13:VAL:O	2.05	0.57
2:A:64:LEU:HD12	2:A:65:LEU:N	2.19	0.57
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.33	0.57
2:A:197:LEU:HD11	2:A:201:MET:CE	2.34	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:CG	2.35	0.57
2:A:118:GLY:C	2:A:140:ILE:HD11	2.30	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:145:MET:HE3	2:A:301:ALA:CB	2.36	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: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:236:GLN:HB2	2:A:237:PRO:HD3	1.88	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
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.38	0.54
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.72	0.54
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.72	0.54
2:A:142:MET:HG2	2:A:155:THR:HG23	1.90	0.54
2:A:144:VAL:HG21	2:A:147:TRP:CE2	2.43	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:64:LEU:HD12	2:A:64:LEU:C	2.33	0.53
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.39	0.53
2:A:200:PHE:HD2	2:A:201:MET:HE1	1.74	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:106:ALA:O	2:A:110:MET:HG3	2.10	0.52
2:A:278:ARG:HG3	2:A:278:ARG:NH1	2.24	0.51
2:A:8:ALA:HB2	2:A:15:THR:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:212:PRO:HG2	2:A:215:TRP:CB	2.36	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:210:LYS:O	2:A:210:LYS:HG2	2.11	0.51
2:A:237:PRO:HG2	2:A:238:HIS:H	1.74	0.51
2:A:135:GLU:HG2	2:A:138:ARG:HD2	1.93	0.50
2:A:105:ARG:N	2:A:133:MET:HE1	2.26	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:325:LEU:CD1	2:A:327:GLU:HG3	2.41	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:200:PHE:CD2	2:A:201:MET:HE2	2.47	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:310:VAL:CG2	2:A:311:ASN:N	2.75	0.49
2:A:265:VAL:HG13	2:A:266:PRO:HA	1.94	0.49
2:A:336:PHE:N	2:A:336:PHE:CD1	2.80	0.49
2:A:128:GLU:N	2:A:129:PRO:CD	2.75	0.49
2:A:197:LEU:O	2:A:200:PHE:HB3	2.12	0.49
2:A:297:LEU:HD23	2:A:297:LEU:C	2.37	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:325:LEU:C	2:A:325:LEU:HD13	2.38	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:100:ASN:HB3	2:A:103:LYS:CB	2.43	0.48
2:A:286:ALA:HB3	2:A:329:ARG:HG2	1.94	0.48
2:A:294:LYS:H	2:A:294:LYS:HG2	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
2:A:224:GLU:HG3	2:A:224:GLU:O	2.12	0.47
1:B:714:DG:C5'	1:B:714:DG:H8	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:ILE:CG2	2:A:41:LYS:HD3	2.45	0.47
2:A:101:LEU:O	2:A:104:GLN:HG2	2.14	0.47
2:A:304:MET:CE	2:A:317:GLN:HB3	2.43	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:3:THR:HG23	2:A:45:TYR:CD1	2.51	0.46
2:A:30:GLU:HG2	2:A:33:ARG:HH12	1.77	0.46
2:A:110:MET:HE2	2:A:110:MET:HB3	1.58	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:197:LEU:CD1	2:A:201:MET:HE1	2.43	0.46
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.46	0.46
2:A:108:LEU:HD23	2:A:133:MET:HE3	1.98	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:57:ASN:O	2:A:58:HIS:HB3	2.16	0.46
2:A:140:ILE:O	2:A:140:ILE:HG13	2.10	0.45
2:A:158:VAL:HG13	2:A:158:VAL:O	2.16	0.45
2:A:216:ILE:O	2:A:216:ILE:HG12	2.16	0.45
2:A:32:THR:O	2:A:35:ALA:HB3	2.16	0.45
2:A:252:MET:CB	2:A:283:PHE:CE2	2.99	0.45
2:A:144:VAL:HG12	2:A:155:THR:HG21	1.99	0.45
2:A:167:TYR:CE2	2:A:202:LYS:HG2	2.51	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: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:HH11	2:A:10:ARG:CG	2.16	0.44
2:A:201:MET:HE3	2:A:201:MET:HB2	1.57	0.44
2:A:152:ALA:HB1	2:A:154:PHE:CD1	2.52	0.44
2:A:310:VAL:C	2:A:312:LYS:H	2.25	0.44
2:A:204:MET:HE3	2:A:209:ILE:HG21	2.00	0.44
2:A:263:LEU:N	2:A:263:LEU:CD1	2.79	0.44
2:A:27:PHE:CD1	2:A:27:PHE:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:GLU:O	2:A:168:MET:HG3	2.17	0.44
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.82	0.44
2:A:292:GLN:O	2:A:294:LYS:HG2	2.18	0.44
2:A:215:TRP:CZ2	2:A:239:ARG:C	2.96	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: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
1:B:706:DA:H2''	1:B:707:DC:C6	2.54	0.43
2:A:37:TRP:CE3	2:A:37:TRP:HA	2.53	0.43
2:A:145:MET:H	2:A:145:MET:HG2	1.64	0.43
2:A:163:PHE:CD1	2:A:163:PHE:C	2.97	0.43
2:A:276:ASN:HB2	2:A:291:HIS:HA	1.99	0.43
2:A:215:TRP:CZ2	2:A:239:ARG:HA	2.54	0.43
2:A:161:ASN:C	2:A:163:PHE:H	2.25	0.43
2:A:286:ALA:HB3	2:A:329:ARG:CG	2.49	0.43
2:A:23:ASN:ND2	2:A:23:ASN:N	2.66	0.42
2:A:220:ASP:OD1	2:A:225:SER:HB3	2.19	0.42
2:A:263:LEU:HA	2:A:263:LEU:HD12	1.67	0.42
2:A:266:PRO:HB3	2:A:330:SER:O	2.18	0.42
2:A:20:HIS:HA	2:A:25:THR:HG22	2.01	0.42
2:A:237:PRO:CG	2:A:238:HIS:N	2.79	0.42
2:A:331:VAL:HG12	2:A:332:ALA:N	2.34	0.42
2:A:87:GLN:HE21	2:A:87:GLN:HB2	1.61	0.42
2:A:315:GLU:HA	2:A:316:PRO:HD2	1.71	0.42
2:A:45:TYR:CE2	2:A:47:PRO:HG3	2.55	0.42
2:A:135:GLU:HG2	2:A:135:GLU:O	2.18	0.42
2:A:23:ASN:N	2:A:23:ASN:HD22	2.17	0.42
2:A:215:TRP:CZ2	2:A:240:PRO:N	2.88	0.42
2:A:207:ALA:O	2:A:208:MET:HB2	2.20	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:276:ASN:ND2	2:A:291:HIS:CD2	2.77	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:32:THR:O	2:A:36:VAL:HG23	2.21	0.41
2:A:61:SER:HA	2:A:91:THR:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:197:LEU:HA	2:A:197:LEU:HD12	1.72	0.41
2:A:52:ARG:O	2:A:56:VAL:HG22	2.21	0.41
2:A:170:GLY:O	2:A:173:LEU:HB2	2.20	0.41
2:A:211:VAL:CG2	2:A:216:ILE:HG22	2.50	0.41
2:A:261:MET:HE3	2:A:261:MET:HB3	1.68	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: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:101:LEU:C	2:A:104:GLN:HG2	2.45	0.41
2:A:131:LEU:HD13	2:A:131:LEU:HA	1.59	0.41
2:A:236:GLN:CG	2:A:237:PRO:HD2	2.43	0.41
2:A:239:ARG:HB2	2:A:240:PRO:CD	2.51	0.41
2:A:274:TYR:C	2:A:274:TYR:CD1	2.99	0.41
2:A:286:ALA:CB	2:A:328:ARG:HG2	2.46	0.41
2:A:64:LEU:HD23	2:A:78:ILE:HG12	2.02	0.41
2:A:133:MET:HE3	2:A:133:MET:HB3	1.84	0.40
2:A:204:MET:HG3	2:A:209:ILE:HG21	2.00	0.40
2:A:21:VAL:HG11	2:A:36:VAL:HG21	2.03	0.40
2:A:196:ARG:NH2	3:A:599:HPA:H8	2.36	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
2:A:119:LEU:O	2:A:142:MET:HB2	2.21	0.40
2:A:159:ILE:C	2:A:159:ILE:HD12	2.46	0.40
2:A:174:ILE:HD11	2:A:209:ILE:HD13	2.03	0.40
2:A:42:GLU:C	2:A:44:HIS:N	2.79	0.40
2:A:137:TYR:C	2:A:139:HIS:N	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	6	31

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 ⓘ

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%)	177 (63%)	102 (37%)	0	1

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	ILE
2	A	5	LYS
2	A	7	VAL
2	A	9	LYS
2	A	10	ARG
2	A	12	ASN
2	A	17	THR
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	40	ILE
2	A	41	LYS

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Mol	Chain	Res	Type
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	88	LYS
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	108	LEU
2	A	109	SER
2	A	110	MET
2	A	114	LYS
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	144	VAL
2	A	151	LYS
2	A	155	THR
2	A	159	ILE
2	A	164	GLU
2	A	174	ILE

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Mol	Chain	Res	Type
2	A	183	VAL
2	A	190	ARG
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	217	VAL
2	A	218	GLN
2	A	224	GLU
2	A	228	ARG
2	A	232	GLN
2	A	233	ILE
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	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	272	ILE
2	A	277	VAL
2	A	278	ARG
2	A	279	ASN
2	A	288	THR
2	A	294	LYS
2	A	295	ASP
2	A	296	SER
2	A	299	GLU
2	A	300	THR
2	A	310	VAL
2	A	312	LYS
2	A	315	GLU
2	A	319	ILE
2	A	324	ARG
2	A	328	ARG

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Mol	Chain	Res	Type
2	A	329	ARG
2	A	337	ARG
2	A	339	TYR

Sometimes 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	99	ASN
2	A	100	ASN
2	A	139	HIS
2	A	218	GLN
2	A	231	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 oligosaccharides 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	-	10,11,11	1.23	2 (20%)	11,15,15	1.50	1 (9%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	HPA	C8-N7	-2.53	1.30	1.35
3	A	599	HPA	C8-N9	2.04	1.37	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	HPA	C6-C5-C4	-3.81	119.01	121.61

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 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.