Full wwPDB EM Validation Report

Mar 6, 2025 – 03:11 pm GMT

PDB ID	:	9Q96
EMDB ID	:	EMD-52919
Title	:	Cryo-EM Structure of Bacterial RNA polymerase-sigma54 transcription open complex with wild type sigma54, from RPi(-10-1)
Authors	:	Gao, F.; Zhang, X.
Deposited on	:	2025-02-26
Resolution	:	4.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

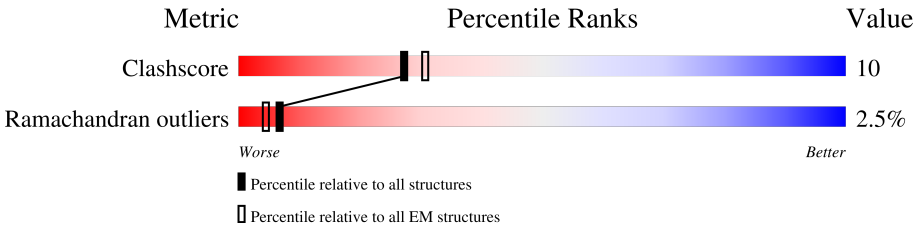
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	329	84% 9% • 6%
1	B	329	67% 5% 29%
2	C	1342	79% 18% •
3	D	1407	77% 15% • • •
4	E	91	74% • • • 18%
5	M	497	52% 9% • 36%
6	N	46	22% 78%
7	T	46	22% 54% 13% 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19633 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	309	Total 1526	C 908	N 309	O 309	0	0
1	B	235	Total 1160	C 690	N 235	O 235	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	1341	Total 6599	C 3917	N 1341	O 1341	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	1345	Total 6619	C 3929	N 1345	O 1345	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	75	Total 371	C 221	N 75	O 75	0	0

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	316	Total 1570	C 938	N 316	O 316	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP A0A377VEN9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-18	GLY	-	expression tag	UNP A0A377VEN9
M	-17	SER	-	expression tag	UNP A0A377VEN9
M	-16	SER	-	expression tag	UNP A0A377VEN9
M	-15	HIS	-	expression tag	UNP A0A377VEN9
M	-14	HIS	-	expression tag	UNP A0A377VEN9
M	-13	HIS	-	expression tag	UNP A0A377VEN9
M	-12	HIS	-	expression tag	UNP A0A377VEN9
M	-11	HIS	-	expression tag	UNP A0A377VEN9
M	-10	HIS	-	expression tag	UNP A0A377VEN9
M	-9	SER	-	expression tag	UNP A0A377VEN9
M	-8	SER	-	expression tag	UNP A0A377VEN9
M	-7	GLY	-	expression tag	UNP A0A377VEN9
M	-6	LEU	-	expression tag	UNP A0A377VEN9
M	-5	VAL	-	expression tag	UNP A0A377VEN9
M	-4	PRO	-	expression tag	UNP A0A377VEN9
M	-3	ARG	-	expression tag	UNP A0A377VEN9
M	-2	GLY	-	expression tag	UNP A0A377VEN9
M	-1	SER	-	expression tag	UNP A0A377VEN9
M	0	HIS	-	expression tag	UNP A0A377VEN9
M	1	MET	-	expression tag	UNP A0A377VEN9
M	2	LYS	-	expression tag	UNP A0A377VEN9
M	3	GLN	-	expression tag	UNP A0A377VEN9
M	4	GLY	-	expression tag	UNP A0A377VEN9
M	5	LEU	-	expression tag	UNP A0A377VEN9
M	6	GLN	-	expression tag	UNP A0A377VEN9
M	7	LEU	-	expression tag	UNP A0A377VEN9
M	8	ARG	-	expression tag	UNP A0A377VEN9
M	9	LEU	-	expression tag	UNP A0A377VEN9
M	10	SER	-	expression tag	UNP A0A377VEN9
M	11	GLN	-	expression tag	UNP A0A377VEN9
M	12	GLN	-	expression tag	UNP A0A377VEN9
M	13	LEU	-	expression tag	UNP A0A377VEN9
M	14	ALA	-	expression tag	UNP A0A377VEN9
M	15	MET	-	expression tag	UNP A0A377VEN9
M	16	THR	-	expression tag	UNP A0A377VEN9
M	17	PRO	-	expression tag	UNP A0A377VEN9
M	18	GLN	-	expression tag	UNP A0A377VEN9
M	19	LEU	-	expression tag	UNP A0A377VEN9
M	20	GLN	-	expression tag	UNP A0A377VEN9
M	21	GLN	-	expression tag	UNP A0A377VEN9
M	22	ALA	-	expression tag	UNP A0A377VEN9
M	23	ILE	-	expression tag	UNP A0A377VEN9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	24	ARG	-	expression tag	UNP A0A377VEN9
M	25	LEU	-	expression tag	UNP A0A377VEN9

- Molecule 6 is a DNA chain called NIFH PROMOTER NON-TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	46	Total	C	N	O	P	0	0
			946	448	173	279	46		

- Molecule 7 is a DNA chain called NIFH PROMOTER TEMPLATE DNA.

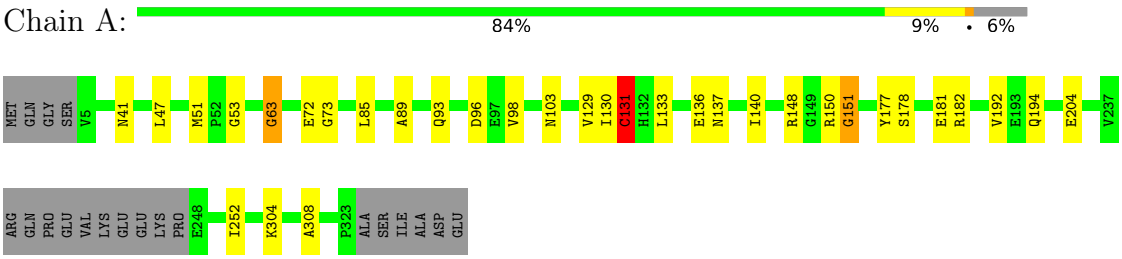
Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	41	Total	C	N	O	P	0	0
			842	396	165	240	41		

3 Residue-property plots (i)

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.

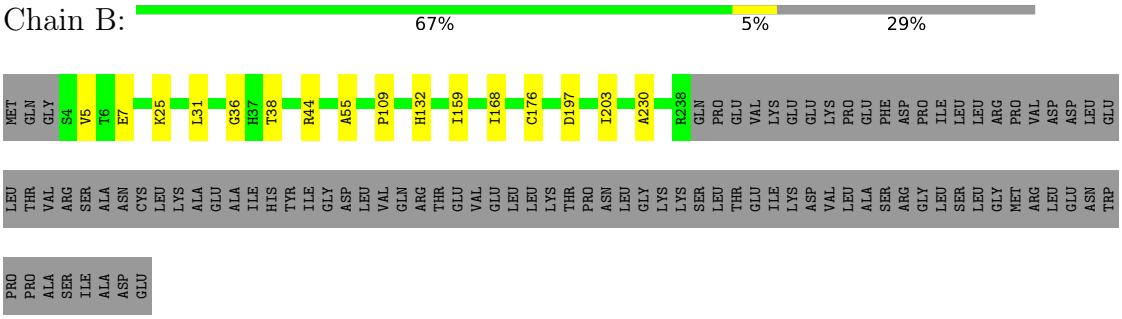
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



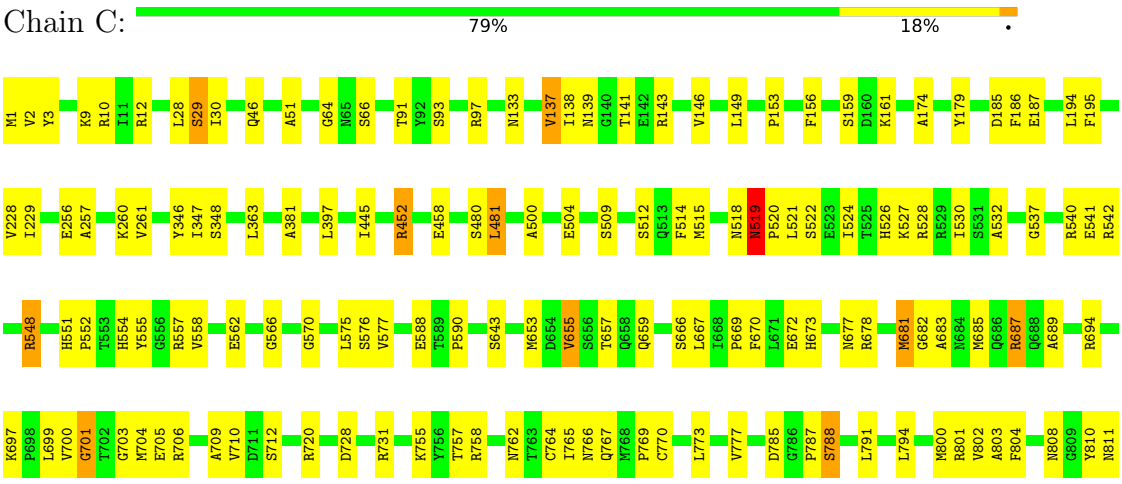
• Molecule 1: DNA-directed RNA polymerase subunit alpha

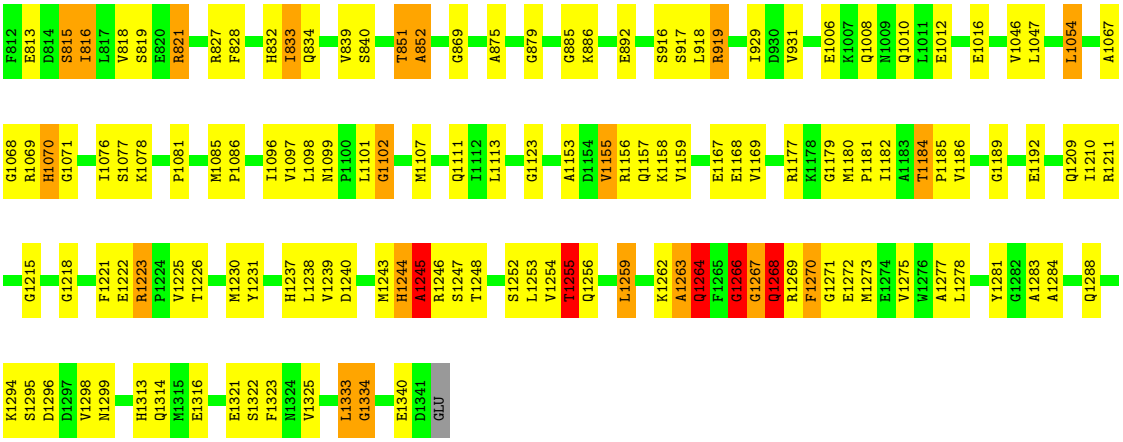
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

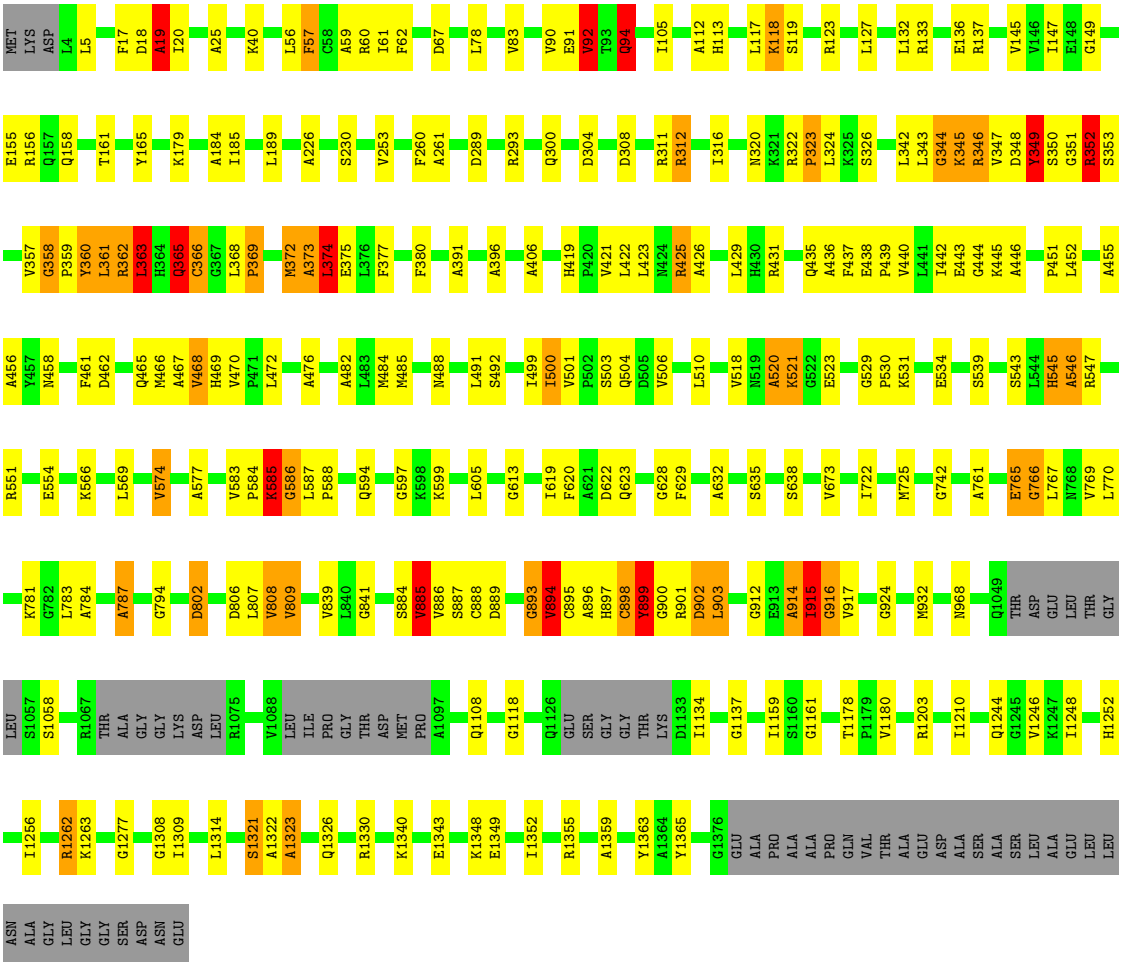
Chain C:





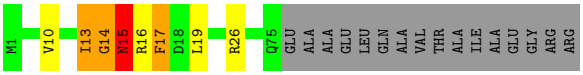
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



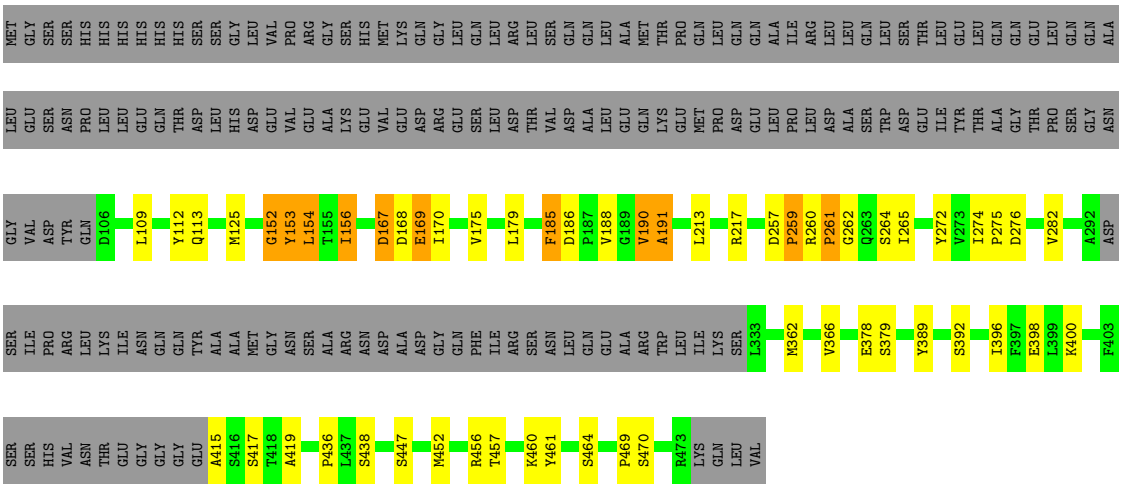
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



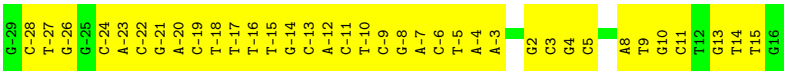
• Molecule 5: RNA polymerase sigma-54 factor

Chain M:



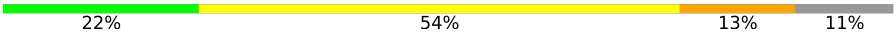
• Molecule 6: NIFH PROMOTER NON-TEMPLATE DNA

Chain N:



• Molecule 7: NIFH PROMOTER TEMPLATE DNA

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	20233, 20233, 79678, 20233	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	A	1.50	13/1524 (0.9%)	1.31	9/2119 (0.4%)
1	B	1.15	5/1159 (0.4%)	1.05	1/1612 (0.1%)
2	C	1.77	159/6598 (2.4%)	1.50	93/9172 (1.0%)
3	D	1.67	133/6614 (2.0%)	1.48	83/9188 (0.9%)
4	E	1.21	2/370 (0.5%)	1.19	1/514 (0.2%)
5	M	0.94	7/1567 (0.4%)	0.98	9/2183 (0.4%)
6	N	0.50	0/1060	0.82	1/1635 (0.1%)
7	T	0.70	1/945 (0.1%)	1.28	14/1453 (1.0%)
All	All	1.53	320/19837 (1.6%)	1.37	211/27876 (0.8%)

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
1	A	0	6
2	C	0	24
3	D	0	24
4	E	0	1
5	M	0	1
All	All	0	56

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	555	TYR	C-O	10.89	1.44	1.23
2	C	526	HIS	C-O	-10.65	1.03	1.23
2	C	1295	SER	CA-CB	10.07	1.68	1.52
3	D	360	TYR	N-CA	9.79	1.66	1.46
2	C	794	LEU	C-O	9.78	1.42	1.23
3	D	369	PRO	N-CA	9.77	1.63	1.47
3	D	359	PRO	CA-CB	9.72	1.73	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1323	ALA	C-O	9.66	1.41	1.23
1	A	151	GLY	N-CA	9.63	1.60	1.46
3	D	429	LEU	C-O	9.61	1.41	1.23
3	D	362	ARG	N-CA	-9.60	1.27	1.46
3	D	597	GLY	C-O	9.59	1.39	1.23
2	C	1225	VAL	C-O	9.52	1.41	1.23
2	C	827	ARG	N-CA	9.51	1.65	1.46
3	D	623	GLN	C-O	9.41	1.41	1.23
2	C	519	ASN	N-CA	9.14	1.64	1.46
2	C	149	LEU	C-O	9.10	1.40	1.23
2	C	143	ARG	C-O	-8.81	1.06	1.23
3	D	451	PRO	C-O	8.70	1.40	1.23
2	C	815	SER	CA-CB	-8.69	1.40	1.52
2	C	879	GLY	C-O	-8.66	1.09	1.23
3	D	543	SER	CA-CB	8.63	1.65	1.52
2	C	1238	LEU	N-CA	8.56	1.63	1.46
2	C	813	GLU	C-O	8.51	1.39	1.23
3	D	841	GLY	N-CA	8.51	1.58	1.46
2	C	1181	PRO	C-O	-8.44	1.06	1.23
3	D	916	GLY	C-O	8.35	1.37	1.23
2	C	1334	GLY	C-O	8.28	1.36	1.23
2	C	699	LEU	C-O	-8.16	1.07	1.23
2	C	1078	LYS	C-O	8.15	1.38	1.23
3	D	352	ARG	N-CA	8.14	1.62	1.46
3	D	345	LYS	CA-CB	8.12	1.71	1.53
3	D	373	ALA	N-CA	8.09	1.62	1.46
2	C	452	ARG	C-O	8.04	1.38	1.23
3	D	1277	GLY	N-CA	8.00	1.58	1.46
3	D	492	SER	C-O	-7.89	1.08	1.23
2	C	1243	MET	CA-C	7.86	1.73	1.52
2	C	577	VAL	C-O	7.84	1.38	1.23
1	B	31	LEU	C-O	7.80	1.38	1.23
2	C	677	ASN	C-O	7.76	1.38	1.23
2	C	697	LYS	N-CA	7.75	1.61	1.46
2	C	518	ASN	N-CA	7.75	1.61	1.46
1	A	181	GLU	N-CA	7.75	1.61	1.46
2	C	683	ALA	C-O	7.72	1.38	1.23
3	D	1365	TYR	C-O	-7.72	1.08	1.23
3	D	1363	TYR	C-O	7.63	1.37	1.23
2	C	803	ALA	C-O	7.60	1.37	1.23
3	D	472	LEU	CA-CB	-7.58	1.36	1.53
2	C	1270	PHE	CA-CB	-7.56	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	515	MET	C-O	7.52	1.37	1.23
2	C	1215	GLY	N-CA	-7.47	1.34	1.46
2	C	1247	SER	N-CA	7.39	1.61	1.46
2	C	1111	GLN	C-O	7.38	1.37	1.23
3	D	924	GLY	N-CA	-7.37	1.35	1.46
2	C	1086	PRO	N-CA	7.35	1.59	1.47
2	C	1113	LEU	C-O	7.31	1.37	1.23
3	D	462	ASP	N-CA	7.28	1.60	1.46
3	D	1340	LYS	C-O	-7.28	1.09	1.23
2	C	667	LEU	C-O	7.26	1.37	1.23
2	C	834	GLN	C-O	7.25	1.37	1.23
2	C	576	SER	CA-CB	-7.20	1.42	1.52
3	D	622	ASP	C-O	7.20	1.37	1.23
5	M	190	VAL	C-O	7.20	1.37	1.23
2	C	818	VAL	CA-CB	7.19	1.69	1.54
2	C	804	PHE	N-CA	7.18	1.60	1.46
2	C	1298	VAL	C-O	7.17	1.36	1.23
3	D	894	VAL	C-O	-7.14	1.09	1.23
3	D	901	ARG	C-O	7.13	1.36	1.23
2	C	133	ASN	N-CA	-7.11	1.32	1.46
3	D	889	ASP	CA-CB	7.10	1.69	1.53
2	C	1268	GLN	CA-CB	7.09	1.69	1.53
2	C	1246	ARG	N-CA	7.05	1.60	1.46
2	C	764	CYS	N-CA	7.05	1.60	1.46
1	A	151	GLY	C-O	-7.03	1.12	1.23
1	B	44	ARG	C-O	7.03	1.36	1.23
2	C	800	MET	CA-CB	7.03	1.69	1.53
3	D	899	TYR	CA-CB	7.01	1.69	1.53
3	D	769	VAL	N-CA	6.99	1.60	1.46
3	D	742	GLY	C-O	-6.98	1.12	1.23
5	M	152	GLY	C-O	-6.97	1.12	1.23
7	T	-3	DG	P-OP2	6.96	1.60	1.49
3	D	476	ALA	CA-CB	-6.95	1.37	1.52
2	C	520	PRO	C-O	6.94	1.37	1.23
2	C	1277	ALA	CA-CB	-6.94	1.37	1.52
3	D	900	GLY	C-O	-6.92	1.12	1.23
3	D	794	GLY	N-CA	-6.92	1.35	1.46
3	D	456	ALA	N-CA	6.91	1.60	1.46
3	D	425	ARG	C-O	-6.90	1.10	1.23
3	D	360	TYR	CA-C	6.81	1.70	1.52
2	C	1177	ARG	C-O	-6.81	1.10	1.23
5	M	262	GLY	N-CA	6.81	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	931	VAL	C-O	6.76	1.36	1.23
3	D	358	GLY	CA-C	6.74	1.62	1.51
3	D	628	GLY	N-CA	6.74	1.56	1.46
2	C	514	PHE	C-O	6.72	1.36	1.23
2	C	552	PRO	CA-CB	-6.71	1.40	1.53
2	C	1215	GLY	CA-C	-6.71	1.41	1.51
3	D	917	VAL	C-O	6.71	1.36	1.23
1	A	51	MET	C-O	6.70	1.36	1.23
2	C	1071	GLY	CA-C	6.69	1.62	1.51
1	A	182	ARG	N-CA	6.68	1.59	1.46
3	D	308	ASP	N-CA	6.67	1.59	1.46
2	C	1068	GLY	N-CA	6.66	1.56	1.46
2	C	1264	GLN	C-O	6.65	1.35	1.23
3	D	458	ASN	C-O	-6.64	1.10	1.23
3	D	770	LEU	C-O	6.63	1.35	1.23
2	C	1231	TYR	C-O	6.63	1.35	1.23
2	C	770	CYS	N-CA	6.61	1.59	1.46
3	D	422	LEU	CA-CB	6.61	1.69	1.53
2	C	153	PRO	C-O	6.60	1.36	1.23
2	C	1101	LEU	C-O	6.59	1.35	1.23
2	C	757	THR	C-O	-6.55	1.10	1.23
3	D	808	VAL	C-O	-6.52	1.10	1.23
3	D	912	GLY	CA-C	6.52	1.62	1.51
2	C	1273	MET	CA-CB	-6.51	1.39	1.53
3	D	784	ALA	C-O	-6.51	1.10	1.23
3	D	808	VAL	CA-CB	6.49	1.68	1.54
1	A	41	ASN	C-O	6.49	1.35	1.23
3	D	365	GLN	CA-CB	6.49	1.68	1.53
2	C	1179	GLY	C-O	6.45	1.33	1.23
3	D	888	CYS	C-O	6.44	1.35	1.23
3	D	506	VAL	C-O	6.44	1.35	1.23
2	C	1218	GLY	N-CA	6.43	1.55	1.46
3	D	360	TYR	CA-CB	-6.42	1.39	1.53
2	C	590	PRO	CA-C	-6.41	1.40	1.52
3	D	351	GLY	N-CA	6.40	1.55	1.46
3	D	841	GLY	C-O	6.39	1.33	1.23
2	C	1299	ASN	CA-C	6.39	1.69	1.52
3	D	112	ALA	CA-CB	6.39	1.65	1.52
3	D	351	GLY	C-O	6.36	1.33	1.23
2	C	701	GLY	C-O	6.34	1.33	1.23
3	D	783	LEU	C-O	6.31	1.35	1.23
2	C	9	LYS	C-O	-6.30	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1334	GLY	N-CA	6.29	1.55	1.46
1	A	178	SER	C-O	-6.28	1.11	1.23
3	D	469	HIS	C-O	6.27	1.35	1.23
3	D	766	GLY	N-CA	6.27	1.55	1.46
1	A	129	VAL	C-O	-6.26	1.11	1.23
2	C	1239	VAL	N-CA	6.22	1.58	1.46
3	D	1256	ILE	N-CA	-6.22	1.33	1.46
2	C	705	GLU	C-O	6.21	1.35	1.23
3	D	1321	SER	C-O	6.21	1.35	1.23
3	D	521	LYS	CA-CB	6.19	1.67	1.53
5	M	153	TYR	CA-CB	6.18	1.67	1.53
3	D	491	LEU	C-O	6.16	1.35	1.23
2	C	1277	ALA	C-O	6.15	1.35	1.23
2	C	537	GLY	C-O	-6.14	1.13	1.23
2	C	548	ARG	CA-CB	6.13	1.67	1.53
2	C	1184	THR	N-CA	6.13	1.58	1.46
2	C	524	ILE	N-CA	-6.12	1.34	1.46
2	C	765	ILE	N-CA	6.12	1.58	1.46
5	M	154	LEU	C-O	-6.11	1.11	1.23
3	D	722	ILE	C-O	6.11	1.34	1.23
2	C	1107	MET	N-CA	6.10	1.58	1.46
3	D	377	PHE	CA-C	6.08	1.68	1.52
1	A	96	ASP	C-O	-6.08	1.11	1.23
2	C	521	LEU	N-CA	-6.08	1.34	1.46
3	D	885	VAL	N-CA	6.07	1.58	1.46
3	D	902	ASP	C-O	6.07	1.34	1.23
2	C	512	SER	C-O	6.06	1.34	1.23
2	C	29	SER	C-O	6.05	1.34	1.23
1	A	63	GLY	CA-C	6.05	1.61	1.51
2	C	562	GLU	CA-CB	6.05	1.67	1.53
3	D	421	VAL	C-O	6.04	1.34	1.23
2	C	1096	ILE	N-CA	6.04	1.58	1.46
3	D	445	LYS	N-CA	-6.04	1.34	1.46
2	C	1271	GLY	C-O	6.03	1.33	1.23
2	C	1246	ARG	CA-C	-6.00	1.37	1.52
2	C	1211	ARG	N-CA	6.00	1.58	1.46
3	D	437	PHE	CA-CB	6.00	1.67	1.53
3	D	357	VAL	CA-C	5.96	1.68	1.52
2	C	1248	THR	C-O	5.95	1.34	1.23
2	C	769	PRO	CA-CB	-5.94	1.41	1.53
2	C	1313	HIS	N-CA	5.94	1.58	1.46
2	C	557	ARG	N-CA	-5.93	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	755	LYS	CA-CB	-5.90	1.41	1.53
3	D	613	GLY	N-CA	5.90	1.54	1.46
3	D	368	LEU	N-CA	5.90	1.58	1.46
3	D	443	GLU	C-O	5.87	1.34	1.23
2	C	1123	GLY	C-O	5.86	1.33	1.23
2	C	522	SER	N-CA	-5.84	1.34	1.46
3	D	462	ASP	CA-C	5.83	1.68	1.52
2	C	828	PHE	N-CA	5.81	1.57	1.46
1	A	204	GLU	C-O	5.81	1.34	1.23
2	C	672	GLU	CA-CB	-5.80	1.41	1.53
3	D	501	VAL	N-CA	-5.79	1.34	1.46
3	D	419	HIS	CA-CB	-5.78	1.41	1.53
3	D	924	GLY	CA-C	-5.78	1.42	1.51
2	C	731	ARG	CA-CB	5.78	1.66	1.53
2	C	138	ILE	C-O	5.78	1.34	1.23
3	D	436	ALA	CA-CB	5.78	1.64	1.52
2	C	93	SER	CA-CB	5.77	1.61	1.52
3	D	585	LYS	C-O	5.75	1.34	1.23
1	B	197	ASP	C-O	5.75	1.34	1.23
3	D	372	MET	C-O	-5.74	1.12	1.23
3	D	781	LYS	C-O	-5.74	1.12	1.23
2	C	1099	ASN	CA-C	-5.73	1.38	1.52
2	C	655	VAL	C-O	5.73	1.34	1.23
3	D	482	ALA	C-O	5.72	1.34	1.23
3	D	452	LEU	C-O	5.72	1.34	1.23
2	C	821	ARG	N-CA	-5.71	1.34	1.46
2	C	1111	GLN	N-CA	-5.68	1.34	1.46
2	C	1322	SER	N-CA	-5.66	1.35	1.46
2	C	452	ARG	CA-CB	5.65	1.66	1.53
3	D	436	ALA	C-O	5.65	1.34	1.23
2	C	1192	GLU	N-CA	5.64	1.57	1.46
3	D	599	LYS	C-O	5.64	1.34	1.23
2	C	762	ASN	CA-C	5.63	1.67	1.52
2	C	1284	ALA	C-O	5.63	1.34	1.23
3	D	787	ALA	C-O	5.58	1.33	1.23
1	B	38	THR	C-O	5.58	1.33	1.23
1	A	133	LEU	N-CA	-5.57	1.35	1.46
3	D	794	GLY	CA-C	-5.57	1.43	1.51
4	E	13	ILE	C-O	5.56	1.33	1.23
2	C	687	ARG	N-CA	-5.56	1.35	1.46
3	D	353	SER	CA-CB	5.55	1.61	1.52
2	C	526	HIS	N-CA	5.55	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	GLY	CA-C	-5.55	1.43	1.51
3	D	917	VAL	N-CA	-5.53	1.35	1.46
2	C	682	GLY	CA-C	5.52	1.60	1.51
3	D	914	ALA	CA-CB	-5.52	1.40	1.52
3	D	588	PRO	N-CA	-5.52	1.37	1.47
3	D	629	PHE	N-CA	-5.52	1.35	1.46
3	D	470	VAL	CA-CB	-5.51	1.43	1.54
2	C	526	HIS	CA-CB	-5.51	1.41	1.53
4	E	26	ARG	C-O	-5.51	1.12	1.23
3	D	620	PHE	C-O	5.50	1.33	1.23
2	C	801	ARG	C-O	5.50	1.33	1.23
3	D	359	PRO	N-CA	5.49	1.56	1.47
3	D	444	GLY	N-CA	5.48	1.54	1.46
2	C	566	GLY	C-O	-5.48	1.14	1.23
2	C	687	ARG	CA-CB	5.46	1.66	1.53
2	C	694	ARG	C-O	5.44	1.33	1.23
2	C	458	GLU	C-O	5.42	1.33	1.23
2	C	808	ASN	C-O	5.41	1.33	1.23
2	C	97	ARG	C-O	-5.41	1.13	1.23
3	D	468	VAL	C-O	5.41	1.33	1.23
3	D	440	VAL	C-O	5.40	1.33	1.23
2	C	1069	ARG	C-O	5.40	1.33	1.23
2	C	659	GLN	CA-C	-5.40	1.39	1.52
2	C	706	ARG	C-O	5.39	1.33	1.23
3	D	488	ASN	C-O	5.38	1.33	1.23
5	M	191	ALA	CA-CB	5.38	1.63	1.52
3	D	1326	GLN	CA-C	-5.38	1.39	1.52
2	C	1316	GLU	N-CA	5.37	1.57	1.46
2	C	551	HIS	C-O	5.37	1.33	1.23
2	C	697	LYS	C-O	5.37	1.33	1.23
2	C	12	ARG	N-CA	5.37	1.57	1.46
3	D	351	GLY	CA-C	-5.36	1.43	1.51
3	D	488	ASN	CA-C	-5.35	1.39	1.52
2	C	1323	PHE	N-CA	5.34	1.57	1.46
2	C	653	MET	C-O	5.33	1.33	1.23
3	D	492	SER	CA-C	-5.33	1.39	1.52
3	D	1248	ILE	C-O	5.33	1.33	1.23
2	C	808	ASN	N-CA	-5.33	1.35	1.46
3	D	725	MET	CA-CB	-5.33	1.42	1.53
2	C	1240	ASP	N-CA	-5.32	1.35	1.46
3	D	113	HIS	CA-C	-5.30	1.39	1.52
3	D	1330	ARG	C-O	5.30	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	GLY	C-O	5.29	1.32	1.23
3	D	374	LEU	N-CA	5.29	1.56	1.46
3	D	484	MET	N-CA	5.27	1.56	1.46
3	D	761	ALA	CA-CB	5.27	1.63	1.52
2	C	685	MET	C-O	-5.26	1.13	1.23
2	C	758	ARG	CA-C	5.26	1.66	1.52
3	D	619	ILE	C-O	5.26	1.33	1.23
2	C	1325	VAL	N-CA	-5.25	1.35	1.46
2	C	1275	VAL	C-O	5.25	1.33	1.23
5	M	152	GLY	N-CA	5.24	1.53	1.46
3	D	518	VAL	C-O	5.24	1.33	1.23
2	C	1047	LEU	C-O	-5.23	1.13	1.23
3	D	421	VAL	N-CA	5.22	1.56	1.46
2	C	681	MET	CA-CB	5.22	1.65	1.53
3	D	1352	ILE	C-O	-5.22	1.13	1.23
2	C	657	THR	C-O	5.21	1.33	1.23
2	C	1283	ALA	N-CA	-5.20	1.35	1.46
2	C	916	SER	C-O	-5.20	1.13	1.23
3	D	802	ASP	C-O	5.19	1.33	1.23
2	C	1226	THR	C-O	5.19	1.33	1.23
3	D	638	SER	C-O	-5.18	1.13	1.23
2	C	1278	LEU	C-O	5.18	1.33	1.23
2	C	777	VAL	C-O	5.17	1.33	1.23
2	C	710	VAL	CA-CB	-5.17	1.43	1.54
2	C	827	ARG	C-O	5.16	1.33	1.23
3	D	914	ALA	C-N	-5.16	1.22	1.34
3	D	465	GLN	C-O	5.16	1.33	1.23
2	C	788	SER	CA-CB	5.15	1.60	1.52
2	C	1123	GLY	N-CA	-5.15	1.38	1.46
3	D	632	ALA	CA-C	-5.15	1.39	1.52
2	C	703	GLY	C-O	5.14	1.31	1.23
3	D	119	SER	N-CA	5.14	1.56	1.46
3	D	431	ARG	CA-CB	-5.13	1.42	1.53
2	C	678	ARG	CA-C	5.12	1.66	1.52
3	D	1252	HIS	C-O	5.11	1.33	1.23
2	C	666	SER	C-O	5.11	1.33	1.23
3	D	349	TYR	C-O	5.11	1.33	1.23
2	C	1259	LEU	C-O	-5.10	1.13	1.23
3	D	1308	GLY	C-O	5.10	1.31	1.23
2	C	832	HIS	C-O	5.09	1.33	1.23
3	D	40	LYS	N-CA	5.08	1.56	1.46
2	C	764	CYS	CA-CB	5.08	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1321	GLU	CA-CB	5.07	1.65	1.53
3	D	1359	ALA	CA-C	-5.07	1.39	1.52
1	A	85	LEU	CA-C	-5.06	1.39	1.52
2	C	1102	GLY	N-CA	5.06	1.53	1.46
3	D	94	GLN	CA-CB	5.06	1.65	1.53
3	D	366	CYS	CA-C	-5.06	1.39	1.52
3	D	406	ALA	C-O	-5.06	1.13	1.23
3	D	766	GLY	C-O	5.05	1.31	1.23
2	C	1158	LYS	N-CA	-5.05	1.36	1.46
2	C	1070	HIS	CA-CB	-5.04	1.42	1.53
2	C	1077	SER	N-CA	-5.04	1.36	1.46
3	D	638	SER	CA-CB	5.04	1.60	1.52
3	D	545	HIS	N-CA	-5.04	1.36	1.46
2	C	669	PRO	CA-C	-5.03	1.42	1.52
2	C	834	GLN	CA-C	-5.03	1.39	1.52
2	C	791	LEU	C-O	5.02	1.32	1.23
3	D	363	LEU	C-O	5.01	1.32	1.23
2	C	703	GLY	CA-C	-5.01	1.43	1.51
2	C	839	VAL	C-O	5.00	1.32	1.23

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	0	DC	O5'-P-OP2	-14.62	92.55	105.70
7	T	-1	DC	O5'-P-OP1	-13.57	93.49	105.70
3	D	353	SER	N-CA-CB	12.88	129.83	110.50
2	C	554	HIS	N-CA-CB	-10.74	91.26	110.60
3	D	765	GLU	C-N-CA	-10.48	100.29	122.30
5	M	186	ASP	N-CA-CB	10.29	129.11	110.60
7	T	-1	DC	O5'-P-OP2	10.05	122.76	110.70
2	C	1246	ARG	CB-CA-C	-9.70	91.01	110.40
2	C	827	ARG	CB-CA-C	-9.40	91.60	110.40
3	D	462	ASP	N-CA-C	-9.25	86.03	111.00
2	C	1267	GLY	C-N-CA	-9.17	98.77	121.70
2	C	1180	MET	CB-CA-C	-9.17	92.06	110.40
3	D	504	GLN	CB-CA-C	8.97	128.34	110.40
5	M	272	TYR	N-CA-CB	-8.87	94.63	110.60
3	D	345	LYS	CB-CA-C	8.63	127.67	110.40
2	C	1268	GLN	CB-CA-C	8.59	127.57	110.40
7	T	-1	DC	P-O5'-C5'	8.31	134.19	120.90
3	D	373	ALA	O-C-N	-8.29	109.43	122.70
3	D	113	HIS	CB-CA-C	-8.29	93.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1288	GLN	CB-CA-C	-8.23	93.94	110.40
2	C	819	SER	N-CA-CB	8.11	122.66	110.50
2	C	1239	VAL	CB-CA-C	-7.98	96.24	111.40
2	C	1159	VAL	CB-CA-C	-7.96	96.28	111.40
7	T	0	DC	N1-C1'-C2'	7.79	127.40	112.60
3	D	539	SER	O-C-N	-7.58	110.31	123.20
2	C	794	LEU	CB-CA-C	-7.54	95.87	110.20
3	D	1323	ALA	O-C-N	7.52	134.73	122.70
2	C	1081	PRO	CB-CA-C	-7.51	93.21	112.00
5	M	261	PRO	N-CA-CB	7.48	112.28	103.30
2	C	1333	LEU	O-C-N	-7.46	110.52	123.20
2	C	700	VAL	CB-CA-C	-7.36	97.41	111.40
3	D	467	ALA	CB-CA-C	-7.35	99.08	110.10
3	D	534	GLU	N-CA-CB	7.34	123.81	110.60
2	C	1263	ALA	CB-CA-C	-7.32	99.12	110.10
2	C	1294	LYS	N-CA-CB	-7.32	97.43	110.60
1	A	73	GLY	N-CA-C	7.31	131.38	113.10
3	D	586	GLY	N-CA-C	7.31	131.37	113.10
2	C	555	TYR	C-N-CA	-7.28	107.01	122.30
2	C	787	PRO	N-CA-C	-7.23	93.30	112.10
3	D	326	SER	N-CA-CB	-7.22	99.67	110.50
5	M	156	ILE	CB-CA-C	7.20	126.01	111.60
3	D	300	GLN	N-CA-CB	7.20	123.56	110.60
3	D	380	PHE	N-CA-CB	-7.16	97.70	110.60
3	D	365	GLN	CB-CA-C	-7.14	96.11	110.40
3	D	377	PHE	N-CA-CB	-7.14	97.74	110.60
2	C	1322	SER	CB-CA-C	7.09	123.57	110.10
2	C	678	ARG	CB-CA-C	7.07	124.53	110.40
2	C	731	ARG	N-CA-CB	6.99	123.18	110.60
3	D	373	ALA	N-CA-C	-6.98	92.16	111.00
3	D	1262	ARG	N-CA-CB	-6.90	98.18	110.60
2	C	810	TYR	N-CA-CB	6.89	123.00	110.60
3	D	451	PRO	N-CA-CB	6.85	111.52	103.30
3	D	885	VAL	N-CA-C	-6.79	92.65	111.00
2	C	527	LYS	O-C-N	-6.77	111.87	122.70
3	D	461	PHE	N-CA-CB	-6.75	98.44	110.60
2	C	813	GLU	C-N-CA	-6.74	104.86	121.70
2	C	532	ALA	CB-CA-C	-6.73	100.01	110.10
3	D	423	LEU	CB-CA-C	-6.72	97.44	110.20
2	C	528	ARG	CB-CA-C	-6.71	96.97	110.40
3	D	485	MET	CB-CA-C	-6.71	96.98	110.40
3	D	374	LEU	N-CA-CB	6.70	123.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	811	ASN	N-CA-C	-6.68	92.97	111.00
2	C	1238	LEU	C-N-CA	-6.67	105.03	121.70
2	C	1169	VAL	CB-CA-C	-6.62	98.83	111.40
2	C	1182	ILE	CB-CA-C	-6.60	98.40	111.60
2	C	577	VAL	C-N-CA	-6.60	105.20	121.70
2	C	555	TYR	N-CA-CB	6.58	122.44	110.60
2	C	764	CYS	N-CA-CB	6.56	122.40	110.60
2	C	681	MET	N-CA-CB	6.54	122.37	110.60
3	D	539	SER	CA-C-N	6.52	129.24	116.20
1	A	181	GLU	N-CA-CB	6.47	122.25	110.60
2	C	828	PHE	N-CA-C	6.43	128.35	111.00
3	D	78	LEU	CB-CA-C	6.42	122.40	110.20
6	N	2	DG	O4'-C4'-C3'	-6.42	101.93	104.50
3	D	468	VAL	CB-CA-C	-6.40	99.24	111.40
3	D	632	ALA	CB-CA-C	-6.39	100.51	110.10
3	D	808	VAL	N-CA-CB	-6.39	97.43	111.50
2	C	1295	SER	N-CA-CB	6.34	120.01	110.50
2	C	697	LYS	CB-CA-C	-6.34	97.72	110.40
2	C	1097	VAL	CB-CA-C	-6.32	99.40	111.40
3	D	808	VAL	CB-CA-C	-6.31	99.41	111.40
3	D	885	VAL	N-CA-CB	-6.31	97.63	111.50
3	D	366	CYS	N-CA-CB	6.30	121.95	110.60
3	D	898	CYS	C-N-CA	-6.29	105.97	121.70
3	D	1355	ARG	N-CA-CB	-6.28	99.29	110.60
3	D	360	TYR	O-C-N	-6.22	112.75	122.70
2	C	519	ASN	CB-CA-C	6.20	122.80	110.40
2	C	1296	ASP	CB-CA-C	-6.17	98.07	110.40
7	T	-4	DC	O5'-P-OP2	-6.09	100.22	105.70
3	D	897	HIS	N-CA-CB	6.07	121.52	110.60
2	C	1231	TYR	O-C-N	6.06	132.40	122.70
2	C	689	ALA	CB-CA-C	-6.05	101.02	110.10
3	D	574	VAL	CB-CA-C	-6.05	99.91	111.40
2	C	137	VAL	CB-CA-C	-6.04	99.93	111.40
2	C	1209	GLN	N-CA-CB	-6.02	99.76	110.60
2	C	875	ALA	CB-CA-C	-6.02	101.08	110.10
3	D	40	LYS	N-CA-CB	5.99	121.38	110.60
7	T	-1	DC	O3'-P-O5'	5.99	115.38	104.00
2	C	1266	GLY	C-N-CA	-5.98	109.73	122.30
3	D	351	GLY	C-N-CA	-5.98	106.75	121.70
2	C	672	GLU	CB-CA-C	-5.97	98.45	110.40
2	C	1192	GLU	CB-CA-C	-5.97	98.46	110.40
2	C	1067	ALA	N-CA-CB	-5.97	101.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	539	SER	C-N-CA	-5.96	109.78	122.30
2	C	1245	ALA	N-CA-C	5.96	127.09	111.00
2	C	1096	ILE	CB-CA-C	5.92	123.44	111.60
3	D	903	LEU	N-CA-C	-5.92	95.01	111.00
2	C	133	ASN	N-CA-CB	-5.91	99.96	110.60
1	A	51	MET	N-CA-CB	5.91	121.23	110.60
2	C	653	MET	CB-CA-C	-5.90	98.60	110.40
3	D	345	LYS	N-CA-C	-5.89	95.09	111.00
2	C	1237	HIS	N-CA-CB	-5.84	100.09	110.60
2	C	1323	PHE	CB-CA-C	-5.83	98.74	110.40
3	D	17	PHE	CB-CA-C	5.80	122.00	110.40
5	M	276	ASP	N-CA-CB	5.79	121.02	110.60
2	C	146	VAL	CB-CA-C	-5.79	100.40	111.40
3	D	806	ASP	N-CA-CB	-5.78	100.19	110.60
7	T	-3	DG	OP1-P-OP2	5.78	128.27	119.60
3	D	765	GLU	O-C-N	-5.77	113.38	123.20
1	A	72	GLU	CB-CA-C	-5.77	98.85	110.40
3	D	17	PHE	N-CA-CB	-5.77	100.22	110.60
3	D	895	CYS	CB-CA-C	-5.76	98.88	110.40
3	D	344	GLY	C-N-CA	-5.76	107.30	121.70
1	A	182	ARG	O-C-N	5.76	131.91	122.70
2	C	766	ASN	CB-CA-C	5.74	121.88	110.40
3	D	446	ALA	CB-CA-C	-5.74	101.50	110.10
2	C	929	ILE	N-CA-CB	-5.70	97.69	110.80
3	D	916	GLY	CA-C-N	-5.70	104.66	117.20
2	C	886	LYS	CB-CA-C	5.69	121.79	110.40
2	C	1244	HIS	C-N-CA	-5.69	107.47	121.70
2	C	788	SER	CB-CA-C	5.69	120.91	110.10
3	D	1246	VAL	CB-CA-C	-5.67	100.62	111.40
2	C	673	HIS	N-CA-CB	-5.65	100.43	110.60
3	D	361	LEU	N-CA-C	5.65	126.26	111.00
3	D	1244	GLN	N-CA-CB	5.62	120.71	110.60
2	C	445	ILE	CB-CA-C	-5.61	100.38	111.60
3	D	807	LEU	O-C-N	-5.61	113.73	122.70
3	D	784	ALA	CB-CA-C	5.59	118.49	110.10
2	C	765	ILE	N-CA-CB	5.57	123.62	110.80
2	C	1231	TYR	N-CA-C	-5.55	96.01	111.00
1	A	182	ARG	CB-CA-C	-5.54	99.33	110.40
2	C	1281	TYR	CB-CA-C	-5.53	99.34	110.40
1	A	89	ALA	N-CA-CB	5.53	117.84	110.10
2	C	1067	ALA	CB-CA-C	-5.51	101.83	110.10
1	B	230	ALA	CB-CA-C	-5.51	101.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	57	PHE	CB-CA-C	5.50	121.39	110.40
3	D	839	VAL	CB-CA-C	-5.49	100.97	111.40
5	M	259	PRO	N-CA-CB	5.49	109.89	103.30
2	C	1107	MET	CA-C-O	5.48	131.62	120.10
2	C	1273	MET	N-CA-CB	-5.48	100.73	110.60
3	D	349	TYR	CB-CA-C	-5.48	99.44	110.40
2	C	1081	PRO	N-CA-CB	-5.46	96.59	102.60
3	D	344	GLY	O-C-N	-5.46	113.96	122.70
7	T	3	DG	C1'-O4'-C4'	-5.46	104.64	110.10
3	D	359	PRO	N-CA-CB	5.46	109.85	103.30
2	C	1314	GLN	CB-CA-C	-5.45	99.49	110.40
3	D	769	VAL	CB-CA-C	-5.45	101.05	111.40
2	C	816	ILE	CB-CA-C	-5.44	100.72	111.60
2	C	149	LEU	CA-C-N	-5.44	105.23	117.20
7	T	0	DC	C1'-O4'-C4'	-5.42	104.68	110.10
2	C	1263	ALA	CA-C-O	-5.41	108.73	120.10
2	C	1054	LEU	N-CA-CB	-5.41	99.58	110.40
3	D	893	GLY	C-N-CA	-5.40	108.20	121.70
3	D	346	ARG	N-CA-C	-5.39	96.44	111.00
2	C	1221	PHE	N-CA-CB	5.39	120.30	110.60
2	C	515	MET	O-C-N	5.36	131.28	122.70
2	C	10	ARG	CB-CA-C	-5.35	99.70	110.40
3	D	19	ALA	O-C-N	-5.35	114.14	122.70
3	D	261	ALA	N-CA-CB	-5.34	102.62	110.10
3	D	488	ASN	N-CA-CB	5.33	120.19	110.60
2	C	530	ILE	N-CA-C	-5.31	96.66	111.00
3	D	583	VAL	CB-CA-C	-5.31	101.31	111.40
7	T	0	DC	C4'-C3'-O3'	-5.30	96.46	109.70
1	A	182	ARG	N-CA-CB	5.29	120.13	110.60
2	C	1107	MET	O-C-N	-5.29	114.23	122.70
3	D	1348	LYS	N-CA-CB	5.29	120.12	110.60
2	C	588	GLU	CB-CA-C	-5.25	99.89	110.40
2	C	802	VAL	N-CA-C	-5.24	96.87	111.00
7	T	12	DT	O5'-P-OP2	5.23	116.98	110.70
3	D	915	ILE	CB-CA-C	5.22	122.05	111.60
2	C	1046	VAL	CB-CA-C	-5.22	101.48	111.40
3	D	442	ILE	CB-CA-C	-5.22	101.16	111.60
3	D	914	ALA	CA-C-O	5.22	131.05	120.10
3	D	492	SER	CA-C-O	-5.21	109.16	120.10
3	D	622	ASP	O-C-N	5.20	131.02	122.70
4	E	17	PHE	CB-CA-C	-5.19	100.02	110.40
2	C	555	TYR	CB-CA-C	5.18	120.77	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	894	VAL	CB-CA-C	5.18	121.25	111.40
2	C	575	LEU	CB-CA-C	-5.18	100.35	110.20
3	D	484	MET	N-CA-C	5.17	124.97	111.00
2	C	1153	ALA	CA-C-O	-5.16	109.26	120.10
5	M	264	SER	CB-CA-C	5.16	119.91	110.10
7	T	11	DG	C4'-C3'-O3'	-5.16	96.80	109.70
7	T	-3	DG	O4'-C1'-N9	5.16	111.61	108.00
3	D	105	ILE	CB-CA-C	5.11	121.81	111.60
2	C	712	SER	CB-CA-C	-5.10	100.41	110.10
3	D	362	ARG	N-CA-CB	-5.10	101.42	110.60
3	D	1365	TYR	O-C-N	-5.08	114.57	122.70
2	C	670	PHE	N-CA-C	5.07	124.70	111.00
1	A	150	ARG	C-N-CA	-5.05	111.69	122.30
2	C	704	MET	N-CA-C	5.05	124.63	111.00
2	C	1255	THR	N-CA-CB	5.05	119.90	110.30
2	C	1270	PHE	C-N-CA	5.05	132.90	122.30
3	D	304	ASP	CB-CA-C	-5.03	100.34	110.40
2	C	833	ILE	N-CA-CB	-5.03	99.23	110.80
5	M	186	ASP	CB-CA-C	-5.02	100.36	110.40
3	D	605	LEU	CB-CA-C	-5.01	100.68	110.20
3	D	889	ASP	N-CA-CB	5.01	119.62	110.60
2	C	1294	LYS	CB-CA-C	-5.00	100.39	110.40
5	M	125	MET	CB-CA-C	5.00	120.41	110.40
3	D	896	ALA	CB-CA-C	-5.00	102.60	110.10

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	CYS	Mainchain
1	A	151	GLY	Peptide,Mainchain
1	A	47	LEU	Mainchain
1	A	63	GLY	Peptide
1	A	93	GLN	Peptide
2	C	1070	HIS	Mainchain
2	C	1085	MET	Mainchain
2	C	1098	LEU	Mainchain
2	C	1102	GLY	Peptide
2	C	1185	PRO	Peptide
2	C	1210	ILE	Mainchain
2	C	1230	MET	Mainchain
2	C	1266	GLY	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
2	C	1270	PHE	Peptide
2	C	1333	LEU	Mainchain
2	C	452	ARG	Mainchain
2	C	519	ASN	Peptide
2	C	548	ARG	Mainchain
2	C	681	MET	Mainchain
2	C	687	ARG	Mainchain
2	C	709	ALA	Mainchain
2	C	788	SER	Mainchain
2	C	815	SER	Peptide,Mainchain
2	C	821	ARG	Mainchain
2	C	840	SER	Peptide
2	C	851	THR	Peptide
2	C	852	ALA	Peptide
3	D	1178	THR	Peptide
3	D	1349	GLU	Mainchain
3	D	19	ALA	Peptide
3	D	345	LYS	Mainchain
3	D	352	ARG	Mainchain
3	D	358	GLY	Peptide
3	D	361	LEU	Mainchain
3	D	365	GLN	Mainchain
3	D	369	PRO	Mainchain
3	D	372	MET	Mainchain
3	D	374	LEU	Mainchain
3	D	425	ARG	Peptide
3	D	435	GLN	Mainchain
3	D	455	ALA	Mainchain
3	D	5	LEU	Peptide
3	D	503	SER	Peptide
3	D	510	LEU	Mainchain
3	D	577	ALA	Mainchain
3	D	802	ASP	Mainchain
3	D	808	VAL	Mainchain
3	D	894	VAL	Mainchain
3	D	90	VAL	Mainchain
3	D	91	GLU	Peptide
3	D	92	VAL	Peptide
4	E	15	ASN	Mainchain
5	M	185	PHE	Peptide

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	A	1526	0	684	6	0
1	B	1160	0	526	4	0
2	C	6599	0	2971	51	0
3	D	6619	0	3083	75	0
4	E	371	0	172	5	0
5	M	1570	0	692	43	0
6	N	946	0	518	62	0
7	T	842	0	457	60	0
All	All	19633	0	9103	274	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 10.

All (274) 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)
6:N:14:DT:H2”	6:N:15:DT:C7	1.31	1.56
5:M:378:GLU:CB	6:N:-16:DT:H73	1.64	1.26
6:N:14:DT:C2’	6:N:15:DT:C7	2.22	1.18
2:C:1262:LYS:O	2:C:1263:ALA:HB3	1.44	1.15
5:M:378:GLU:CB	6:N:-16:DT:C7	2.24	1.15
5:M:379:SER:CB	6:N:-15:DT:C6	2.29	1.15
5:M:379:SER:CB	6:N:-15:DT:C5	2.20	1.15
7:T:4:DG:C1’	7:T:5:DC:H5’	1.79	1.12
7:T:4:DG:H1’	7:T:5:DC:H5’	1.28	1.12
6:N:14:DT:H2”	6:N:15:DT:H73	1.30	1.11
7:T:-9:DA:H2”	7:T:-8:DT:H71	1.26	1.09
6:N:14:DT:H2”	6:N:15:DT:H71	1.08	1.02
7:T:4:DG:H4’	7:T:5:DC:OP1	1.57	1.01
7:T:-9:DA:C2’	7:T:-8:DT:H71	1.90	1.01
2:C:1262:LYS:O	2:C:1263:ALA:CB	2.11	0.99
6:N:8:DA:H2”	6:N:9:DT:H71	1.44	0.99
6:N:14:DT:C2’	6:N:15:DT:H73	1.90	0.98
5:M:415:ALA:HB3	5:M:419:ALA:HB2	1.44	0.96
6:N:14:DT:C2’	6:N:15:DT:H71	1.88	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:12:DT:OP2	7:T:12:DT:H3'	1.68	0.93
6:N:14:DT:H2"	6:N:15:DT:C5	2.05	0.92
7:T:12:DT:H3'	7:T:12:DT:P	2.09	0.92
5:M:366:VAL:HA	6:N:-17:DT:P	2.09	0.92
6:N:-10:DT:H3'	6:N:-9:DC:H5"	1.53	0.89
5:M:447:SER:HA	5:M:452:MET:H	1.38	0.89
7:T:-9:DA:H2"	7:T:-8:DT:C7	2.02	0.89
6:N:8:DA:C2'	6:N:9:DT:H71	2.03	0.88
5:M:389:TYR:HA	5:M:398:GLU:HA	1.53	0.87
3:D:311:ARG:O	3:D:312:ARG:CB	2.23	0.86
6:N:13:DG:H2"	6:N:14:DT:C5	2.13	0.83
2:C:1267:GLY:HA3	3:D:347:VAL:O	1.79	0.82
5:M:378:GLU:CB	6:N:-16:DT:H71	2.11	0.80
5:M:379:SER:CB	6:N:-15:DT:H6	1.96	0.79
6:N:8:DA:H2"	6:N:9:DT:C7	2.13	0.78
7:T:20:DT:H2"	7:T:21:DC:C5	2.18	0.78
2:C:179:TYR:H	2:C:397:LEU:HA	1.48	0.77
7:T:-1:DC:P	7:T:-1:DC:H3'	2.25	0.76
6:N:-8:DG:H3'	6:N:-7:DA:H5"	1.66	0.75
2:C:833:ILE:HA	2:C:1054:LEU:O	1.88	0.74
3:D:117:LEU:O	3:D:118:LYS:CB	2.34	0.73
7:T:13:DG:H2'	7:T:14:DC:C6	2.24	0.72
7:T:-1:DC:H3'	7:T:-1:DC:OP2	1.89	0.72
5:M:109:LEU:CB	7:T:2:DG:O6	2.38	0.72
5:M:366:VAL:CB	6:N:-17:DT:OP2	2.32	0.72
1:A:304:LYS:O	1:A:308:ALA:HB2	1.90	0.71
5:M:447:SER:HA	5:M:452:MET:N	2.05	0.71
5:M:389:TYR:CA	5:M:398:GLU:HA	2.21	0.71
7:T:-3:DG:C2'	7:T:-2:DC:H5'	2.22	0.70
3:D:348:ASP:O	3:D:349:TYR:C	2.30	0.69
6:N:8:DA:C2'	6:N:9:DT:C7	2.70	0.69
7:T:-9:DA:C2'	7:T:-8:DT:C7	2.65	0.69
5:M:168:ASP:O	5:M:169:GLU:CB	2.41	0.69
2:C:1272:GLU:HA	3:D:343:LEU:CB	2.23	0.69
5:M:190:VAL:O	5:M:191:ALA:HB3	1.93	0.68
7:T:4:DG:OP2	7:T:4:DG:H3'	1.93	0.67
6:N:15:DT:H3	7:T:-15:DA:H61	1.42	0.67
5:M:457:THR:HA	5:M:460:LYS:CB	2.26	0.66
6:N:3:DC:H2"	6:N:4:DG:H5"	1.78	0.66
5:M:457:THR:N	7:T:23:DT:H71	2.12	0.65
5:M:392:SER:H	5:M:396:ILE:CB	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1253:LEU:CB	5:M:113:GLN:O	2.46	0.64
3:D:529:GLY:N	3:D:530:PRO:HA	2.13	0.64
6:N:-13:DC:H2"	6:N:-12:DA:O4'	1.98	0.64
6:N:-7:DA:H2'	6:N:-6:DC:C2	2.33	0.63
7:T:11:DG:H2'	7:T:12:DT:H71	1.81	0.63
3:D:898:CYS:O	3:D:899:TYR:CB	2.46	0.63
2:C:256:GLU:HA	2:C:261:VAL:HA	1.82	0.62
5:M:366:VAL:HA	6:N:-17:DT:OP1	1.99	0.62
6:N:-8:DG:H3'	6:N:-7:DA:C5'	2.28	0.61
3:D:914:ALA:O	3:D:915:ILE:CB	2.42	0.61
7:T:1:DA:H2'	7:T:1:DA:N3	2.16	0.61
4:E:14:GLY:O	4:E:15:ASN:C	2.36	0.60
2:C:540:ARG:C	2:C:542:ARG:H	2.04	0.60
3:D:59:ALA:O	3:D:60:ARG:CB	2.49	0.60
6:N:-21:DG:C2	6:N:-20:DA:C2	2.90	0.60
6:N:-5:DT:H1'	6:N:-4:DA:C8	2.37	0.60
3:D:1262:ARG:O	3:D:1263:LYS:CB	2.49	0.60
6:N:-21:DG:H2"	6:N:-20:DA:C8	2.38	0.59
7:T:-9:DA:H2'	7:T:-8:DT:H71	1.82	0.59
6:N:-10:DT:H3'	6:N:-9:DC:C5'	2.29	0.59
5:M:213:LEU:O	5:M:217:ARG:CB	2.51	0.58
6:N:-17:DT:C6	6:N:-16:DT:H72	2.38	0.58
6:N:-7:DA:H4'	6:N:-7:DA:OP1	2.03	0.58
7:T:0:DC:OP2	7:T:0:DC:H4'	2.03	0.58
7:T:0:DC:OP2	7:T:0:DC:C4'	2.50	0.58
7:T:-9:DA:H2"	7:T:-8:DT:C5	2.38	0.58
3:D:19:ALA:HA	3:D:1343:GLU:H	1.69	0.57
6:N:8:DA:H2"	6:N:9:DT:C5	2.38	0.57
6:N:-10:DT:H2'	6:N:-9:DC:H4'	1.85	0.57
5:M:362:MET:O	5:M:415:ALA:HB1	2.04	0.57
6:N:-5:DT:H4'	6:N:-4:DA:OP1	2.04	0.57
6:N:-9:DC:H4'	6:N:-8:DG:OP1	2.05	0.57
2:C:1155:VAL:O	2:C:1157:GLN:N	2.38	0.57
3:D:123:ARG:O	3:D:127:LEU:CB	2.53	0.56
5:M:366:VAL:CA	6:N:-17:DT:P	2.78	0.56
2:C:1267:GLY:O	3:D:347:VAL:O	2.22	0.56
6:N:13:DG:H2"	6:N:14:DT:C6	2.39	0.56
7:T:-7:DG:H2"	7:T:-6:DC:C6	2.40	0.56
7:T:-11:DG:H2"	7:T:-10:DC:C5	2.40	0.56
3:D:289:ASP:O	3:D:293:ARG:CB	2.54	0.56
1:A:53:GLY:O	1:A:148:ARG:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:LEU:O	2:C:30:ILE:N	2.39	0.55
2:C:1222:GLU:O	2:C:1223:ARG:CB	2.51	0.55
3:D:56:LEU:O	3:D:57:PHE:CB	2.50	0.55
3:D:373:ALA:C	3:D:375:GLU:H	2.08	0.55
7:T:-3:DG:H2'	7:T:-2:DC:H5'	1.88	0.55
3:D:1321:SER:C	3:D:1323:ALA:H	2.10	0.55
7:T:-11:DG:H2"	7:T:-10:DC:C6	2.42	0.55
3:D:185:ILE:O	3:D:189:LEU:CB	2.54	0.55
3:D:366:CYS:O	3:D:439:PRO:HA	2.07	0.55
3:D:585:LYS:O	3:D:587:LEU:N	2.40	0.55
3:D:179:LYS:CB	3:D:184:ALA:HB2	2.38	0.54
2:C:540:ARG:O	2:C:542:ARG:N	2.33	0.54
7:T:15:DA:H2"	7:T:16:DA:C8	2.43	0.54
5:M:457:THR:O	5:M:461:TYR:N	2.34	0.54
7:T:-3:DG:H4'	7:T:-2:DC:OP1	2.08	0.54
7:T:3:DG:H2'	7:T:4:DG:C8	2.43	0.54
5:M:456:ARG:CB	7:T:23:DT:H73	2.37	0.54
5:M:460:LYS:O	5:M:464:SER:N	2.41	0.54
2:C:1252:SER:O	2:C:1256:GLN:HA	2.07	0.53
6:N:15:DT:O2	7:T:-15:DA:N1	2.40	0.53
7:T:12:DT:H2"	7:T:13:DG:H5"	1.90	0.53
3:D:551:ARG:HA	3:D:569:LEU:HA	1.89	0.53
5:M:457:THR:H	7:T:23:DT:H71	1.73	0.53
3:D:92:VAL:O	3:D:94:GLN:N	2.37	0.53
3:D:885:VAL:C	3:D:887:SER:H	2.12	0.53
6:N:8:DA:H2"	6:N:9:DT:C6	2.44	0.53
7:T:-9:DA:H2"	7:T:-8:DT:C6	2.44	0.53
7:T:3:DG:H3'	7:T:4:DG:H3'	1.91	0.53
2:C:918:LEU:O	2:C:919:ARG:C	2.46	0.53
7:T:20:DT:H2"	7:T:21:DC:H5	1.74	0.53
3:D:765:GLU:O	3:D:766:GLY:C	2.42	0.52
7:T:4:DG:O4'	7:T:5:DC:H5'	2.08	0.52
3:D:809:VAL:HA	3:D:893:GLY:O	2.09	0.52
3:D:499:ILE:O	3:D:500:ILE:CB	2.54	0.52
3:D:902:ASP:O	3:D:903:LEU:CB	2.56	0.52
2:C:1263:ALA:O	2:C:1264:GLN:CB	2.57	0.52
7:T:4:DG:C2'	7:T:5:DC:H5'	2.40	0.52
1:A:130:ILE:O	1:A:131:CYS:C	2.46	0.51
7:T:-15:DA:H2'	7:T:-14:DA:C8	2.45	0.51
3:D:226:ALA:O	3:D:230:SER:CB	2.59	0.51
3:D:546:ALA:O	3:D:547:ARG:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:-14:DG:H2”	6:N:-13:DC:O4’	2.10	0.51
2:C:64:GLY:C	2:C:66:SER:H	2.14	0.51
3:D:893:GLY:O	3:D:894:VAL:CB	2.52	0.51
6:N:-16:DT:H2’	6:N:-15:DT:H71	1.91	0.51
2:C:500:ALA:O	2:C:504:GLU:CB	2.59	0.51
2:C:701:GLY:O	2:C:1184:THR:N	2.39	0.51
7:T:4:DG:H3’	7:T:4:DG:P	2.50	0.51
5:M:417:SER:CB	7:T:21:DC:H3’	2.41	0.51
3:D:523:GLU:HA	3:D:546:ALA:HB1	1.93	0.50
4:E:16:ARG:O	4:E:19:LEU:N	2.44	0.50
7:T:24:DG:H2”	7:T:25:DC:C6	2.47	0.50
3:D:1161:GLY:HA3	3:D:1203:ARG:HA	1.93	0.50
6:N:8:DA:H2’	6:N:9:DT:H71	1.88	0.50
2:C:1254:VAL:O	2:C:1255:THR:CB	2.59	0.50
6:N:13:DG:H2”	6:N:14:DT:C7	2.41	0.50
7:T:3:DG:H2”	7:T:4:DG:H5’	1.93	0.50
2:C:1267:GLY:O	2:C:1268:GLN:CB	2.52	0.50
5:M:470:SER:N	6:N:-26:DG:H5”	2.25	0.50
5:M:366:VAL:CB	6:N:-17:DT:P	3.00	0.50
6:N:14:DT:H2’	6:N:15:DT:H73	1.83	0.49
3:D:350:SER:HA	3:D:468:VAL:O	2.12	0.49
2:C:851:THR:CB	2:C:869:GLY:HA3	2.41	0.49
3:D:530:PRO:N	3:D:531:LYS:HA	2.27	0.49
7:T:-7:DG:H2”	7:T:-6:DC:H6	1.77	0.49
2:C:346:TYR:C	2:C:348:SER:H	2.16	0.49
1:A:103:ASN:HA	1:A:140:ILE:O	2.12	0.49
3:D:1058:SER:HA	3:D:1108:GLN:HA	1.94	0.49
5:M:447:SER:HA	5:M:452:MET:CA	2.42	0.49
6:N:13:DG:H2”	6:N:14:DT:H72	1.94	0.49
7:T:23:DT:H2”	7:T:24:DG:C8	2.47	0.49
2:C:767:GLN:HA	2:C:785:ASP:O	2.13	0.48
7:T:11:DG:C4	7:T:12:DT:H73	2.49	0.48
7:T:27:DA:H2”	7:T:28:DG:C8	2.49	0.48
2:C:1167:GLU:O	2:C:1168:GLU:CB	2.61	0.48
3:D:1321:SER:O	3:D:1323:ALA:N	2.47	0.48
2:C:257:ALA:N	2:C:260:LYS:O	2.43	0.47
5:M:152:GLY:O	5:M:154:LEU:N	2.45	0.47
3:D:884:SER:C	3:D:885:VAL:O	2.48	0.47
5:M:167:ASP:O	5:M:168:ASP:CB	2.62	0.47
3:D:373:ALA:O	3:D:375:GLU:N	2.48	0.47
7:T:1:DA:OP2	7:T:1:DA:O3’	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:SER:C	2:C:161:LYS:H	2.18	0.47
3:D:902:ASP:C	3:D:903:LEU:O	2.44	0.47
4:E:16:ARG:O	4:E:17:PHE:C	2.48	0.47
3:D:342:LEU:C	3:D:344:GLY:N	2.68	0.47
2:C:186:PHE:HA	2:C:195:PHE:O	2.15	0.47
3:D:391:ALA:HB1	3:D:396:ALA:HB3	1.97	0.46
2:C:1244:HIS:O	2:C:1245:ALA:HB3	2.15	0.46
2:C:1006:GLU:O	2:C:1010:GLN:CB	2.63	0.46
3:D:92:VAL:C	3:D:94:GLN:H	2.18	0.46
2:C:91:THR:HA	2:C:139:ASN:H	1.81	0.46
5:M:457:THR:CB	7:T:23:DT:O4	2.64	0.46
6:N:-19:DC:H2"	6:N:-18:DT:C6	2.51	0.46
2:C:187:GLU:O	2:C:194:LEU:HA	2.16	0.46
3:D:352:ARG:HA	3:D:466:MET:O	2.16	0.46
1:B:55:ALA:HB2	1:B:176:CYS:O	2.15	0.46
2:C:46:GLN:HA	2:C:51:ALA:HB2	1.98	0.46
7:T:0:DC:O4'	7:T:0:DC:P	2.73	0.46
6:N:-11:DC:H2"	6:N:-10:DT:C5'	2.46	0.46
6:N:8:DA:H2'	6:N:9:DT:C7	2.44	0.45
1:B:25:LYS:HA	1:B:203:ILE:O	2.15	0.45
2:C:816:ILE:O	2:C:1076:ILE:HA	2.16	0.45
2:C:885:GLY:HA2	2:C:917:SER:CB	2.46	0.45
3:D:530:PRO:CB	3:D:531:LYS:C	2.84	0.45
2:C:363:LEU:CB	2:C:381:ALA:HB1	2.47	0.45
7:T:0:DC:H2"	7:T:1:DA:H5'	1.98	0.45
2:C:1340:GLU:O	3:D:18:ASP:O	2.35	0.45
7:T:1:DA:OP2	7:T:1:DA:H3'	2.17	0.45
2:C:1:MET:C	2:C:3:TYR:H	2.20	0.45
2:C:137:VAL:HA	2:C:141:THR:O	2.16	0.45
3:D:584:PRO:O	3:D:585:LYS:CB	2.65	0.45
5:M:415:ALA:CB	5:M:419:ALA:HB2	2.32	0.45
6:N:-23:DA:H2"	6:N:-22:DC:C6	2.51	0.45
6:N:10:DG:H2"	6:N:11:DC:C6	2.52	0.45
2:C:156:PHE:O	2:C:174:ALA:HA	2.17	0.44
3:D:362:ARG:O	3:D:363:LEU:C	2.55	0.44
4:E:10:VAL:O	4:E:13:ILE:O	2.35	0.44
7:T:4:DG:C4'	7:T:5:DC:C5'	2.95	0.44
5:M:398:GLU:C	5:M:400:LYS:H	2.21	0.44
3:D:1321:SER:C	3:D:1323:ALA:N	2.69	0.44
2:C:1259:LEU:O	2:C:1266:GLY:HA2	2.18	0.44
3:D:529:GLY:N	3:D:530:PRO:CA	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:13:DG:C2'	6:N:14:DT:H72	2.48	0.44
3:D:133:ARG:O	3:D:137:ARG:CB	2.66	0.44
1:B:109:PRO:HA	1:B:132:HIS:HA	2.00	0.44
2:C:540:ARG:C	2:C:542:ARG:N	2.71	0.44
2:C:1267:GLY:CA	3:D:347:VAL:O	2.59	0.44
6:N:-24:DC:H2"	6:N:-23:DA:C8	2.53	0.43
3:D:914:ALA:C	3:D:916:GLY:H	2.21	0.43
5:M:447:SER:HA	5:M:452:MET:HA	2.01	0.43
5:M:378:GLU:CB	6:N:-15:DT:H73	2.48	0.43
3:D:155:GLU:O	3:D:156:ARG:C	2.57	0.43
3:D:322:ARG:O	3:D:324:LEU:N	2.52	0.43
3:D:545:HIS:O	3:D:546:ALA:HB3	2.17	0.43
7:T:-1:DC:H6	7:T:-1:DC:H2'	1.63	0.43
3:D:132:LEU:O	3:D:136:GLU:CB	2.66	0.43
3:D:161:THR:O	3:D:165:TYR:N	2.46	0.43
7:T:12:DT:H1'	7:T:13:DG:C8	2.54	0.43
3:D:520:ALA:HB3	3:D:545:HIS:CB	2.48	0.43
1:B:5:VAL:C	1:B:7:GLU:H	2.23	0.42
3:D:968:ASN:HA	3:D:1118:GLY:HA3	2.01	0.42
7:T:1:DA:H3'	7:T:1:DA:P	2.58	0.42
2:C:1012:GLU:O	2:C:1016:GLU:CB	2.66	0.42
3:D:19:ALA:CB	3:D:1343:GLU:H	2.33	0.42
3:D:61:ILE:O	3:D:62:PHE:CB	2.67	0.42
3:D:323:PRO:O	3:D:324:LEU:CB	2.63	0.42
3:D:932:MET:O	3:D:1137:GLY:HA3	2.19	0.42
5:M:175:VAL:O	5:M:179:LEU:CB	2.68	0.42
2:C:480:SER:O	2:C:481:LEU:CB	2.68	0.42
2:C:1269:ARG:HA	3:D:346:ARG:HA	2.02	0.42
3:D:893:GLY:O	3:D:894:VAL:C	2.53	0.42
5:M:438:SER:HA	6:N:-27:DT:H3'	2.01	0.42
1:A:136:GLU:O	1:A:137:ASN:CB	2.67	0.42
7:T:2:DG:H2"	7:T:3:DG:H1'	2.02	0.42
6:N:-28:DC:H2'	6:N:-27:DT:H72	2.01	0.42
5:M:436:PRO:O	5:M:469:PRO:HA	2.20	0.41
6:N:4:DG:C4	6:N:5:DC:C5	3.08	0.41
1:A:192:VAL:C	1:A:194:GLN:H	2.24	0.41
2:C:1222:GLU:O	3:D:635:SER:O	2.37	0.41
3:D:19:ALA:HB2	3:D:1343:GLU:HA	2.02	0.41
2:C:174:ALA:O	2:C:185:ASP:HA	2.20	0.41
4:E:15:ASN:O	4:E:16:ARG:C	2.57	0.41
3:D:1314:LEU:HA	3:D:1322:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1334:GLY:C	3:D:25:ALA:HB3	2.41	0.41
7:T:-3:DG:C4'	7:T:-2:DC:OP1	2.69	0.41
3:D:253:VAL:HA	5:M:112:TYR:CB	2.51	0.40
3:D:147:ILE:O	3:D:149:GLY:N	2.54	0.40
3:D:554:GLU:N	3:D:566:LYS:O	2.54	0.40
2:C:1008:GLN:O	2:C:1012:GLU:CB	2.69	0.40
3:D:365:GLN:HA	3:D:438:GLU:O	2.21	0.40
3:D:373:ALA:O	3:D:374:LEU:CB	2.69	0.40
6:N:-4:DA:H2"	6:N:-3:DA:H8	1.87	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 PDB entries followed by that with respect to all EM entries.

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
1	A	305/329 (93%)	269 (88%)	32 (10%)	4 (1%)	10 42
1	B	233/329 (71%)	209 (90%)	22 (9%)	2 (1%)	14 51
2	C	1339/1342 (100%)	1183 (88%)	128 (10%)	28 (2%)	5 30
3	D	1335/1407 (95%)	1133 (85%)	163 (12%)	39 (3%)	3 23
4	E	73/91 (80%)	68 (93%)	3 (4%)	2 (3%)	4 26
5	M	310/497 (62%)	254 (82%)	41 (13%)	15 (5%)	2 17
All	All	3595/3995 (90%)	3116 (87%)	389 (11%)	90 (2%)	7 27

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ILE
2	C	29	SER
2	C	347	ILE

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Mol	Chain	Res	Type
2	C	541	GLU
2	C	1155	VAL
3	D	118	LYS
3	D	158	GLN
3	D	312	ARG
3	D	426	ALA
3	D	500	ILE
3	D	521	LYS
3	D	586	GLY
3	D	886	VAL
3	D	1134	ILE
4	E	15	ASN
5	M	153	TYR
5	M	259	PRO
5	M	260	ARG
5	M	261	PRO
5	M	274	ILE
5	M	275	PRO
2	C	2	VAL
2	C	228	VAL
2	C	570	GLY
2	C	728	ASP
2	C	773	LEU
2	C	919	ARG
2	C	1156	ARG
2	C	1189	GLY
2	C	1264	GLN
2	C	1268	GLN
3	D	94	GLN
3	D	349	TYR
3	D	574	VAL
3	D	915	ILE
3	D	1159	ILE
3	D	1309	ILE
5	M	169	GLU
5	M	282	VAL
1	A	98	VAL
1	A	177	TYR
1	B	168	ILE
2	C	481	LEU
2	C	509	SER
2	C	852	ALA

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Mol	Chain	Res	Type
2	C	1255	THR
3	D	360	TYR
3	D	363	LEU
3	D	585	LYS
3	D	594	GLN
3	D	767	LEU
3	D	787	ALA
3	D	1210	ILE
4	E	14	GLY
5	M	156	ILE
5	M	167	ASP
5	M	188	VAL
1	A	131	CYS
2	C	519	ASN
2	C	655	VAL
2	C	720	ARG
3	D	20	ILE
3	D	316	ILE
3	D	320	ASN
3	D	520	ALA
3	D	899	TYR
2	C	643	SER
2	C	1223	ARG
3	D	67	ASP
3	D	323	PRO
3	D	546	ALA
3	D	1180	VAL
5	M	185	PHE
2	C	892	GLU
2	C	1245	ALA
3	D	92	VAL
3	D	260	PHE
5	M	257	ASP
5	M	265	ILE
3	D	83	VAL
3	D	809	VAL
3	D	885	VAL
2	C	229	ILE
3	D	673	VAL
5	M	170	ILE
1	B	159	ILE
2	C	558	VAL

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Mol	Chain	Res	Type
2	C	1186	VAL
3	D	145	VAL
3	D	894	VAL

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.