



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 22, 2018 – 07:03 PM EST

PDB ID : 5NZR  
EMDB ID: : EMD-3720  
Title : The structure of the COPI coat leaf  
Authors : Dodonova, S.O.; Aderhold, P.; Kopp, J.; Ganeva, I.; Roehling, S.; Hagen, W.J.H.; Sinning, I.; Wieland, F.; Briggs, J.A.G.  
Deposited on : 2017-05-15  
Resolution : 9.20 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

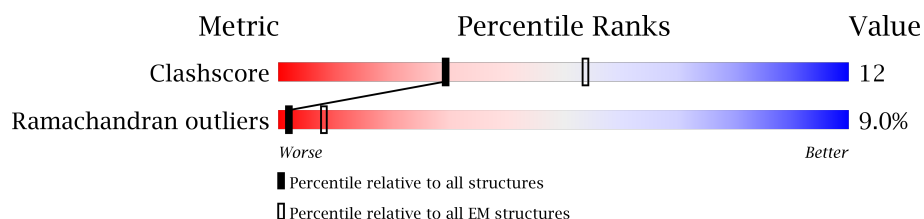
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*








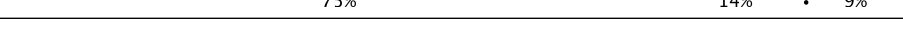
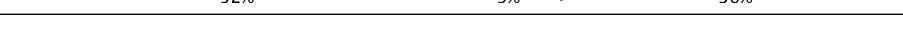
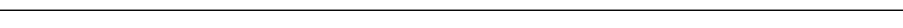
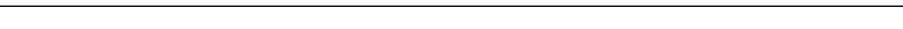
The reported resolution of this entry is 9.20 Å.

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	125131	1336
Ramachandran outliers	121729	1120

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1262	 49% 14% • 36%
2	B	968	 66% 13% • 17%
3	C	905	 77% 14% • 7%
4	D	511	 29% 5% • 65%
5	F	181	 77% 8% • 12%
5	M	181	 65% 19% • 12%
5	R	181	 54% 27% 7% 12%
6	G	874	 75% 14% • 9%
6	K	874	 52% 9% • 36%
7	L	177	 66% 12% • 21%
7	Z	177	 66% 12% • 21%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18970 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	813	Total	C	N	O	0	0
			3251	1626	813	812		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1225	LEU	-	expression tag	UNP Q8CIE6
A	1226	GLU	-	expression tag	UNP Q8CIE6
A	1227	VAL	-	expression tag	UNP Q8CIE6
A	1228	LEU	-	expression tag	UNP Q8CIE6
A	1229	PHE	-	expression tag	UNP Q8CIE6
A	1230	GLN	-	expression tag	UNP Q8CIE6
A	1231	GLY	-	expression tag	UNP Q8CIE6
A	1232	PRO	-	expression tag	UNP Q8CIE6
A	1233	SER	-	expression tag	UNP Q8CIE6
A	1234	ALA	-	expression tag	UNP Q8CIE6
A	1235	TRP	-	expression tag	UNP Q8CIE6
A	1236	SER	-	expression tag	UNP Q8CIE6
A	1237	HIS	-	expression tag	UNP Q8CIE6
A	1238	PRO	-	expression tag	UNP Q8CIE6
A	1239	GLN	-	expression tag	UNP Q8CIE6
A	1240	PHE	-	expression tag	UNP Q8CIE6
A	1241	GLU	-	expression tag	UNP Q8CIE6
A	1242	LYS	-	expression tag	UNP Q8CIE6
A	1243	GLY	-	expression tag	UNP Q8CIE6
A	1244	GLY	-	expression tag	UNP Q8CIE6
A	1245	GLY	-	expression tag	UNP Q8CIE6
A	1246	SER	-	expression tag	UNP Q8CIE6
A	1247	GLY	-	expression tag	UNP Q8CIE6
A	1248	GLY	-	expression tag	UNP Q8CIE6
A	1249	GLY	-	expression tag	UNP Q8CIE6
A	1250	SER	-	expression tag	UNP Q8CIE6
A	1251	GLY	-	expression tag	UNP Q8CIE6
A	1252	GLY	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1253	SER	-	expression tag	UNP Q8CIE6
A	1254	ALA	-	expression tag	UNP Q8CIE6
A	1255	TRP	-	expression tag	UNP Q8CIE6
A	1256	SER	-	expression tag	UNP Q8CIE6
A	1257	HIS	-	expression tag	UNP Q8CIE6
A	1258	PRO	-	expression tag	UNP Q8CIE6
A	1259	GLN	-	expression tag	UNP Q8CIE6
A	1260	PHE	-	expression tag	UNP Q8CIE6
A	1261	GLU	-	expression tag	UNP Q8CIE6
A	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 2 is a protein called Coatomer subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	800	Total	C	N	O	0	0
			3198	1600	800	798		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9JIF7
B	2	HIS	-	expression tag	UNP Q9JIF7
B	3	HIS	-	expression tag	UNP Q9JIF7
B	4	HIS	-	expression tag	UNP Q9JIF7
B	5	HIS	-	expression tag	UNP Q9JIF7
B	6	HIS	-	expression tag	UNP Q9JIF7
B	7	HIS	-	expression tag	UNP Q9JIF7
B	8	GLU	-	expression tag	UNP Q9JIF7
B	9	ASN	-	expression tag	UNP Q9JIF7
B	10	LEU	-	expression tag	UNP Q9JIF7
B	11	TYR	-	expression tag	UNP Q9JIF7
B	12	PHE	-	expression tag	UNP Q9JIF7
B	13	GLN	-	expression tag	UNP Q9JIF7
B	14	GLY	-	expression tag	UNP Q9JIF7
B	15	HIS	-	expression tag	UNP Q9JIF7

- Molecule 3 is a protein called Coatomer subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	843	Total	C	N	O	0	0
			3371	1686	843	842		

- Molecule 4 is a protein called Coatomer subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	177	Total	C	N	O	0	0
			706	354	177	175		

- Molecule 5 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	159	Total	C	N	O	0	0
			635	318	159	158		
5	R	159	Total	C	N	O	0	0
			635	318	159	158		
5	M	159	Total	C	N	O	0	0
			635	318	159	158		

- Molecule 6 is a protein called Coatomer subunit gamma-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	798	Total	C	N	O	0	0
			3190	1596	798	796		
6	K	560	Total	C	N	O	0	0
			2239	1120	560	559		

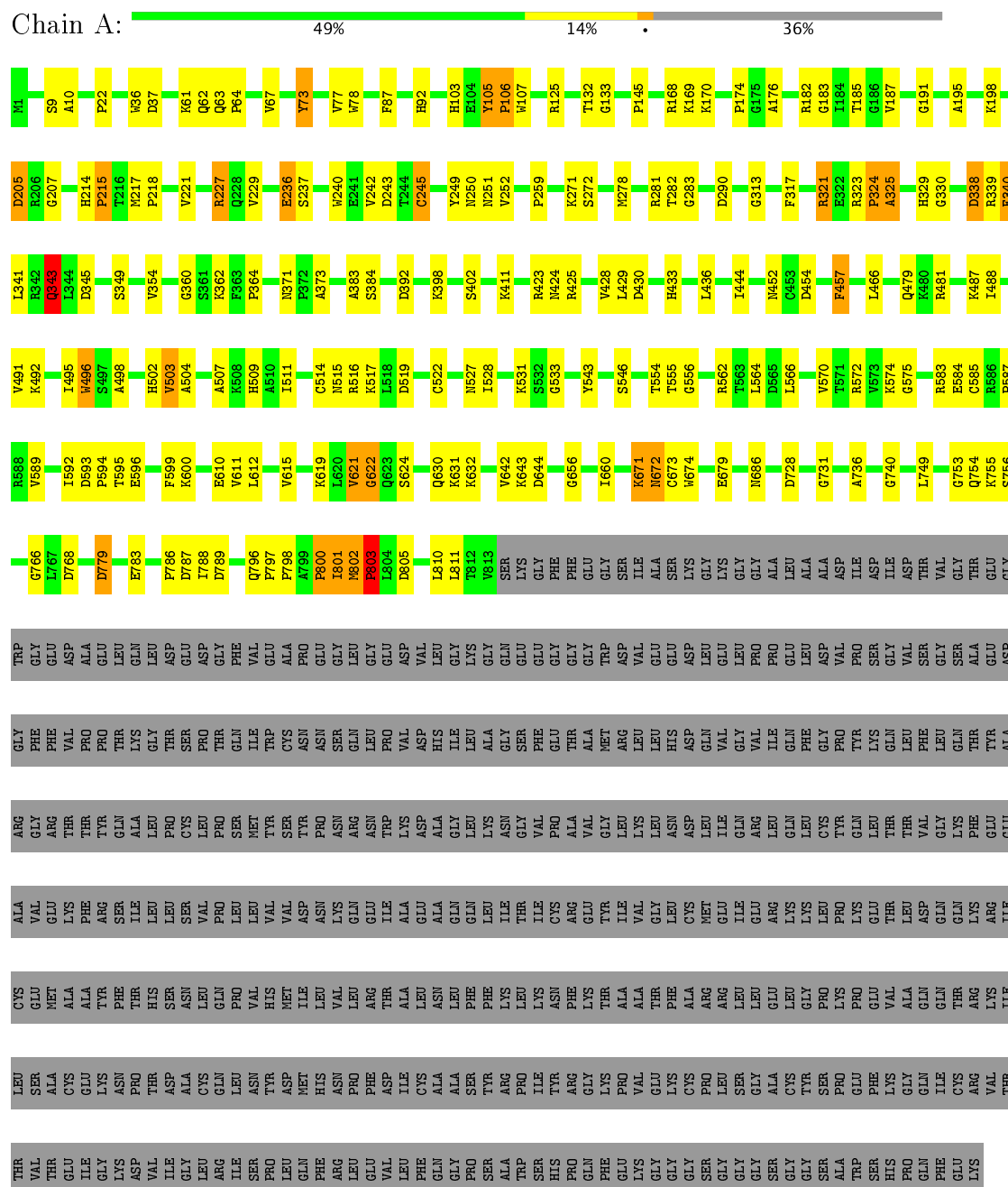
- Molecule 7 is a protein called Coatomer subunit zeta-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	139	Total	C	N	O	0	0
			555	278	139	138		
7	L	139	Total	C	N	O	0	0
			555	278	139	138		

### 3 Residue-property plots

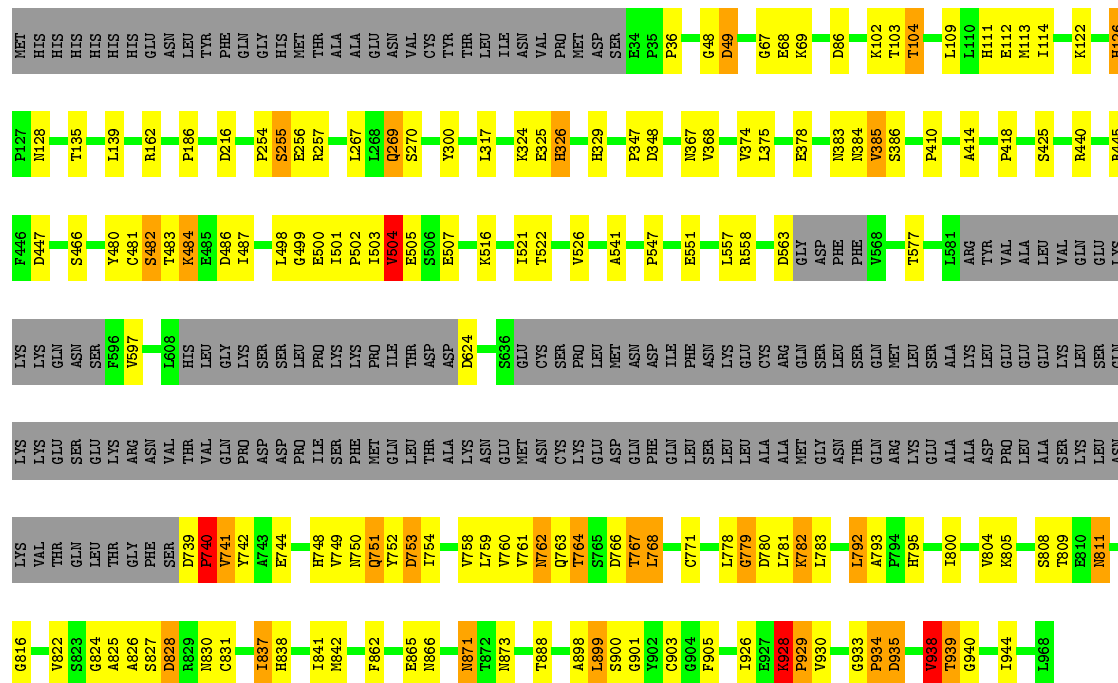
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Coatomer subunit alpha



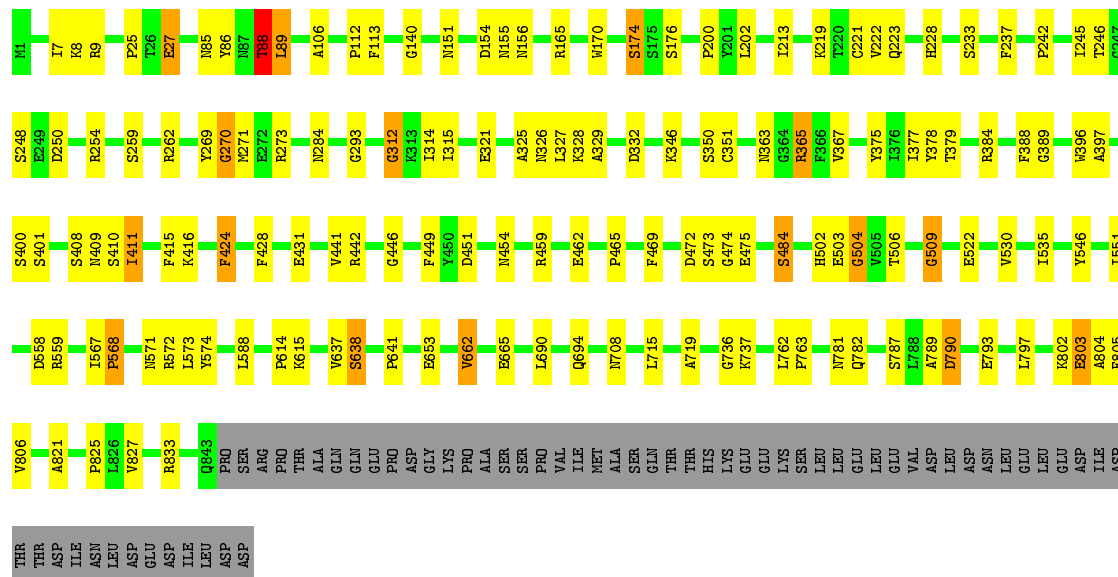
- Molecule 2: Coatomer subunit beta

Chain B:  66% 13% • 17%



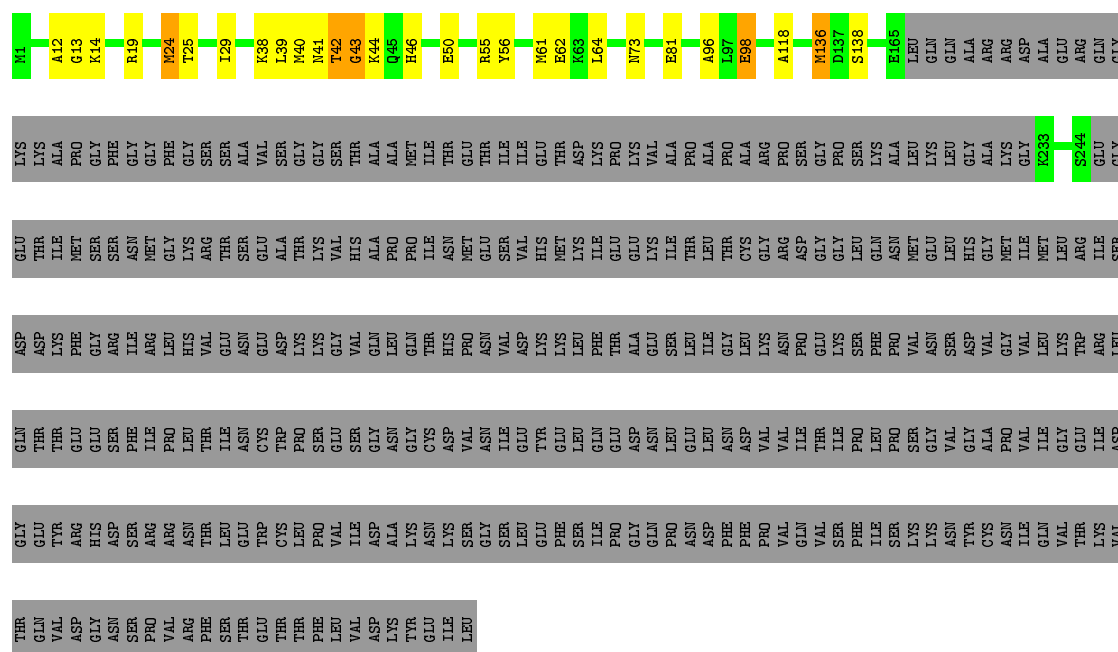
- Molecule 3: Coatomer subunit beta'

Chain C:  77% 14% • 7%

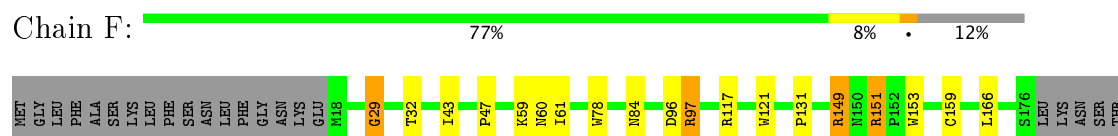


- Molecule 4: Coatomer subunit delta

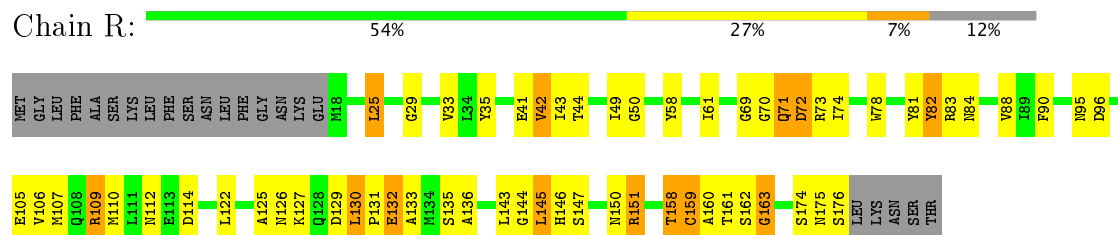
Chain D:  29% 5% 65%



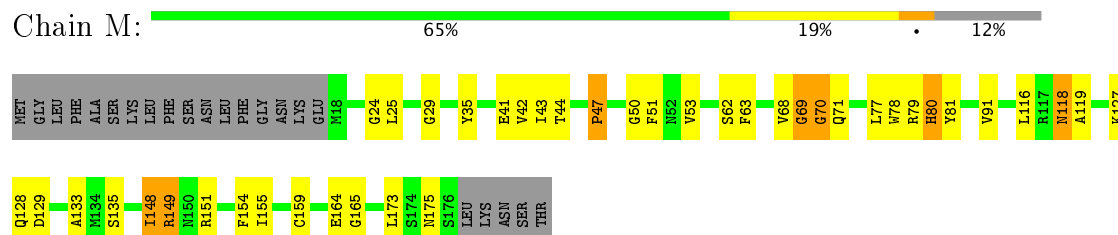
- Molecule 5: ADP-ribosylation factor 1



- Molecule 5: ADP-ribosylation factor 1



- Molecule 5: ADP-ribosylation factor 1



- Molecule 6: Coatomer subunit gamma-1









● Molecule 7: Coatomer subunit zeta-1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	38498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF-determination for each individual tilt image was performed using CTFFIND4. Strip-based CTF-correction and tomogram reconstruction was performed in Imod.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k 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  >2	RMSZ	# Z  >2
1	A	1.56	15/3250 (0.5%)	1.81	74/4061 (1.8%)
2	B	1.71	19/3193 (0.6%)	1.55	45/3983 (1.1%)
3	C	1.76	23/3370 (0.7%)	1.70	60/4211 (1.4%)
4	D	1.67	3/704 (0.4%)	1.65	10/877 (1.1%)
5	F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
6	G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	K	1.72	9/2237 (0.4%)	1.69	44/2793 (1.6%)
7	L	2.05	3/554 (0.5%)	1.72	7/691 (1.0%)
7	Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
All	All	1.69	101/18952 (0.5%)	1.68	329/23662 (1.4%)

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	B	0	3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	940	GLY	N-CA	-7.80	1.34	1.46
5	R	29	GLY	CA-C	-7.62	1.39	1.51
5	R	35	TYR	CA-C	-7.33	1.33	1.52
1	A	191	GLY	CA-C	-7.04	1.40	1.51
3	C	572	ARG	CA-C	-6.59	1.35	1.52
2	B	418	PRO	CA-C	-6.57	1.39	1.52
6	G	215	ILE	CA-C	-6.56	1.35	1.52
1	A	594	PRO	CA-C	-6.55	1.39	1.52
6	K	235	VAL	N-CA	-6.52	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	55	ARG	CA-C	-6.44	1.36	1.52
1	A	612	LEU	N-CA	-6.41	1.33	1.46
5	R	109	ARG	CA-C	-6.34	1.36	1.52
6	G	839	ASP	CA-C	-6.34	1.36	1.52
1	A	766	GLY	CA-C	-6.34	1.41	1.51
6	K	839	ASP	CA-C	-6.32	1.36	1.52
6	K	211	VAL	CA-C	-6.31	1.36	1.52
6	K	214	MET	CA-C	-6.21	1.36	1.52
7	Z	19	LEU	N-CA	-6.18	1.33	1.46
3	C	293	GLY	CA-C	-6.18	1.42	1.51
3	C	416	LYS	CA-C	-6.12	1.37	1.52
3	C	378	TYR	CA-C	-6.11	1.37	1.52
5	M	29	GLY	CA-C	-6.07	1.42	1.51
5	M	47	PRO	CA-C	-6.03	1.40	1.52
5	M	70	GLY	CA-C	-6.03	1.42	1.51
1	A	596	GLU	N-CA	-6.03	1.34	1.46
6	G	774	ALA	N-CA	-5.99	1.34	1.46
7	L	23	GLY	CA-C	-5.99	1.42	1.51
6	K	774	ALA	N-CA	-5.96	1.34	1.46
2	B	762	ASN	CA-C	-5.95	1.37	1.52
3	C	641	PRO	CA-C	-5.92	1.41	1.52
3	C	384	ARG	CA-C	-5.88	1.37	1.52
6	K	105	VAL	N-CA	-5.79	1.34	1.46
2	B	126	HIS	CA-C	-5.76	1.38	1.52
2	B	940	GLY	CA-C	-5.76	1.42	1.51
3	C	377	ILE	CA-C	-5.70	1.38	1.52
5	F	29	GLY	N-CA	-5.66	1.37	1.46
3	C	245	ILE	N-CA	-5.60	1.35	1.46
1	A	660	ILE	CA-C	-5.57	1.38	1.52
3	C	568	PRO	CA-C	-5.55	1.41	1.52
6	G	235	VAL	N-CA	-5.54	1.35	1.46
2	B	378	GLU	CA-C	-5.54	1.38	1.52
1	A	679	GLU	CA-C	-5.51	1.38	1.52
6	G	442	PHE	CA-C	-5.50	1.38	1.52
6	K	165	HIS	CA-C	-5.49	1.38	1.52
1	A	360	GLY	CA-C	-5.48	1.43	1.51
6	K	203	VAL	N-CA	-5.47	1.35	1.46
7	Z	65	LEU	N-CA	-5.47	1.35	1.46
2	B	753	ASP	N-CA	-5.45	1.35	1.46
1	A	600	LYS	CA-C	-5.43	1.38	1.52
3	C	449	PHE	CA-C	-5.43	1.38	1.52
1	A	599	PHE	N-CA	-5.42	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	180	GLU	N-CA	-5.41	1.35	1.46
1	A	595	THR	N-CA	-5.40	1.35	1.46
6	G	112	ASP	CA-C	-5.38	1.39	1.52
5	R	90	PHE	N-CA	-5.38	1.35	1.46
2	B	749	VAL	CA-C	-5.37	1.39	1.52
4	D	56	TYR	CA-C	-5.37	1.39	1.52
1	A	612	LEU	CA-C	-5.36	1.39	1.52
2	B	938	VAL	CA-C	-5.36	1.39	1.52
4	D	81	GLU	CA-C	-5.34	1.39	1.52
2	B	783	LEU	CA-C	-5.33	1.39	1.52
5	R	107	MET	CA-C	-5.32	1.39	1.52
2	B	754	ILE	N-CA	-5.32	1.35	1.46
3	C	312	GLY	CA-C	-5.31	1.43	1.51
3	C	223	GLN	CA-C	-5.31	1.39	1.52
3	C	8	LYS	CA-C	-5.30	1.39	1.52
7	Z	19	LEU	CA-C	-5.29	1.39	1.52
3	C	315	ILE	N-CA	-5.28	1.35	1.46
2	B	368	VAL	N-CA	-5.27	1.35	1.46
1	A	283	GLY	CA-C	-5.27	1.43	1.51
7	L	49	PHE	CA-C	-5.27	1.39	1.52
3	C	85	ASN	N-CA	-5.25	1.35	1.46
1	A	610	GLU	N-CA	-5.24	1.35	1.46
2	B	759	LEU	N-CA	-5.24	1.35	1.46
3	C	415	PHE	CA-C	-5.23	1.39	1.52
3	C	736	GLY	CA-C	-5.23	1.43	1.51
5	R	105	GLU	CA-C	-5.22	1.39	1.52
2	B	440	ARG	CA-C	-5.21	1.39	1.52
3	C	379	THR	N-CA	-5.20	1.35	1.46
2	B	750	ASN	N-CA	-5.17	1.36	1.46
6	G	499	GLY	CA-C	-5.15	1.43	1.51
6	G	174	VAL	CA-C	-5.13	1.39	1.52
2	B	375	LEU	CA-C	-5.12	1.39	1.52
2	B	317	LEU	CA-C	-5.11	1.39	1.52
3	C	573	LEU	CA-C	-5.11	1.39	1.52
1	A	631	LYS	N-CA	-5.11	1.36	1.46
3	C	367	VAL	CA-C	-5.11	1.39	1.52
5	M	35	TYR	CA-C	-5.11	1.39	1.52
5	R	110	MET	CA-C	-5.10	1.39	1.52
6	G	460	GLY	CA-C	-5.09	1.43	1.51
5	R	33	VAL	N-CA	-5.08	1.36	1.46
7	L	139	PRO	CA-C	-5.07	1.42	1.52
6	G	91	THR	N-CA	-5.04	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	96	ASP	CA-C	-5.04	1.39	1.52
3	C	314	ILE	CA-C	-5.03	1.39	1.52
3	C	588	LEU	N-CA	-5.03	1.36	1.46
3	C	535	ILE	N-CA	-5.02	1.36	1.46
6	K	234	ARG	CA-C	-5.02	1.39	1.52
5	R	106	VAL	N-CA	-5.02	1.36	1.46
2	B	374	VAL	N-CA	-5.02	1.36	1.46
2	B	300	TYR	CA-C	-5.00	1.40	1.52

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLN	N-CA-C	-9.86	84.38	111.00
6	K	117	GLU	C-N-CA	9.76	146.10	121.70
2	B	326	HIS	N-CA-C	-9.59	85.12	111.00
6	G	96	SER	N-CA-C	9.10	135.56	111.00
2	B	940	GLY	N-CA-C	-9.03	90.52	113.10
3	C	416	LYS	N-CA-C	-8.89	87.00	111.00
2	B	760	VAL	N-CA-C	-8.57	87.86	111.00
1	A	229	VAL	N-CA-C	-8.57	87.87	111.00
4	D	61	MET	N-CA-C	-8.53	87.97	111.00
2	B	67	GLY	N-CA-C	-8.51	91.83	113.10
5	R	150	ASN	C-N-CA	8.40	142.71	121.70
1	A	740	GLY	N-CA-C	-8.37	92.17	113.10
5	F	59	LYS	C-N-CA	8.28	142.41	121.70
1	A	631	LYS	N-CA-C	-8.21	88.84	111.00
5	R	122	LEU	N-CA-C	-8.18	88.91	111.00
1	A	491	VAL	C-N-CA	8.16	142.10	121.70
2	B	759	LEU	N-CA-C	-8.07	89.20	111.00
1	A	504	ALA	N-CA-C	-7.99	89.43	111.00
4	D	56	TYR	N-CA-C	-7.91	89.65	111.00
1	A	789	ASP	N-CA-C	-7.90	89.67	111.00
6	G	829	LEU	N-CA-C	-7.82	89.89	111.00
6	K	829	LEU	N-CA-C	-7.81	89.91	111.00
1	A	371	ASN	N-CA-C	-7.77	90.02	111.00
1	A	779	ASP	N-CA-C	-7.76	90.04	111.00
5	R	144	GLY	N-CA-C	-7.74	93.75	113.10
3	C	441	VAL	N-CA-C	-7.67	90.30	111.00
1	A	803	PRO	N-CA-C	7.66	132.02	112.10
1	A	321	ARG	N-CA-C	-7.62	90.43	111.00
2	B	255	SER	C-N-CA	7.62	140.74	121.70
2	B	750	ASN	N-CA-C	-7.61	90.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	41	GLU	C-N-CA	7.58	140.65	121.70
5	R	159	CYS	N-CA-C	-7.54	90.63	111.00
5	F	97	ARG	N-CA-C	-7.53	90.67	111.00
1	A	622	GLY	N-CA-C	-7.53	94.28	113.10
5	F	61	ILE	N-CA-C	-7.48	90.80	111.00
6	G	117	GLU	N-CA-C	-7.46	90.87	111.00
4	D	118	ALA	N-CA-C	-7.45	90.88	111.00
1	A	198	LYS	N-CA-C	-7.42	90.96	111.00
3	C	559	ARG	N-CA-C	-7.32	91.24	111.00
3	C	221	CYS	N-CA-C	-7.30	91.29	111.00
4	D	136	MET	N-CA-C	-7.30	91.29	111.00
6	G	693	VAL	C-N-CA	-7.26	91.52	122.00
2	B	749	VAL	N-CA-C	-7.25	91.42	111.00
1	A	338	ASP	N-CA-C	-7.24	91.45	111.00
2	B	761	VAL	N-CA-C	-7.18	91.60	111.00
1	A	519	ASP	N-CA-C	-7.18	91.62	111.00
2	B	837	ILE	N-CA-C	-7.16	91.68	111.00
5	M	69	GLY	N-CA-C	-7.11	95.33	113.10
2	B	269	GLN	N-CA-C	-7.11	91.81	111.00
2	B	48	GLY	N-CA-C	-7.07	95.42	113.10
5	F	121	TRP	N-CA-C	7.07	130.09	111.00
6	K	244	ASP	N-CA-C	-7.05	91.98	111.00
2	B	49	ASP	N-CA-C	-7.03	92.01	111.00
2	B	811	ASN	N-CA-C	-7.02	92.06	111.00
6	G	609	ARG	C-N-CA	7.01	139.24	121.70
6	K	609	ARG	C-N-CA	7.00	139.20	121.70
1	A	339	ARG	N-CA-C	-7.00	92.11	111.00
2	B	871	ASN	N-CA-C	-6.94	92.25	111.00
1	A	36	TRP	N-CA-C	-6.88	92.42	111.00
1	A	240	TRP	C-N-CA	6.88	138.89	121.70
1	A	243	ASP	N-CA-C	-6.87	92.44	111.00
1	A	236	GLU	N-CA-C	-6.80	92.63	111.00
3	C	653	GLU	N-CA-C	-6.79	92.67	111.00
1	A	528	ILE	N-CA-C	-6.76	92.74	111.00
1	A	430	ASP	N-CA-C	-6.75	92.78	111.00
3	C	27	GLU	N-CA-C	-6.72	92.84	111.00
1	A	766	GLY	N-CA-C	-6.69	96.37	113.10
6	G	828	LEU	N-CA-C	-6.67	93.00	111.00
6	K	828	LEU	N-CA-C	-6.66	93.02	111.00
6	K	629	LEU	C-N-CA	6.65	138.33	121.70
6	G	629	LEU	C-N-CA	6.63	138.29	121.70
5	F	159	CYS	N-CA-C	-6.63	93.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	379	THR	N-CA-C	-6.59	93.20	111.00
7	Z	11	TYR	N-CA-C	-6.59	93.20	111.00
2	B	740	PRO	N-CA-C	-6.57	95.02	112.10
1	A	457	PHE	N-CA-C	-6.57	93.27	111.00
7	Z	62	LEU	N-CA-C	-6.56	93.28	111.00
4	D	14	LYS	C-N-CA	6.56	138.09	121.70
6	K	667	ASN	N-CA-C	-6.55	93.32	111.00
1	A	242	VAL	N-CA-C	-6.54	93.33	111.00
6	G	667	ASN	N-CA-C	-6.54	93.33	111.00
5	M	155	ILE	N-CA-C	-6.50	93.46	111.00
2	B	792	LEU	N-CA-C	-6.48	93.50	111.00
1	A	105	TYR	N-CA-C	-6.48	93.50	111.00
4	D	19	ARG	C-N-CA	6.44	137.79	121.70
6	K	849	LEU	N-CA-C	-6.43	93.63	111.00
6	G	849	LEU	N-CA-C	-6.42	93.65	111.00
1	A	317	PHE	C-N-CA	6.41	137.73	121.70
1	A	589	VAL	N-CA-C	-6.41	93.69	111.00
2	B	754	ILE	N-CA-C	-6.40	93.72	111.00
6	G	484	HIS	N-CA-C	-6.37	93.80	111.00
3	C	546	TYR	N-CA-C	-6.37	93.80	111.00
3	C	154	ASP	N-CA-C	-6.36	93.82	111.00
4	D	29	ILE	N-CA-C	-6.36	93.83	111.00
6	G	150	ASP	C-N-CA	6.35	137.57	121.70
2	B	414	ALA	C-N-CA	6.34	137.55	121.70
7	Z	29	LYS	N-CA-C	-6.33	93.92	111.00
5	M	149	ARG	N-CA-C	-6.32	93.93	111.00
6	K	838	HIS	C-N-CA	6.32	137.50	121.70
6	K	206	ASN	N-CA-C	-6.32	93.94	111.00
6	G	704	GLY	N-CA-C	-6.32	97.31	113.10
6	G	838	HIS	C-N-CA	6.32	137.49	121.70
6	K	704	GLY	N-CA-C	-6.31	97.32	113.10
6	K	117	GLU	CA-C-N	-6.31	103.32	117.20
6	K	96	SER	N-CA-C	6.29	127.99	111.00
1	A	768	ASP	C-N-CA	6.29	137.42	121.70
1	A	73	TYR	N-CA-C	-6.27	94.06	111.00
3	C	155	ASN	C-N-CA	6.26	137.36	121.70
6	G	665	CYS	N-CA-C	6.24	127.86	111.00
5	M	62	SER	C-N-CA	6.24	137.31	121.70
2	B	816	GLY	N-CA-C	-6.24	97.50	113.10
3	C	113	PHE	N-CA-C	6.23	127.83	111.00
3	C	736	GLY	N-CA-C	-6.19	97.61	113.10
3	C	546	TYR	O-C-N	6.19	132.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	277	LEU	C-N-CA	-6.19	96.02	122.00
7	L	30	TYR	N-CA-C	-6.17	94.34	111.00
2	B	933	GLY	C-N-CA	-6.16	96.12	122.00
3	C	85	ASN	N-CA-C	-6.15	94.41	111.00
5	R	42	VAL	C-N-CA	6.14	137.06	121.70
6	K	665	CYS	N-CA-C	6.14	127.58	111.00
7	Z	25	ARG	N-CA-C	-6.13	94.45	111.00
1	A	511	ILE	N-CA-C	-6.09	94.55	111.00
2	B	905	PHE	C-N-CA	6.09	136.93	121.70
3	C	396	TRP	N-CA-C	-6.09	94.55	111.00
3	C	315	ILE	N-CA-C	-6.09	94.57	111.00
3	C	546	TYR	CA-C-N	-6.08	103.81	117.20
5	R	58	TYR	N-CA-C	-6.07	94.60	111.00
7	Z	30	TYR	N-CA-C	-6.07	94.62	111.00
3	C	170	TRP	C-N-CA	6.06	136.86	121.70
7	Z	129	VAL	N-CA-C	-6.06	94.65	111.00
6	G	207	ASP	N-CA-C	6.05	127.33	111.00
3	C	551	ILE	N-CA-C	-6.04	94.68	111.00
7	L	80	ILE	C-N-CA	6.04	134.98	122.30
4	D	50	GLU	N-CA-C	-6.03	94.72	111.00
2	B	385	VAL	C-N-CA	6.03	136.77	121.70
3	C	424	PHE	N-CA-C	-6.01	94.78	111.00
6	G	731	THR	N-CA-C	-6.01	94.78	111.00
6	K	731	THR	N-CA-C	-6.01	94.78	111.00
3	C	504	GLY	N-CA-C	5.99	128.08	113.10
5	M	53	VAL	N-CA-C	-5.99	94.83	111.00
5	R	71	GLN	N-CA-C	-5.98	94.85	111.00
6	K	80	ASN	N-CA-C	-5.98	94.84	111.00
6	G	640	THR	N-CA-C	-5.98	94.86	111.00
1	A	599	PHE	CA-C-N	5.97	130.33	117.20
3	C	245	ILE	N-CA-C	-5.97	94.89	111.00
6	K	640	THR	N-CA-C	-5.96	94.90	111.00
1	A	554	THR	N-CA-C	5.96	127.09	111.00
3	C	174	SER	N-CA-C	-5.96	94.91	111.00
6	K	736	ASP	N-CA-C	-5.96	94.92	111.00
6	G	736	ASP	N-CA-C	-5.95	94.94	111.00
6	K	222	GLY	N-CA-C	-5.94	98.24	113.10
6	G	506	LEU	N-CA-C	5.94	127.05	111.00
5	R	96	ASP	N-CA-C	-5.94	94.96	111.00
3	C	151	ASN	N-CA-C	-5.94	94.97	111.00
3	C	88	THR	N-CA-C	-5.93	94.98	111.00
1	A	392	ASP	N-CA-C	-5.93	94.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	61	LEU	C-N-CA	-5.91	106.92	121.70
6	K	240	LEU	C-N-CA	5.91	136.47	121.70
2	B	795	HIS	C-N-CA	5.91	136.46	121.70
2	B	928	LYS	N-CA-C	5.90	126.92	111.00
6	G	858	ALA	N-CA-C	-5.88	95.13	111.00
6	K	858	ALA	N-CA-C	-5.88	95.12	111.00
6	G	300	LYS	N-CA-C	-5.85	95.20	111.00
1	A	429	LEU	N-CA-C	-5.83	95.26	111.00
3	C	446	GLY	N-CA-C	-5.83	98.53	113.10
6	K	695	ALA	N-CA-C	-5.83	95.27	111.00
1	A	496	TRP	N-CA-C	-5.82	95.27	111.00
1	A	325	ALA	N-CA-C	5.81	126.69	111.00
6	K	845	ARG	N-CA-C	-5.80	95.34	111.00
6	G	845	ARG	N-CA-C	-5.79	95.37	111.00
6	K	749	ASP	N-CA-C	-5.78	95.41	111.00
2	B	748	HIS	N-CA-C	-5.77	95.43	111.00
4	D	98	GLU	N-CA-C	-5.77	95.43	111.00
2	B	325	GLU	C-N-CA	5.76	136.11	121.70
6	G	749	ASP	N-CA-C	-5.76	95.43	111.00
2	B	410	PRO	N-CA-C	-5.75	97.15	112.10
3	C	530	VAL	N-CA-C	-5.74	95.49	111.00
1	A	509	HIS	N-CA-C	-5.74	95.50	111.00
5	R	61	ILE	N-CA-C	-5.74	95.51	111.00
6	K	40	ASN	N-CA-C	-5.73	95.52	111.00
1	A	507	ALA	N-CA-C	-5.72	95.56	111.00
2	B	804	VAL	N-CA-C	-5.72	95.56	111.00
6	G	95	MET	N-CA-C	5.72	126.43	111.00
6	G	178	VAL	N-CA-C	5.70	126.38	111.00
1	A	67	VAL	N-CA-C	-5.69	95.63	111.00
4	D	24	MET	C-N-CA	5.69	135.93	121.70
1	A	77	VAL	N-CA-C	-5.68	95.66	111.00
2	B	841	ILE	N-CA-C	5.68	126.34	111.00
1	A	522	CYS	N-CA-C	-5.67	95.69	111.00
6	K	853	THR	N-CA-C	-5.67	95.69	111.00
5	F	151	ARG	N-CA-C	-5.66	95.71	111.00
6	G	853	THR	N-CA-C	-5.66	95.72	111.00
5	R	41	GLU	C-N-CA	5.66	135.84	121.70
1	A	87	PHE	N-CA-C	-5.65	95.74	111.00
2	B	926	ILE	N-CA-C	5.65	126.25	111.00
3	C	411	ILE	N-CA-C	-5.65	95.75	111.00
1	A	324	PRO	C-N-CA	5.64	135.81	121.70
2	B	414	ALA	O-C-N	5.64	131.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	VAL	CA-C-N	-5.62	104.83	117.20
3	C	442	ARG	N-CA-C	-5.62	95.83	111.00
1	A	227	ARG	N-CA-C	-5.61	95.84	111.00
7	Z	58	GLU	N-CA-C	-5.61	95.86	111.00
5	R	151	ARG	N-CA-C	5.60	126.12	111.00
1	A	621	VAL	C-N-CA	5.59	134.04	122.30
5	R	88	VAL	N-CA-C	5.59	126.09	111.00
1	A	423	ARG	C-N-CA	5.58	135.64	121.70
3	C	9	ARG	N-CA-C	-5.58	95.94	111.00
1	A	487	LYS	C-N-CA	5.56	135.60	121.70
2	B	800	ILE	N-CA-C	-5.55	96.00	111.00
5	M	63	PHE	N-CA-C	5.54	125.97	111.00
3	C	246	THR	C-N-CA	5.54	133.94	122.30
3	C	662	VAL	N-CA-C	-5.54	96.03	111.00
5	M	148	ILE	C-N-CA	5.54	135.56	121.70
1	A	78	TRP	N-CA-C	-5.54	96.04	111.00
3	C	202	LEU	O-C-N	5.52	131.53	122.70
6	K	279	GLY	N-CA-C	-5.52	99.30	113.10
5	M	154	PHE	N-CA-C	-5.52	96.10	111.00
3	C	202	LEU	N-CA-C	-5.52	96.10	111.00
6	G	132	THR	N-CA-C	5.51	125.89	111.00
1	A	574	LYS	C-N-CA	5.51	133.88	122.30
2	B	828	ASP	N-CA-C	-5.51	96.13	111.00
3	C	89	LEU	N-CA-C	-5.50	96.15	111.00
3	C	365	ARG	N-CA-C	5.50	125.85	111.00
3	C	472	ASP	N-CA-C	-5.50	96.16	111.00
7	Z	16	ILE	N-CA-C	-5.49	96.17	111.00
6	K	831	ALA	C-N-CA	5.49	133.82	122.30
6	K	673	THR	N-CA-C	-5.49	96.19	111.00
1	A	736	ALA	N-CA-C	5.49	125.81	111.00
6	G	116	LYS	N-CA-C	5.49	125.81	111.00
6	G	831	ALA	C-N-CA	5.49	133.82	122.30
1	A	516	ARG	C-N-CA	5.48	135.40	121.70
1	A	132	THR	N-CA-C	-5.48	96.21	111.00
3	C	327	LEU	N-CA-C	-5.48	96.21	111.00
6	G	673	THR	N-CA-C	-5.47	96.22	111.00
2	B	256	GLU	N-CA-C	5.47	125.78	111.00
1	A	587	PRO	N-CA-C	5.46	126.30	112.10
7	L	29	LYS	N-CA-C	-5.46	96.26	111.00
2	B	103	THR	C-N-CA	5.44	135.31	121.70
3	C	202	LEU	CA-C-N	-5.44	105.23	117.20
2	B	758	VAL	N-CA-C	-5.44	96.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	257	ARG	N-CA-C	5.43	125.66	111.00
2	B	939	THR	N-CA-C	-5.41	96.38	111.00
6	G	459	LEU	C-N-CA	5.41	133.67	122.30
1	A	533	GLY	N-CA-C	-5.41	99.58	113.10
2	B	482	SER	N-CA-C	5.40	125.58	111.00
6	G	844	SER	N-CA-C	-5.39	96.44	111.00
1	A	444	ILE	N-CA-C	-5.39	96.45	111.00
1	A	656	GLY	N-CA-C	-5.39	99.63	113.10
6	G	274	ILE	N-CA-C	5.39	125.55	111.00
6	K	814	GLU	N-CA-C	-5.38	96.47	111.00
7	L	60	ALA	C-N-CA	5.38	135.14	121.70
6	K	844	SER	N-CA-C	-5.37	96.49	111.00
2	B	744	GLU	N-CA-C	-5.36	96.54	111.00
5	M	91	VAL	C-N-CA	5.35	135.08	121.70
3	C	262	ARG	N-CA-C	-5.34	96.58	111.00
1	A	272	SER	N-CA-C	5.33	125.38	111.00
2	B	763	GLN	C-N-CA	5.31	134.97	121.70
3	C	509	GLY	N-CA-C	-5.31	99.83	113.10
3	C	106	ALA	N-CA-C	-5.30	96.68	111.00
1	A	329	HIS	N-CA-C	-5.30	96.69	111.00
7	L	13	VAL	N-CA-C	-5.30	96.69	111.00
1	A	630	GLN	N-CA-C	-5.30	96.69	111.00
3	C	378	TYR	CA-C-N	-5.30	105.54	117.20
3	C	378	TYR	O-C-N	5.29	131.16	122.70
6	G	686	ALA	N-CA-C	5.29	125.28	111.00
1	A	383	ALA	C-N-CA	5.29	134.91	121.70
6	K	686	ALA	N-CA-C	5.27	125.24	111.00
1	A	340	PHE	C-N-CA	5.27	134.87	121.70
5	F	166	LEU	C-N-CA	5.27	134.87	121.70
1	A	402	SER	N-CA-C	-5.26	96.78	111.00
6	K	131	ILE	N-CA-C	5.25	125.17	111.00
5	F	60	ASN	CA-C-N	-5.24	105.67	117.20
6	K	120	TYR	CA-C-N	-5.24	105.68	117.20
3	C	237	PHE	N-CA-C	-5.23	96.87	111.00
6	G	838	HIS	CA-C-N	-5.23	105.70	117.20
6	K	297	SER	N-CA-C	5.22	125.09	111.00
6	K	247	ARG	N-CA-C	-5.21	96.92	111.00
6	K	838	HIS	CA-C-N	-5.21	105.73	117.20
5	R	25	LEU	CA-C-N	-5.21	105.73	117.20
3	C	574	TYR	N-CA-C	-5.21	96.93	111.00
6	G	683	PRO	N-CA-C	5.20	125.62	112.10
2	B	822	VAL	N-CA-C	-5.20	96.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	VAL	CA-C-N	5.19	128.62	117.20
6	K	683	PRO	N-CA-C	5.18	125.58	112.10
1	A	245	CYS	N-CA-C	-5.18	97.02	111.00
3	C	254	ARG	N-CA-C	-5.18	97.02	111.00
1	A	436	LEU	N-CA-C	-5.17	97.03	111.00
6	K	176	ARG	C-N-CA	5.17	134.63	121.70
3	C	474	GLY	C-N-CA	5.16	134.60	121.70
3	C	588	LEU	N-CA-C	-5.16	97.08	111.00
5	F	96	ASP	N-CA-C	-5.15	97.09	111.00
2	B	504	VAL	N-CA-C	5.15	124.90	111.00
6	G	39	ILE	N-CA-C	-5.15	97.10	111.00
3	C	469	PHE	N-CA-C	-5.14	97.11	111.00
5	R	146	HIS	C-N-CA	5.14	134.55	121.70
1	A	221	VAL	N-CA-C	-5.13	97.14	111.00
6	G	296	CYS	C-N-CA	5.12	134.51	121.70
3	C	155	ASN	CA-C-N	-5.12	105.94	117.20
2	B	782	LYS	N-CA-C	-5.12	97.19	111.00
6	G	703	PRO	C-N-CA	5.10	133.02	122.30
3	C	802	LYS	N-CA-C	5.10	124.77	111.00
1	A	515	ASN	N-CA-C	-5.10	97.24	111.00
7	L	18	ILE	O-C-N	5.10	130.85	122.70
3	C	803	GLU	N-CA-C	5.09	124.75	111.00
3	C	802	LYS	CA-C-N	5.09	128.40	117.20
3	C	827	VAL	C-N-CA	5.09	134.43	121.70
6	G	804	ILE	N-CA-C	5.09	124.74	111.00
5	R	29	GLY	N-CA-C	-5.09	100.38	113.10
6	K	703	PRO	C-N-CA	5.08	132.97	122.30
3	C	7	ILE	N-CA-C	-5.08	97.28	111.00
3	C	314	ILE	N-CA-C	-5.08	97.29	111.00
7	Z	18	ILE	CA-C-N	-5.08	106.03	117.20
3	C	567	ILE	N-CA-C	-5.07	97.31	111.00
6	G	118	ASP	CA-C-N	-5.07	106.05	117.20
1	A	37	ASP	N-CA-C	-5.07	97.33	111.00
6	G	141	GLU	N-CA-C	5.07	124.67	111.00
7	Z	56	ASP	N-CA-C	-5.06	97.33	111.00
6	G	435	GLY	C-N-CA	5.06	134.36	121.70
6	K	804	ILE	N-CA-C	5.06	124.67	111.00
6	K	120	TYR	C-N-CA	5.05	134.33	121.70
1	A	543	TYR	N-CA-C	-5.05	97.36	111.00
3	C	790	ASP	CA-C-N	5.04	131.21	117.10
6	G	815	ARG	N-CA-C	-5.04	97.40	111.00
1	A	562	ARG	N-CA-C	-5.03	97.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	813	CYS	N-CA-C	5.03	124.59	111.00
1	A	249	TYR	N-CA-C	-5.01	97.47	111.00
6	K	221	HIS	C-N-CA	5.01	132.82	122.30
1	A	428	VAL	N-CA-C	-5.00	97.49	111.00
3	C	397	ALA	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	898	ALA	Peptide
2	B	903	CYS	Peptide
2	B	938	VAL	Mainchain

## 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	A	3251	0	869	36	0
2	B	3198	0	810	58	0
3	C	3371	0	919	23	0
4	D	706	0	182	9	0
5	F	635	0	181	3	0
5	M	635	0	181	19	0
5	R	635	0	181	37	0
6	G	3190	0	822	57	0
6	K	2239	0	572	39	0
7	L	555	0	148	2	0
7	Z	555	0	147	15	0
All	All	18970	0	5012	279	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 12.

All (279) 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:K:107:SER:N	5:M:50:GLY:HA3	1.28	1.43
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.43
6:G:107:SER:H	5:R:50:GLY:CA	1.31	1.41
6:K:167:LEU:CA	6:K:170:SER:O	1.73	1.35
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.30
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.26
3:C:269:TYR:O	3:C:271:MET:N	1.69	1.25
5:R:143:LEU:C	5:R:145:LEU:H	1.23	1.25
5:R:71:GLN:O	5:R:74:ILE:N	1.74	1.20
6:K:107:SER:H	5:M:50:GLY:CA	1.53	1.19
2:B:778:LEU:O	2:B:809:THR:O	1.58	1.17
4:D:13:GLY:HA2	4:D:38:LYS:CA	1.75	1.16
6:G:167:LEU:CA	6:G:170:SER:O	1.95	1.14
2:B:781:LEU:O	2:B:808:SER:O	1.63	1.14
6:K:190:ILE:CA	6:K:225:SER:CA	2.26	1.13
2:B:778:LEU:O	2:B:809:THR:C	1.91	1.09
5:R:143:LEU:C	5:R:145:LEU:N	1.99	1.08
7:L:31:TYR:CA	7:L:131:GLY:O	2.03	1.07
7:Z:11:TYR:CA	7:Z:132:GLY:HA3	1.84	1.06
5:R:159:CYS:O	5:R:162:SER:N	1.88	1.04
2:B:526:VAL:CA	2:B:597:VAL:CA	2.35	1.04
6:G:276:ASN:O	6:G:281:SER:O	1.75	1.03
5:R:130:LEU:O	5:R:132:GLU:N	1.92	1.02
7:Z:12:THR:H	7:Z:132:GLY:CA	1.72	1.02
5:R:126:ASN:CA	5:R:158:THR:O	2.10	0.99
6:K:677:VAL:O	6:K:694:PRO:CA	2.11	0.98
6:K:167:LEU:C	6:K:170:SER:O	2.03	0.96
7:Z:11:TYR:CA	7:Z:132:GLY:CA	2.41	0.96
2:B:541:ALA:CA	2:B:624:ASP:N	2.29	0.96
2:B:766:ASP:O	2:B:768:LEU:N	2.00	0.95
2:B:778:LEU:C	2:B:809:THR:O	2.04	0.95
6:K:190:ILE:C	6:K:225:SER:CA	2.34	0.95
7:Z:12:THR:N	7:Z:132:GLY:CA	2.30	0.94
2:B:824:GLY:CA	2:B:830:ASN:O	2.16	0.93
6:G:107:SER:N	5:R:50:GLY:CA	2.05	0.92
7:Z:12:THR:N	7:Z:132:GLY:O	2.02	0.92
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.90
5:R:125:ALA:O	5:R:158:THR:O	1.89	0.90
6:K:107:SER:CA	5:M:50:GLY:HA3	2.00	0.90
2:B:767:THR:CA	2:B:792:LEU:H	1.85	0.90
2:B:781:LEU:CA	2:B:805:LYS:O	2.22	0.88
6:K:167:LEU:O	6:K:170:SER:O	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.88
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.87
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.86
6:G:301:ALA:C	6:G:303:LEU:H	1.79	0.86
6:G:198:GLY:O	6:G:201:TYR:N	2.07	0.86
6:K:190:ILE:O	6:K:225:SER:CA	2.23	0.86
6:K:190:ILE:CA	6:K:225:SER:N	2.40	0.85
5:R:78:TRP:O	5:R:81:TYR:O	1.95	0.85
6:G:107:SER:H	5:R:50:GLY:C	1.79	0.84
2:B:483:THR:O	2:B:487:ILE:N	2.09	0.84
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.84
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.84
2:B:824:GLY:HA2	2:B:830:ASN:O	1.78	0.84
6:G:106:THR:C	5:R:50:GLY:HA3	1.98	0.83
5:R:130:LEU:C	5:R:132:GLU:H	1.82	0.83
1:A:214:HIS:O	1:A:217:MET:N	2.10	0.83
2:B:739:ASP:O	2:B:740:PRO:O	1.96	0.83
4:D:41:ASN:O	4:D:43:GLY:N	2.12	0.82
2:B:483:THR:O	2:B:484:LYS:C	2.18	0.82
5:M:79:ARG:O	5:M:81:TYR:N	2.13	0.82
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.81
2:B:767:THR:C	2:B:792:LEU:H	1.84	0.81
7:Z:11:TYR:C	7:Z:132:GLY:HA3	2.02	0.80
6:K:107:SER:N	5:M:50:GLY:CA	2.24	0.80
4:D:13:GLY:CA	4:D:38:LYS:CA	2.60	0.79
7:Z:13:VAL:H	7:Z:132:GLY:HA2	1.46	0.79
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.78
7:Z:12:THR:H	7:Z:132:GLY:C	1.86	0.78
2:B:483:THR:O	2:B:486:ASP:N	2.17	0.78
6:G:105:VAL:O	6:G:107:SER:N	2.17	0.77
3:C:637:VAL:O	3:C:638:SER:O	2.03	0.76
6:G:277:LEU:O	6:G:280:CYS:N	2.16	0.76
2:B:740:PRO:O	2:B:741:VAL:C	2.18	0.76
7:Z:12:THR:N	7:Z:132:GLY:HA3	2.00	0.76
7:Z:12:THR:H	7:Z:132:GLY:HA2	1.51	0.76
2:B:766:ASP:C	2:B:768:LEU:H	1.89	0.76
5:R:174:SER:O	5:R:176:SER:N	2.21	0.74
6:G:301:ALA:C	6:G:303:LEU:N	2.41	0.73
5:M:77:LEU:O	5:M:80:HIS:N	2.20	0.73
1:A:800:PRO:O	3:C:805:PHE:O	2.05	0.73
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:143:LEU:O	5:R:145:LEU:N	2.22	0.72
6:G:247:ARG:O	6:G:248:ASP:C	2.24	0.72
2:B:928:LYS:O	2:B:934:PRO:O	2.08	0.71
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.71
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.70
5:F:29:GLY:HA2	5:F:32:THR:H	1.56	0.70
4:D:41:ASN:C	4:D:43:GLY:H	1.95	0.70
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.70
6:G:337:ASN:O	6:G:340:ILE:N	2.25	0.69
1:A:801:ILE:O	3:C:805:PHE:N	2.24	0.69
6:G:167:LEU:C	6:G:170:SER:O	2.30	0.69
6:G:215:ILE:O	6:G:219:THR:N	2.22	0.69
6:G:215:ILE:O	6:G:217:LYS:N	2.25	0.69
6:K:133:ASP:O	6:K:134:SER:O	2.10	0.68
6:G:247:ARG:O	6:G:248:ASP:O	2.12	0.68
6:G:172:ASP:O	6:G:175:LYS:N	2.26	0.68
7:Z:12:THR:N	7:Z:132:GLY:C	2.44	0.67
6:K:107:SER:CA	5:M:50:GLY:O	2.43	0.67
7:Z:10:LEU:O	7:Z:11:TYR:C	2.32	0.67
2:B:779:GLY:O	2:B:808:SER:O	2.14	0.66
2:B:929:PRO:CA	2:B:935:ASP:O	2.44	0.66
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.66
6:G:277:LEU:CA	6:G:280:CYS:CA	2.74	0.66
7:Z:10:LEU:O	7:Z:11:TYR:O	2.13	0.66
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.66
4:D:39:LEU:C	4:D:41:ASN:H	2.00	0.66
2:B:766:ASP:C	2:B:768:LEU:N	2.45	0.65
2:B:563:ASP:C	2:B:577:THR:C	2.55	0.65
5:R:71:GLN:O	5:R:74:ILE:CA	2.44	0.65
2:B:112:GLU:O	2:B:114:ILE:N	2.30	0.64
6:G:167:LEU:O	6:G:170:SER:O	2.15	0.64
3:C:269:TYR:C	3:C:271:MET:N	2.44	0.64
6:K:135:THR:C	6:K:137:LEU:H	2.00	0.64
2:B:824:GLY:HA3	2:B:830:ASN:O	1.96	0.64
5:R:71:GLN:C	5:R:74:ILE:H	2.00	0.63
2:B:766:ASP:O	2:B:792:LEU:O	2.16	0.63
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.63
1:A:803:PRO:N	3:C:803:GLU:H	1.97	0.63
6:K:243:GLU:O	6:K:245:GLY:N	2.31	0.63
5:M:116:LEU:O	5:M:118:ASN:N	2.32	0.62
2:B:739:ASP:O	2:B:740:PRO:C	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:24:GLY:O	5:M:68:VAL:O	2.17	0.62
1:A:227:ARG:O	1:A:245:CYS:O	2.17	0.62
5:R:71:GLN:O	5:R:72:ASP:C	2.39	0.60
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.60
6:K:135:THR:O	6:K:137:LEU:N	2.35	0.60
5:R:69:GLY:C	5:R:71:GLN:H	2.04	0.59
6:G:215:ILE:O	6:G:218:PHE:N	2.36	0.59
6:G:215:ILE:C	6:G:217:LYS:H	2.05	0.59
2:B:557:LEU:O	2:B:558:ARG:C	2.41	0.59
5:R:159:CYS:O	5:R:162:SER:CA	2.50	0.59
2:B:740:PRO:O	2:B:742:TYR:N	2.35	0.59
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.59
2:B:563:ASP:C	2:B:577:THR:CA	2.71	0.59
3:C:269:TYR:O	3:C:271:MET:CA	2.49	0.59
6:G:215:ILE:C	6:G:217:LYS:N	2.55	0.58
5:M:128:GLN:H	5:M:159:CYS:CA	2.16	0.58
6:G:277:LEU:CA	6:G:280:CYS:C	2.72	0.58
2:B:563:ASP:C	2:B:577:THR:O	2.43	0.57
2:B:767:THR:CA	2:B:792:LEU:N	2.65	0.57
2:B:526:VAL:CA	2:B:597:VAL:N	2.67	0.57
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.57
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.57
2:B:504:VAL:O	2:B:507:GLU:N	2.37	0.57
5:R:82:TYR:O	5:R:83:ARG:C	2.39	0.57
6:K:107:SER:CA	5:M:50:GLY:CA	2.75	0.57
6:G:387:CYS:O	6:G:391:PRO:CA	2.53	0.56
6:G:337:ASN:O	6:G:338:ARG:C	2.39	0.56
2:B:541:ALA:N	2:B:624:ASP:N	2.53	0.56
3:C:269:TYR:C	3:C:271:MET:H	2.02	0.56
6:K:274:ILE:O	6:K:276:ASN:N	2.39	0.56
2:B:779:GLY:HA2	2:B:811:ASN:H	1.70	0.56
6:G:172:ASP:O	6:G:173:VAL:C	2.36	0.56
5:R:69:GLY:O	5:R:71:GLN:N	2.34	0.56
6:G:198:GLY:C	6:G:201:TYR:H	2.07	0.56
6:K:135:THR:C	6:K:137:LEU:N	2.58	0.55
2:B:899:LEU:O	2:B:900:SER:C	2.44	0.55
6:G:277:LEU:CA	6:G:280:CYS:N	2.69	0.55
3:C:506:THR:C	3:C:509:GLY:H	2.10	0.55
6:K:665:CYS:O	6:K:703:PRO:CA	2.55	0.54
6:G:726:CYS:O	6:G:753:LEU:O	2.25	0.54
6:G:106:THR:CA	5:R:50:GLY:HA3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:LYS:C	2:B:104:THR:H	2.09	0.54
3:C:375:TYR:O	3:C:388:PHE:CA	2.56	0.54
2:B:112:GLU:C	2:B:114:ILE:H	2.12	0.53
2:B:779:GLY:N	2:B:809:THR:O	2.22	0.53
5:R:130:LEU:C	5:R:132:GLU:N	2.51	0.53
7:Z:11:TYR:C	7:Z:132:GLY:CA	2.69	0.53
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.53
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.53
1:A:496:TRP:CA	1:A:502:HIS:H	2.20	0.53
5:M:25:LEU:C	5:M:69:GLY:HA2	2.29	0.53
5:M:47:PRO:C	5:M:69:GLY:HA3	2.29	0.53
3:C:174:SER:C	3:C:176:SER:H	2.12	0.53
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.53
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.52
5:R:135:SER:O	5:R:136:ALA:C	2.48	0.52
6:G:198:GLY:C	6:G:200:LEU:N	2.58	0.52
2:B:483:THR:O	2:B:484:LYS:O	2.28	0.52
6:G:665:CYS:O	6:G:703:PRO:CA	2.57	0.52
6:G:666:THR:O	6:G:668:THR:N	2.43	0.52
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.52
5:M:78:TRP:O	5:M:79:ARG:C	2.46	0.52
5:R:71:GLN:O	5:R:73:ARG:N	2.43	0.52
6:G:666:THR:O	6:G:667:ASN:C	2.49	0.51
2:B:767:THR:CA	2:B:793:ALA:N	2.73	0.51
5:R:71:GLN:C	5:R:73:ARG:N	2.60	0.51
6:G:274:ILE:O	6:G:275:VAL:C	2.48	0.51
5:M:77:LEU:O	5:M:80:HIS:CA	2.59	0.51
1:A:802:MET:O	3:C:804:ALA:CA	2.58	0.51
2:B:324:LYS:C	2:B:326:HIS:H	2.15	0.51
2:B:767:THR:O	2:B:768:LEU:C	2.49	0.51
5:M:173:LEU:C	5:M:175:ASN:H	2.15	0.51
6:G:247:ARG:O	6:G:251:LEU:N	2.37	0.50
5:R:69:GLY:C	5:R:71:GLN:N	2.65	0.50
5:R:127:LYS:H	5:R:159:CYS:CA	2.24	0.50
6:G:172:ASP:C	6:G:175:LYS:H	2.14	0.50
6:G:211:VAL:O	6:G:215:ILE:N	2.45	0.50
3:C:459:ARG:CA	3:C:509:GLY:HA3	2.42	0.49
6:G:277:LEU:C	6:G:280:CYS:N	2.66	0.49
4:D:39:LEU:C	4:D:41:ASN:N	2.66	0.49
4:D:42:THR:O	4:D:43:GLY:C	2.50	0.49
6:G:277:LEU:CA	6:G:280:CYS:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:928:LYS:C	2:B:934:PRO:O	2.51	0.49
3:C:568:PRO:C	3:C:571:ASN:H	2.16	0.49
4:D:41:ASN:C	4:D:43:GLY:N	2.60	0.48
6:K:172:ASP:O	6:K:175:LYS:N	2.46	0.48
6:G:198:GLY:O	6:G:199:LEU:C	2.49	0.48
3:C:375:TYR:N	3:C:389:GLY:O	2.41	0.48
5:F:29:GLY:CA	5:F:32:THR:H	2.26	0.48
6:G:441:GLU:O	6:G:444:GLU:O	2.32	0.48
6:K:666:THR:O	6:K:668:THR:N	2.47	0.48
6:G:460:GLY:HA2	6:G:494:ALA:CA	2.44	0.48
6:G:301:ALA:O	6:G:303:LEU:N	2.48	0.47
2:B:767:THR:CA	2:B:792:LEU:C	2.83	0.47
6:G:116:LYS:O	6:G:118:ASP:N	2.48	0.47
6:G:726:CYS:O	6:G:753:LEU:N	2.44	0.47
6:K:274:ILE:O	6:K:275:VAL:C	2.52	0.47
5:M:173:LEU:C	5:M:175:ASN:N	2.68	0.47
3:C:637:VAL:O	3:C:638:SER:C	2.52	0.47
6:G:246:SER:C	6:G:248:ASP:N	2.66	0.47
5:F:149:ARG:C	5:F:151:ARG:H	2.16	0.47
3:C:86:TYR:C	3:C:88:THR:H	2.19	0.46
6:K:666:THR:O	6:K:667:ASN:C	2.53	0.46
3:C:233:SER:H	3:C:248:SER:CA	2.29	0.46
2:B:842:MET:O	2:B:888:THR:O	2.34	0.46
6:G:665:CYS:O	6:G:703:PRO:N	2.48	0.46
6:K:665:CYS:O	6:K:702:GLN:C	2.54	0.46
6:K:665:CYS:O	6:K:702:GLN:O	2.34	0.45
6:K:133:ASP:O	6:K:134:SER:C	2.53	0.45
2:B:751:GLN:C	2:B:753:ASP:H	2.19	0.45
6:K:244:ASP:O	6:K:245:GLY:C	2.54	0.45
6:K:695:ALA:O	6:K:696:ARG:C	2.55	0.45
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.45
6:K:243:GLU:C	6:K:245:GLY:N	2.69	0.45
5:R:159:CYS:C	5:R:161:THR:N	2.68	0.45
6:G:298:SER:O	6:G:300:LYS:N	2.50	0.44
6:K:166:LEU:O	6:K:170:SER:N	2.42	0.44
6:G:172:ASP:C	6:G:174:VAL:N	2.66	0.44
6:K:273:ALA:C	6:K:275:VAL:H	2.21	0.44
2:B:762:ASN:C	2:B:764:THR:H	2.18	0.44
6:K:181:ALA:O	6:K:185:ALA:N	2.51	0.44
7:L:49:PHE:O	7:L:53:HIS:N	2.51	0.43
1:A:749:LEU:O	1:A:753:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:269:TYR:O	3:C:270:GLY:C	2.48	0.43
6:G:529:THR:O	6:G:533:ASN:N	2.52	0.43
6:G:274:ILE:O	6:G:275:VAL:O	2.37	0.43
6:K:135:THR:O	6:K:136:MET:C	2.54	0.43
5:R:70:GLY:O	5:R:72:ASP:N	2.52	0.43
2:B:482:SER:C	2:B:484:LYS:N	2.71	0.43
3:C:484:SER:CA	3:C:522:GLU:H	2.32	0.42
6:K:107:SER:H	5:M:50:GLY:HA3	0.67	0.42
2:B:135:THR:O	2:B:139:LEU:N	2.52	0.42
6:K:226:PRO:O	6:K:229:TYR:N	2.51	0.42
3:C:690:LEU:O	3:C:694:GLN:N	2.53	0.42
5:R:109:ARG:C	5:R:112:ASN:H	2.23	0.42
3:C:715:LEU:O	3:C:719:ALA:N	2.51	0.42
4:D:62:GLU:C	4:D:64:LEU:H	2.23	0.42
6:G:176:ARG:C	6:G:178:VAL:H	2.21	0.42
6:K:171:PHE:O	6:K:174:VAL:N	2.52	0.41
2:B:267:LEU:C	2:B:269:GLN:H	2.24	0.41
2:B:866:ASN:O	2:B:944:ILE:O	2.39	0.41
6:G:107:SER:CA	5:R:50:GLY:CA	2.92	0.41
6:G:107:SER:N	5:R:50:GLY:C	2.59	0.41
6:K:232:MET:O	6:K:236:ALA:N	2.53	0.41
2:B:779:GLY:O	2:B:808:SER:C	2.58	0.41
2:B:778:LEU:O	2:B:809:THR:CA	2.65	0.41
5:R:25:LEU:C	5:R:70:GLY:H	2.24	0.41
5:M:79:ARG:O	5:M:81:TYR:O	2.39	0.41
5:R:160:ALA:C	5:R:163:GLY:H	2.24	0.41
1:A:9:SER:N	1:A:313:GLY:HA3	2.36	0.40
2:B:122:LYS:O	2:B:126:HIS:N	2.54	0.40
7:Z:12:THR:N	7:Z:132:GLY:HA2	2.20	0.40
3:C:213:ILE:O	3:C:222:VAL:N	2.54	0.40
2:B:767:THR:CA	2:B:793:ALA:CA	2.99	0.40
2:B:782:LYS:N	2:B:805:LYS:O	2.55	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	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0	6
2	B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	1	14
3	C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1	16
4	D	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1	18
5	F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	2	24
5	M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0	8
5	R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	7
6	G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1	20
6	K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1	19
7	L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	21
7	Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	26
All	All	4710/6291 (75%)	3832 (81%)	456 (10%)	422 (9%)	2	15

All (422) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	64	PRO
1	A	92	HIS
1	A	106	PRO
1	A	125	ARG
1	A	169	LYS
1	A	174	PRO
1	A	187	VAL
1	A	215	PRO
1	A	237	SER
1	A	250	ASN
1	A	252	VAL
1	A	271	LYS
1	A	278	MET
1	A	281	ARG
1	A	324	PRO
1	A	325	ALA
1	A	341	LEU
1	A	343	GLN

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Mol	Chain	Res	Type
1	A	384	SER
1	A	454	ASP
1	A	457	PHE
1	A	466	LEU
1	A	479	GLN
1	A	492	LYS
1	A	566	LEU
1	A	583	ARG
1	A	584	GLU
1	A	592	ILE
1	A	593	ASP
1	A	619	LYS
1	A	642	VAL
1	A	671	LYS
1	A	728	ASP
1	A	779	ASP
1	A	788	ILE
1	A	796	GLN
1	A	797	PRO
1	A	798	PRO
1	A	803	PRO
1	A	805	ASP
1	A	811	LEU
2	B	36	PRO
2	B	68	GLU
2	B	109	LEU
2	B	111	HIS
2	B	113	MET
2	B	254	PRO
2	B	255	SER
2	B	329	HIS
2	B	348	ASP
2	B	367	ASN
2	B	385	VAL
2	B	386	SER
2	B	466	SER
2	B	480	TYR
2	B	484	LYS
2	B	500	GLU
2	B	501	ILE
2	B	502	PRO
2	B	503	ILE

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Mol	Chain	Res	Type
2	B	505	GLU
2	B	521	ILE
2	B	522	THR
2	B	547	PRO
2	B	767	THR
2	B	771	CYS
2	B	826	ALA
2	B	831	CYS
2	B	865	GLU
2	B	899	LEU
2	B	929	PRO
2	B	930	VAL
2	B	934	PRO
2	B	935	ASP
2	B	938	VAL
3	C	27	GLU
3	C	89	LEU
3	C	200	PRO
3	C	228	HIS
3	C	270	GLY
3	C	273	ARG
3	C	325	ALA
3	C	326	ASN
3	C	328	LYS
3	C	329	ALA
3	C	332	ASP
3	C	350	SER
3	C	363	ASN
3	C	365	ARG
3	C	400	SER
3	C	410	SER
3	C	411	ILE
3	C	424	PHE
3	C	451	ASP
3	C	462	GLU
3	C	475	GLU
3	C	484	SER
3	C	502	HIS
3	C	614	PRO
3	C	615	LYS
3	C	638	SER
3	C	762	LEU

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Mol	Chain	Res	Type
3	C	781	ASN
3	C	782	GLN
3	C	789	ALA
3	C	790	ASP
3	C	806	VAL
3	C	825	PRO
3	C	833	ARG
4	D	12	ALA
4	D	44	LYS
4	D	73	ASN
4	D	96	ALA
5	F	97	ARG
5	F	117	ARG
5	F	131	PRO
6	G	77	PHE
6	G	100	GLU
6	G	106	THR
6	G	132	THR
6	G	151	LYS
6	G	171	PHE
6	G	243	GLU
6	G	261	ASN
6	G	275	VAL
6	G	277	LEU
6	G	283	LYS
6	G	299	PRO
6	G	373	ASP
6	G	394	HIS
6	G	446	CYS
6	G	484	HIS
6	G	608	THR
6	G	621	PRO
6	G	686	ALA
6	G	741	GLU
5	R	42	VAL
5	R	43	ILE
5	R	130	LEU
5	R	131	PRO
5	R	145	LEU
5	R	147	SER
5	R	151	ARG
5	R	175	ASN

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Mol	Chain	Res	Type
7	Z	36	PRO
7	Z	37	SER
7	Z	84	TYR
6	K	134	SER
6	K	135	THR
6	K	170	SER
6	K	171	PHE
6	K	207	ASP
6	K	221	HIS
6	K	225	SER
6	K	226	PRO
6	K	227	PHE
6	K	243	GLU
6	K	275	VAL
6	K	299	PRO
6	K	608	THR
6	K	621	PRO
6	K	686	ALA
6	K	741	GLU
6	K	813	CYS
7	L	37	SER
7	L	84	TYR
7	L	147	ALA
5	M	42	VAL
5	M	43	ILE
5	M	44	THR
5	M	51	PHE
5	M	71	GLN
5	M	80	HIS
5	M	118	ASN
5	M	149	ARG
1	A	10	ALA
1	A	185	THR
1	A	282	THR
1	A	290	ASP
1	A	345	ASP
1	A	373	ALA
1	A	425	ARG
1	A	498	ALA
1	A	546	SER
1	A	564	LEU
1	A	572	ARG

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Mol	Chain	Res	Type
1	A	622	GLY
1	A	624	SER
1	A	632	LYS
1	A	672	ASN
1	A	787	ASP
1	A	800	PRO
2	B	49	ASP
2	B	69	LYS
2	B	162	ARG
2	B	186	PRO
2	B	383	ASN
2	B	445	ARG
2	B	498	LEU
2	B	499	GLY
2	B	551	GLU
2	B	740	PRO
2	B	741	VAL
2	B	751	GLN
2	B	764	THR
2	B	828	ASP
2	B	838	HIS
2	B	862	PHE
2	B	873	ASN
2	B	939	THR
3	C	88	THR
3	C	219	LYS
3	C	428	PHE
3	C	465	PRO
3	C	503	GLU
3	C	504	GLY
3	C	558	ASP
3	C	665	GLU
3	C	787	SER
3	C	793	GLU
3	C	797	LEU
4	D	24	MET
4	D	25	THR
4	D	42	THR
4	D	98	GLU
4	D	136	MET
6	G	96	SER
6	G	98	ILE

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Mol	Chain	Res	Type
6	G	105	VAL
6	G	116	LYS
6	G	216	SER
6	G	278	PRO
6	G	310	THR
6	G	463	GLY
6	G	467	ASN
6	G	522	ASN
6	G	633	SER
6	G	718	THR
5	R	72	ASP
5	R	82	TYR
5	R	84	ASN
5	R	95	ASN
5	R	132	GLU
5	R	133	ALA
7	Z	73	ILE
6	K	38	PRO
6	K	116	LYS
6	K	245	GLY
6	K	297	SER
6	K	633	SER
6	K	718	THR
7	L	12	THR
7	L	69	TYR
7	L	132	GLY
5	M	70	GLY
5	M	129	ASP
5	M	164	GLU
1	A	61	LYS
1	A	62	GLN
1	A	168	ARG
1	A	176	ALA
1	A	183	GLY
1	A	218	PRO
1	A	251	ASN
1	A	323	ARG
1	A	340	PHE
1	A	349	SER
1	A	362	LYS
1	A	433	HIS
1	A	481	ARG

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Mol	Chain	Res	Type
1	A	527	ASN
1	A	555	THR
1	A	585	CYS
1	A	686	ASN
1	A	731	GLY
1	A	755	LYS
2	B	216	ASP
2	B	779	GLY
2	B	871	ASN
3	C	140	GLY
3	C	156	ASN
3	C	250	ASP
3	C	259	SER
3	C	351	CYS
3	C	408	SER
3	C	454	ASN
3	C	708	ASN
3	C	763	PRO
4	D	46	HIS
4	D	138	SER
5	F	47	PRO
5	F	84	ASN
5	F	149	ARG
6	G	170	SER
6	G	282	ALA
6	G	297	SER
6	G	391	PRO
6	G	393	LYS
6	G	445	ASP
6	G	447	GLU
6	G	504	GLU
6	G	505	MET
6	G	628	PRO
6	G	641	GLU
6	G	687	TYR
6	G	720	VAL
6	G	761	ALA
5	R	114	ASP
7	Z	147	ALA
6	K	96	SER
6	K	248	ASP
6	K	628	PRO

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Mol	Chain	Res	Type
6	K	641	GLU
6	K	687	TYR
6	K	720	VAL
6	K	761	ALA
7	L	36	PRO
5	M	127	LYS
5	M	135	SER
5	M	165	GLY
1	A	73	TYR
1	A	103	HIS
1	A	170	LYS
1	A	205	ASP
1	A	236	GLU
1	A	330	GLY
1	A	398	LYS
1	A	411	LYS
1	A	424	ASN
1	A	488	ILE
1	A	556	GLY
1	A	783	GLU
1	A	786	PRO
1	A	801	ILE
2	B	128	ASN
2	B	384	ASN
2	B	425	SER
2	B	447	ASP
2	B	481	CYS
2	B	504	VAL
2	B	752	TYR
2	B	768	LEU
2	B	780	ASP
2	B	827	SER
2	B	837	ILE
2	B	901	GLY
2	B	928	LYS
3	C	165	ARG
3	C	321	GLU
3	C	346	LYS
3	C	401	SER
3	C	409	ASN
3	C	431	GLU
3	C	662	VAL

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Mol	Chain	Res	Type
3	C	821	ALA
5	F	153	TRP
6	G	23	GLU
6	G	428	ASN
6	G	623	PHE
5	R	44	THR
5	R	129	ASP
7	Z	34	THR
6	K	76	LEU
6	K	623	PHE
7	L	86	ASN
5	M	119	ALA
5	M	133	ALA
1	A	182	ARG
1	A	195	ALA
1	A	364	PRO
1	A	452	ASN
1	A	517	LYS
1	A	531	LYS
1	A	621	VAL
1	A	644	ASP
1	A	810	LEU
2	B	270	SER
2	B	347	PRO
2	B	825	ALA
3	C	242	PRO
3	C	284	ASN
3	C	473	SER
3	C	737	LYS
4	D	40	MET
4	D	43	GLY
5	F	78	TRP
6	G	99	ALA
6	G	226	PRO
6	G	248	ASP
5	R	158	THR
6	K	40	ASN
6	K	81	ASP
7	L	63	GLU
5	M	151	ARG
1	A	643	LYS
1	A	802	MET

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Mol	Chain	Res	Type
2	B	86	ASP
2	B	104	THR
3	C	25	PRO
6	G	152	VAL
5	R	49	ILE
7	Z	54	ARG
6	K	37	THR
6	K	310	THR
6	K	694	PRO
3	C	312	GLY
6	K	274	ILE
1	A	22	PRO
1	A	503	VAL
1	A	615	VAL
3	C	112	PRO
5	R	163	GLY
5	M	148	ILE
1	A	133	GLY
1	A	259	PRO
5	F	43	ILE
6	G	820	PRO
6	K	820	PRO
6	G	694	PRO
1	A	575	GLY
2	B	516	LYS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.