



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:04 PM UTC

PDB ID : 1PNR / pdb_00001pnr
Title : PURINE REPRESSOR-HYPOXANTHINE-PURF-OPERATOR COMPLEX
Authors : Schumacher, M.A.; Choi, K.Y.; Zalkin, H.; Brennan, R.G.
Deposited on : 1995-03-29
Resolution : 2.70 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

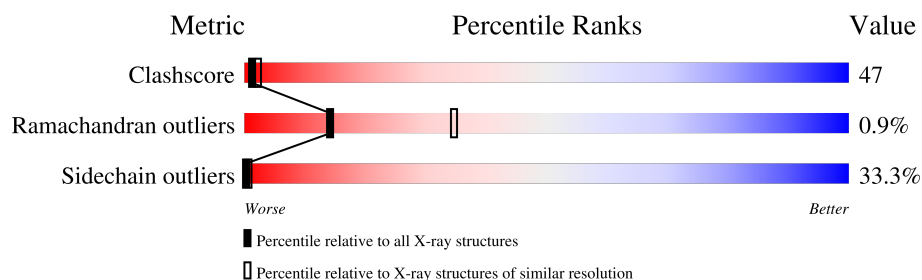
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	
2	A	340	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3054 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.

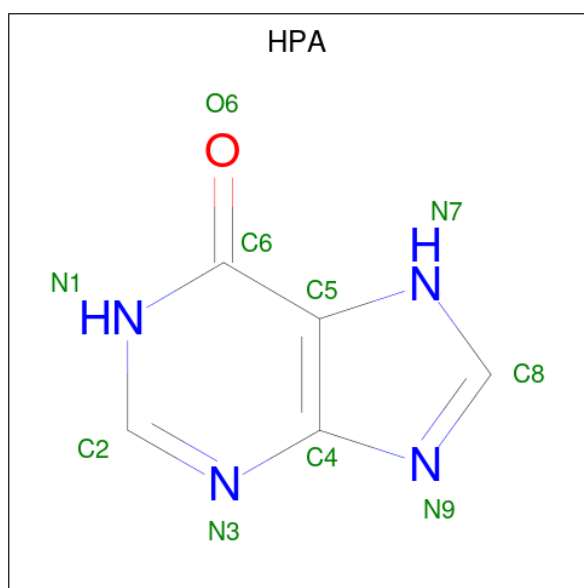
- Molecule 1 is a DNA chain called DNA (5'-D(*AP*AP*CP*GP*AP*AP*AP*AP*CP*GP*TP*TP*TP*TP*CP*GP*T)-3').

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 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	B	2	Total 2	O 2	0	0
4	A	44	Total 44	O 44	0	0

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.

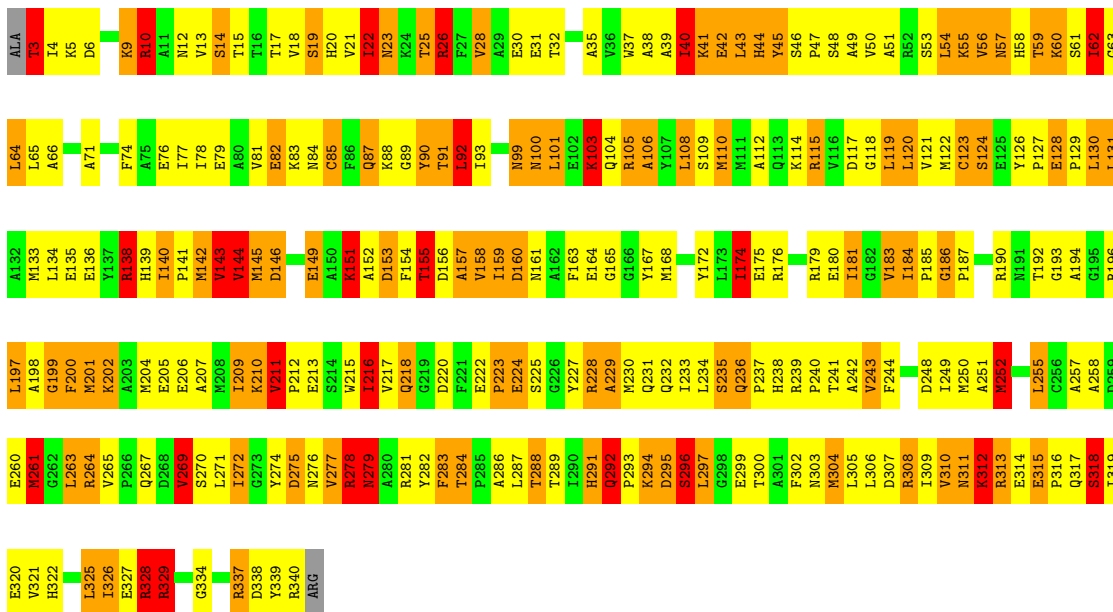
- Molecule 1: DNA (5'-D(*AP*AP*CP*GP*AP*AP*AP*AP*CP*GP*TP*TP*TP*TP*CP*GP*T)-3')

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	175.85Å 94.79Å 81.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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	0.43	0/388	2.84	26/597 (4.4%)
2	A	1.68	35/2706 (1.3%)	2.16	128/3660 (3.5%)
All	All	1.57	35/3094 (1.1%)	2.27	154/4257 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	2	0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	40	ILE	CA-CB	-9.23	1.43	1.54
2	A	81	VAL	CA-CB	-8.20	1.45	1.54
2	A	77	ILE	CA-CB	-8.11	1.45	1.54
2	A	184	ILE	CA-CB	-7.75	1.44	1.54
2	A	243	VAL	CA-CB	-7.70	1.44	1.54
2	A	158	VAL	CA-CB	-7.33	1.45	1.54
2	A	319	ILE	CA-CB	-7.09	1.44	1.54
2	A	78	ILE	CA-CB	-6.96	1.46	1.54
2	A	322	HIS	CA-CB	-6.81	1.43	1.53
2	A	229	ALA	CA-C	6.54	1.61	1.52
2	A	158	VAL	C-O	6.52	1.31	1.24
2	A	241	THR	CA-C	-6.34	1.44	1.52
2	A	6	ASP	CA-C	-6.17	1.44	1.52
2	A	13	VAL	CA-CB	-6.05	1.46	1.55
2	A	66	ALA	CA-CB	-6.01	1.44	1.53
2	A	53	SER	CA-C	-6.00	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	93	ILE	CA-CB	-5.96	1.46	1.54
2	A	251	ALA	CA-C	-5.82	1.45	1.52
2	A	272	ILE	C-O	5.71	1.30	1.24
2	A	269	VAL	CA-CB	-5.59	1.46	1.54
2	A	198	ALA	CA-CB	-5.56	1.44	1.53
2	A	272	ILE	CA-CB	-5.53	1.47	1.54
2	A	59	THR	CA-CB	-5.48	1.44	1.53
2	A	282	TYR	CA-CB	-5.38	1.45	1.53
2	A	174	ILE	CA-CB	-5.34	1.48	1.54
2	A	28	VAL	C-O	-5.32	1.18	1.24
2	A	106	ALA	CA-CB	-5.26	1.45	1.53
2	A	136	GLU	CA-C	-5.21	1.45	1.52
2	A	159	ILE	CA-C	5.17	1.58	1.52
2	A	328	ARG	CA-C	5.16	1.59	1.52
2	A	157	ALA	CA-CB	-5.09	1.45	1.53
2	A	124	SER	CA-C	-5.08	1.46	1.52
2	A	84	ASN	N-CA	-5.07	1.40	1.46
2	A	295	ASP	CA-C	5.06	1.59	1.52
2	A	28	VAL	CA-C	-5.01	1.46	1.52

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	DA	C4-N9-C1'	-22.77	92.89	127.05
1	B	703	DA	C8-N9-C1'	22.42	160.68	127.05
2	A	139	HIS	CA-CB-CG	19.03	132.83	113.80
1	B	705	DA	C4-N9-C1'	-16.71	101.98	127.05
1	B	705	DA	C8-N9-C1'	16.69	152.08	127.05
1	B	706	DA	C8-N9-C1'	15.37	150.11	127.05
1	B	706	DA	C4-N9-C1'	-15.05	104.47	127.05
1	B	699	DA	C8-N9-C1'	-13.06	107.46	127.05
1	B	699	DA	C4-N9-C1'	12.96	146.49	127.05
1	B	711	DT	C2-N1-C1'	-12.72	100.26	119.35
1	B	700	DA	C4-N9-C1'	-12.70	108.01	127.05
1	B	700	DA	C8-N9-C1'	12.30	145.50	127.05
1	B	711	DT	C6-N1-C1'	12.22	137.68	119.35
2	A	155	THR	CB-CA-C	-10.88	89.84	111.17
1	B	715	DT	C6-N1-C1'	-10.81	103.14	119.35
1	B	715	DT	C2-N1-C1'	10.60	135.24	119.35
1	B	704	DA	C4-N9-C1'	-10.43	111.41	127.05
1	B	704	DA	C8-N9-C1'	10.34	142.56	127.05
1	B	709	DT	C6-N1-C1'	-10.17	104.10	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	709	DT	C2-N1-C1'	10.14	134.56	119.35
2	A	54	LEU	N-CA-CB	9.81	124.55	110.12
2	A	45	TYR	N-CA-C	9.62	124.40	109.96
1	B	712	DT	C6-N1-C1'	9.55	133.68	119.35
2	A	57	ASN	N-CA-C	9.39	124.50	111.92
1	B	713	DC	C2-N1-C1'	-9.29	105.76	119.70
2	A	144	VAL	N-CA-CB	9.28	121.58	111.00
2	A	287	LEU	N-CA-C	8.99	123.44	109.96
2	A	294	LYS	CB-CA-C	8.98	125.88	110.79
2	A	146	ASP	N-CA-C	8.94	121.79	110.61
1	B	712	DT	C2-N1-C1'	-8.89	106.02	119.35
2	A	297	LEU	N-CA-C	-8.88	101.68	111.36
2	A	142	MET	N-CA-C	8.81	122.83	108.99
2	A	322	HIS	N-CA-C	8.80	125.94	107.91
2	A	283	PHE	N-CA-C	-8.61	99.82	110.41
1	B	701	DC	C2-N1-C1'	-8.51	106.94	119.70
2	A	158	VAL	N-CA-C	-8.26	96.61	108.17
1	B	701	DC	C6-N1-C1'	8.10	131.84	119.70
1	B	713	DC	C6-N1-C1'	8.09	131.83	119.70
2	A	106	ALA	N-CA-C	8.01	119.92	111.03
2	A	243	VAL	N-CA-C	7.92	120.26	108.46
2	A	269	VAL	CB-CA-C	-7.78	97.25	110.71
2	A	200	PHE	CB-CA-C	-7.66	97.83	110.85
2	A	264	ARG	CA-C-N	-7.50	116.81	123.33
2	A	264	ARG	C-N-CA	-7.50	116.81	123.33
2	A	209	ILE	N-CA-C	-7.40	97.69	108.71
2	A	123	CYS	N-CA-C	7.37	122.46	113.17
2	A	160	ASP	N-CA-C	7.30	122.02	113.18
2	A	296	SER	N-CA-C	-7.24	104.25	113.23
2	A	261	MET	N-CA-C	-7.12	104.47	113.02
2	A	143	VAL	N-CA-C	7.09	118.34	108.12
2	A	49	ALA	CA-C-N	-7.02	110.46	120.42
2	A	49	ALA	C-N-CA	-7.02	110.46	120.42
2	A	326	ILE	CB-CA-C	-7.02	100.95	110.42
2	A	121	VAL	N-CA-C	7.01	117.97	107.80
2	A	197	LEU	CB-CA-C	-7.00	99.18	110.79
2	A	329	ARG	N-CA-C	6.83	121.28	112.41
2	A	313	ARG	N-CA-C	6.82	120.12	110.50
2	A	318	SER	CA-C-N	-6.78	113.52	122.94
2	A	318	SER	C-N-CA	-6.78	113.52	122.94
2	A	303	ASN	N-CA-C	6.76	118.44	111.14
2	A	25	THR	N-CA-CB	-6.57	100.69	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	139	HIS	N-CA-CB	-6.56	99.50	110.39
2	A	174	ILE	N-CA-C	6.55	116.71	110.42
2	A	40	ILE	CB-CA-C	-6.54	103.47	112.04
2	A	216	ILE	CB-CA-C	6.49	119.98	110.77
2	A	292	GLN	CB-CA-C	-6.49	101.33	109.31
1	B	707	DC	C6-N1-C1'	6.44	129.36	119.70
2	A	250	MET	N-CA-C	-6.44	104.36	111.82
1	B	707	DC	C2-N1-C1'	-6.34	110.19	119.70
2	A	18	VAL	CB-CA-C	-6.23	103.88	112.04
2	A	48	SER	N-CA-C	6.19	118.73	109.25
2	A	278	ARG	CA-C-N	-6.18	109.82	121.81
2	A	278	ARG	C-N-CA	-6.18	109.82	121.81
2	A	159	ILE	N-CA-C	6.17	116.81	108.17
2	A	194	ALA	N-CA-C	6.09	118.42	111.11
2	A	199	GLY	N-CA-C	-6.00	105.53	112.73
2	A	252	MET	N-CA-C	-6.00	104.74	111.28
2	A	3	THR	CB-CA-C	5.98	122.26	109.10
2	A	51	ALA	N-CA-C	-5.96	104.48	110.97
2	A	181	ILE	N-CA-C	5.96	117.17	108.53
2	A	236	GLN	C-N-CD	-5.95	100.62	125.00
2	A	153	ASP	CA-C-N	-5.94	113.68	122.83
2	A	153	ASP	C-N-CA	-5.94	113.68	122.83
2	A	241	THR	CB-CA-C	-5.94	100.14	110.17
2	A	89	GLY	N-CA-C	5.93	123.42	115.59
2	A	46	SER	CA-C-O	5.91	125.18	119.62
2	A	121	VAL	CB-CA-C	-5.85	102.42	110.96
2	A	291	HIS	CA-CB-CG	5.81	119.61	113.80
2	A	115	ARG	CB-CA-C	-5.80	103.64	112.11
2	A	181	ILE	CA-C-N	-5.78	117.33	122.47
2	A	181	ILE	C-N-CA	-5.78	117.33	122.47
2	A	279	ASN	N-CA-C	5.75	119.41	111.71
2	A	312	LYS	N-CA-C	5.74	123.03	110.80
2	A	294	LYS	N-CA-C	5.73	118.39	111.40
2	A	340	ARG	CA-C-O	-5.72	111.08	120.80
2	A	62	ILE	CB-CA-C	5.71	119.13	110.62
2	A	223	PRO	CA-C-N	-5.71	111.64	120.31
2	A	223	PRO	C-N-CA	-5.71	111.64	120.31
2	A	9	LYS	N-CA-C	5.70	119.42	112.23
2	A	28	VAL	CB-CA-C	-5.68	100.88	110.71
2	A	155	THR	N-CA-C	5.68	116.89	108.60
2	A	252	MET	CA-C-N	-5.67	113.02	120.22
2	A	252	MET	C-N-CA	-5.67	113.02	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	258	ALA	N-CA-C	-5.66	104.32	111.11
2	A	10	ARG	N-CA-C	-5.66	105.26	111.82
2	A	99	ASN	CA-C-N	-5.64	115.15	123.05
2	A	99	ASN	C-N-CA	-5.64	115.15	123.05
2	A	229	ALA	N-CA-C	5.62	117.21	111.14
2	A	192	THR	N-CA-C	-5.60	106.15	112.87
2	A	248	ASP	N-CA-C	5.57	117.35	111.28
2	A	22	ILE	CA-C-N	-5.56	113.92	122.60
2	A	22	ILE	C-N-CA	-5.56	113.92	122.60
2	A	103	LYS	CA-C-N	-5.56	111.42	120.71
2	A	103	LYS	C-N-CA	-5.56	111.42	120.71
2	A	103	LYS	N-CA-C	-5.55	105.32	111.71
2	A	241	THR	CA-C-N	-5.55	112.03	121.85
2	A	241	THR	C-N-CA	-5.55	112.03	121.85
2	A	211	VAL	CB-CA-C	5.51	121.38	111.36
2	A	340	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	A	236	GLN	CB-CA-C	5.47	118.14	109.55
2	A	334	GLY	CA-C-N	5.46	126.67	119.84
2	A	334	GLY	C-N-CA	5.46	126.67	119.84
2	A	119	LEU	N-CA-C	5.46	117.29	108.34
2	A	90	TYR	N-CA-C	5.45	117.72	110.53
2	A	62	ILE	CA-C-N	-5.44	117.67	122.73
2	A	62	ILE	C-N-CA	-5.44	117.67	122.73
2	A	228	ARG	NE-CZ-NH2	5.41	124.07	119.20
2	A	56	VAL	CA-CB-CG2	-5.40	101.22	110.40
2	A	165	GLY	N-CA-C	-5.40	100.38	113.18
2	A	174	ILE	CB-CA-C	-5.40	105.06	111.97
2	A	4	ILE	N-CA-C	-5.39	105.12	110.62
2	A	304	MET	N-CA-C	-5.37	105.43	111.28
2	A	151	LYS	N-CA-C	5.37	117.88	111.71
2	A	58	HIS	N-CA-C	-5.34	100.40	108.52
2	A	149	GLU	N-CA-C	-5.33	102.02	109.69
2	A	328	ARG	CA-C-N	-5.32	114.14	122.49
2	A	328	ARG	C-N-CA	-5.32	114.14	122.49
2	A	85	CYS	N-CA-C	-5.30	105.40	111.07
2	A	126	TYR	N-CA-C	5.29	118.79	108.21
2	A	338	ASP	N-CA-C	5.27	117.77	111.71
2	A	339	TYR	CB-CA-C	-5.26	104.47	111.88
2	A	124	SER	CA-C-N	-5.23	115.35	122.93
2	A	124	SER	C-N-CA	-5.23	115.35	122.93
2	A	92	LEU	CA-C-N	-5.23	116.15	123.10
2	A	92	LEU	C-N-CA	-5.23	116.15	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	26	ARG	CB-CA-C	5.19	118.35	109.99
2	A	15	THR	N-CA-C	-5.12	105.13	111.33
2	A	211	VAL	N-CA-CB	5.12	118.38	111.21
2	A	186	GLY	CA-C-N	5.11	125.39	119.93
2	A	186	GLY	C-N-CA	5.11	125.39	119.93
2	A	279	ASN	CB-CA-C	5.09	120.88	110.75
2	A	138	ARG	CA-C-N	-5.04	112.31	120.72
2	A	138	ARG	C-N-CA	-5.04	112.31	120.72
2	A	142	MET	CB-CG-SD	-5.02	97.63	112.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	211	VAL	CA
2	A	294	LYS	CA

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	25	2
2	A	2652	0	2636	254	0
3	A	10	0	4	0	0
4	A	44	0	0	0	1
4	B	2	0	0	0	0
All	All	3054	0	2834	275	3

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 (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:DC:H2''	1:B:714:DG:H5''	1.25	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.16	1.08
2:A:61:SER:HB2	2:A:91:THR:HG22	1.16	1.08
2:A:337:ARG:HG2	2:A:337:ARG:HH11	1.26	1.01
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.81	0.95
2:A:20:HIS:HD1	2:A:25:THR:HG23	1.31	0.94
2:A:210:LYS:H	2:A:210:LYS:HD3	1.31	0.94
2:A:200:PHE:CZ	2:A:204:MET:HE2	2.04	0.92
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.85	0.91
2:A:292:GLN:HG3	2:A:293:PRO:HD2	1.51	0.91
2:A:292:GLN:HG3	2:A:293:PRO:CD	2.02	0.89
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.01	0.89
2:A:140:ILE:HD12	2:A:141:PRO:CD	2.05	0.86
2:A:181:ILE:HD13	2:A:204:MET:HE1	1.58	0.85
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.57	0.85
1:B:713:DC:C2'	1:B:714:DG:H5''	2.05	0.83
2:A:135:GLU:O	2:A:138:ARG:HG2	1.78	0.83
2:A:61:SER:CB	2:A:91:THR:HG22	2.07	0.83
1:B:712:DT:H2''	1:B:713:DC:H5''	1.58	0.83
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.61	0.83
2:A:61:SER:HB2	2:A:91:THR:CG2	2.07	0.81
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.61	0.81
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.64	0.78
1:B:713:DC:H2''	1:B:714:DG:H8	1.49	0.78
2:A:200:PHE:HD2	2:A:201:MET:CE	1.96	0.78
2:A:167:TYR:CD1	2:A:202:LYS:HG2	2.19	0.78
1:B:713:DC:H2''	1:B:714:DG:C8	2.19	0.77
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.67	0.77
2:A:20:HIS:HA	2:A:25:THR:CG2	2.15	0.77
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.66	0.76
1:B:706:DA:C2	2:A:55:LYS:HE2	2.20	0.76
2:A:23:ASN:N	2:A:23:ASN:HD22	1.82	0.76
2:A:159:ILE:HD12	2:A:159:ILE:O	1.85	0.76
2:A:3:THR:HG23	2:A:45:TYR:CE1	2.22	0.75
1:B:714:DG:C2'	1:B:715:DT:H5'	2.17	0.75
2:A:277:VAL:HG12	2:A:279:ASN:H	1.51	0.74
2:A:164:GLU:O	2:A:168:MET:HG3	1.89	0.73
2:A:167:TYR:HD1	2:A:202:LYS:HG2	1.54	0.73
1:B:700:DA:H2''	1:B:701:DC:O5'	1.88	0.72
2:A:201:MET:CA	2:A:201:MET:HE2	2.19	0.72
2:A:325:LEU:HD11	2:A:327:GLU:HG3	1.72	0.72
2:A:101:LEU:HA	2:A:104:GLN:HG2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:PHE:HD2	2:A:201:MET:HE1	1.55	0.71
2:A:286:ALA:HB1	2:A:328:ARG:HG2	1.70	0.71
2:A:337:ARG:HG2	2:A:337:ARG:NH1	2.03	0.71
2:A:23:ASN:ND2	2:A:23:ASN:N	2.38	0.71
2:A:257:ALA:O	2:A:261:MET:HG3	1.91	0.70
2:A:101:LEU:HA	2:A:104:GLN:CG	2.21	0.70
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.23	0.69
2:A:105:ARG:HA	2:A:133:MET:CE	2.22	0.69
2:A:159:ILE:HD12	2:A:159:ILE:C	2.17	0.69
1:B:706:DA:H2	2:A:55:LYS:HE2	1.57	0.69
2:A:224:GLU:O	2:A:224:GLU:HG3	1.93	0.68
2:A:40:ILE:HG22	2:A:41:LYS:HD3	1.74	0.68
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.29	0.68
2:A:105:ARG:HA	2:A:133:MET:HE1	1.77	0.67
2:A:210:LYS:HD3	2:A:210:LYS:N	2.07	0.67
2:A:210:LYS:H	2:A:210:LYS:CD	2.06	0.66
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.13	0.66
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.61	0.66
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.09	0.66
2:A:155:THR:HG22	2:A:156:ASP:N	2.11	0.65
2:A:306:LEU:O	2:A:310:VAL:N	2.29	0.65
2:A:304:MET:HE3	2:A:317:GLN:HG2	1.77	0.65
2:A:237:PRO:HG2	2:A:238:HIS:H	1.61	0.65
2:A:309:ILE:HG22	2:A:310:VAL:N	2.12	0.65
2:A:140:ILE:HD12	2:A:141:PRO:N	2.11	0.65
1:B:714:DG:H5''	1:B:714:DG:H8	1.62	0.65
2:A:130:LEU:HD22	2:A:130:LEU:O	1.96	0.65
2:A:201:MET:HE2	2:A:201:MET:HA	1.77	0.65
2:A:174:ILE:HG22	2:A:175:GLU:N	2.12	0.64
1:B:702:DG:H5'	1:B:702:DG:H8	1.62	0.64
2:A:122:MET:HE2	2:A:145:MET:HE2	1.79	0.64
1:B:714:DG:H2''	1:B:715:DT:H5'	1.80	0.63
2:A:10:ARG:NE	2:A:42:GLU:OE1	2.30	0.63
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.28	0.63
2:A:62:ILE:HD12	2:A:63:GLY:N	2.14	0.63
2:A:252:MET:HE2	2:A:283:PHE:CE1	2.34	0.63
2:A:181:ILE:CD1	2:A:204:MET:HE1	2.29	0.63
2:A:281:ARG:O	2:A:281:ARG:NH1	2.27	0.62
2:A:149:GLU:HG2	2:A:151:LYS:HD2	1.82	0.62
1:B:714:DG:H8	1:B:714:DG:C5'	2.13	0.61
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.83	0.61
2:A:100:ASN:O	2:A:104:GLN:HG2	2.01	0.61
2:A:265:VAL:HG13	2:A:269:VAL:O	2.00	0.61
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.01	0.61
2:A:23:ASN:HD22	2:A:23:ASN:H	1.48	0.60
2:A:183:VAL:HG13	2:A:216:ILE:HB	1.84	0.60
2:A:231:GLN:O	2:A:235:SER:HB2	2.02	0.60
2:A:237:PRO:CG	2:A:238:HIS:H	2.15	0.60
2:A:19:SER:O	2:A:23:ASN:ND2	2.34	0.60
2:A:39:ALA:O	2:A:43:LEU:HB2	2.02	0.59
2:A:105:ARG:CA	2:A:133:MET:HE1	2.31	0.59
2:A:325:LEU:HD13	2:A:326:ILE:N	2.17	0.59
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.67	0.59
1:B:703:DA:H5'	1:B:703:DA:N9	2.19	0.58
2:A:63:GLY:O	2:A:119:LEU:HD12	2.03	0.58
2:A:157:ALA:O	2:A:318:SER:HA	2.04	0.58
2:A:155:THR:HG22	2:A:156:ASP:H	1.68	0.58
2:A:163:PHE:O	2:A:199:GLY:HA3	2.04	0.58
2:A:286:ALA:HB3	2:A:329:ARG:CG	2.34	0.58
2:A:28:VAL:HG12	2:A:32:THR:HB	1.85	0.57
2:A:243:VAL:HG12	2:A:244:PHE:N	2.18	0.57
2:A:101:LEU:HD13	2:A:104:GLN:HE21	1.69	0.57
2:A:82:GLU:HG3	2:A:83:LYS:N	2.20	0.57
2:A:196:ARG:HD3	2:A:274:TYR:CD2	2.40	0.57
2:A:62:ILE:HD12	2:A:62:ILE:C	2.31	0.56
2:A:35:ALA:O	2:A:38:ALA:HB3	2.06	0.56
2:A:112:ALA:O	2:A:115:ARG:N	2.37	0.56
2:A:310:VAL:HG22	2:A:311:ASN:OD1	2.04	0.56
2:A:234:LEU:N	2:A:234:LEU:HD23	2.21	0.55
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.33	0.55
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.87	0.55
2:A:200:PHE:CZ	2:A:204:MET:CE	2.86	0.55
2:A:284:THR:O	2:A:284:THR:HG22	2.07	0.55
2:A:135:GLU:O	2:A:135:GLU:HG2	2.07	0.55
2:A:279:ASN:HD22	2:A:279:ASN:C	2.13	0.55
2:A:278:ARG:HG3	2:A:278:ARG:NH1	2.22	0.55
1:B:702:DG:H5'	1:B:702:DG:C8	2.42	0.54
1:B:714:DG:C8	1:B:714:DG:C5'	2.90	0.54
2:A:22:ILE:HG22	2:A:23:ASN:HD21	1.69	0.54
2:A:90:TYR:N	2:A:90:TYR:CD1	2.74	0.54
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:PHE:CD2	2:A:201:MET:HE1	2.39	0.54
2:A:310:VAL:HG22	2:A:311:ASN:N	2.22	0.54
2:A:313:ARG:HG3	2:A:314:GLU:N	2.23	0.54
2:A:197:LEU:O	2:A:200:PHE:HB3	2.09	0.53
2:A:286:ALA:HB3	2:A:329:ARG:HG3	1.90	0.53
2:A:222:GLU:HB3	2:A:223:PRO:HD2	1.90	0.53
2:A:274:TYR:HD1	2:A:275:ASP:N	2.07	0.53
2:A:64:LEU:C	2:A:64:LEU:HD12	2.31	0.53
2:A:179:ARG:HA	2:A:209:ILE:CD1	2.38	0.53
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.54	0.53
2:A:152:ALA:HB1	2:A:154:PHE:CE1	2.44	0.53
2:A:337:ARG:HH11	2:A:337:ARG:CG	2.10	0.53
2:A:10:ARG:HG3	2:A:10:ARG:NH1	2.24	0.53
2:A:239:ARG:HB2	2:A:240:PRO:CD	2.38	0.53
2:A:41:LYS:O	2:A:44:HIS:N	2.39	0.52
2:A:142:MET:CG	2:A:155:THR:HG23	2.39	0.52
2:A:130:LEU:HD22	2:A:134:LEU:HG	1.90	0.52
2:A:304:MET:HE1	2:A:317:GLN:C	2.35	0.52
2:A:276:ASN:ND2	2:A:291:HIS:HD2	2.08	0.52
2:A:114:LYS:O	2:A:115:ARG:HB2	2.10	0.51
2:A:183:VAL:HA	2:A:244:PHE:O	2.10	0.51
2:A:236:GLN:CB	2:A:237:PRO:CD	2.88	0.51
2:A:296:SER:O	2:A:300:THR:HB	2.10	0.51
2:A:14:SER:O	2:A:17:THR:HB	2.10	0.51
2:A:140:ILE:HD12	2:A:140:ILE:C	2.35	0.51
2:A:236:GLN:HB2	2:A:237:PRO:CD	2.40	0.51
2:A:252:MET:HB2	2:A:283:PHE:CE2	2.45	0.51
2:A:3:THR:HG23	2:A:45:TYR:CD1	2.46	0.51
2:A:101:LEU:C	2:A:104:GLN:HG2	2.36	0.51
2:A:184:ILE:HD13	2:A:229:ALA:HB3	1.93	0.51
2:A:236:GLN:HB2	2:A:237:PRO:HD3	1.93	0.51
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.75	0.51
2:A:145:MET:HA	2:A:158:VAL:CG1	2.41	0.51
2:A:28:VAL:CG1	2:A:32:THR:HB	2.41	0.50
2:A:160:ASP:O	2:A:161:ASN:HB2	2.11	0.50
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.94	0.50
2:A:308:ARG:HH21	2:A:316:PRO:HA	1.76	0.50
1:B:709:DT:H2''	1:B:710:DT:H5'	1.92	0.50
1:B:714:DG:H5''	1:B:714:DG:C8	2.45	0.50
2:A:101:LEU:HD12	2:A:104:GLN:HG3	1.94	0.49
2:A:179:ARG:NH2	2:A:207:ALA:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:DC:H2''	1:B:702:DG:H5''	1.95	0.49
2:A:179:ARG:HA	2:A:209:ILE:HD13	1.94	0.49
2:A:233:ILE:O	2:A:236:GLN:HG2	2.12	0.49
2:A:286:ALA:CB	2:A:328:ARG:HG2	2.41	0.49
2:A:210:LYS:O	2:A:210:LYS:HG2	2.13	0.48
1:B:707:DC:H2''	2:A:54:LEU:HD11	1.95	0.48
2:A:120:LEU:HD13	2:A:305:LEU:HD22	1.95	0.48
2:A:112:ALA:O	2:A:115:ARG:HD3	2.14	0.48
2:A:144:VAL:HG23	2:A:146:ASP:H	1.79	0.48
2:A:140:ILE:CD1	2:A:141:PRO:HD2	2.40	0.48
2:A:60:LYS:N	2:A:117:ASP:OD2	2.39	0.47
2:A:304:MET:O	2:A:307:ASP:HB3	2.13	0.47
1:B:703:DA:H5'	1:B:703:DA:C8	2.49	0.47
2:A:54:LEU:HD12	2:A:54:LEU:O	2.13	0.47
2:A:211:VAL:HG23	2:A:212:PRO:HD2	1.97	0.47
2:A:304:MET:CE	2:A:317:GLN:HG2	2.44	0.47
2:A:325:LEU:HD13	2:A:326:ILE:C	2.40	0.47
2:A:211:VAL:CB	2:A:212:PRO:HD2	2.44	0.47
2:A:64:LEU:HD12	2:A:65:LEU:N	2.30	0.47
2:A:252:MET:CE	2:A:283:PHE:CE1	2.97	0.47
2:A:105:ARG:N	2:A:133:MET:HE1	2.30	0.46
2:A:123:CYS:O	2:A:124:SER:HB2	2.13	0.46
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.45	0.46
2:A:243:VAL:CG1	2:A:244:PHE:N	2.77	0.46
2:A:274:TYR:N	2:A:289:THR:OG1	2.48	0.46
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.45	0.46
2:A:184:ILE:HA	2:A:217:VAL:O	2.15	0.46
2:A:281:ARG:O	2:A:281:ARG:HG2	2.15	0.46
1:B:706:DA:N3	2:A:55:LYS:HE2	2.31	0.46
2:A:45:TYR:CZ	2:A:47:PRO:HA	2.50	0.46
2:A:131:LEU:O	2:A:134:LEU:HB2	2.15	0.46
2:A:222:GLU:O	2:A:225:SER:N	2.47	0.46
2:A:237:PRO:CG	2:A:238:HIS:N	2.79	0.46
2:A:152:ALA:CB	2:A:154:PHE:CE1	2.99	0.46
2:A:272:ILE:HG21	2:A:272:ILE:HD13	1.64	0.46
2:A:142:MET:HG3	2:A:155:THR:HG23	1.97	0.45
2:A:185:PRO:HD2	2:A:218:GLN:HA	1.98	0.45
1:B:715:DT:H6	1:B:715:DT:H2'	1.30	0.45
2:A:277:VAL:CG1	2:A:278:ARG:N	2.78	0.45
2:A:310:VAL:C	2:A:312:LYS:H	2.24	0.45
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:43:LEU:HA	2:A:43:LEU:HD22	1.18	0.45
2:A:183:VAL:O	2:A:216:ILE:HA	2.17	0.45
2:A:180:GLU:HB3	2:A:240:PRO:HA	1.98	0.45
2:A:227:TYR:OH	2:A:260:GLU:OE1	2.29	0.45
2:A:163:PHE:CD1	2:A:163:PHE:C	2.94	0.44
2:A:167:TYR:CE1	2:A:202:LYS:CG	3.00	0.44
2:A:20:HIS:CE1	2:A:26:ARG:HB3	2.52	0.44
2:A:117:ASP:O	2:A:141:PRO:HG2	2.17	0.44
2:A:142:MET:HG2	2:A:155:THR:HG23	1.98	0.44
2:A:187:PRO:O	2:A:193:GLY:HA3	2.17	0.44
2:A:291:HIS:CE1	2:A:293:PRO:HA	2.52	0.44
2:A:106:ALA:O	2:A:110:MET:HG3	2.17	0.44
2:A:184:ILE:HD13	2:A:229:ALA:CB	2.48	0.44
2:A:110:MET:HE2	2:A:110:MET:HB3	1.93	0.44
2:A:128:GLU:N	2:A:129:PRO:CD	2.80	0.44
2:A:37:TRP:O	2:A:40:ILE:HB	2.17	0.44
2:A:42:GLU:C	2:A:44:HIS:N	2.74	0.44
2:A:152:ALA:HB1	2:A:154:PHE:CD1	2.52	0.44
2:A:313:ARG:NH1	2:A:315:GLU:O	2.47	0.44
2:A:64:LEU:HB2	2:A:92:LEU:HD21	2.00	0.44
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.99	0.44
2:A:325:LEU:HD13	2:A:325:LEU:C	2.43	0.44
2:A:142:MET:O	2:A:155:THR:HG22	2.18	0.43
2:A:212:PRO:HG2	2:A:215:TRP:CD2	2.52	0.43
2:A:105:ARG:HA	2:A:133:MET:HE3	1.97	0.43
2:A:87:GLN:OE1	2:A:88:LYS:HD3	2.18	0.43
2:A:59:THR:HG21	2:A:115:ARG:O	2.18	0.43
2:A:56:VAL:HG23	2:A:57:ASN:N	2.26	0.43
2:A:134:LEU:HD23	2:A:134:LEU:HA	1.70	0.43
2:A:274:TYR:CD1	2:A:274:TYR:C	2.97	0.43
2:A:181:ILE:HA	2:A:242:ALA:O	2.19	0.43
2:A:210:LYS:N	2:A:210:LYS:CD	2.75	0.43
2:A:263:LEU:N	2:A:263:LEU:HD13	2.32	0.43
2:A:71:ALA:O	2:A:74:PHE:HB2	2.19	0.42
2:A:313:ARG:CG	2:A:314:GLU:N	2.81	0.42
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.53	0.42
2:A:304:MET:HE2	2:A:317:GLN:HB3	2.01	0.42
2:A:85:CYS:HA	2:A:302:PHE:CZ	2.55	0.42
2:A:200:PHE:CE1	2:A:204:MET:HE2	2.53	0.42
2:A:297:LEU:HD23	2:A:297:LEU:C	2.44	0.42
2:A:20:HIS:HA	2:A:25:THR:HG22	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:186:GLY:C	2:A:218:GLN:HE22	2.27	0.42
1:B:713:DC:C2'	1:B:714:DG:C8	2.97	0.42
2:A:154:PHE:CD1	2:A:154:PHE:N	2.87	0.42
2:A:281:ARG:HG2	2:A:281:ARG:HH11	1.83	0.42
2:A:143:VAL:HG23	2:A:144:VAL:N	2.35	0.41
2:A:161:ASN:HB3	2:A:164:GLU:HG2	2.03	0.41
2:A:202:LYS:HE3	2:A:206:GLU:HG3	2.02	0.41
2:A:212:PRO:CG	2:A:215:TRP:CE3	3.03	0.41
2:A:252:MET:CE	2:A:283:PHE:CZ	3.02	0.41
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.15	0.41
2:A:143:VAL:HA	2:A:155:THR:HG22	2.01	0.41
2:A:297:LEU:HD23	2:A:297:LEU:O	2.21	0.41
2:A:267:GLN:CD	2:A:267:GLN:H	2.28	0.41
2:A:315:GLU:HB3	2:A:316:PRO:HD2	2.01	0.41
2:A:131:LEU:HD12	2:A:131:LEU:HA	1.58	0.41
2:A:161:ASN:HD21	2:A:320:GLU:HB3	1.85	0.41
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.01	0.41
2:A:277:VAL:O	2:A:279:ASN:N	2.54	0.41
2:A:288:THR:OG1	2:A:328:ARG:N	2.30	0.41
2:A:337:ARG:NH1	2:A:337:ARG:O	2.53	0.41
1:B:702:DG:H5'	1:B:702:DG:H2'	1.94	0.40
2:A:149:GLU:CG	2:A:151:LYS:HD2	2.49	0.40
2:A:212:PRO:HG2	2:A:215:TRP:CE3	2.56	0.40
2:A:274:TYR:CD1	2:A:275:ASP:N	2.88	0.40
2:A:14:SER:O	2:A:17:THR:N	2.54	0.40
2:A:329:ARG:CZ	2:A:329:ARG:CB	2.98	0.40
2:A:236:GLN:HG3	2:A:237:PRO:HD2	2.04	0.40
2:A:278:ARG:HH11	2:A:278:ARG:CG	2.34	0.40

All (3) 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)
4:A:718:HOH:O	4:A:718:HOH:O[4_555]	1.83	0.37
1:B:703:DA:N6	1:B:712:DT:O4[4_555]	2.07	0.13
1:B:702:DG:O6	1:B:713:DC:N4[4_555]	2.19	0.01

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%)	302 (90%)	31 (9%)	3 (1%)	14	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	278	ARG
2	A	311	ASN

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%)	186 (67%)	93 (33%)	0	1

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR
2	A	5	LYS
2	A	9	LYS
2	A	10	ARG
2	A	12	ASN
2	A	14	SER
2	A	19	SER
2	A	21	VAL

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Mol	Chain	Res	Type
2	A	22	ILE
2	A	23	ASN
2	A	26	ARG
2	A	30	GLU
2	A	31	GLU
2	A	40	ILE
2	A	41	LYS
2	A	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	76	GLU
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	101	LEU
2	A	103	LYS
2	A	105	ARG
2	A	108	LEU
2	A	109	SER
2	A	110	MET
2	A	120	LEU
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	138	ARG
2	A	140	ILE
2	A	143	VAL
2	A	144	VAL
2	A	145	MET
2	A	151	LYS
2	A	153	ASP
2	A	155	THR
2	A	174	ILE

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Mol	Chain	Res	Type
2	A	176	ARG
2	A	183	VAL
2	A	190	ARG
2	A	201	MET
2	A	202	LYS
2	A	205	GLU
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	230	MET
2	A	232	GLN
2	A	235	SER
2	A	249	ILE
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	270	SER
2	A	277	VAL
2	A	278	ARG
2	A	279	ASN
2	A	284	THR
2	A	288	THR
2	A	292	GLN
2	A	294	LYS
2	A	295	ASP
2	A	296	SER
2	A	299	GLU
2	A	308	ARG
2	A	310	VAL
2	A	312	LYS
2	A	315	GLU
2	A	318	SER
2	A	325	LEU
2	A	328	ARG
2	A	329	ARG

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Mol	Chain	Res	Type
2	A	337	ARG

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	99	ASN
2	A	104	GLN
2	A	161	ASN
2	A	218	GLN
2	A	231	GLN
2	A	279	ASN
2	A	291	HIS
2	A	292	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	1.20	2 (20%)	11,15,15	1.37	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-N9	2.30	1.38	1.33
3	A	599	HPA	C8-N7	-2.16	1.31	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	HPA	C6-C5-C4	-3.21	119.42	121.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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.