



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:05 PM UTC

PDB ID : 1QP0 / pdb_00001qp0
Title : PURINE REPRESSOR-HYPOXANTHINE-PALINDROMIC OPERATOR
COMPLEX
Authors : Glasfeld, A.; Koehler, A.N.; Schumacher, M.A.; Brennan, R.G.
Deposited on : 1999-06-01
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

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

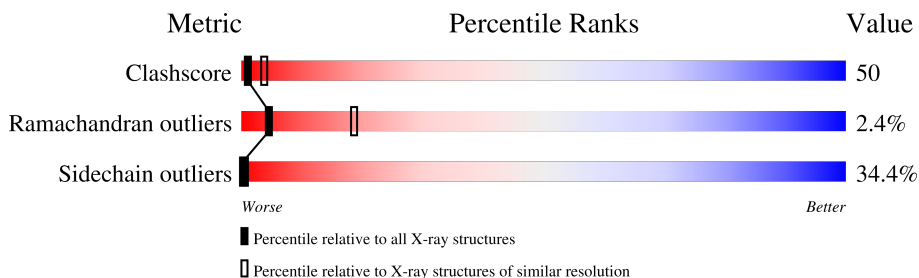
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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	M	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	HPA	A	599	-	-	X	-

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.

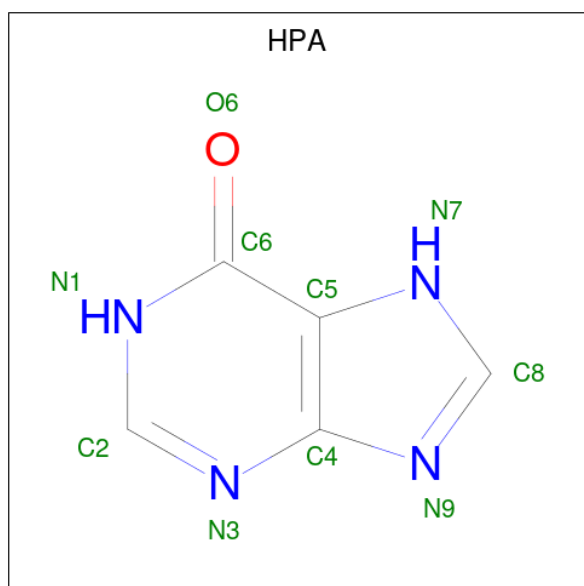
- Molecule 1 is a DNA chain called DNA (5'-D(*TP*AP*CP*GP*CP*AP*AP*CP*CP*GP*GP*TP*TP*GP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			

- Molecule 2 is a protein called PROTEIN (PURINE NUCLEOTIDE SYNTHESIS 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.

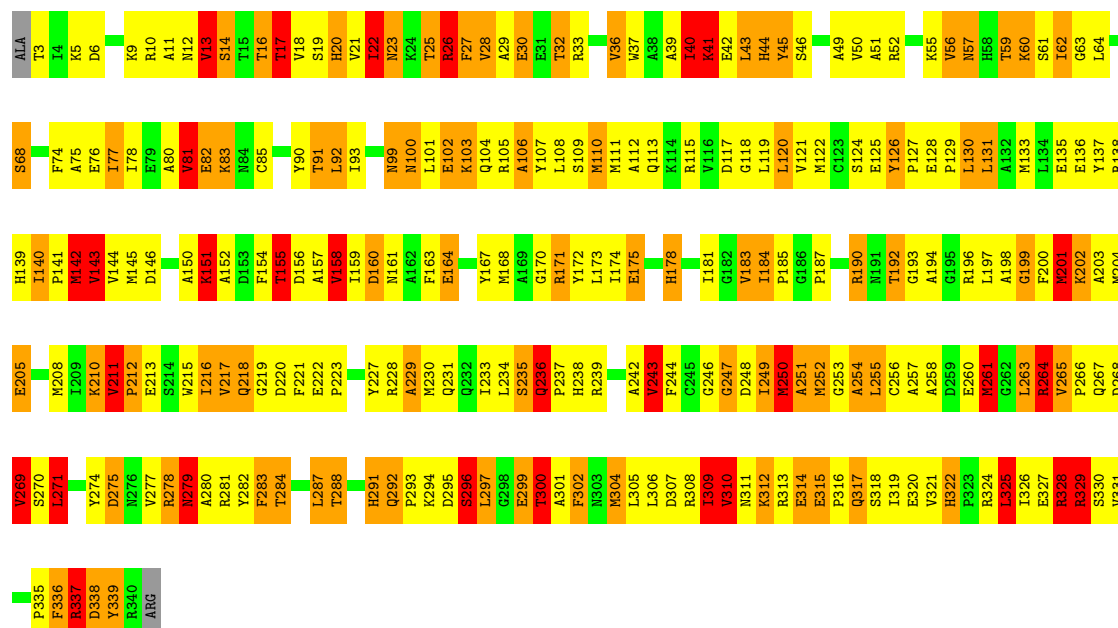
- Molecule 1: DNA (5'-D(*TP*AP*CP*GP*CP*AP*AP*CP*CP*GP*GP*TP*TP*GP*CP*GP*T)-3')

Chain M: 



- Molecule 2: PROTEIN (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, α , β , γ	176.47Å 95.02Å 81.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	8.91	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3009	wwPDB-VP
Average B, all atoms (Å ²)	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	M	0.48	0/386	0.95	0/594
2	A	1.56	34/2706 (1.3%)	1.75	69/3660 (1.9%)
All	All	1.47	34/3092 (1.1%)	1.66	69/4254 (1.6%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	211	VAL	CA-C	-9.53	1.44	1.53
2	A	328	ARG	CA-C	8.54	1.64	1.52
2	A	291	HIS	CA-CB	-8.32	1.41	1.53
2	A	174	ILE	CA-CB	-7.74	1.46	1.54
2	A	36	VAL	CA-CB	-7.40	1.45	1.54
2	A	81	VAL	CA-CB	-7.22	1.44	1.54
2	A	93	ILE	CA-CB	-7.02	1.44	1.53
2	A	78	ILE	CA-CB	-6.91	1.46	1.54
2	A	212	PRO	C-O	6.40	1.31	1.23
2	A	287	LEU	C-O	-6.24	1.16	1.23
2	A	198	ALA	CA-CB	-6.06	1.43	1.53
2	A	150	ALA	CA-CB	-5.87	1.45	1.53
2	A	17	THR	CA-CB	-5.86	1.44	1.53
2	A	28	VAL	CA-CB	-5.84	1.46	1.54
2	A	142	MET	SD-CE	-5.75	1.65	1.79
2	A	201	MET	SD-CE	-5.53	1.65	1.79
2	A	184	ILE	CA-CB	-5.51	1.47	1.54
2	A	229	ALA	CA-CB	-5.47	1.44	1.53
2	A	139	HIS	CA-CB	-5.47	1.44	1.53
2	A	13	VAL	CA-CB	-5.46	1.47	1.54
2	A	56	VAL	CA-CB	-5.39	1.45	1.54
2	A	247	GLY	CA-C	5.37	1.56	1.51
2	A	75	ALA	CA-CB	-5.33	1.44	1.53
2	A	113	GLN	N-CA	-5.28	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	243	VAL	CA-CB	-5.27	1.47	1.54
2	A	251	ALA	CA-C	-5.25	1.46	1.52
2	A	59	THR	CA-CB	-5.21	1.44	1.53
2	A	319	ILE	CA-CB	-5.19	1.48	1.54
2	A	46	SER	C-O	-5.15	1.20	1.25
2	A	329	ARG	CA-C	-5.11	1.45	1.53
2	A	211	VAL	N-CA	-5.06	1.41	1.46
2	A	300	THR	CA-C	5.05	1.59	1.52
2	A	282	TYR	N-CA	-5.03	1.40	1.46
2	A	74	PHE	CA-C	-5.01	1.46	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	211	VAL	CB-CA-C	13.14	125.96	110.85
2	A	146	ASP	N-CA-C	10.40	124.20	110.88
2	A	322	HIS	N-CA-C	9.88	125.21	109.40
2	A	261	MET	N-CA-C	-9.24	102.12	112.57
2	A	250	MET	N-CA-C	-9.02	101.36	111.82
2	A	267	GLN	N-CA-C	8.98	121.89	111.11
2	A	142	MET	N-CA-C	8.93	123.06	109.23
2	A	57	ASN	N-CA-C	8.06	122.72	111.92
2	A	283	PHE	N-CA-C	-7.97	100.61	110.41
2	A	248	ASP	N-CA-C	7.84	120.82	111.33
2	A	16	THR	N-CA-C	-7.58	103.02	111.28
2	A	41	LYS	N-CA-C	7.49	119.35	111.03
2	A	160	ASP	N-CA-C	7.49	122.52	113.23
2	A	243	VAL	N-CA-C	7.41	118.79	108.12
2	A	236	GLN	N-CA-C	7.37	120.82	110.20
2	A	45	TYR	N-CA-C	7.24	121.05	109.24
2	A	158	VAL	N-CA-C	-7.21	98.02	108.11
2	A	155	THR	CB-CA-C	-7.16	94.71	110.67
2	A	51	ALA	N-CA-C	-7.10	103.23	110.97
2	A	264	ARG	CA-C-N	-6.83	117.39	123.33
2	A	264	ARG	C-N-CA	-6.83	117.39	123.33
2	A	269	VAL	CB-CA-C	-6.82	98.68	111.30
2	A	296	SER	N-CA-C	-6.73	104.33	112.54
2	A	297	LEU	N-CA-C	-6.63	103.98	111.14
2	A	271	LEU	CA-C-N	-6.63	114.45	123.14
2	A	271	LEU	C-N-CA	-6.63	114.45	123.14
2	A	287	LEU	N-CA-C	6.49	119.89	110.28
2	A	174	ILE	N-CA-C	6.45	116.94	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	304	MET	N-CA-C	-6.36	104.28	111.14
2	A	181	ILE	N-CA-C	6.35	117.62	108.48
2	A	310	VAL	N-CA-C	6.29	122.43	109.34
2	A	199	GLY	N-CA-C	-6.23	105.25	112.73
2	A	44	HIS	N-CA-C	-6.13	103.73	110.91
2	A	27	PHE	N-CA-C	6.11	118.19	110.24
2	A	178	HIS	N-CA-C	6.09	119.53	110.52
2	A	279	ASN	CB-CA-C	-6.08	100.44	110.72
2	A	121	VAL	N-CA-C	6.06	116.66	108.17
2	A	143	VAL	N-CA-CB	6.04	119.74	111.41
2	A	258	ALA	N-CA-C	-6.00	104.65	111.07
2	A	288	THR	N-CA-C	-5.95	99.54	109.24
2	A	106	ALA	N-CA-C	5.93	118.25	111.02
2	A	36	VAL	CB-CA-C	-5.81	104.54	111.97
2	A	325	LEU	N-CA-C	5.70	118.83	109.76
2	A	338	ASP	N-CA-C	5.67	119.45	112.54
2	A	337	ARG	N-CA-C	5.64	117.90	111.02
2	A	302	PHE	CB-CA-C	-5.63	101.96	110.92
2	A	211	VAL	N-CA-CB	5.62	118.48	111.39
2	A	212	PRO	N-CA-C	-5.62	102.37	111.14
2	A	151	LYS	N-CA-C	5.58	120.08	113.16
2	A	22	ILE	CA-C-N	-5.54	113.79	122.49
2	A	22	ILE	C-N-CA	-5.54	113.79	122.49
2	A	254	ALA	N-CA-C	-5.53	105.66	112.90
2	A	40	ILE	CB-CA-C	-5.50	103.63	112.16
2	A	329	ARG	CB-CA-C	-5.48	101.07	111.97
2	A	330	SER	N-CA-C	-5.47	104.88	113.02
2	A	183	VAL	N-CA-C	5.42	115.69	108.27
2	A	68	SER	N-CA-C	-5.40	100.87	109.07
2	A	328	ARG	O-C-N	-5.38	118.11	122.03
2	A	17	THR	CB-CA-C	5.33	119.17	110.96
2	A	25	THR	N-CA-C	5.32	119.87	113.17
2	A	92	LEU	N-CA-C	5.24	118.02	109.59
2	A	265	VAL	CA-C-O	5.22	122.75	119.51
2	A	26	ARG	CB-CA-C	5.21	118.38	109.99
2	A	299	GLU	CA-C-N	-5.19	112.81	120.28
2	A	299	GLU	C-N-CA	-5.19	112.81	120.28
2	A	126	TYR	N-CA-C	5.16	118.02	108.94
2	A	32	THR	CB-CA-C	5.07	118.77	110.96
2	A	49	ALA	CA-C-N	-5.07	112.44	120.55
2	A	49	ALA	C-N-CA	-5.07	112.44	120.55

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	M	345	0	193	10	0
2	A	2652	0	2636	284	0
3	A	10	0	4	6	0
4	A	2	0	0	0	0
All	All	3009	0	2833	293	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 50.

All (293) 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:M:713:DC:H2''	1:M:714:DG:H5''	1.26	1.10
2:A:337:ARG:HG2	2:A:337:ARG:HH11	1.23	1.00
2:A:265:VAL:HG22	2:A:269:VAL:HG23	1.48	0.95
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.84	0.92
2:A:61:SER:HB2	2:A:91:THR:HG22	1.50	0.91
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.50	0.91
2:A:140:ILE:HD12	2:A:141:PRO:CD	1.99	0.91
2:A:30:GLU:HG2	2:A:33:ARG:HH12	1.34	0.90
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.03	0.89
1:M:712:DG:H2''	1:M:713:DC:H5''	1.56	0.88
2:A:105:ARG:HA	2:A:133:MET:HE1	1.54	0.88
2:A:108:LEU:HD12	2:A:133:MET:HE2	1.56	0.87
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.88	0.87
2:A:236:GLN:HB3	2:A:237:PRO:HD2	1.57	0.87
1:M:713:DC:C2'	1:M:714:DG:H5''	2.04	0.86
1:M:713:DC:H2''	1:M:714:DG:C5'	2.05	0.86
2:A:100:ASN:ND2	2:A:103:LYS:H	1.74	0.86
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.58	0.84
2:A:82:GLU:HG3	2:A:83:LYS:N	1.93	0.83
2:A:105:ARG:HA	2:A:133:MET:CE	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:237:PRO:HG2	2:A:238:HIS:H	1.43	0.82
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.15	0.82
2:A:140:ILE:HD12	2:A:141:PRO:N	1.95	0.80
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.63	0.80
2:A:164:GLU:O	2:A:168:MET:HG3	1.83	0.79
2:A:183:VAL:HG13	2:A:216:ILE:HB	1.63	0.79
2:A:52:ARG:O	2:A:56:VAL:HG22	1.82	0.79
1:M:714:DG:H2''	1:M:715:DT:H5'	1.63	0.78
2:A:107:TYR:O	2:A:111:MET:HG3	1.82	0.78
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.13	0.78
2:A:325:LEU:HD12	2:A:326:ILE:N	1.98	0.78
2:A:39:ALA:O	2:A:43:LEU:HB2	1.84	0.77
2:A:20:HIS:CE1	2:A:26:ARG:HG2	2.19	0.77
2:A:200:PHE:HD2	2:A:201:MET:CE	1.97	0.77
2:A:192:THR:O	2:A:196:ARG:HD2	1.84	0.77
2:A:20:HIS:ND1	2:A:26:ARG:HG2	2.01	0.76
2:A:184:ILE:HD13	2:A:229:ALA:HB3	1.67	0.76
2:A:337:ARG:HG2	2:A:337:ARG:NH1	1.91	0.75
1:M:700:DA:H2''	1:M:701:DC:O5'	1.85	0.75
1:M:714:DG:H2''	1:M:715:DT:C5'	2.17	0.75
2:A:108:LEU:HD12	2:A:133:MET:CE	2.16	0.75
2:A:270:SER:HB3	2:A:331:VAL:HA	1.69	0.74
2:A:155:THR:HG22	2:A:156:ASP:H	1.51	0.74
2:A:101:LEU:HA	2:A:104:GLN:HG2	1.69	0.74
2:A:30:GLU:CG	2:A:33:ARG:HH12	1.99	0.74
2:A:32:THR:O	2:A:36:VAL:HG23	1.88	0.74
2:A:13:VAL:HG23	2:A:14:SER:O	1.88	0.73
2:A:192:THR:CB	3:A:599:HPA:HN7	2.02	0.73
2:A:216:ILE:HD13	2:A:216:ILE:O	1.89	0.72
2:A:192:THR:HG21	3:A:599:HPA:HN7	1.54	0.72
2:A:212:PRO:HG2	2:A:215:TRP:HB2	1.71	0.72
2:A:3:THR:HG23	2:A:45:TYR:CE1	2.25	0.72
2:A:192:THR:HG21	3:A:599:HPA:N7	2.04	0.72
2:A:101:LEU:HA	2:A:104:GLN:CG	2.19	0.71
2:A:125:GLU:HG2	2:A:190:ARG:HD2	1.73	0.71
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.72	0.71
2:A:3:THR:HA	2:A:6:ASP:OD2	1.90	0.71
2:A:201:MET:CA	2:A:201:MET:HE2	2.21	0.70
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.18	0.70
2:A:184:ILE:HA	2:A:217:VAL:O	1.91	0.70
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:HIS:HA	2:A:25:THR:HG22	1.73	0.70
2:A:309:ILE:HG22	2:A:310:VAL:N	2.05	0.70
2:A:61:SER:CB	2:A:91:THR:HG22	2.20	0.69
2:A:159:ILE:HG13	2:A:159:ILE:O	1.94	0.68
2:A:20:HIS:HA	2:A:25:THR:CG2	2.24	0.68
2:A:210:LYS:H	2:A:210:LYS:HD3	1.58	0.68
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.24	0.67
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.22	0.67
2:A:292:GLN:HG3	2:A:293:PRO:HD2	1.75	0.67
2:A:247:GLY:HA2	2:A:274:TYR:O	1.94	0.67
2:A:41:LYS:N	2:A:41:LYS:HD2	2.09	0.67
2:A:160:ASP:O	2:A:161:ASN:HB2	1.94	0.67
2:A:257:ALA:O	2:A:261:MET:HG2	1.95	0.66
2:A:192:THR:CG2	3:A:599:HPA:HN7	2.07	0.66
2:A:100:ASN:HD22	2:A:103:LYS:H	1.44	0.66
2:A:155:THR:HG22	2:A:156:ASP:N	2.10	0.66
2:A:184:ILE:HD13	2:A:229:ALA:CB	2.24	0.66
2:A:30:GLU:HG2	2:A:33:ARG:NH1	2.10	0.65
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.59	0.64
2:A:62:ILE:HD12	2:A:63:GLY:N	2.13	0.64
2:A:101:LEU:O	2:A:104:GLN:HG2	1.98	0.64
2:A:304:MET:CE	2:A:317:GLN:HB3	2.28	0.64
2:A:293:PRO:HG2	2:A:321:VAL:HG22	1.80	0.63
2:A:106:ALA:O	2:A:110:MET:HG2	1.97	0.63
2:A:218:GLN:CA	2:A:218:GLN:HE21	2.11	0.63
1:M:702:DG:OP2	2:A:14:SER:HB3	1.99	0.62
2:A:264:ARG:H	2:A:268:ASP:HB2	1.63	0.62
2:A:284:THR:O	2:A:284:THR:HG22	1.97	0.62
2:A:200:PHE:HD2	2:A:201:MET:HE1	1.64	0.62
2:A:100:ASN:HD22	2:A:100:ASN:C	2.06	0.62
2:A:237:PRO:CG	2:A:238:HIS:H	2.12	0.62
2:A:100:ASN:HD21	2:A:102:GLU:HB2	1.64	0.62
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.29	0.62
2:A:167:TYR:CD1	2:A:202:LYS:HG2	2.35	0.62
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.81	0.61
2:A:187:PRO:O	2:A:193:GLY:HA3	2.01	0.61
2:A:325:LEU:HD12	2:A:326:ILE:C	2.26	0.61
2:A:137:TYR:HB3	2:A:140:ILE:CG2	2.30	0.60
2:A:293:PRO:HB2	2:A:296:SER:OG	2.01	0.60
2:A:256:CYS:O	2:A:260:GLU:HG3	2.01	0.60
2:A:76:GLU:OE1	2:A:294:LYS:HE3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:LEU:C	2:A:104:GLN:HG2	2.26	0.60
2:A:223:PRO:HG3	2:A:249:ILE:HG22	1.83	0.60
2:A:252:MET:HB3	2:A:283:PHE:CE2	2.37	0.60
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.31	0.60
2:A:274:TYR:HD1	2:A:275:ASP:N	2.00	0.60
2:A:145:MET:HA	2:A:158:VAL:CG1	2.32	0.60
2:A:187:PRO:HD2	2:A:221:PHE:CE2	2.37	0.60
2:A:85:CYS:HA	2:A:302:PHE:CZ	2.37	0.60
2:A:210:LYS:H	2:A:210:LYS:CD	2.14	0.59
2:A:218:GLN:HE21	2:A:219:GLY:N	2.00	0.59
2:A:314:GLU:HA	2:A:314:GLU:OE1	2.02	0.59
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.67	0.59
2:A:40:ILE:HG23	2:A:45:TYR:HB3	1.83	0.59
1:M:699:DT:H2''	1:M:700:DA:O5'	2.02	0.59
2:A:40:ILE:C	2:A:41:LYS:HD2	2.28	0.59
2:A:210:LYS:HD3	2:A:210:LYS:N	2.17	0.58
2:A:105:ARG:HG3	2:A:106:ALA:N	2.18	0.58
2:A:167:TYR:HD1	2:A:202:LYS:HG2	1.68	0.58
2:A:62:ILE:HD12	2:A:62:ILE:C	2.27	0.58
2:A:63:GLY:O	2:A:119:LEU:HD12	2.04	0.58
2:A:201:MET:HE2	2:A:201:MET:HA	1.84	0.58
2:A:163:PHE:O	2:A:199:GLY:HA3	2.03	0.58
2:A:101:LEU:HD13	2:A:104:GLN:HE21	1.69	0.58
2:A:223:PRO:HG3	2:A:249:ILE:CG2	2.34	0.57
2:A:313:ARG:HD2	2:A:315:GLU:O	2.05	0.57
2:A:277:VAL:HG12	2:A:279:ASN:H	1.68	0.57
2:A:137:TYR:O	2:A:140:ILE:HG23	2.05	0.56
2:A:142:MET:O	2:A:155:THR:HG22	2.05	0.56
2:A:171:ARG:O	2:A:175:GLU:HG3	2.05	0.56
2:A:184:ILE:HG23	2:A:217:VAL:O	2.05	0.56
2:A:185:PRO:HD2	2:A:217:VAL:O	2.05	0.56
2:A:293:PRO:HG2	2:A:321:VAL:CG2	2.35	0.56
2:A:296:SER:O	2:A:300:THR:HB	2.04	0.56
2:A:100:ASN:ND2	2:A:100:ASN:C	2.63	0.56
2:A:161:ASN:HB3	2:A:164:GLU:HG2	1.88	0.56
2:A:274:TYR:CD1	2:A:274:TYR:C	2.84	0.56
2:A:336:PHE:N	2:A:336:PHE:CD1	2.73	0.56
2:A:11:ALA:O	2:A:13:VAL:HG13	2.06	0.56
2:A:280:ALA:HA	2:A:283:PHE:CD1	2.41	0.56
1:M:714:DG:H2''	1:M:715:DT:O5'	2.07	0.55
2:A:200:PHE:CD2	2:A:201:MET:CE	2.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:243:VAL:HG12	2:A:271:LEU:CD1	2.37	0.55
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.88	0.55
2:A:178:HIS:ND1	2:A:242:ALA:HB2	2.22	0.54
2:A:325:LEU:HD12	2:A:325:LEU:C	2.32	0.54
2:A:187:PRO:HB2	2:A:190:ARG:HD3	1.90	0.54
2:A:159:ILE:HG12	2:A:320:GLU:HG2	1.86	0.53
2:A:304:MET:HE3	2:A:317:GLN:HB3	1.91	0.53
2:A:313:ARG:HG3	2:A:314:GLU:N	2.23	0.53
2:A:274:TYR:HD1	2:A:274:TYR:C	2.16	0.53
2:A:337:ARG:HH11	2:A:337:ARG:CG	2.08	0.53
2:A:36:VAL:O	2:A:40:ILE:HG13	2.09	0.53
2:A:56:VAL:HG23	2:A:57:ASN:N	2.23	0.53
2:A:200:PHE:CD2	2:A:201:MET:HE1	2.44	0.53
2:A:135:GLU:C	2:A:137:TYR:H	2.17	0.53
2:A:310:VAL:CG2	2:A:311:ASN:N	2.73	0.52
2:A:138:ARG:NH2	2:A:154:PHE:HB3	2.25	0.52
2:A:218:GLN:HE21	2:A:219:GLY:H	1.57	0.52
2:A:105:ARG:CA	2:A:133:MET:HE1	2.32	0.52
2:A:313:ARG:CG	2:A:314:GLU:N	2.72	0.52
2:A:80:ALA:O	2:A:83:LYS:HB2	2.09	0.51
2:A:264:ARG:HB2	2:A:268:ASP:OD2	2.10	0.51
2:A:202:LYS:HG3	2:A:203:ALA:N	2.18	0.51
2:A:119:LEU:HB3	2:A:142:MET:HB2	1.92	0.51
2:A:310:VAL:C	2:A:312:LYS:H	2.19	0.51
2:A:325:LEU:CD1	2:A:326:ILE:N	2.71	0.51
2:A:130:LEU:HD22	2:A:130:LEU:O	2.10	0.51
2:A:220:ASP:OD1	2:A:222:GLU:HB2	2.11	0.50
2:A:234:LEU:HB2	2:A:261:MET:HE2	1.93	0.50
2:A:13:VAL:HG23	2:A:14:SER:N	2.26	0.50
2:A:137:TYR:HB3	2:A:140:ILE:HG23	1.93	0.50
2:A:160:ASP:HA	2:A:321:VAL:CG1	2.41	0.50
2:A:243:VAL:O	2:A:271:LEU:HD12	2.12	0.50
2:A:292:GLN:HG3	2:A:293:PRO:CD	2.40	0.50
2:A:117:ASP:O	2:A:141:PRO:HG2	2.12	0.50
2:A:37:TRP:HA	2:A:37:TRP:HE3	1.72	0.50
2:A:101:LEU:CD1	2:A:104:GLN:HE21	2.24	0.50
2:A:297:LEU:HD23	2:A:297:LEU:O	2.12	0.50
2:A:108:LEU:CD1	2:A:133:MET:HE2	2.36	0.49
2:A:41:LYS:N	2:A:41:LYS:CD	2.73	0.49
2:A:77:ILE:O	2:A:80:ALA:HB3	2.12	0.49
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:218:GLN:HE21	2:A:218:GLN:HA	1.76	0.49
2:A:16:THR:HG22	2:A:20:HIS:HD2	1.78	0.49
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.95	0.49
2:A:101:LEU:HA	2:A:104:GLN:CD	2.38	0.49
2:A:27:PHE:CD1	2:A:27:PHE:C	2.91	0.48
2:A:152:ALA:HB1	2:A:154:PHE:CE2	2.48	0.48
2:A:90:TYR:N	2:A:90:TYR:CD1	2.81	0.48
2:A:185:PRO:HB3	2:A:197:LEU:HD13	1.95	0.48
2:A:263:LEU:HD13	2:A:263:LEU:N	2.27	0.48
2:A:59:THR:HG21	2:A:115:ARG:O	2.13	0.48
2:A:144:VAL:HG23	2:A:155:THR:HG21	1.96	0.48
2:A:277:VAL:CG1	2:A:278:ARG:N	2.77	0.48
2:A:100:ASN:ND2	2:A:102:GLU:N	2.62	0.48
2:A:62:ILE:HD13	2:A:120:LEU:HD22	1.96	0.48
2:A:43:LEU:HD22	2:A:43:LEU:HA	1.53	0.47
2:A:142:MET:HG2	2:A:155:THR:HG23	1.95	0.47
2:A:159:ILE:HG13	2:A:320:GLU:HG2	1.94	0.47
2:A:213:GLU:C	2:A:215:TRP:N	2.72	0.47
2:A:159:ILE:O	2:A:320:GLU:HA	2.13	0.47
2:A:40:ILE:HB	2:A:41:LYS:HD3	1.97	0.47
2:A:161:ASN:ND2	2:A:322:HIS:CE1	2.83	0.47
2:A:81:VAL:HG12	2:A:82:GLU:N	2.30	0.47
2:A:281:ARG:HD3	2:A:281:ARG:C	2.39	0.47
2:A:251:ALA:C	2:A:253:GLY:N	2.70	0.47
2:A:212:PRO:HG2	2:A:215:TRP:CB	2.44	0.46
2:A:192:THR:HG21	3:A:599:HPA:C8	2.44	0.46
2:A:213:GLU:C	2:A:215:TRP:H	2.21	0.46
2:A:280:ALA:O	2:A:283:PHE:HB2	2.15	0.46
2:A:281:ARG:HD3	2:A:281:ARG:O	2.15	0.46
2:A:291:HIS:CD2	2:A:291:HIS:C	2.87	0.46
2:A:157:ALA:O	2:A:318:SER:HA	2.16	0.45
2:A:304:MET:HE2	2:A:317:GLN:HB3	1.97	0.45
2:A:237:PRO:CG	2:A:238:HIS:N	2.78	0.45
2:A:135:GLU:C	2:A:137:TYR:N	2.74	0.45
2:A:313:ARG:HG3	2:A:314:GLU:H	1.82	0.45
2:A:339:TYR:CD1	2:A:339:TYR:N	2.84	0.45
2:A:212:PRO:CG	2:A:215:TRP:CE3	2.99	0.45
2:A:218:GLN:CA	2:A:218:GLN:NE2	2.80	0.45
2:A:231:GLN:O	2:A:235:SER:HB2	2.17	0.45
2:A:236:GLN:CB	2:A:237:PRO:CD	2.93	0.45
2:A:212:PRO:HG3	2:A:215:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:304:MET:O	2:A:307:ASP:HB3	2.17	0.45
2:A:219:GLY:HA3	2:A:250:MET:SD	2.56	0.44
2:A:233:ILE:O	2:A:236:GLN:HG3	2.16	0.44
2:A:237:PRO:HG2	2:A:238:HIS:N	2.20	0.44
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.76	0.44
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.46	0.44
2:A:126:TYR:CD2	2:A:130:LEU:HD12	2.52	0.44
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.17	0.44
2:A:197:LEU:O	2:A:200:PHE:HB3	2.17	0.44
2:A:131:LEU:HA	2:A:131:LEU:HD22	1.23	0.44
2:A:140:ILE:HD12	2:A:140:ILE:C	2.42	0.44
2:A:135:GLU:O	2:A:138:ARG:HG3	2.17	0.44
2:A:266:PRO:HA	2:A:269:VAL:O	2.18	0.44
2:A:27:PHE:CD1	2:A:28:VAL:N	2.86	0.44
2:A:59:THR:CG2	2:A:115:ARG:O	2.65	0.44
2:A:308:ARG:HH21	2:A:316:PRO:HA	1.83	0.44
2:A:30:GLU:HA	2:A:33:ARG:NH1	2.33	0.44
2:A:136:GLU:C	2:A:137:TYR:CD1	2.95	0.44
2:A:168:MET:HE1	2:A:324:ARG:HA	1.99	0.44
2:A:168:MET:HE1	2:A:325:LEU:N	2.33	0.43
2:A:211:VAL:HA	2:A:212:PRO:HD2	1.51	0.43
2:A:99:ASN:HD22	2:A:99:ASN:HA	1.61	0.43
2:A:145:MET:HE3	2:A:301:ALA:CB	2.49	0.43
2:A:196:ARG:NH2	3:A:599:HPA:H8	2.32	0.43
2:A:220:ASP:O	2:A:221:PHE:HB2	2.18	0.43
2:A:274:TYR:CD1	2:A:275:ASP:N	2.84	0.43
2:A:23:ASN:N	2:A:23:ASN:HD22	2.16	0.43
2:A:201:MET:HE2	2:A:201:MET:N	2.33	0.43
2:A:243:VAL:HG12	2:A:271:LEU:HD11	1.99	0.43
2:A:126:TYR:CD2	2:A:130:LEU:CD1	3.02	0.43
2:A:218:GLN:HA	2:A:218:GLN:NE2	2.34	0.43
2:A:107:TYR:HA	2:A:110:MET:HG3	2.01	0.42
2:A:310:VAL:HG22	2:A:311:ASN:N	2.34	0.42
2:A:328:ARG:C	2:A:329:ARG:HG2	2.42	0.42
2:A:216:ILE:HD13	2:A:216:ILE:C	2.44	0.42
2:A:278:ARG:HG3	2:A:278:ARG:NH1	2.34	0.42
2:A:60:LYS:N	2:A:117:ASP:OD2	2.49	0.42
2:A:120:LEU:HD12	2:A:120:LEU:HA	1.94	0.42
2:A:187:PRO:HD2	2:A:221:PHE:HE2	1.83	0.42
2:A:16:THR:HG22	2:A:20:HIS:CD2	2.54	0.42
2:A:230:MET:HG2	2:A:254:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:9:LYS:HE3	2:A:9:LYS:HB2	1.56	0.42
2:A:264:ARG:O	2:A:268:ASP:N	2.42	0.42
2:A:287:LEU:O	2:A:328:ARG:HB2	2.20	0.42
2:A:335:PRO:HB2	2:A:336:PHE:CD1	2.54	0.42
2:A:143:VAL:HB	2:A:156:ASP:HB2	2.01	0.42
2:A:85:CYS:HA	2:A:302:PHE:HZ	1.82	0.42
2:A:252:MET:CE	2:A:283:PHE:CE1	3.03	0.42
2:A:297:LEU:HD23	2:A:297:LEU:C	2.44	0.42
2:A:28:VAL:HG12	2:A:29:ALA:O	2.19	0.42
2:A:170:GLY:O	2:A:173:LEU:HB2	2.20	0.42
2:A:17:THR:O	2:A:18:VAL:C	2.63	0.41
2:A:204:MET:O	2:A:205:GLU:C	2.63	0.41
2:A:131:LEU:N	2:A:131:LEU:HD23	2.32	0.41
2:A:151:LYS:HZ3	2:A:151:LYS:HG2	1.23	0.41
2:A:212:PRO:HG2	2:A:215:TRP:CG	2.55	0.41
2:A:305:LEU:HG	2:A:309:ILE:CD1	2.50	0.41
2:A:36:VAL:HG23	2:A:36:VAL:H	1.25	0.41
2:A:244:PHE:CD1	2:A:244:PHE:C	2.95	0.41
2:A:265:VAL:HA	2:A:266:PRO:HA	1.70	0.41
2:A:23:ASN:ND2	2:A:23:ASN:N	2.69	0.41
2:A:110:MET:HG2	2:A:110:MET:H	1.56	0.41
2:A:167:TYR:CD1	2:A:202:LYS:CG	3.03	0.41
2:A:27:PHE:C	2:A:28:VAL:HG23	2.46	0.40
2:A:112:ALA:O	2:A:115:ARG:HD3	2.22	0.40
2:A:212:PRO:O	2:A:215:TRP:HB2	2.21	0.40
2:A:36:VAL:O	2:A:40:ILE:CG1	2.69	0.40
2:A:328:ARG:HB2	2:A:328:ARG:HE	1.73	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%)	294 (88%)	34 (10%)	8 (2%)	4	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	309	ILE
2	A	227	TYR
2	A	19	SER
2	A	20	HIS
2	A	124	SER
2	A	194	ALA
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%)	183 (66%)	96 (34%)	0	0

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	LYS
2	A	10	ARG
2	A	12	ASN
2	A	13	VAL
2	A	14	SER
2	A	17	THR
2	A	21	VAL
2	A	22	ILE
2	A	23	ASN
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	62	ILE
2	A	64	LEU
2	A	68	SER
2	A	77	ILE
2	A	81	VAL
2	A	82	GLU
2	A	83	LYS
2	A	91	THR
2	A	92	LEU
2	A	99	ASN
2	A	100	ASN
2	A	102	GLU
2	A	103	LYS
2	A	109	SER
2	A	110	MET
2	A	120	LEU
2	A	122	MET
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	140	ILE
2	A	142	MET
2	A	143	VAL
2	A	151	LYS
2	A	155	THR
2	A	158	VAL
2	A	164	GLU
2	A	171	ARG
2	A	175	GLU
2	A	190	ARG
2	A	192	THR
2	A	201	MET
2	A	202	LYS
2	A	205	GLU
2	A	208	MET
2	A	210	LYS

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Mol	Chain	Res	Type
2	A	211	VAL
2	A	216	ILE
2	A	217	VAL
2	A	218	GLN
2	A	228	ARG
2	A	235	SER
2	A	236	GLN
2	A	239	ARG
2	A	243	VAL
2	A	249	ILE
2	A	250	MET
2	A	252	MET
2	A	255	LEU
2	A	261	MET
2	A	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	271	LEU
2	A	278	ARG
2	A	279	ASN
2	A	284	THR
2	A	288	THR
2	A	292	GLN
2	A	295	ASP
2	A	296	SER
2	A	299	GLU
2	A	300	THR
2	A	306	LEU
2	A	309	ILE
2	A	310	VAL
2	A	312	LYS
2	A	314	GLU
2	A	315	GLU
2	A	317	GLN
2	A	325	LEU
2	A	328	ARG
2	A	329	ARG
2	A	336	PHE
2	A	337	ARG
2	A	338	ASP
2	A	339	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	ASN
2	A	34	ASN
2	A	58	HIS
2	A	96	ASN
2	A	100	ASN
2	A	104	GLN
2	A	113	GLN
2	A	161	ASN
2	A	218	GLN
2	A	231	GLN
2	A	322	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	1.35	2 (20%)	11,15,15	1.46	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	-2.65	1.30	1.35
3	A	599	HPA	C8-N9	2.10	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	-3.12	119.48	121.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	599	HPA	6	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.