Full wwPDB EM Validation Report

Nov 5, 2024 – 10:30 AM JST

PDB ID	:	8JHO
EMDB ID	:	EMD-36283
Title	:	Cryo-EM structure of the histone deacetylase complex Rpd3S in complex with di-nucleosome
Authors	:	Wang, H.
Deposited on	:	2023-05-25
Resolution	:	7.60 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:

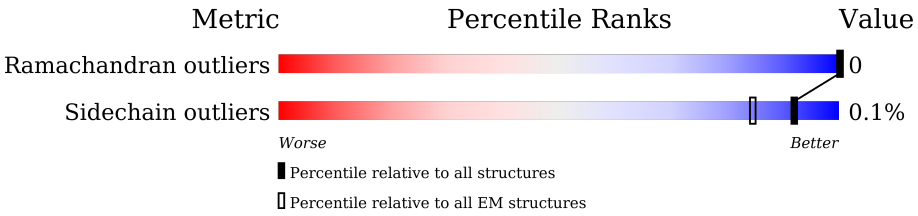
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 7.60 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	135	73% · 24%
1	E	135	81% · · 13%
1	a	135	76% 24%
1	e	135	70% · 27%
2	B	102	77% ·· 21%
2	F	102	73% 5% · 22%
2	b	102	80% 20%
2	f	102	78% 22%
3	C	129	79% 5% 16%
3	G	129	81% · 18%

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Mol	Chain	Length	Quality of chain
3	c	129	
3	g	129	
4	D	122	
4	H	122	
4	d	122	
4	h	122	
5	I	350	
6	J	350	
7	K	1536	
8	L	433	
9	M	401	
9	O	401	
10	N	684	
10	P	684	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 42813 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	102	Total 837	C 529	N 162	O 143	S 3	0	0
1	E	117	Total 954	C 597	N 191	O 164	S 2	0	0
1	a	102	Total 837	C 529	N 162	O 143	S 3	0	0
1	e	98	Total 810	C 512	N 157	O 139	S 2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
E	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
a	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
e	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total 646	C 407	N 126	O 112	S 1	0	0
2	F	80	Total 638	C 401	N 125	O 111	S 1	0	0
2	b	82	Total 653	C 412	N 127	O 113	S 1	0	0
2	f	80	Total 638	C 401	N 125	O 111	S 1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total 843	C 531	N 167	O 145	0	0
3	G	106	Total 818	C 516	N 160	O 142	0	0
3	c	109	Total 843	C 531	N 167	O 145	0	0
3	g	106	Total 818	C 516	N 160	O 142	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total 757	C 475	N 140	O 140	S 2	0	0
4	H	95	Total 745	C 469	N 134	O 140	S 2	0	0
4	d	96	Total 757	C 475	N 140	O 140	S 2	0	0
4	h	95	Total 745	C 469	N 134	O 140	S 2	0	0

- Molecule 5 is a DNA chain called Di-nucleosome template foward.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	340	Total 6937	C 3299	N 1252	O 2046	P 340	0	0

- Molecule 6 is a DNA chain called Di-nucleosome template reverse.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	340	Total 7003	C 3319	N 1310	O 2034	P 340	0	0

- Molecule 7 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	549	Total 4597	C 2954	N 774	O 854	S 15	0	0

- Molecule 8 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	384	Total	C	N	O	S	0	0
			3048	1941	512	569	26		

- Molecule 9 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	294	Total	C	N	O	S	0	0
			2398	1541	394	449	14		
9	O	267	Total	C	N	O	S	0	0
			2190	1414	359	404	13		

- Molecule 10 is a protein called RCO1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	372	Total	C	N	O	S	0	0
			3045	1935	526	566	18		
10	P	151	Total	C	N	O	S	0	0
			1249	802	206	231	10		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	L	1	Total	Zn	0
			1	1	
11	N	4	Total	Zn	0
			4	4	
11	P	2	Total	Zn	0
			2	2	

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: Histone H3

Chain A:

- Molecule 1: Histone H3

Chain E:

- Molecule 1: Histone H3

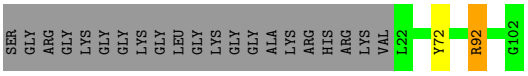
Chain a:

- Molecule 1: Histone H3

Chain e:

- Molecule 2: Histone H4

Chain B:

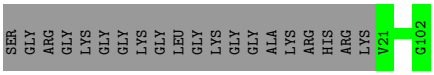


- Molecule 2: Histone H4

Chain F:

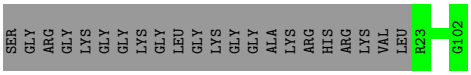
• Molecule 2: Histone H4

Chain b:



• Molecule 2: Histone H4

Chain f:

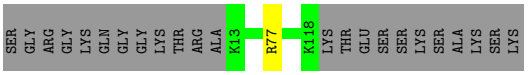


• Molecule 3: Histone H2A

Chain C:

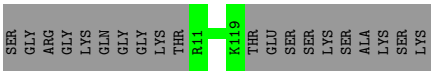
• Molecule 3: Histone H2A

Chain G:



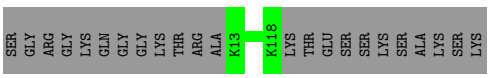
• Molecule 3: Histone H2A

Chain c:



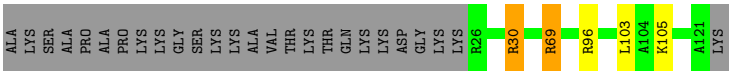
• Molecule 3: Histone H2A

Chain g:



• Molecule 4: Histone H2B

Chain D:

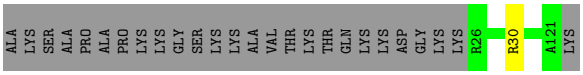


• Molecule 4: Histone H2B

Chain H:

• Molecule 4: Histone H2B

Chain d:

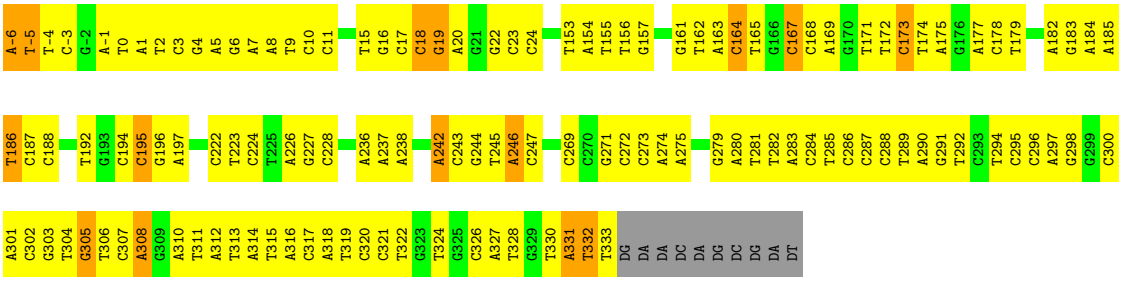


• Molecule 4: Histone H2B

Chain h:

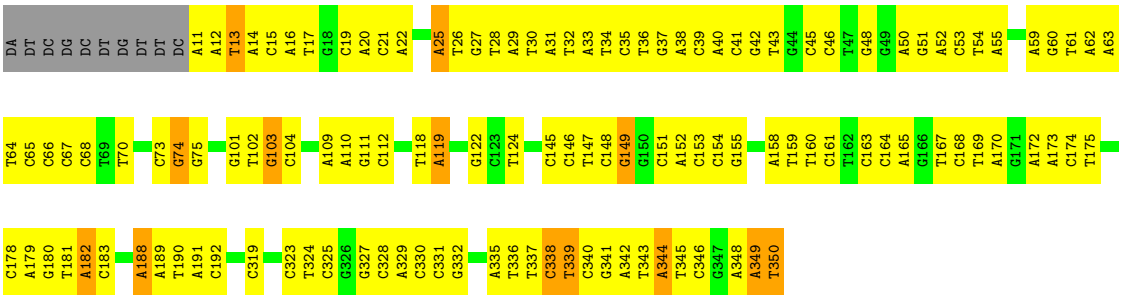
• Molecule 5: Di-nucleosome template foward

Chain I:



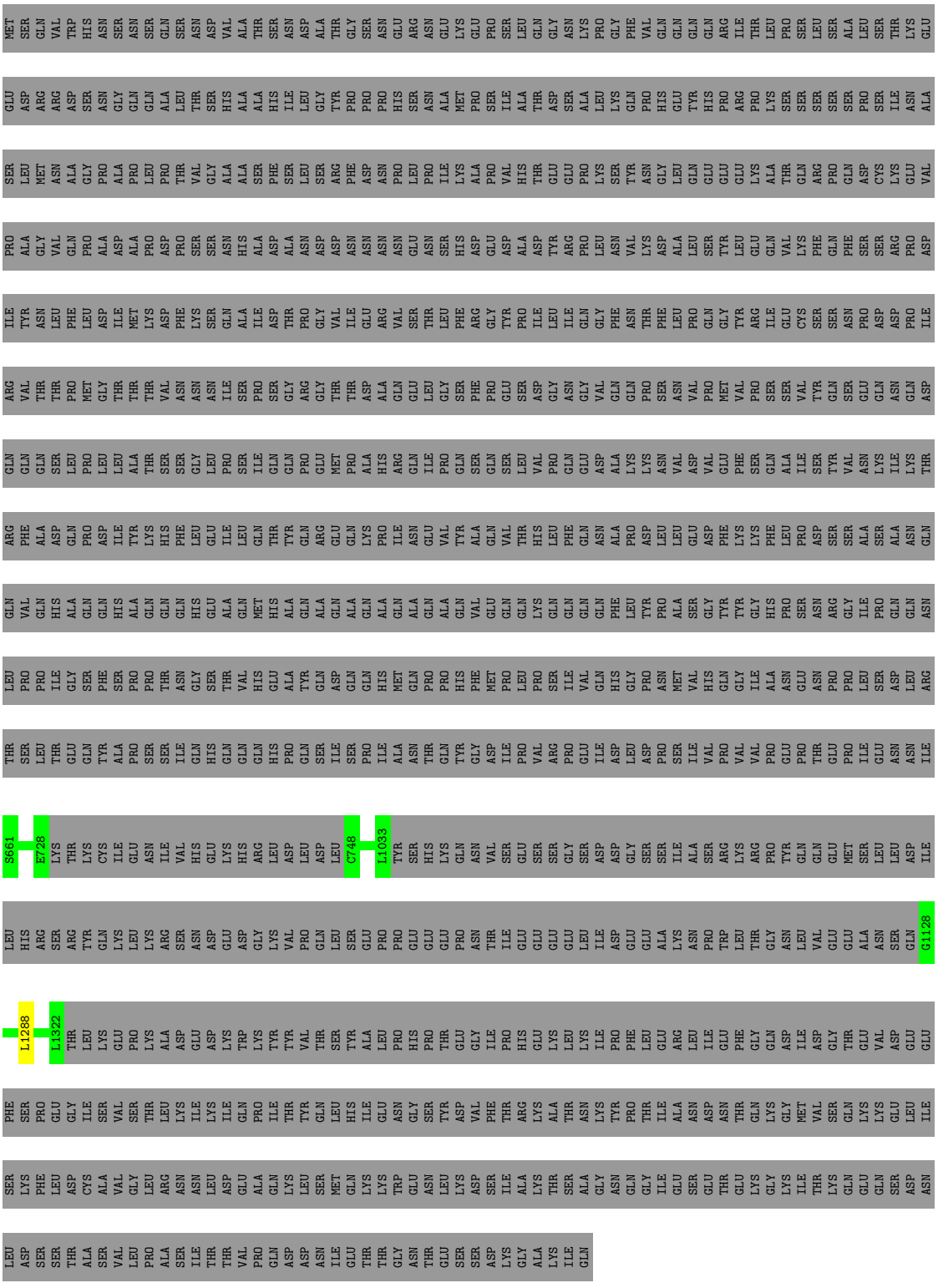
• Molecule 6: Di-nucleosome template reverse

Chain J:



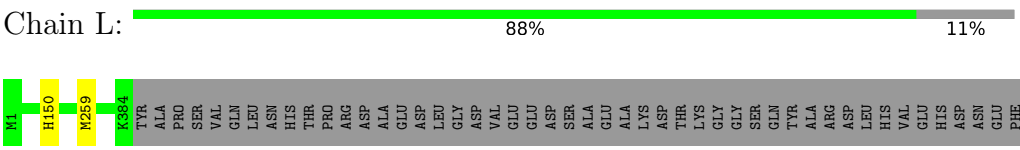
• Molecule 7: Transcriptional regulatory protein SIN3

Chain K:



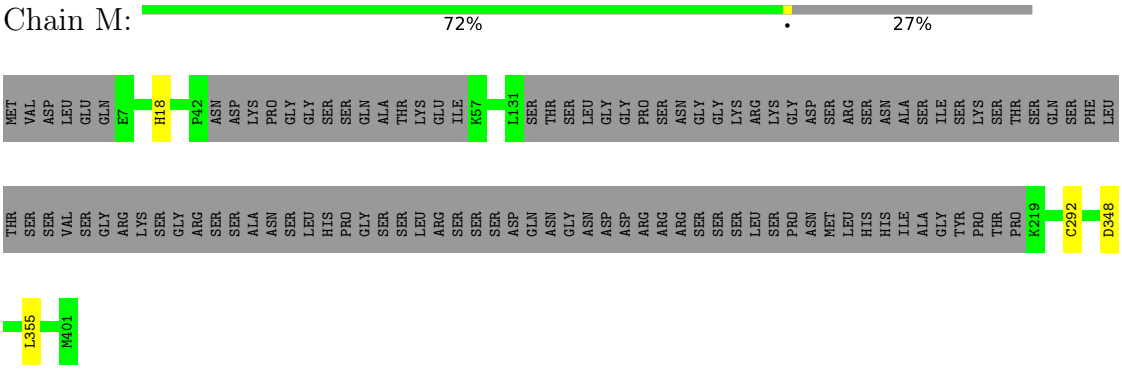
• Molecule 8: Histone deacetylase RPD3

Chain L:



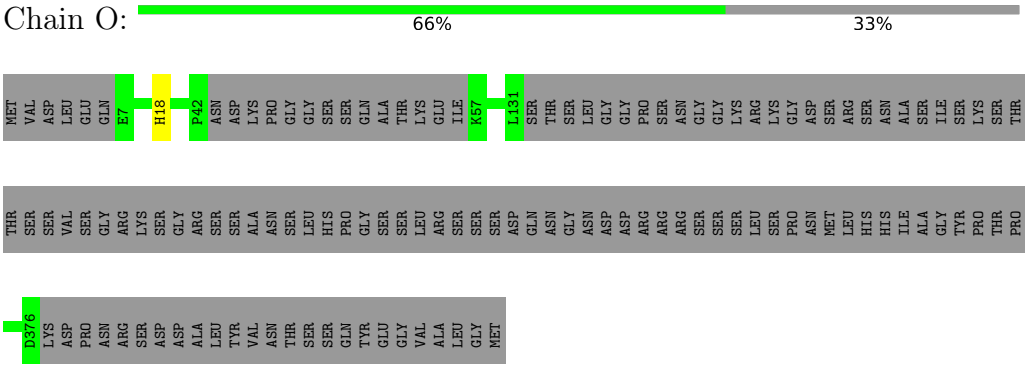
• Molecule 9: Chromatin modification-related protein EAF3

Chain M:



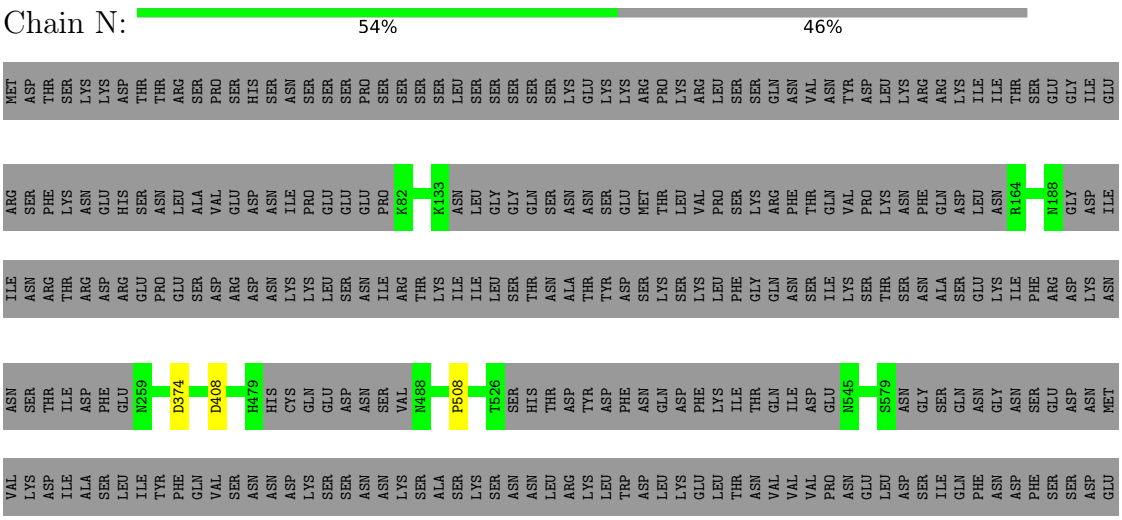
• Molecule 9: Chromatin modification-related protein EAF3

Chain O:



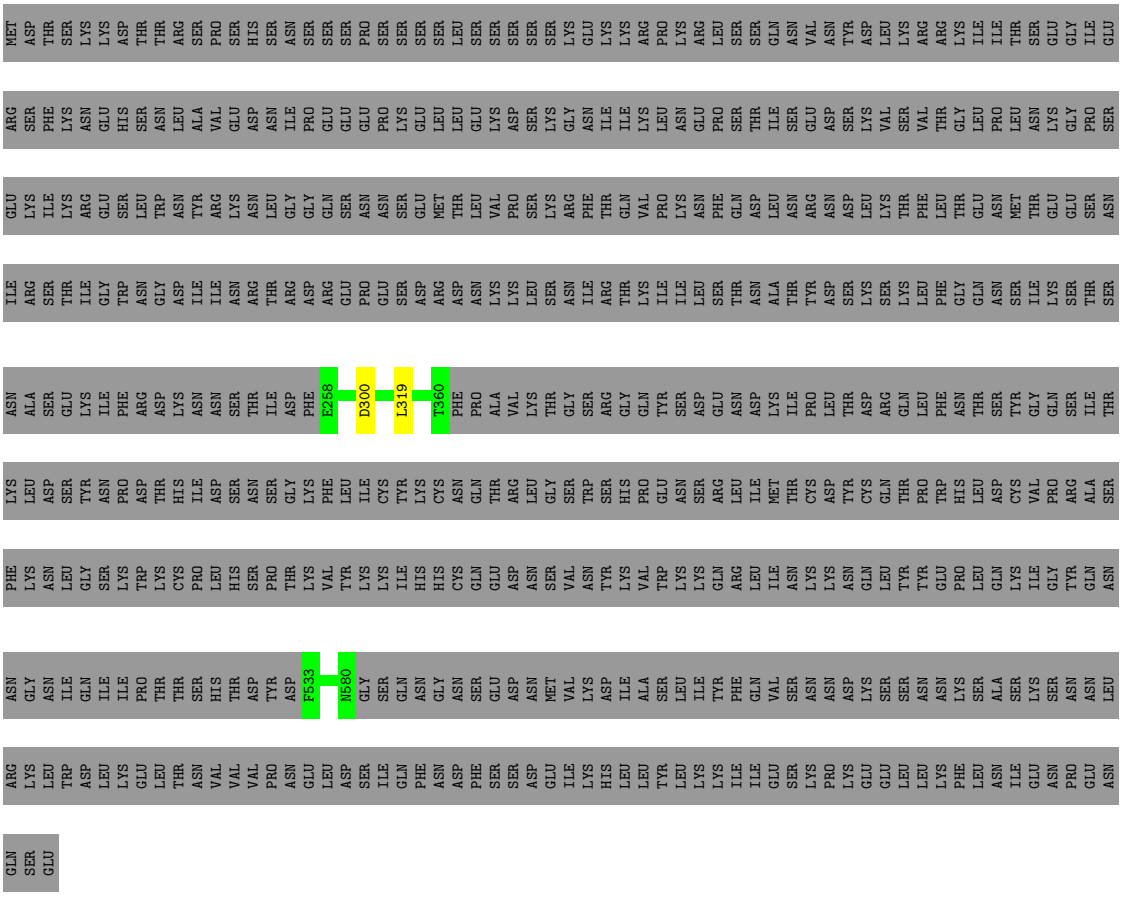
• Molecule 10: RCO1 isoform 1

Chain N:



• Molecule 10: RCO1 isoform 1

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31310	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ML3

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	0.57	0/836	1.03	3/1120 (0.3%)
1	E	0.60	0/966	1.13	7/1291 (0.5%)
1	a	0.34	0/836	0.80	0/1120
1	e	0.43	0/822	0.86	3/1103 (0.3%)
2	B	0.54	0/653	0.95	3/873 (0.3%)
2	F	0.61	0/645	1.33	8/862 (0.9%)
2	b	0.34	0/660	0.80	0/883
2	f	0.40	0/645	0.83	0/862
3	C	0.66	0/853	1.25	5/1149 (0.4%)
3	G	0.44	0/828	0.77	0/1117
3	c	0.37	0/853	0.76	0/1149
3	g	0.33	0/828	0.68	0/1117
4	D	0.68	0/768	1.25	3/1032 (0.3%)
4	H	0.44	0/756	0.74	0/1015
4	d	0.44	0/768	0.78	0/1032
4	h	0.36	0/756	0.69	2/1015 (0.2%)
5	I	1.14	1/7773 (0.0%)	1.66	231/11987 (1.9%)
6	J	1.12	3/7865 (0.0%)	1.64	232/12145 (1.9%)
7	K	0.32	0/4699	0.54	1/6334 (0.0%)
8	L	0.34	0/3127	0.51	0/4231
9	M	0.32	0/2446	0.57	3/3292 (0.1%)
9	O	0.30	0/2235	0.58	2/3008 (0.1%)
10	N	0.32	0/3115	0.56	3/4195 (0.1%)
10	P	0.31	0/1278	0.60	2/1716 (0.1%)
All	All	0.74	4/45011 (0.0%)	1.17	508/63648 (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	1
1	E	0	1
2	B	0	1
2	F	0	1
3	C	0	2
3	G	0	1
4	D	0	4
4	d	0	1
5	I	0	23
6	J	0	18
All	All	0	53

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	42	DG	C2-N2	-5.38	1.29	1.34
6	J	67	DC	C4-N4	-5.34	1.29	1.33
5	I	22	DG	C2-N2	-5.11	1.29	1.34
6	J	60	DG	C2-N2	-5.11	1.29	1.34

All (508) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	78	ARG	NE-CZ-NH2	10.19	125.39	120.30
1	A	72	ARG	NE-CZ-NH2	9.84	125.22	120.30
5	I	5	DA	N1-C6-N6	-9.59	112.85	118.60
6	J	31	DA	N1-C6-N6	-9.36	112.99	118.60
6	J	14	DA	N1-C6-N6	-9.28	113.03	118.60
6	J	349	DA	N1-C6-N6	-9.10	113.14	118.60
5	I	163	DA	C5-C6-N1	8.40	121.90	117.70
6	J	25	DA	N1-C6-N6	-8.37	113.58	118.60
7	K	1288	LEU	CA-CB-CG	8.36	134.54	115.30
6	J	170	DA	N1-C6-N6	-8.36	113.58	118.60
1	E	116	ARG	NE-CZ-NH2	8.28	124.44	120.30
5	I	-6	DA	N1-C6-N6	-8.25	113.65	118.60
5	I	236	DA	C5-C6-N1	8.25	121.83	117.70
5	I	237	DA	C5-C6-N1	8.18	121.79	117.70
6	J	20	DA	C5-C6-N1	8.13	121.77	117.70
6	J	172	DA	N1-C6-N6	-8.11	113.73	118.60
6	J	182	DA	C5-C6-N1	8.08	121.74	117.70
6	J	75	DG	P-O3'-C3'	8.04	129.35	119.70
10	P	300	ASP	CB-CG-OD1	7.99	125.49	118.30
5	I	185	DA	C5-C6-N1	7.88	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	11	DA	N1-C6-N6	-7.86	113.88	118.60
5	I	274	DA	C5-C6-N1	7.83	121.62	117.70
6	J	109	DA	C5-C6-N1	7.81	121.60	117.70
5	I	182	DA	C5-C6-N1	7.79	121.59	117.70
5	I	-1	DA	N1-C6-N6	-7.76	113.94	118.60
6	J	173	DA	N1-C6-N6	-7.71	113.97	118.60
5	I	310	DA	N1-C6-N6	-7.69	113.99	118.60
6	J	31	DA	C4-C5-C6	-7.65	113.18	117.00
5	I	7	DA	O4'-C1'-N9	7.63	113.34	108.00
6	J	192	DC	O4'-C1'-N1	7.58	113.31	108.00
6	J	344	DA	N1-C6-N6	-7.58	114.05	118.60
6	J	182	DA	N1-C6-N6	-7.56	114.06	118.60
6	J	63	DA	N1-C6-N6	-7.55	114.07	118.60
6	J	59	DA	C5-C6-N1	7.55	121.47	117.70
5	I	161	DG	O4'-C1'-N9	7.54	113.28	108.00
5	I	-6	DA	C4-C5-C6	-7.52	113.24	117.00
5	I	163	DA	N1-C6-N6	-7.51	114.10	118.60
6	J	342	DA	N1-C6-N6	-7.50	114.10	118.60
5	I	169	DA	N1-C6-N6	-7.48	114.11	118.60
6	J	62	DA	C4-C5-C6	-7.44	113.28	117.00
5	I	5	DA	C4-C5-C6	-7.42	113.29	117.00
6	J	348	DA	N1-C6-N6	-7.40	114.16	118.60
6	J	325	DC	N3-C2-O2	-7.39	116.72	121.90
5	I	237	DA	C4-C5-C6	-7.39	113.30	117.00
5	I	301	DA	N1-C6-N6	-7.30	114.22	118.60
6	J	344	DA	C4-C5-C6	-7.29	113.35	117.00
5	I	1	DA	N1-C6-N6	-7.27	114.24	118.60
5	I	8	DA	N1-C6-N6	-7.25	114.25	118.60
5	I	275	DA	C4-C5-C6	-7.23	113.39	117.00
6	J	179	DA	N1-C6-N6	-7.22	114.27	118.60
5	I	177	DA	C4-C5-C6	-7.22	113.39	117.00
5	I	8	DA	C5-C6-N1	7.21	121.31	117.70
5	I	316	DA	C5-C6-N1	7.20	121.30	117.70
5	I	290	DA	N1-C6-N6	-7.17	114.30	118.60
6	J	29	DA	C5-C6-N1	7.17	121.28	117.70
6	J	16	DA	N1-C6-N6	-7.16	114.31	118.60
6	J	50	DA	C4-C5-C6	-7.14	113.43	117.00
6	J	119	DA	C5-C6-N1	7.11	121.25	117.70
6	J	158	DA	N1-C6-N6	-7.11	114.34	118.60
6	J	335	DA	N1-C6-N6	-7.11	114.34	118.60
6	J	52	DA	C4-C5-C6	-7.10	113.45	117.00
3	C	77	ARG	NE-CZ-NH2	7.09	123.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	40	DA	C5-C6-N1	7.09	121.25	117.70
6	J	348	DA	C5-C6-N1	7.08	121.24	117.70
5	I	197	DA	C5-C6-N1	7.07	121.23	117.70
5	I	184	DA	C5-C6-N1	7.07	121.23	117.70
5	I	194	DC	N3-C2-O2	-7.06	116.96	121.90
6	J	164	DC	N3-C2-O2	-7.06	116.96	121.90
6	J	63	DA	C4-C5-C6	-7.04	113.48	117.00
3	C	29	ARG	NE-CZ-NH2	7.00	123.80	120.30
6	J	158	DA	C5-C6-N1	6.99	121.20	117.70
6	J	12	DA	C5-C6-N1	6.99	121.19	117.70
5	I	184	DA	N1-C6-N6	-6.96	114.42	118.60
5	I	280	DA	C4-C5-C6	-6.95	113.53	117.00
5	I	177	DA	C5-C6-N1	6.95	121.17	117.70
6	J	52	DA	C5-C6-N1	6.93	121.16	117.70
6	J	172	DA	C4-C5-C6	-6.93	113.54	117.00
6	J	349	DA	C5-C6-N1	6.91	121.16	117.70
2	B	92	ARG	NE-CZ-NH2	6.91	123.75	120.30
5	I	318	DA	N1-C6-N6	-6.90	114.46	118.60
2	F	39	ARG	NE-CZ-NH2	6.90	123.75	120.30
6	J	190	DT	O4'-C1'-N1	6.89	112.82	108.00
5	I	169	DA	C5-C6-N1	6.88	121.14	117.70
6	J	109	DA	N1-C6-N6	-6.88	114.47	118.60
6	J	11	DA	C5-C6-N1	6.87	121.14	117.70
6	J	40	DA	N1-C6-N6	-6.86	114.49	118.60
6	J	342	DA	C5-C6-N1	6.84	121.12	117.70
6	J	22	DA	N1-C6-N6	-6.83	114.50	118.60
6	J	40	DA	C4-C5-C6	-6.82	113.59	117.00
5	I	195	DC	N3-C2-O2	-6.82	117.13	121.90
5	I	327	DA	C5-C6-N1	6.80	121.10	117.70
5	I	173	DC	N3-C2-O2	-6.79	117.15	121.90
6	J	110	DA	C5-C6-N1	6.77	121.09	117.70
5	I	17	DC	N3-C2-O2	-6.77	117.16	121.90
5	I	246	DA	C5-C6-N1	6.77	121.08	117.70
6	J	182	DA	C4-C5-C6	-6.76	113.62	117.00
6	J	319	DC	N3-C2-O2	-6.76	117.17	121.90
5	I	20	DA	N1-C6-N6	-6.75	114.55	118.60
6	J	170	DA	C4-C5-C6	-6.75	113.63	117.00
2	F	39	ARG	NE-CZ-NH1	-6.74	116.93	120.30
5	I	175	DA	C5-C6-N1	6.74	121.07	117.70
5	I	327	DA	C4-C5-C6	-6.73	113.64	117.00
5	I	3	DC	N3-C2-O2	-6.73	117.19	121.90
6	J	189	DA	C5-C6-N1	6.72	121.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	316	DA	N1-C6-N6	-6.72	114.57	118.60
6	J	67	DC	N3-C4-C5	6.72	124.59	121.90
6	J	59	DA	C4-C5-C6	-6.70	113.65	117.00
6	J	179	DA	C4-C5-C6	-6.69	113.66	117.00
5	I	163	DA	C4-C5-C6	-6.68	113.66	117.00
5	I	310	DA	C5-C6-N1	6.68	121.04	117.70
5	I	297	DA	C5-C6-N1	6.68	121.04	117.70
6	J	349	DA	C4-C5-C6	-6.67	113.66	117.00
6	J	39	DC	N3-C2-O2	-6.67	117.23	121.90
5	I	312	DA	C4-C5-C6	-6.65	113.67	117.00
6	J	173	DA	C4-C5-C6	-6.64	113.68	117.00
6	J	146	DC	N3-C2-O2	-6.63	117.26	121.90
6	J	340	DC	N3-C2-O2	-6.63	117.26	121.90
3	C	11	ARG	NE-CZ-NH2	6.63	123.61	120.30
5	I	274	DA	C4-C5-C6	-6.62	113.69	117.00
5	I	-6	DA	C5-C6-N1	6.62	121.01	117.70
6	J	179	DA	C5-C6-N1	6.60	121.00	117.70
5	I	314	DA	N1-C6-N6	-6.60	114.64	118.60
5	I	18	DC	N3-C2-O2	-6.59	117.28	121.90
6	J	25	DA	C4-C5-C6	-6.59	113.71	117.00
5	I	177	DA	N1-C6-N6	-6.59	114.65	118.60
10	N	374	ASP	CB-CG-OD1	6.58	124.22	118.30
4	h	97	LEU	CA-CB-CG	6.57	130.42	115.30
5	I	226	DA	N1-C6-N6	-6.57	114.66	118.60
6	J	25	DA	C5-C6-N1	6.56	120.98	117.70
10	N	408	ASP	CB-CG-OD1	6.56	124.20	118.30
5	I	185	DA	C4-C5-C6	-6.56	113.72	117.00
5	I	197	DA	N1-C6-N6	-6.56	114.67	118.60
5	I	185	DA	N1-C6-N6	-6.55	114.67	118.60
6	J	329	DA	C5-C6-N1	6.55	120.97	117.70
5	I	280	DA	C5-C6-N1	6.50	120.95	117.70
5	I	182	DA	C4-C5-C6	-6.50	113.75	117.00
5	I	292	DT	C6-C5-C7	-6.48	119.01	122.90
6	J	173	DA	C5-C6-N1	6.47	120.94	117.70
6	J	74	DG	N3-C2-N2	-6.47	115.37	119.90
5	I	328	DT	C6-C5-C7	-6.45	119.03	122.90
6	J	33	DA	C4-C5-C6	-6.45	113.77	117.00
6	J	55	DA	C5-C6-N1	6.44	120.92	117.70
6	J	165	DA	C5-C6-N1	6.44	120.92	117.70
6	J	172	DA	C5-C6-N1	6.44	120.92	117.70
5	I	280	DA	N1-C6-N6	-6.43	114.74	118.60
6	J	36	DT	C6-C5-C7	-6.42	119.05	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	317	DC	N3-C2-O2	-6.42	117.41	121.90
6	J	50	DA	C5-C6-N1	6.41	120.90	117.70
6	J	170	DA	C5-C6-N1	6.40	120.90	117.70
5	I	175	DA	N1-C6-N6	-6.39	114.77	118.60
2	F	98	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	E	42	ARG	NE-CZ-NH2	6.39	123.49	120.30
6	J	175	DT	C6-C5-C7	-6.39	119.07	122.90
5	I	275	DA	N1-C6-N6	-6.38	114.77	118.60
5	I	-3	DC	N3-C2-O2	-6.38	117.43	121.90
9	O	234	ASP	CB-CG-OD1	6.37	124.03	118.30
5	I	238	DA	O4'-C1'-N9	6.37	112.46	108.00
6	J	330	DC	N3-C2-O2	-6.37	117.44	121.90
5	I	175	DA	C4-C5-C6	-6.36	113.82	117.00
5	I	164	DC	N3-C2-O2	-6.36	117.45	121.90
6	J	188	DA	C5-C6-N1	6.36	120.88	117.70
6	J	168	DC	N3-C2-O2	-6.33	117.47	121.90
6	J	46	DC	N3-C2-O2	-6.33	117.47	121.90
5	I	168	DC	N3-C2-O2	-6.33	117.47	121.90
5	I	242	DA	C4-C5-C6	-6.32	113.84	117.00
6	J	103	DG	N3-C2-N2	-6.32	115.47	119.90
6	J	16	DA	C4-C5-C6	-6.32	113.84	117.00
9	M	348	ASP	CB-CG-OD1	6.32	123.98	118.30
2	F	39	ARG	CD-NE-CZ	6.31	132.43	123.60
2	F	67	ARG	NE-CZ-NH2	6.31	123.45	120.30
5	I	237	DA	N1-C6-N6	-6.30	114.82	118.60
5	I	10	DC	N3-C2-O2	-6.30	117.49	121.90
5	I	247	DC	N3-C2-O2	-6.30	117.49	121.90
5	I	2	DT	C6-C5-C7	-6.29	119.12	122.90
5	I	5	DA	C5-C6-N1	6.29	120.85	117.70
5	I	187	DC	N3-C2-O2	-6.29	117.50	121.90
5	I	226	DA	C4-C5-C6	-6.28	113.86	117.00
5	I	269	DC	N3-C2-O2	-6.28	117.50	121.90
6	J	152	DA	C5-C6-N1	6.28	120.84	117.70
6	J	29	DA	C4-C5-C6	-6.27	113.87	117.00
6	J	50	DA	N1-C6-N6	-6.27	114.84	118.60
5	I	316	DA	C4-C5-C6	-6.26	113.87	117.00
5	I	154	DA	C5-C6-N1	6.26	120.83	117.70
6	J	11	DA	C4-C5-C6	-6.25	113.88	117.00
5	I	169	DA	C4-C5-C6	-6.24	113.88	117.00
5	I	7	DA	C5-C6-N1	6.23	120.82	117.70
5	I	269	DC	N1-C2-O2	6.23	122.64	118.90
2	F	35	ARG	NE-CZ-NH2	6.23	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	20	DA	C5-C6-N1	6.23	120.81	117.70
6	J	328	DC	N3-C2-O2	-6.23	117.54	121.90
6	J	188	DA	N1-C6-N6	-6.22	114.87	118.60
6	J	350	DT	C6-C5-C7	-6.21	119.17	122.90
6	J	12	DA	C4-C5-C6	-6.21	113.90	117.00
5	I	283	DA	C4-C5-C6	-6.18	113.91	117.00
5	I	312	DA	N1-C6-N6	-6.18	114.89	118.60
6	J	64	DT	C6-C5-C7	-6.18	119.19	122.90
5	I	238	DA	C5-C6-N1	6.17	120.79	117.70
6	J	31	DA	C5-C6-N1	6.17	120.78	117.70
5	I	333	DT	N3-C2-O2	-6.17	118.60	122.30
6	J	346	DC	N3-C2-O2	-6.16	117.59	121.90
5	I	-4	DT	C6-C5-C7	-6.15	119.21	122.90
5	I	331	DA	C5-C6-N1	6.15	120.78	117.70
6	J	62	DA	C5-C6-N1	6.15	120.78	117.70
5	I	306	DT	C6-C5-C7	-6.15	119.21	122.90
6	J	110	DA	C4-C5-C6	-6.15	113.93	117.00
6	J	158	DA	C4-C5-C6	-6.14	113.93	117.00
6	J	153	DC	N3-C2-O2	-6.13	117.61	121.90
4	D	69	ARG	NE-CZ-NH2	6.12	123.36	120.30
6	J	342	DA	C4-C5-C6	-6.12	113.94	117.00
6	J	323	DC	N3-C2-O2	-6.11	117.62	121.90
5	I	161	DG	N1-C6-O6	-6.10	116.24	119.90
5	I	269	DC	O4'-C1'-C2'	-6.10	101.02	105.90
6	J	33	DA	C5-C6-N1	6.10	120.75	117.70
5	I	167	DC	N3-C2-O2	-6.10	117.63	121.90
5	I	0	DT	C6-C5-C7	-6.08	119.25	122.90
5	I	300	DC	N3-C2-O2	-6.08	117.64	121.90
5	I	242	DA	N1-C6-N6	-6.08	114.95	118.60
5	I	153	DT	O4'-C1'-N1	6.07	112.25	108.00
6	J	345	DT	C6-C5-C7	-6.07	119.26	122.90
6	J	159	DT	C6-C5-C7	-6.06	119.26	122.90
6	J	331	DC	N3-C4-C5	6.05	124.32	121.90
6	J	112	DC	N3-C2-O2	-6.04	117.67	121.90
6	J	163	DC	O4'-C4'-C3'	6.03	109.61	106.00
6	J	183	DC	N3-C2-O2	-6.02	117.68	121.90
5	I	228	DC	N3-C2-O2	-6.02	117.69	121.90
6	J	21	DC	N3-C2-O2	-6.02	117.69	121.90
5	I	308	DA	C5-C6-N1	6.01	120.71	117.70
5	I	332	DT	C6-C5-C7	-6.01	119.30	122.90
5	I	275	DA	C5-C6-N1	6.00	120.70	117.70
6	J	103	DG	N9-C4-C5	5.99	107.80	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	11	DC	N3-C2-O2	-5.99	117.71	121.90
5	I	318	DA	C5-C6-N1	5.98	120.69	117.70
5	I	283	DA	C5-C6-N1	5.98	120.69	117.70
5	I	1	DA	C5-C6-N1	5.97	120.69	117.70
6	J	164	DC	N1-C2-O2	5.97	122.48	118.90
5	I	238	DA	C5'-C4'-C3'	-5.97	103.36	114.10
5	I	310	DA	C4-C5-C6	-5.96	114.02	117.00
5	I	8	DA	C4-C5-C6	-5.96	114.02	117.00
6	J	12	DA	N1-C6-N6	-5.96	115.03	118.60
6	J	163	DC	N3-C2-O2	-5.96	117.73	121.90
6	J	336	DT	C6-C5-C7	-5.95	119.33	122.90
5	I	294	DT	C6-C5-C7	-5.94	119.34	122.90
6	J	60	DG	N3-C2-N2	-5.94	115.74	119.90
6	J	154	DC	N3-C4-C5	5.94	124.27	121.90
1	E	63	ARG	NE-CZ-NH2	5.93	123.27	120.30
5	I	7	DA	C4-C5-C6	-5.93	114.04	117.00
6	J	61	DT	C6-C5-C7	-5.92	119.35	122.90
6	J	174	DC	N3-C2-O2	-5.92	117.76	121.90
5	I	322	DT	C6-C5-C7	-5.91	119.35	122.90
6	J	337	DT	C6-C5-C7	-5.91	119.35	122.90
6	J	14	DA	C5-C6-N1	5.91	120.66	117.70
5	I	192	DT	C6-C5-C7	-5.91	119.36	122.90
2	B	92	ARG	NE-CZ-NH1	-5.90	117.35	120.30
6	J	103	DG	N1-C6-O6	-5.90	116.36	119.90
6	J	66	DC	N3-C2-O2	-5.90	117.77	121.90
6	J	34	DT	C6-C5-C7	-5.89	119.36	122.90
5	I	282	DT	C6-C5-C7	-5.88	119.37	122.90
5	I	331	DA	N1-C6-N6	-5.88	115.07	118.60
6	J	147	DT	C6-C5-C7	-5.88	119.37	122.90
1	e	42	ARG	NE-CZ-NH2	5.88	123.24	120.30
5	I	15	DT	C1'-O4'-C4'	-5.87	104.23	110.10
5	I	324	DT	C1'-O4'-C4'	-5.86	104.24	110.10
6	J	119	DA	N1-C6-N6	-5.86	115.08	118.60
5	I	315	DT	C6-C5-C7	-5.86	119.39	122.90
5	I	184	DA	C4-C5-C6	-5.86	114.07	117.00
6	J	339	DT	C6-C5-C7	-5.85	119.39	122.90
6	J	32	DT	C6-C5-C7	-5.85	119.39	122.90
10	N	508	PRO	CA-N-CD	-5.85	103.31	111.50
5	I	281	DT	C6-C5-C7	-5.85	119.39	122.90
5	I	289	DT	O4'-C1'-C2'	-5.85	101.22	105.90
5	I	24	DC	N3-C2-O2	-5.85	117.81	121.90
2	B	72	TYR	CB-CG-CD2	-5.84	117.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	188	DA	C4-C5-C6	-5.84	114.08	117.00
6	J	147	DT	N3-C2-O2	-5.83	118.80	122.30
5	I	153	DT	C6-C5-C7	-5.82	119.41	122.90
5	I	271	DG	C1'-O4'-C4'	-5.81	104.29	110.10
5	I	311	DT	C6-C5-C7	-5.81	119.42	122.90
5	I	-5	DT	C6-C5-C7	-5.81	119.42	122.90
5	I	9	DT	C6-C5-C7	-5.79	119.42	122.90
6	J	67	DC	N3-C2-O2	-5.79	117.85	121.90
6	J	178	DC	N3-C2-O2	-5.79	117.85	121.90
5	I	289	DT	C6-C5-C7	-5.79	119.43	122.90
6	J	331	DC	N3-C2-O2	-5.79	117.85	121.90
5	I	237	DA	P-O3'-C3'	5.78	126.64	119.70
6	J	154	DC	N3-C2-O2	-5.78	117.85	121.90
5	I	186	DT	C6-C5-C7	-5.78	119.43	122.90
5	I	290	DA	C4-C5-C6	-5.78	114.11	117.00
5	I	171	DT	C6-C5-C7	-5.77	119.44	122.90
6	J	329	DA	N1-C6-N6	-5.77	115.14	118.60
5	I	303	DG	N3-C2-N2	-5.76	115.87	119.90
6	J	15	DC	N3-C2-O2	-5.76	117.87	121.90
5	I	326	DC	N3-C2-O2	-5.76	117.87	121.90
6	J	35	DC	N3-C2-O2	-5.76	117.87	121.90
6	J	55	DA	C4-C5-C6	-5.76	114.12	117.00
5	I	304	DT	C6-C5-C7	-5.73	119.46	122.90
6	J	16	DA	C5-C6-N1	5.73	120.56	117.70
6	J	65	DC	N3-C2-O2	-5.73	117.89	121.90
5	I	319	DT	O4'-C1'-N1	5.71	112.00	108.00
5	I	319	DT	C6-C5-C7	-5.71	119.47	122.90
6	J	13	DT	C6-C5-C7	-5.71	119.47	122.90
5	I	274	DA	N1-C6-N6	-5.71	115.17	118.60
6	J	189	DA	C4-C5-C6	-5.71	114.15	117.00
5	I	20	DA	C4-C5-C6	-5.70	114.15	117.00
6	J	319	DC	O4'-C1'-N1	5.70	111.99	108.00
5	I	244	DG	C5-C6-N1	5.70	114.35	111.50
6	J	38	DA	C5-C6-N1	5.70	120.55	117.70
6	J	20	DA	C4-C5-C6	-5.69	114.15	117.00
6	J	191	DA	C5-C6-N1	5.69	120.55	117.70
5	I	222	DC	N3-C4-C5	5.69	124.17	121.90
5	I	324	DT	C6-C5-C7	-5.68	119.49	122.90
6	J	344	DA	C5-C6-N1	5.68	120.54	117.70
6	J	151	DC	N3-C4-C5	5.66	124.17	121.90
5	I	164	DC	C1'-O4'-C4'	-5.65	104.45	110.10
5	I	312	DA	C5-C6-N1	5.65	120.53	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	287	DC	N3-C2-O2	-5.65	117.95	121.90
6	J	341	DG	O4'-C1'-N9	5.64	111.95	108.00
5	I	226	DA	C5-C6-N1	5.64	120.52	117.70
5	I	290	DA	C5-C6-N1	5.64	120.52	117.70
6	J	348	DA	C4-C5-C6	-5.64	114.18	117.00
6	J	102	DT	C6-C5-C7	-5.64	119.52	122.90
5	I	162	DT	N3-C2-O2	-5.63	118.92	122.30
4	D	30	ARG	NE-CZ-NH2	5.63	123.11	120.30
4	h	77	LEU	CA-CB-CG	5.63	128.24	115.30
6	J	324	DT	C6-C5-C7	-5.62	119.53	122.90
2	F	79	LYS	CB-CA-C	5.62	121.63	110.40
5	I	327	DA	N1-C6-N6	-5.61	115.23	118.60
6	J	29	DA	N1-C6-N6	-5.61	115.24	118.60
6	J	41	DC	N3-C2-O2	-5.61	117.98	121.90
6	J	119	DA	C4-C5-C6	-5.60	114.20	117.00
5	I	-1	DA	C5-C6-N1	5.60	120.50	117.70
5	I	155	DT	O4'-C4'-C3'	5.60	109.36	106.00
5	I	1	DA	C4-C5-C6	-5.59	114.20	117.00
10	P	319	LEU	CA-CB-CG	5.59	128.17	115.30
6	J	62	DA	N1-C6-N6	-5.59	115.25	118.60
6	J	17	DT	C6-C5-C7	-5.59	119.55	122.90
6	J	327	DG	O4'-C4'-C3'	5.58	109.35	106.00
6	J	329	DA	C4-C5-C6	-5.58	114.21	117.00
5	I	243	DC	N3-C2-O2	-5.58	118.00	121.90
1	E	69	ARG	NE-CZ-NH2	5.57	123.08	120.30
5	I	330	DT	C6-C5-C7	-5.57	119.56	122.90
5	I	318	DA	C4-C5-C6	-5.57	114.22	117.00
5	I	296	DC	N3-C4-C5	5.57	124.13	121.90
6	J	38	DA	C4-C5-C6	-5.56	114.22	117.00
5	I	223	DT	C6-C5-C7	-5.55	119.57	122.90
5	I	178	DC	N3-C2-O2	-5.55	118.02	121.90
6	J	118	DT	C6-C5-C7	-5.54	119.57	122.90
6	J	45	DC	N3-C2-O2	-5.53	118.03	121.90
5	I	174	DT	C6-C5-C7	-5.53	119.58	122.90
6	J	169	DT	C6-C5-C7	-5.53	119.58	122.90
5	I	289	DT	N3-C2-O2	-5.53	118.98	122.30
9	O	18	HIS	N-CA-C	-5.53	96.08	111.00
1	e	40	ARG	NE-CZ-NH2	5.52	123.06	120.30
6	J	112	DC	O4'-C4'-C3'	5.52	109.31	106.00
9	M	18	HIS	N-CA-C	-5.52	96.10	111.00
6	J	20	DA	N1-C6-N6	-5.52	115.29	118.60
1	A	40	ARG	NE-CZ-NH2	5.51	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	14	DA	C4-C5-C6	-5.51	114.25	117.00
6	J	66	DC	N3-C4-C5	5.51	124.10	121.90
5	I	179	DT	C6-C5-C7	-5.51	119.59	122.90
5	I	308	DA	C4-C5-C6	-5.50	114.25	117.00
5	I	301	DA	C5-C6-N1	5.49	120.44	117.70
6	J	59	DA	N1-C6-N6	-5.48	115.31	118.60
5	I	224	DC	N3-C2-O2	-5.48	118.06	121.90
6	J	335	DA	C5-C6-N1	5.48	120.44	117.70
6	J	55	DA	N1-C6-N6	-5.48	115.31	118.60
5	I	23	DC	N3-C2-O2	-5.47	118.07	121.90
6	J	65	DC	N3-C4-C5	5.47	124.09	121.90
5	I	0	DT	P-O3'-C3'	5.46	126.25	119.70
6	J	67	DC	N1-C2-O2	5.46	122.17	118.90
6	J	181	DT	N3-C2-O2	-5.46	119.03	122.30
5	I	289	DT	O4'-C1'-N1	5.45	111.82	108.00
5	I	285	DT	C1'-O4'-C4'	-5.45	104.65	110.10
6	J	167	DT	C6-C5-C7	-5.45	119.63	122.90
6	J	43	DT	C6-C5-C7	-5.45	119.63	122.90
5	I	314	DA	C4-C5-C6	-5.44	114.28	117.00
6	J	160	DT	C6-C5-C7	-5.44	119.64	122.90
5	I	-1	DA	C4-C5-C6	-5.44	114.28	117.00
6	J	26	DT	C6-C5-C7	-5.44	119.64	122.90
9	M	355	LEU	CA-CB-CG	5.44	127.81	115.30
5	I	3	DC	O4'-C4'-C3'	5.44	109.26	106.00
6	J	70	DT	N3-C2-O2	-5.42	119.05	122.30
5	I	156	DT	C6-C5-C7	-5.42	119.65	122.90
5	I	333	DT	C6-C5-C7	-5.42	119.65	122.90
6	J	325	DC	N1-C2-O2	5.42	122.15	118.90
5	I	15	DT	C6-C5-C7	-5.41	119.65	122.90
6	J	190	DT	C6-C5-C7	-5.41	119.66	122.90
5	I	297	DA	C4-C5-C6	-5.40	114.30	117.00
5	I	155	DT	C6-C5-C7	-5.40	119.66	122.90
5	I	182	DA	N1-C6-N6	-5.40	115.36	118.60
5	I	-5	DT	C5-C6-N1	-5.39	120.46	123.70
5	I	165	DT	N3-C2-O2	-5.39	119.06	122.30
5	I	165	DT	C6-C5-C7	-5.39	119.67	122.90
6	J	101	DG	C8-N9-C4	-5.38	104.25	106.40
5	I	313	DT	C6-C5-C7	-5.37	119.68	122.90
6	J	22	DA	C4-C5-C6	-5.37	114.31	117.00
6	J	54	DT	C6-C5-C7	-5.37	119.68	122.90
5	I	168	DC	N1-C2-O2	5.36	122.12	118.90
5	I	305	DG	P-O3'-C3'	5.36	126.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	295	DC	N3-C2-O2	-5.36	118.15	121.90
6	J	191	DA	N1-C6-N6	-5.35	115.39	118.60
6	J	109	DA	C4-C5-C6	-5.34	114.33	117.00
6	J	39	DC	N3-C4-C5	5.34	124.03	121.90
6	J	164	DC	N3-C4-C5	5.34	124.03	121.90
6	J	27	DG	N1-C6-O6	-5.33	116.70	119.90
6	J	335	DA	C4-C5-C6	-5.33	114.34	117.00
6	J	30	DT	C6-C5-C7	-5.32	119.71	122.90
5	I	195	DC	N1-C2-O2	5.31	122.09	118.90
5	I	19	DG	N3-C2-N2	-5.31	116.19	119.90
6	J	48	DG	O4'-C4'-C3'	5.31	109.18	106.00
6	J	27	DG	O4'-C4'-C3'	5.30	109.18	106.00
5	I	282	DT	C5-C6-N1	-5.30	120.52	123.70
5	I	222	DC	O4'-C4'-C3'	5.28	109.17	106.00
6	J	65	DC	N1-C2-O2	5.28	122.07	118.90
5	I	302	DC	N3-C2-O2	-5.28	118.20	121.90
5	I	321	DC	N3-C2-O2	-5.28	118.20	121.90
6	J	190	DT	O4'-C1'-C2'	-5.27	101.68	105.90
1	E	60	LEU	CB-CA-C	5.27	120.22	110.20
6	J	178	DC	N3-C4-C5	5.27	124.01	121.90
6	J	165	DA	C4-C5-C6	-5.27	114.37	117.00
6	J	30	DT	O4'-C4'-C3'	5.26	109.16	106.00
5	I	281	DT	C5-C6-N1	-5.26	120.55	123.70
5	I	172	DT	O4'-C4'-C3'	5.26	109.15	106.00
4	D	103	LEU	CB-CG-CD1	5.25	119.92	111.00
5	I	246	DA	C4-C5-C6	-5.24	114.38	117.00
5	I	272	DC	N3-C4-C5	5.24	124.00	121.90
5	I	238	DA	N1-C6-N6	-5.23	115.46	118.60
5	I	283	DA	N1-C6-N6	-5.23	115.46	118.60
6	J	190	DT	C1'-O4'-C4'	-5.23	104.87	110.10
6	J	19	DC	N3-C4-C5	5.22	123.99	121.90
5	I	288	DC	N3-C2-O2	-5.22	118.25	121.90
6	J	60	DG	N9-C4-C5	5.22	107.49	105.40
6	J	343	DT	C6-C5-C7	-5.22	119.77	122.90
5	I	172	DT	C6-C5-C7	-5.22	119.77	122.90
1	A	49	ARG	NE-CZ-NH2	5.21	122.91	120.30
6	J	39	DC	O4'-C4'-C3'	5.21	109.13	106.00
6	J	70	DT	C6-C5-C7	-5.21	119.77	122.90
5	I	320	DC	N3-C2-O2	-5.21	118.25	121.90
6	J	319	DC	O4'-C1'-C2'	-5.21	101.74	105.90
6	J	191	DA	C4-C5-C6	-5.20	114.40	117.00
6	J	151	DC	N3-C2-O2	-5.20	118.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	285	DT	P-O3'-C3'	5.20	125.93	119.70
5	I	15	DT	O4'-C1'-N1	5.19	111.64	108.00
6	J	180	DG	N1-C6-O6	-5.19	116.79	119.90
5	I	242	DA	C5-C6-N1	5.18	120.29	117.70
3	C	20	ARG	NE-CZ-NH2	5.18	122.89	120.30
5	I	-3	DC	O4'-C1'-N1	5.18	111.63	108.00
5	I	314	DA	C5-C6-N1	5.18	120.29	117.70
6	J	154	DC	N1-C2-O2	5.17	122.00	118.90
5	I	162	DT	C6-C5-C7	-5.17	119.80	122.90
6	J	169	DT	O4'-C4'-C3'	5.17	109.10	106.00
5	I	286	DC	N3-C2-O2	-5.16	118.29	121.90
5	I	301	DA	C4-C5-C6	-5.16	114.42	117.00
6	J	148	DC	N3-C2-O2	-5.16	118.29	121.90
5	I	177	DA	P-O3'-C3'	5.16	125.89	119.70
6	J	330	DC	N1-C2-O2	5.15	121.99	118.90
6	J	68	DC	N3-C2-O2	-5.15	118.30	121.90
5	I	307	DC	N3-C4-C5	5.15	123.96	121.90
6	J	104	DC	N3-C2-O2	-5.15	118.30	121.90
5	I	247	DC	O4'-C1'-N1	5.14	111.60	108.00
6	J	337	DT	O4'-C4'-C3'	5.14	109.08	106.00
5	I	307	DC	N3-C2-O2	-5.14	118.30	121.90
5	I	285	DT	C6-C5-C7	-5.13	119.82	122.90
5	I	243	DC	N3-C4-C5	5.13	123.95	121.90
6	J	104	DC	O4'-C4'-C3'	5.12	109.07	106.00
6	J	145	DC	N3-C2-O2	-5.11	118.32	121.90
1	E	122	LYS	CA-CB-CG	5.11	124.63	113.40
6	J	53	DC	O4'-C4'-C3'	5.10	109.06	106.00
5	I	24	DC	N3-C4-C5	5.10	123.94	121.90
6	J	28	DT	C6-C5-C7	-5.10	119.84	122.90
1	E	72	ARG	NE-CZ-NH2	5.09	122.85	120.30
5	I	286	DC	N3-C4-C5	5.09	123.94	121.90
6	J	52	DA	N1-C6-N6	-5.08	115.55	118.60
6	J	149	DG	C8-N9-C4	-5.08	104.37	106.40
6	J	22	DA	C5-C6-N1	5.08	120.24	117.70
6	J	111	DG	C5-C6-N1	5.08	114.04	111.50
5	I	296	DC	N1-C2-O2	5.08	121.94	118.90
6	J	189	DA	N1-C6-N6	-5.08	115.56	118.60
5	I	330	DT	N3-C2-O2	-5.07	119.26	122.30
1	e	122	LYS	CA-CB-CG	5.07	124.55	113.40
5	I	245	DT	C6-C5-C7	-5.06	119.86	122.90
6	J	19	DC	N3-C2-O2	-5.06	118.36	121.90
3	C	88	ARG	NE-CZ-NH2	5.06	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	194	DC	C6-N1-C2	-5.06	118.28	120.30
6	J	151	DC	N1-C2-O2	5.05	121.93	118.90
5	I	308	DA	N1-C6-N6	-5.05	115.57	118.60
6	J	178	DC	N1-C2-O2	5.05	121.93	118.90
6	J	173	DA	O4'-C4'-C3'	5.05	109.03	106.00
5	I	15	DT	O4'-C1'-C2'	-5.04	101.87	105.90
5	I	168	DC	O4'-C1'-N1	5.04	111.53	108.00
5	I	17	DC	C6-N1-C2	-5.03	118.29	120.30
5	I	4	DG	C5-C6-N1	5.03	114.01	111.50
6	J	175	DT	N3-C2-O2	-5.03	119.28	122.30
5	I	273	DC	N3-C2-O2	-5.03	118.38	121.90
6	J	161	DC	N3-C4-C5	5.03	123.91	121.90
5	I	196	DG	P-O3'-C3'	5.02	125.73	119.70
5	I	284	DC	N3-C2-O2	-5.02	118.38	121.90
6	J	192	DC	N3-C2-O2	-5.02	118.38	121.90
6	J	324	DT	N3-C2-O2	-5.02	119.29	122.30
6	J	122	DG	C5-C6-N1	5.02	114.01	111.50
5	I	228	DC	N3-C4-C5	5.02	123.91	121.90
6	J	73	DC	N3-C4-C5	5.01	123.90	121.90
6	J	74	DG	O4'-C1'-C2'	5.01	109.91	105.90
6	J	153	DC	N1-C2-O2	5.01	121.91	118.90
5	I	188	DC	O4'-C4'-C3'	5.00	109.00	106.00
5	I	289	DT	C4-C5-C6	5.00	121.00	118.00
5	I	296	DC	N3-C2-O2	-5.00	118.40	121.90
6	J	159	DT	O4'-C4'-C3'	5.00	109.00	106.00
6	J	338	DC	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	ARG	Sidechain
2	B	92	ARG	Sidechain
3	C	32	ARG	Sidechain
3	C	50	TYR	Sidechain
4	D	105	LYS	Mainchain
4	D	30	ARG	Sidechain
4	D	69	ARG	Sidechain
4	D	96	ARG	Sidechain
1	E	63	ARG	Sidechain
2	F	35	ARG	Sidechain
3	G	77	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	I	-5	DT	Sidechain
5	I	-6	DA	Sidechain
5	I	157	DG	Sidechain
5	I	16	DG	Sidechain
5	I	164	DC	Sidechain
5	I	167	DC	Sidechain
5	I	173	DC	Sidechain
5	I	18	DC	Sidechain
5	I	183	DG	Sidechain
5	I	186	DT	Sidechain
5	I	19	DG	Sidechain
5	I	195	DC	Sidechain
5	I	227	DG	Sidechain
5	I	242	DA	Sidechain
5	I	246	DA	Sidechain
5	I	279	DG	Sidechain
5	I	291	DG	Sidechain
5	I	298	DG	Sidechain
5	I	305	DG	Sidechain
5	I	308	DA	Sidechain
5	I	331	DA	Sidechain
5	I	332	DT	Sidechain
5	I	6	DG	Sidechain
6	J	103	DG	Sidechain
6	J	119	DA	Sidechain
6	J	124	DT	Sidechain
6	J	13	DT	Sidechain
6	J	149	DG	Sidechain
6	J	155	DG	Sidechain
6	J	182	DA	Sidechain
6	J	188	DA	Sidechain
6	J	25	DA	Sidechain
6	J	332	DG	Sidechain
6	J	338	DC	Sidechain
6	J	339	DT	Sidechain
6	J	344	DA	Sidechain
6	J	349	DA	Sidechain
6	J	350	DT	Sidechain
6	J	37	DG	Sidechain
6	J	51	DG	Sidechain
6	J	74	DG	Sidechain
4	d	30	ARG	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	99/135 (73%)	92 (93%)	7 (7%)	0	100	100
1	E	113/135 (84%)	110 (97%)	3 (3%)	0	100	100
1	a	99/135 (73%)	96 (97%)	3 (3%)	0	100	100
1	e	96/135 (71%)	94 (98%)	2 (2%)	0	100	100
2	B	79/102 (78%)	77 (98%)	2 (2%)	0	100	100
2	F	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
2	b	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
2	f	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
3	C	107/129 (83%)	104 (97%)	3 (3%)	0	100	100
3	G	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
3	c	107/129 (83%)	105 (98%)	2 (2%)	0	100	100
3	g	104/129 (81%)	101 (97%)	3 (3%)	0	100	100
4	D	94/122 (77%)	90 (96%)	4 (4%)	0	100	100
4	H	93/122 (76%)	84 (90%)	9 (10%)	0	100	100
4	d	94/122 (77%)	92 (98%)	2 (2%)	0	100	100
4	h	93/122 (76%)	84 (90%)	9 (10%)	0	100	100
7	K	543/1536 (35%)	526 (97%)	17 (3%)	0	100	100
8	L	382/433 (88%)	369 (97%)	13 (3%)	0	100	100
9	M	288/401 (72%)	284 (99%)	4 (1%)	0	100	100
9	O	261/401 (65%)	255 (98%)	6 (2%)	0	100	100
10	N	362/684 (53%)	347 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	P	147/684 (22%)	140 (95%)	7 (5%)	0	100	100
All	All	3501/6091 (58%)	3382 (97%)	119 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	
1	A	86/108 (80%)	86 (100%)	0	100	100
1	E	99/108 (92%)	98 (99%)	1 (1%)	73	82
1	a	86/108 (80%)	86 (100%)	0	100	100
1	e	85/108 (79%)	85 (100%)	0	100	100
2	B	66/78 (85%)	66 (100%)	0	100	100
2	F	65/78 (83%)	65 (100%)	0	100	100
2	b	67/78 (86%)	67 (100%)	0	100	100
2	f	65/78 (83%)	65 (100%)	0	100	100
3	C	86/101 (85%)	86 (100%)	0	100	100
3	G	84/101 (83%)	84 (100%)	0	100	100
3	c	86/101 (85%)	86 (100%)	0	100	100
3	g	84/101 (83%)	84 (100%)	0	100	100
4	D	82/102 (80%)	82 (100%)	0	100	100
4	H	81/102 (79%)	81 (100%)	0	100	100
4	d	82/102 (80%)	82 (100%)	0	100	100
4	h	81/102 (79%)	81 (100%)	0	100	100
7	K	510/1391 (37%)	510 (100%)	0	100	100
8	L	326/367 (89%)	324 (99%)	2 (1%)	84	88
9	M	268/359 (75%)	267 (100%)	1 (0%)	89	91
9	O	245/359 (68%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	N	353/653 (54%)	353 (100%)	0	100 100
10	P	146/653 (22%)	146 (100%)	0	100 100
All	All	3133/5338 (59%)	3129 (100%)	4 (0%)	92 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	63	ARG
8	L	150	HIS
8	L	259	MET
9	M	292	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
2	B	93	GLN
1	E	19	GLN
4	H	81	ASN
7	K	690	ASN
7	K	937	GLN
7	K	1311	HIS
9	M	389	ASN
10	N	304	ASN
10	N	393	GLN
10	N	517	ASN
9	O	275	GLN
2	b	93	GLN
3	c	38	ASN
1	e	108	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	ML3	A	36	1	10,11,12	0.77	0	10,14,16	0.83	0
1	ML3	a	36	1	10,11,12	0.76	0	10,14,16	0.82	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
1	ML3	A	36	1	-	5/8/10/12	-
1	ML3	a	36	1	-	5/8/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	36	ML3	SG-CD-CE-NZ
1	a	36	ML3	SG-CD-CE-NZ
1	A	36	ML3	CD-CE-NZ-CM1
1	A	36	ML3	CD-CE-NZ-CM2
1	a	36	ML3	CD-CE-NZ-CM1
1	a	36	ML3	CD-CE-NZ-CM2
1	A	36	ML3	CD-CE-NZ-CM3
1	a	36	ML3	CD-CE-NZ-CM3
1	A	36	ML3	CA-CB-SG-CD
1	a	36	ML3	CA-CB-SG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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.

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.