



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:20 AM UTC

PDB ID : 1WET / pdb_00001wet
Title : STRUCTURE OF THE PURR-GUANINE-PURF OPERATOR COMPLEX
Authors : Schumacher, M.A.; Glasfeld, A.; Zalkin, H.; Brennan, R.G.
Deposited on : 1997-04-27
Resolution : 2.60 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

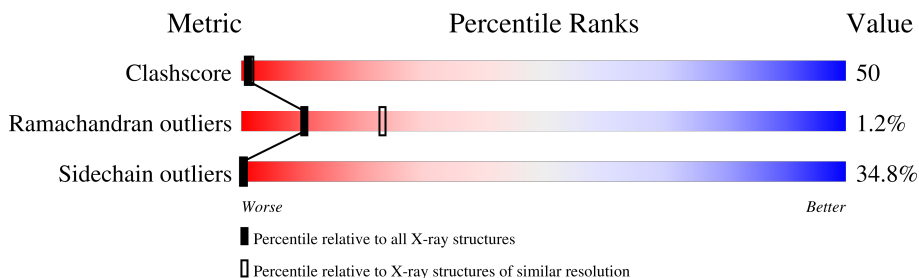
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

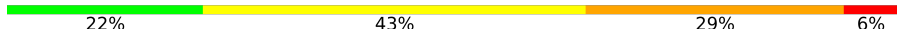
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 3055 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.

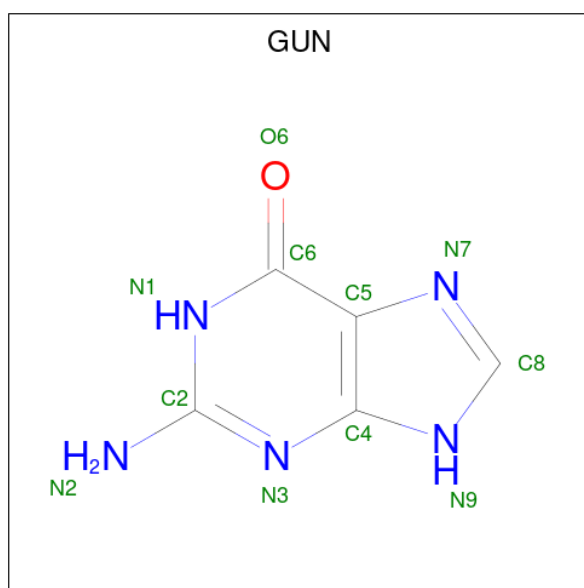
- Molecule 1 is a DNA chain called DNA (5'-D(*AP*AP*CP*GP*AP*AP*AP*AP*CP*GP*TP*TP*TP*TP*CP*GP*T)-3').

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 GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	5	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

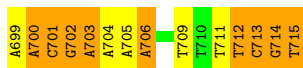
3 Residue-property plots

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.

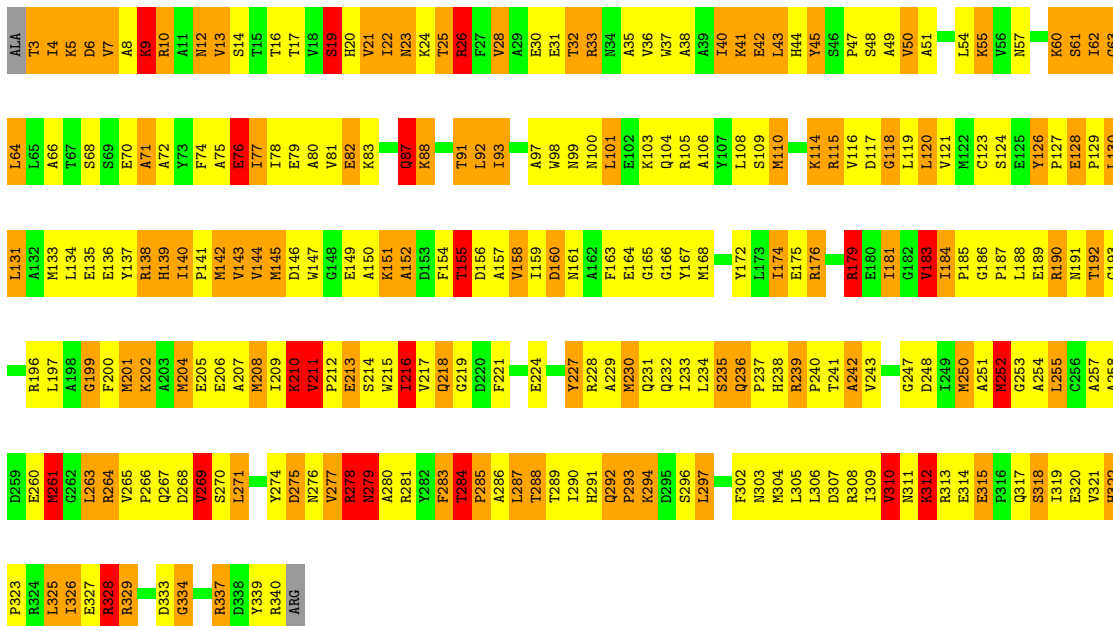
- Molecule 1: DNA (5'-D(*AP*AP*CP*GP*AP*AP*AP*AP*CP*GP*TP*TP*TP*TP*CP*GP*T)-3')

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	175.99Å 95.08Å 81.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3055	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: GUN

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	0.49	0/388	2.83	28/597 (4.7%)
2	A	1.42	21/2706 (0.8%)	1.85	95/3660 (2.6%)
All	All	1.34	21/3094 (0.7%)	2.02	123/4257 (2.9%)

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	1	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	284	THR	CA-C	-13.80	1.41	1.52
2	A	78	ILE	CA-CB	-8.23	1.44	1.54
2	A	81	VAL	CA-CB	-8.12	1.45	1.54
2	A	204	MET	SD-CE	-7.87	1.59	1.79
2	A	243	VAL	CA-CB	-7.35	1.45	1.54
2	A	116	VAL	CA-CB	-6.76	1.47	1.54
2	A	32	THR	CA-C	6.67	1.61	1.52
2	A	339	TYR	CA-C	-6.14	1.46	1.53
2	A	271	LEU	CA-C	-5.95	1.45	1.52
2	A	283	PHE	CA-C	-5.91	1.45	1.53
2	A	152	ALA	CA-C	-5.82	1.45	1.52
2	A	139	HIS	CA-CB	-5.57	1.44	1.53
2	A	184	ILE	CA-CB	-5.49	1.47	1.54
2	A	250	MET	CG-SD	5.47	1.94	1.80
2	A	284	THR	N-CA	-5.42	1.37	1.45
2	A	77	ILE	CA-CB	-5.38	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	242	ALA	N-CA	-5.35	1.39	1.46
2	A	118	GLY	CA-C	5.29	1.57	1.51
2	A	114	LYS	CA-C	5.25	1.60	1.52
2	A	319	ILE	CA-CB	-5.16	1.48	1.54
2	A	75	ALA	CA-C	-5.04	1.46	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	711	DT	C2-N1-C1'	-18.12	92.17	119.35
1	B	711	DT	C6-N1-C1'	17.75	145.98	119.35
1	B	700	DA	C4-N9-C1'	-16.93	101.65	127.05
1	B	703	DA	C4-N9-C1'	-16.93	101.66	127.05
1	B	705	DA	C8-N9-C1'	16.85	152.32	127.05
1	B	705	DA	C4-N9-C1'	-16.58	102.19	127.05
1	B	703	DA	C8-N9-C1'	16.53	151.84	127.05
1	B	700	DA	C8-N9-C1'	16.49	151.78	127.05
1	B	706	DA	C4-N9-C1'	-14.49	105.31	127.05
1	B	706	DA	C8-N9-C1'	13.99	148.03	127.05
2	A	284	THR	C-N-CD	-13.78	90.28	120.60
1	B	699	DA	C8-N9-C1'	-10.96	110.60	127.05
1	B	699	DA	C4-N9-C1'	10.87	143.36	127.05
1	B	709	DT	C6-N1-C1'	-10.66	103.36	119.35
1	B	709	DT	C2-N1-C1'	9.87	134.16	119.35
1	B	701	DC	C2-N1-C1'	-9.78	105.03	119.70
2	A	243	VAL	N-CA-C	9.73	122.14	108.12
2	A	310	VAL	N-CA-C	9.66	119.67	110.30
1	B	704	DA	C4-N9-C1'	-9.60	112.65	127.05
1	B	713	DC	C2-N1-C1'	-9.54	105.39	119.70
1	B	701	DC	C6-N1-C1'	9.30	133.66	119.70
1	B	704	DA	C8-N9-C1'	9.07	140.66	127.05
2	A	284	THR	CA-C-N	8.84	148.22	127.00
2	A	284	THR	C-N-CA	8.84	148.22	127.00
2	A	283	PHE	CA-C-N	-8.54	107.36	122.48
2	A	283	PHE	C-N-CA	-8.54	107.36	122.48
2	A	326	ILE	CB-CA-C	-8.30	98.99	110.77
1	B	713	DC	C6-N1-C1'	8.23	132.04	119.70
2	A	284	THR	CB-CA-C	-8.14	97.81	110.02
2	A	211	VAL	CB-CA-C	7.99	120.03	110.85
2	A	283	PHE	N-CA-C	-7.86	100.75	110.41
2	A	87	GLN	N-CA-C	7.58	120.21	111.11
2	A	210	LYS	CA-C-N	-7.47	111.50	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	210	LYS	C-N-CA	-7.47	111.50	123.46
1	B	712	DT	C2-N1-C1'	-7.39	108.26	119.35
2	A	252	MET	N-CA-C	-7.37	102.31	111.75
2	A	160	ASP	N-CA-C	7.33	122.05	113.18
2	A	149	GLU	N-CA-C	-7.25	98.89	109.18
1	B	715	DT	C6-N1-C1'	-7.23	108.50	119.35
2	A	57	ASN	N-CA-C	7.20	121.00	111.28
1	B	712	DT	C6-N1-C1'	7.14	130.06	119.35
1	B	714	DG	C8-N9-C1'	7.12	137.68	127.00
2	A	211	VAL	CA-C-N	7.10	128.22	119.98
2	A	211	VAL	C-N-CA	7.10	128.22	119.98
2	A	36	VAL	CB-CA-C	-7.01	103.00	111.97
1	B	714	DG	C4-N9-C1'	-6.99	116.52	127.00
2	A	287	LEU	N-CA-C	6.85	120.23	109.96
2	A	258	ALA	N-CA-C	-6.77	103.83	111.07
2	A	192	THR	N-CA-C	-6.70	104.83	112.87
1	B	715	DT	C2-N1-C1'	6.66	129.34	119.35
2	A	269	VAL	CB-CA-C	-6.63	99.03	111.30
2	A	315	GLU	CA-C-N	6.62	126.59	120.03
2	A	315	GLU	C-N-CA	6.62	126.59	120.03
2	A	183	VAL	N-CA-C	6.57	117.76	108.17
2	A	328	ARG	CA-C-N	-6.51	112.34	122.37
2	A	328	ARG	C-N-CA	-6.51	112.34	122.37
2	A	42	GLU	N-CA-C	-6.50	103.47	111.40
2	A	284	THR	N-CA-C	-6.39	96.12	108.45
2	A	121	VAL	CB-CA-C	-6.38	101.32	110.83
2	A	87	GLN	CB-CA-C	6.37	121.00	110.81
2	A	293	PRO	CA-C-N	-6.34	110.51	121.66
2	A	293	PRO	C-N-CA	-6.34	110.51	121.66
2	A	279	ASN	N-CA-C	6.33	118.98	110.88
2	A	181	ILE	N-CA-C	6.24	118.45	108.85
2	A	166	GLY	N-CA-C	-6.18	105.33	112.50
2	A	49	ALA	CA-C-N	-6.17	111.65	120.42
2	A	49	ALA	C-N-CA	-6.17	111.65	120.42
2	A	285	PRO	CA-N-CD	6.17	120.14	111.50
2	A	76	GLU	CB-CA-C	6.12	120.57	110.90
2	A	76	GLU	N-CA-CB	6.08	118.89	110.07
2	A	146	ASP	N-CA-C	6.03	121.65	112.54
2	A	236	GLN	N-CA-C	5.99	117.89	108.55
2	A	4	ILE	N-CA-C	-5.90	103.72	111.09
2	A	115	ARG	N-CA-C	5.89	119.24	111.28
2	A	318	SER	N-CA-C	5.86	118.22	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	87	GLN	N-CA-CB	5.85	118.66	109.94
2	A	241	THR	N-CA-C	-5.83	106.21	113.38
2	A	45	TYR	N-CA-C	5.82	119.01	109.76
2	A	126	TYR	N-CA-C	5.78	119.11	108.94
2	A	236	GLN	CB-CA-C	5.72	119.10	109.32
2	A	340	ARG	CA-C-O	-5.69	111.12	120.80
2	A	303	ASN	N-CA-C	5.67	117.14	111.07
2	A	121	VAL	N-CA-C	5.65	116.07	108.17
2	A	93	ILE	N-CA-C	-5.64	99.62	107.80
1	B	701	DC	O3'-P-O5'	-5.59	95.61	104.00
2	A	179	ARG	N-CA-C	-5.59	106.14	114.64
2	A	297	LEU	N-CA-C	-5.58	105.28	111.36
2	A	261	MET	N-CA-C	-5.58	106.36	112.72
2	A	165	GLY	CA-C-N	5.57	126.13	119.94
2	A	165	GLY	C-N-CA	5.57	126.13	119.94
2	A	322	HIS	N-CA-C	5.57	119.21	108.45
2	A	70	GLU	N-CA-C	-5.57	104.85	111.03
2	A	278	ARG	CA-C-N	-5.53	112.68	123.13
2	A	278	ARG	C-N-CA	-5.53	112.68	123.13
2	A	155	THR	CB-CA-C	-5.50	101.20	110.43
2	A	232	GLN	CA-C-N	-5.46	114.06	120.72
2	A	232	GLN	C-N-CA	-5.46	114.06	120.72
2	A	340	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	A	150	ALA	N-CA-C	5.38	118.01	107.57
2	A	98	TRP	N-CA-CB	-5.38	103.93	111.62
2	A	50	VAL	CB-CA-C	5.37	119.63	112.22
1	B	702	DG	C8-N9-C1'	-5.35	118.97	127.00
2	A	216	ILE	CB-CA-C	5.35	118.36	110.77
2	A	9	LYS	N-CA-C	5.31	116.88	111.14
2	A	334	GLY	CA-C-N	5.27	126.42	119.84
2	A	334	GLY	C-N-CA	5.27	126.42	119.84
2	A	142	MET	N-CA-C	5.25	116.51	108.42
2	A	227	TYR	N-CA-C	-5.21	105.30	110.97
2	A	284	THR	O-C-N	-5.18	116.40	121.38
2	A	66	ALA	N-CA-C	5.18	118.39	110.36
2	A	26	ARG	N-CA-C	-5.12	100.53	108.42
2	A	28	VAL	CB-CA-C	-5.11	101.88	110.71
2	A	199	GLY	N-CA-C	-5.09	106.59	112.50
2	A	211	VAL	O-C-N	5.06	125.83	121.12
2	A	63	GLY	N-CA-C	5.04	118.42	110.71
2	A	24	LYS	CA-C-N	-5.03	114.70	122.49
2	A	24	LYS	C-N-CA	-5.03	114.70	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	214	SER	N-CA-C	-5.03	107.21	113.19
2	A	241	THR	CA-C-N	-5.02	112.00	121.63
2	A	241	THR	C-N-CA	-5.02	112.00	121.63
2	A	19	SER	CA-C-N	-5.01	112.01	120.58
2	A	19	SER	C-N-CA	-5.01	112.01	120.58
2	A	57	ASN	CB-CA-C	-5.00	104.81	112.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	87	GLN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	284	THR	Mainchain,Peptide

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	346	0	194	23	0
2	A	2652	0	2636	274	0
3	A	11	0	5	1	0
4	A	44	0	0	4	0
4	B	2	0	0	1	0
All	All	3055	0	2835	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:B:713:DC:H2"	1:B:714:DG:H5"	1.24	1.12
2:A:61:SER:HB2	2:A:91:THR:HG22	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.31	1.09
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.42	1.00
2:A:210:LYS:H	2:A:210:LYS:HD3	1.30	0.96
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.82	0.95
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.50	0.93
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.51	0.93
2:A:286:ALA:HB3	2:A:329:ARG:HG3	1.51	0.92
2:A:140:ILE:HD12	2:A:141:PRO:CD	2.00	0.91
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.52	0.89
2:A:230:MET:HG2	2:A:254:ALA:HB1	1.55	0.89
1:B:713:DC:C2'	1:B:714:DG:H5''	2.03	0.89
2:A:236:GLN:HB2	2:A:237:PRO:HD2	1.54	0.88
2:A:61:SER:HB2	2:A:91:THR:CG2	2.02	0.87
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.57	0.87
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.58	0.85
2:A:276:ASN:HD22	2:A:291:HIS:CD2	1.94	0.85
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.08	0.83
2:A:100:ASN:HB3	2:A:103:LYS:CB	2.09	0.82
1:B:702:DG:H5'	1:B:702:DG:H8	1.45	0.82
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.94	0.81
2:A:210:LYS:HD3	2:A:210:LYS:N	1.95	0.81
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.10	0.81
2:A:23:ASN:N	2:A:23:ASN:HD22	1.79	0.80
2:A:88:LYS:HG3	2:A:302:PHE:HE2	1.48	0.79
2:A:237:PRO:HG2	2:A:238:HIS:H	1.47	0.79
1:B:712:DT:H2''	1:B:713:DC:H5''	1.65	0.78
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.28	0.77
2:A:167:TYR:CD1	2:A:202:LYS:HG2	2.20	0.77
2:A:200:PHE:CZ	2:A:204:MET:HE3	2.19	0.77
1:B:713:DC:H2''	1:B:714:DG:C8	2.20	0.76
2:A:3:THR:HG23	2:A:45:TYR:CE1	2.21	0.76
2:A:337:ARG:HG2	2:A:337:ARG:HH11	1.49	0.76
1:B:714:DG:C2'	1:B:715:DT:H5'	2.16	0.75
2:A:87:GLN:OE1	2:A:88:LYS:HD2	1.87	0.74
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.16	0.74
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.50	0.74
2:A:22:ILE:HD11	2:A:40:ILE:CD1	2.19	0.73
2:A:101:LEU:HA	2:A:104:GLN:HG2	1.71	0.72
2:A:252:MET:HE2	2:A:283:PHE:CE1	2.23	0.72
2:A:145:MET:HA	2:A:158:VAL:CG1	2.19	0.72
2:A:62:ILE:HD13	2:A:120:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:ASN:ND2	2:A:23:ASN:N	2.31	0.72
1:B:714:DG:H2''	1:B:715:DT:H5'	1.70	0.72
2:A:88:LYS:HG3	2:A:302:PHE:CE2	2.25	0.72
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.72	0.71
2:A:22:ILE:HD11	2:A:40:ILE:HD11	1.73	0.71
2:A:278:ARG:HG3	2:A:278:ARG:NH1	2.06	0.71
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.22	0.70
2:A:200:PHE:HD2	2:A:201:MET:CE	2.04	0.69
1:B:702:DG:H5'	1:B:702:DG:C8	2.25	0.69
2:A:101:LEU:O	2:A:101:LEU:HD12	1.92	0.69
2:A:63:GLY:O	2:A:119:LEU:HD12	1.92	0.69
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.57	0.69
2:A:310:VAL:HG22	2:A:311:ASN:OD1	1.92	0.69
2:A:167:TYR:CE1	2:A:202:LYS:HG2	2.29	0.68
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.76	0.68
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.23	0.67
2:A:179:ARG:NH2	2:A:207:ALA:O	2.28	0.67
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.28	0.67
2:A:281:ARG:O	2:A:281:ARG:NH1	2.25	0.67
1:B:713:DC:H2''	1:B:714:DG:H8	1.59	0.66
2:A:264:ARG:O	2:A:268:ASP:N	2.24	0.66
2:A:230:MET:HG2	2:A:254:ALA:CB	2.25	0.66
2:A:257:ALA:O	2:A:261:MET:HG2	1.94	0.66
2:A:276:ASN:ND2	2:A:291:HIS:HD2	1.94	0.66
1:B:700:DA:H2''	1:B:701:DC:O5'	1.96	0.66
2:A:329:ARG:NH1	4:A:732:HOH:O	2.28	0.65
2:A:186:GLY:C	2:A:218:GLN:HE22	2.04	0.65
2:A:210:LYS:H	2:A:210:LYS:CD	2.06	0.65
2:A:101:LEU:O	2:A:104:GLN:HG2	1.97	0.65
2:A:61:SER:CB	2:A:91:THR:HG22	2.21	0.64
2:A:10:ARG:NE	2:A:42:GLU:OE1	2.29	0.64
2:A:105:ARG:HA	2:A:133:MET:HE3	1.78	0.64
2:A:19:SER:O	2:A:23:ASN:ND2	2.30	0.64
2:A:157:ALA:O	2:A:318:SER:HA	1.98	0.64
2:A:184:ILE:HA	2:A:217:VAL:O	1.97	0.64
2:A:252:MET:HE2	2:A:283:PHE:CZ	2.32	0.64
2:A:255:LEU:HD13	2:A:271:LEU:CD2	2.29	0.63
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.63	0.63
2:A:72:ALA:O	2:A:76:GLU:HG2	1.98	0.63
2:A:138:ARG:NH2	2:A:154:PHE:HB3	2.13	0.62
2:A:192:THR:O	2:A:196:ARG:HD2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:22:ILE:HG22	2:A:23:ASN:HD21	1.62	0.62
2:A:77:ILE:O	2:A:80:ALA:HB3	1.99	0.61
2:A:286:ALA:HB3	2:A:329:ARG:CG	2.28	0.61
2:A:309:ILE:HG22	2:A:310:VAL:N	2.15	0.61
2:A:3:THR:O	2:A:7:VAL:HG23	2.01	0.60
2:A:117:ASP:O	2:A:141:PRO:HG2	2.02	0.60
2:A:101:LEU:HD12	2:A:101:LEU:C	2.26	0.60
2:A:231:GLN:O	2:A:235:SER:HB2	2.02	0.60
2:A:22:ILE:CD1	2:A:40:ILE:HD11	2.31	0.60
2:A:105:ARG:HA	2:A:133:MET:CE	2.32	0.59
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.33	0.59
2:A:126:TYR:HB3	2:A:131:LEU:CD1	2.33	0.58
2:A:266:PRO:HA	2:A:269:VAL:O	2.04	0.58
2:A:40:ILE:HG22	2:A:41:LYS:HD3	1.84	0.58
2:A:185:PRO:HD2	2:A:217:VAL:O	2.03	0.58
2:A:101:LEU:HA	2:A:104:GLN:CG	2.34	0.57
2:A:188:LEU:HG	2:A:218:GLN:OE1	2.04	0.57
2:A:106:ALA:O	2:A:110:MET:HG3	2.04	0.57
2:A:130:LEU:HD22	2:A:130:LEU:O	2.04	0.57
2:A:164:GLU:O	2:A:168:MET:HG3	2.05	0.57
2:A:284:THR:HG22	2:A:285:PRO:HD3	1.85	0.57
2:A:237:PRO:CG	2:A:238:HIS:H	2.17	0.57
2:A:140:ILE:CD1	2:A:141:PRO:HD2	2.19	0.57
2:A:279:ASN:HD22	2:A:279:ASN:C	2.12	0.57
2:A:304:MET:HE3	2:A:317:GLN:HG2	1.87	0.56
2:A:60:LYS:N	2:A:117:ASP:OD2	2.38	0.56
2:A:151:LYS:HE2	4:A:727:HOH:O	2.04	0.56
1:B:701:DC:H5	4:B:744:HOH:O	1.88	0.56
2:A:181:ILE:HD13	2:A:204:MET:HE1	1.87	0.56
2:A:64:LEU:HB2	2:A:92:LEU:HD21	1.87	0.56
2:A:280:ALA:HA	2:A:283:PHE:CD1	2.41	0.56
2:A:71:ALA:HB3	2:A:74:PHE:CD2	2.40	0.56
2:A:101:LEU:HD13	2:A:104:GLN:HE21	1.69	0.56
2:A:152:ALA:HB1	2:A:154:PHE:CE1	2.41	0.56
2:A:234:LEU:N	2:A:234:LEU:HD23	2.20	0.56
2:A:14:SER:O	2:A:17:THR:HB	2.06	0.55
2:A:51:ALA:O	2:A:54:LEU:HB3	2.06	0.55
2:A:308:ARG:O	2:A:312:LYS:HA	2.07	0.55
2:A:278:ARG:HH11	2:A:278:ARG:CG	2.20	0.55
2:A:147:TRP:CE3	2:A:151:LYS:HB2	2.42	0.55
2:A:71:ALA:HB3	2:A:74:PHE:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:ALA:O	2:A:42:GLU:HG3	2.08	0.54
2:A:161:ASN:HD21	2:A:320:GLU:HB3	1.73	0.54
2:A:163:PHE:O	2:A:199:GLY:HA3	2.08	0.54
2:A:30:GLU:HG3	2:A:33:ARG:NH1	2.22	0.54
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.90	0.54
2:A:100:ASN:HB3	2:A:103:LYS:HB3	1.90	0.53
1:B:706:DA:C2	2:A:55:LYS:HE2	2.42	0.53
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.42	0.53
2:A:144:VAL:HG21	2:A:147:TRP:CD2	2.43	0.53
2:A:274:TYR:N	2:A:289:THR:OG1	2.42	0.53
2:A:3:THR:HA	2:A:6:ASP:OD2	2.09	0.53
2:A:181:ILE:HA	2:A:242:ALA:O	2.08	0.53
2:A:287:LEU:O	2:A:328:ARG:NE	2.37	0.53
1:B:714:DG:H8	1:B:714:DG:C5'	2.22	0.52
2:A:248:ASP:O	2:A:251:ALA:HB3	2.09	0.52
2:A:184:ILE:HG12	2:A:229:ALA:HB1	1.90	0.52
2:A:234:LEU:CD1	2:A:263:LEU:HD23	2.35	0.52
2:A:239:ARG:HB2	2:A:240:PRO:CD	2.40	0.52
1:B:701:DC:H2"	1:B:702:DG:C8	2.44	0.52
2:A:143:VAL:HA	2:A:155:THR:HG22	1.92	0.52
2:A:152:ALA:HB1	2:A:154:PHE:CD1	2.45	0.52
2:A:277:VAL:HG12	2:A:279:ASN:H	1.74	0.52
2:A:288:THR:OG1	2:A:328:ARG:N	2.33	0.51
2:A:306:LEU:O	2:A:310:VAL:N	2.34	0.51
2:A:10:ARG:NH2	2:A:42:GLU:OE1	2.44	0.51
2:A:23:ASN:HD22	2:A:23:ASN:H	1.52	0.51
2:A:142:MET:CG	2:A:155:THR:HG23	2.39	0.51
2:A:183:VAL:O	2:A:216:ILE:HA	2.11	0.51
2:A:310:VAL:HG22	2:A:311:ASN:N	2.24	0.50
2:A:108:LEU:HD12	2:A:133:MET:CE	2.41	0.50
2:A:120:LEU:HD13	2:A:305:LEU:HD22	1.93	0.50
2:A:45:TYR:CZ	2:A:47:PRO:HA	2.47	0.50
2:A:325:LEU:HD22	2:A:326:ILE:N	2.26	0.50
1:B:706:DA:H2	2:A:55:LYS:HE2	1.77	0.50
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.41	0.50
2:A:147:TRP:CZ3	2:A:151:LYS:HB2	2.46	0.50
2:A:167:TYR:HD1	2:A:202:LYS:HG2	1.74	0.50
2:A:218:GLN:HE21	2:A:219:GLY:N	2.10	0.50
2:A:101:LEU:C	2:A:104:GLN:HG2	2.37	0.50
2:A:247:GLY:HA2	2:A:274:TYR:O	2.11	0.50
2:A:145:MET:HA	2:A:158:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:227:TYR:OH	2:A:260:GLU:OE1	2.26	0.49
2:A:71:ALA:O	2:A:74:PHE:HB2	2.13	0.49
2:A:142:MET:HG3	2:A:155:THR:HG23	1.95	0.49
2:A:35:ALA:O	2:A:38:ALA:HB3	2.13	0.49
1:B:713:DC:C3'	1:B:714:DG:H5''	2.43	0.49
2:A:234:LEU:HD22	2:A:239:ARG:HD3	1.95	0.49
2:A:97:ALA:HA	2:A:103:LYS:HG2	1.94	0.48
2:A:128:GLU:N	2:A:129:PRO:CD	2.76	0.48
2:A:191:ASN:C	2:A:193:GLY:N	2.72	0.48
2:A:274:TYR:CD1	2:A:274:TYR:C	2.91	0.48
2:A:100:ASN:HD22	2:A:103:LYS:H	1.60	0.48
2:A:167:TYR:OH	2:A:206:GLU:OE1	2.31	0.48
2:A:200:PHE:HD2	2:A:201:MET:HE1	1.78	0.48
2:A:236:GLN:HB2	2:A:237:PRO:CD	2.34	0.48
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.44	0.48
2:A:289:THR:HG22	2:A:328:ARG:HH21	1.77	0.47
1:B:714:DG:H5''	1:B:714:DG:H8	1.79	0.47
2:A:8:ALA:HB1	2:A:13:VAL:O	2.14	0.47
1:B:703:DA:H5'	1:B:703:DA:N9	2.29	0.47
2:A:135:GLU:O	2:A:138:ARG:HG2	2.13	0.47
2:A:118:GLY:C	2:A:140:ILE:HD11	2.39	0.47
2:A:137:TYR:HA	2:A:139:HIS:CD2	2.49	0.47
1:B:714:DG:C8	1:B:714:DG:C5'	2.98	0.47
1:B:703:DA:H5'	1:B:703:DA:C8	2.50	0.47
2:A:274:TYR:HD1	2:A:275:ASP:N	2.13	0.47
2:A:212:PRO:O	2:A:215:TRP:HB2	2.15	0.46
2:A:234:LEU:HB2	2:A:261:MET:HE2	1.98	0.46
2:A:297:LEU:HD23	2:A:297:LEU:O	2.15	0.46
2:A:322:HIS:N	4:A:722:HOH:O	2.33	0.46
2:A:191:ASN:C	2:A:193:GLY:H	2.22	0.46
2:A:284:THR:HG22	2:A:284:THR:O	2.15	0.46
2:A:306:LEU:O	2:A:309:ILE:HB	2.16	0.46
2:A:161:ASN:HA	4:A:747:HOH:O	2.15	0.46
2:A:237:PRO:HG2	2:A:238:HIS:N	2.24	0.46
2:A:276:ASN:HA	2:A:289:THR:HG21	1.97	0.46
2:A:310:VAL:C	2:A:312:LYS:H	2.23	0.46
2:A:200:PHE:CD2	2:A:201:MET:CE	2.93	0.46
2:A:284:THR:HG22	2:A:285:PRO:CD	2.46	0.46
2:A:287:LEU:O	2:A:328:ARG:HB2	2.16	0.46
2:A:200:PHE:CZ	2:A:204:MET:CE	2.94	0.45
2:A:313:ARG:CG	2:A:314:GLU:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:176:ARG:NH1	2:A:333:ASP:OD1	2.41	0.45
2:A:210:LYS:O	2:A:210:LYS:HG2	2.15	0.45
2:A:236:GLN:CB	2:A:237:PRO:CD	2.93	0.45
2:A:10:ARG:CZ	2:A:42:GLU:OE1	2.64	0.45
2:A:21:VAL:HG12	2:A:28:VAL:HG21	1.98	0.45
2:A:192:THR:HG21	3:A:599:GUN:C8	2.47	0.45
2:A:211:VAL:HA	2:A:212:PRO:HD3	1.70	0.45
2:A:250:MET:O	2:A:253:GLY:N	2.49	0.44
2:A:181:ILE:CD1	2:A:204:MET:HE1	2.47	0.44
2:A:190:ARG:HH11	2:A:190:ARG:HD2	1.64	0.44
2:A:20:HIS:CE1	2:A:26:ARG:HB3	2.53	0.44
2:A:137:TYR:C	2:A:139:HIS:N	2.74	0.44
2:A:291:HIS:CE1	2:A:293:PRO:HA	2.52	0.44
2:A:62:ILE:CD1	2:A:120:LEU:HD22	2.45	0.44
2:A:292:GLN:O	2:A:294:LYS:HE3	2.18	0.44
2:A:237:PRO:CG	2:A:238:HIS:N	2.80	0.44
2:A:187:PRO:HB2	2:A:190:ARG:HD3	2.00	0.44
2:A:213:GLU:C	2:A:215:TRP:H	2.25	0.44
2:A:110:MET:HE2	2:A:110:MET:HB3	1.89	0.43
2:A:201:MET:HE3	2:A:201:MET:HB2	1.75	0.43
2:A:176:ARG:O	2:A:334:GLY:N	2.40	0.43
2:A:201:MET:HE2	2:A:201:MET:CA	2.48	0.43
1:B:713:DC:C2'	1:B:714:DG:C8	2.96	0.43
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.42	0.43
2:A:114:LYS:O	2:A:115:ARG:HB2	2.17	0.43
2:A:181:ILE:HG21	2:A:200:PHE:HZ	1.83	0.43
2:A:252:MET:HB2	2:A:283:PHE:CE2	2.54	0.43
2:A:82:GLU:HG3	2:A:83:LYS:N	2.33	0.43
2:A:123:CYS:O	2:A:124:SER:HB2	2.19	0.43
2:A:135:GLU:C	2:A:137:TYR:N	2.76	0.43
2:A:255:LEU:HA	2:A:255:LEU:HD12	1.57	0.43
2:A:135:GLU:C	2:A:137:TYR:H	2.26	0.43
2:A:37:TRP:O	2:A:40:ILE:HB	2.18	0.42
2:A:100:ASN:O	2:A:104:GLN:HG2	2.19	0.42
2:A:119:LEU:HB3	2:A:142:MET:HB2	2.01	0.42
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.49	0.42
2:A:185:PRO:HD2	2:A:218:GLN:HA	2.01	0.42
2:A:265:VAL:HG13	2:A:269:VAL:O	2.19	0.42
2:A:274:TYR:C	2:A:274:TYR:HD1	2.27	0.42
2:A:164:GLU:OE2	2:A:322:HIS:ND1	2.45	0.42
2:A:329:ARG:CZ	2:A:329:ARG:CB	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:119:LEU:O	2:A:142:MET:HB2	2.19	0.42
2:A:267:GLN:H	2:A:267:GLN:CD	2.27	0.42
2:A:140:ILE:HD12	2:A:141:PRO:N	2.34	0.42
2:A:101:LEU:HA	2:A:104:GLN:NE2	2.33	0.42
2:A:160:ASP:HA	2:A:321:VAL:CG1	2.40	0.42
2:A:239:ARG:HB2	2:A:240:PRO:HD2	2.00	0.42
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.43	0.42
1:B:702:DG:OP2	2:A:17:THR:OG1	2.31	0.42
2:A:108:LEU:HD12	2:A:133:MET:HE2	2.00	0.42
2:A:134:LEU:HD23	2:A:134:LEU:HA	1.75	0.42
2:A:211:VAL:CG2	2:A:216:ILE:HG22	2.50	0.42
2:A:216:ILE:O	2:A:216:ILE:HG12	2.19	0.42
2:A:233:ILE:O	2:A:236:GLN:HG2	2.20	0.42
2:A:290:ILE:HD13	2:A:325:LEU:HD23	2.02	0.42
2:A:100:ASN:CB	2:A:103:LYS:HB2	2.34	0.42
2:A:304:MET:CE	2:A:317:GLN:HB3	2.50	0.42
2:A:147:TRP:CD2	2:A:151:LYS:HB2	2.55	0.41
2:A:159:ILE:HD11	2:A:320:GLU:CD	2.45	0.41
2:A:174:ILE:HG22	2:A:175:GLU:N	2.32	0.41
2:A:158:VAL:HG13	2:A:158:VAL:O	2.21	0.41
2:A:207:ALA:O	2:A:208:MET:HB2	2.20	0.41
2:A:313:ARG:HG3	2:A:314:GLU:H	1.84	0.41
2:A:163:PHE:CD1	2:A:163:PHE:C	2.97	0.41
2:A:264:ARG:O	2:A:268:ASP:HB2	2.19	0.41
2:A:313:ARG:HG3	2:A:314:GLU:N	2.36	0.41
2:A:108:LEU:HD23	2:A:108:LEU:HA	1.90	0.41
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.21	0.41
2:A:276:ASN:HB2	2:A:291:HIS:HA	2.03	0.41
2:A:8:ALA:O	2:A:12:ASN:N	2.54	0.41
2:A:43:LEU:N	2:A:43:LEU:HD23	2.35	0.41
2:A:250:MET:C	2:A:253:GLY:H	2.29	0.41
2:A:4:ILE:CG2	2:A:5:LYS:N	2.84	0.41
2:A:105:ARG:CA	2:A:133:MET:CE	2.99	0.41
2:A:291:HIS:HE1	2:A:293:PRO:HA	1.85	0.41
2:A:322:HIS:HA	2:A:323:PRO:HD3	1.95	0.41
2:A:280:ALA:O	2:A:283:PHE:HB2	2.21	0.41
2:A:127:PRO:CB	2:A:129:PRO:HD2	2.37	0.40
2:A:9:LYS:HE3	2:A:9:LYS:HB2	1.50	0.40
2:A:197:LEU:O	2:A:200:PHE:HB3	2.21	0.40
2:A:307:ASP:O	2:A:311:ASN:N	2.55	0.40
1:B:701:DC:OP1	2:A:32:THR:OG1	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:ASN:ND2	2:A:100:ASN:C	2.80	0.40
2:A:215:TRP:CZ2	2:A:239:ARG:C	3.00	0.40
2:A:308:ARG:HH11	2:A:308:ARG:HD3	1.75	0.40
2:A:221:PHE:HA	2:A:250:MET:HG3	2.03	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%)	293 (87%)	39 (12%)	4 (1%)	10 23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	278	ARG
2	A	312	LYS
2	A	71	ALA

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%)	182 (65%)	97 (35%)	0 0

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR
2	A	5	LYS
2	A	6	ASP
2	A	7	VAL
2	A	9	LYS
2	A	10	ARG
2	A	12	ASN
2	A	13	VAL
2	A	16	THR
2	A	19	SER
2	A	21	VAL
2	A	22	ILE
2	A	23	ASN
2	A	25	THR
2	A	26	ARG
2	A	31	GLU
2	A	33	ARG
2	A	40	ILE
2	A	41	LYS
2	A	43	LEU
2	A	44	HIS
2	A	48	SER
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	76	GLU
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	93	ILE
2	A	99	ASN
2	A	101	LEU
2	A	109	SER
2	A	110	MET
2	A	120	LEU

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Mol	Chain	Res	Type
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	136	GLU
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	155	THR
2	A	158	VAL
2	A	174	ILE
2	A	176	ARG
2	A	179	ARG
2	A	183	VAL
2	A	189	GLU
2	A	190	ARG
2	A	201	MET
2	A	202	LYS
2	A	205	GLU
2	A	208	MET
2	A	209	ILE
2	A	210	LYS
2	A	211	VAL
2	A	213	GLU
2	A	216	ILE
2	A	218	GLN
2	A	224	GLU
2	A	228	ARG
2	A	230	MET
2	A	235	SER
2	A	239	ARG
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

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Mol	Chain	Res	Type
2	A	279	ASN
2	A	284	THR
2	A	288	THR
2	A	292	GLN
2	A	294	LYS
2	A	296	SER
2	A	310	VAL
2	A	312	LYS
2	A	315	GLU
2	A	325	LEU
2	A	328	ARG
2	A	329	ARG
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	12	ASN
2	A	23	ASN
2	A	99	ASN
2	A	100	ASN
2	A	104	GLN
2	A	113	GLN
2	A	139	HIS
2	A	218	GLN
2	A	231	GLN
2	A	279	ASN
2	A	291	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 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	GUN	A	599	-	12,12,12	0.61	0	15,17,17	0.50	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
3	GUN	A	599	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

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	GUN	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.