



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 5, 2020 – 06:34 PM EST

PDB ID : 6V8O
EMDB ID: : EMD-21107
Title : RSC core
Authors : Patel, A.B.; Moore, C.M.; Greber, B.J.; Nogales, E.
Deposited on : 2019-12-11
Resolution : 3.07 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

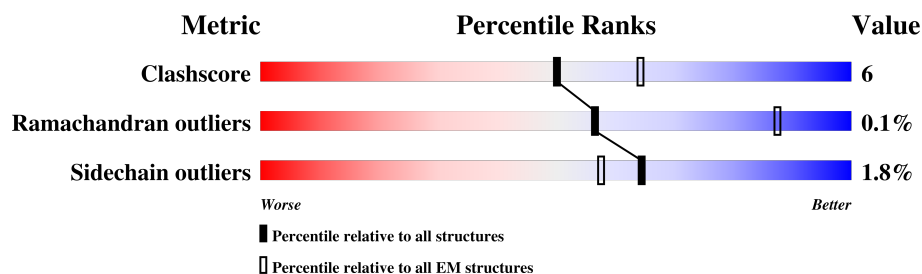
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 ≥ 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	C	78	
2	D	180	
3	E	435	
4	F	889	
5	G	885	
6	H	625	
7	I	557	
7	J	557	
7	K	557	

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Mol	Chain	Length	Quality of chain
7	L	557	 44%9%46%
8	M	483	 51%13%36%
9	N	581	 57%13%29%
10	O	502	 63%13%24%
11	Q	426	 48%12%38%
12	R	1359	 16%81%
13	S	883	 96%
14	2	28	 96%
15	3	19	 100%
15	4	19	 95%5%
16	5	14	 100%
17	6	15	 100%
18	7	49	 96%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 25103 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 High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	60	Total	C	N	O	S	0	0
			493	301	92	96	4		

- Molecule 2 is a protein called Chromatin structure-remodeling complex protein RSC14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	100	Total	C	N	O	S	0	0
			772	490	132	148	2		

- Molecule 3 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	120	Total	C	N	O	S	0	0
			978	610	166	200	2		

- Molecule 4 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	67	Total	C	N	O	S	0	0
			536	346	94	95	1		

- Molecule 5 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	53	Total	C	N	O	S	0	0
			422	270	71	79	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	767	SER	THR	conflict	UNP Q06639

- Molecule 6 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1083	696	175	205	7		

- Molecule 7 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	293	Total	C	N	O	S	0	0
			2416	1537	423	448	8		
7	J	115	Total	C	N	O	S	0	0
			924	579	149	190	6		
7	K	109	Total	C	N	O	S	0	0
			878	554	139	179	6		
7	L	298	Total	C	N	O	S	0	0
			2445	1557	428	452	8		

- Molecule 8 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	310	Total	C	N	O	S	0	0
			2474	1558	414	496	6		

- Molecule 9 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	412	Total	C	N	O	S	0	0
			3275	2105	540	612	18		

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	384	Total	C	N	O	S	0	0
			3145	2025	529	581	10		

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	264	Total	C	N	O	S	0	0
			2137	1349	362	418	8		

- Molecule 12 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	262	Total	C	N	O	S	0	0
			2126	1339	378	407	2		

- Molecule 13 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	34	Total	C	N	O	S	0	0
			278	182	41	54	1		

- Molecule 14 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	2	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 15 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	3	19	Total	C	N	O	0	0
			95	57	19	19		
15	4	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	5	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 17 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	6	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 18 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	7	49	Total	C	N	O	0	0
			245	147	49	49		

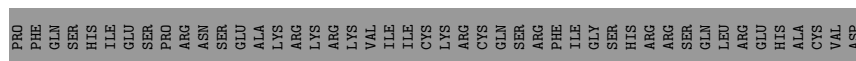
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	I	1	Total	Zn	0
			1	1	

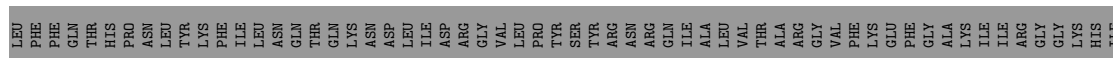
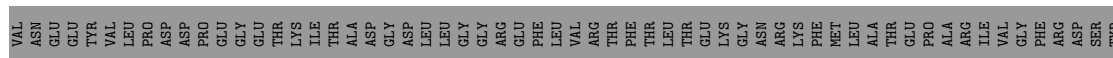
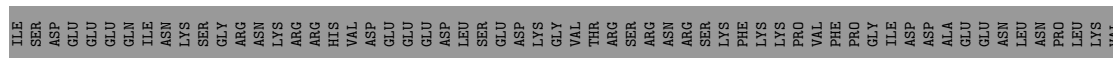
- Molecule 1: High temperature lethal protein 1



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|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|
| MET | SER | GLY | ASN | K6 | Q36 | GLN | SER | HIS | ALA | ALA | THR | ASP | LYS | ILE | GLU | GLY | SER | GLU | ASN | LYS | ALA | VAL | LYS | LYS | SER | PRO | R59 | A62 | V63 | H64 | G65 | Y66 | V71 | H85 | Q96 | L97 | E98 | H10 | C115 | D123 | A127 | GLY | ALA | GLY | GLN | LEU | SER |
|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|

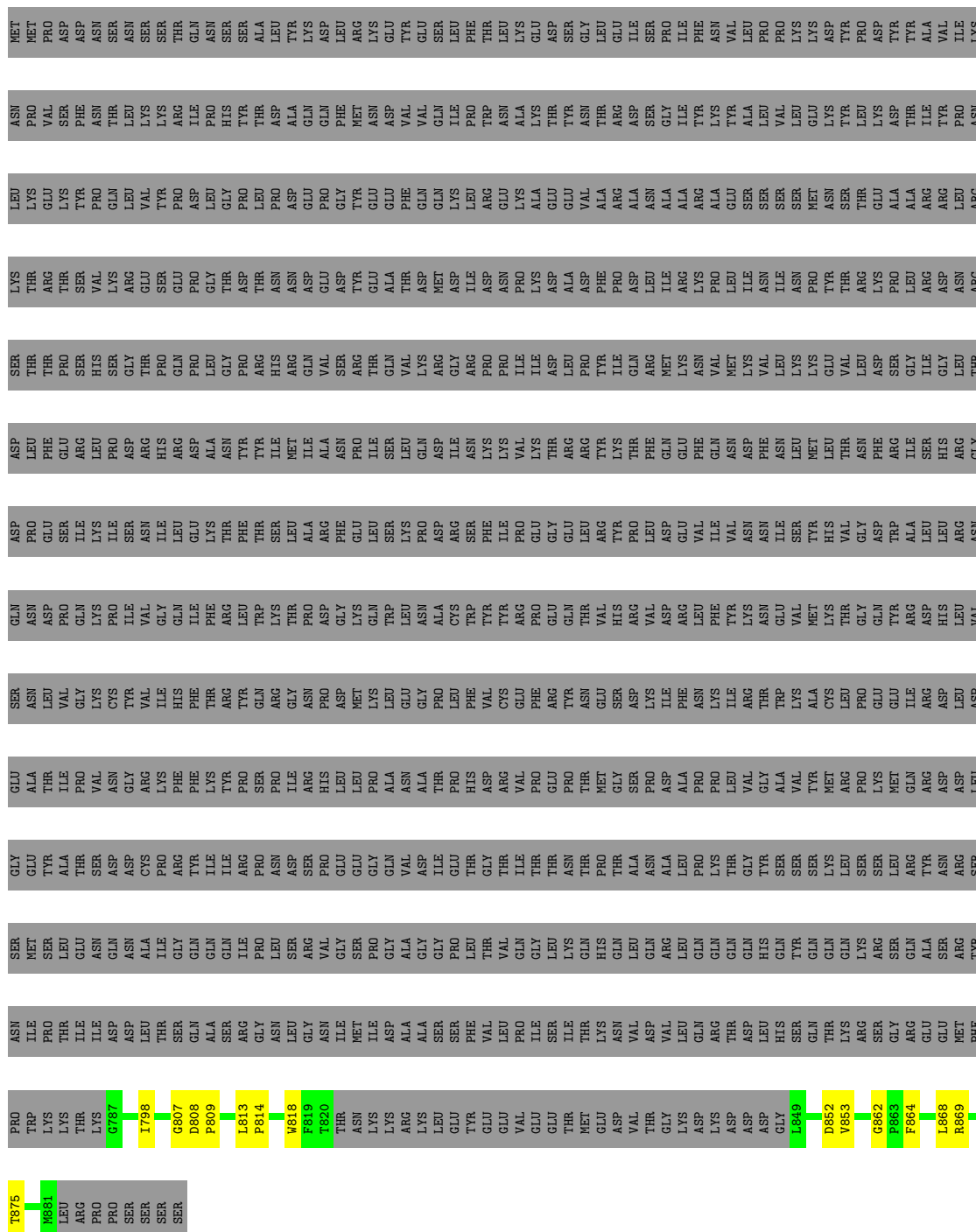


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| MET | SER | ASP | SER | GLU | GLY | LEU | ALA | SER | SER | VAL | GLU | GLU | HIS | GLU | LYS | ARG | SER | ARG | SER | THR | ASN | ARG | PRO | ASN | TYR | ALA | ILE | ASP | THR | GLU | GLU | ASN | ASP | ASP | GLP | ASP | ASN | GLU | ASP | ASP | TYR | ARG | GLU | GLU | ALA | ASN | GLN | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



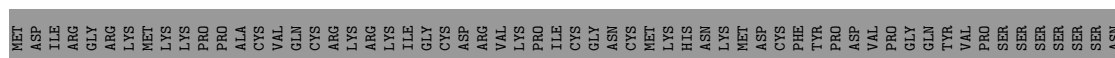
- Molecule 4: Chromatin structure-remodeling complex subunit RSC2

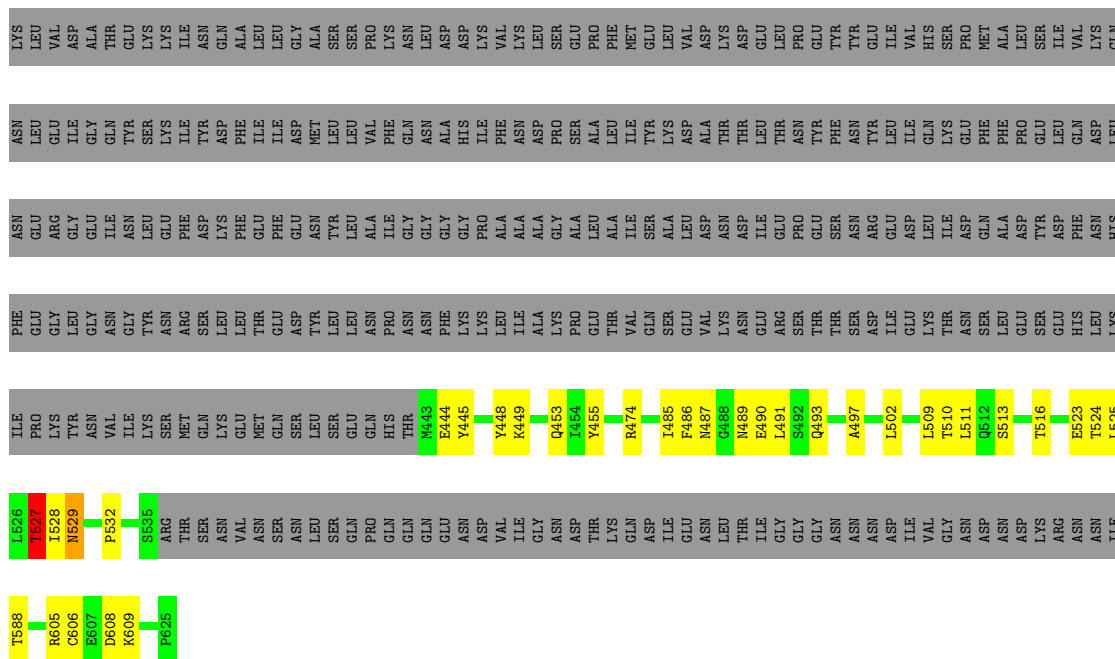
Chain F: 6% . 92%



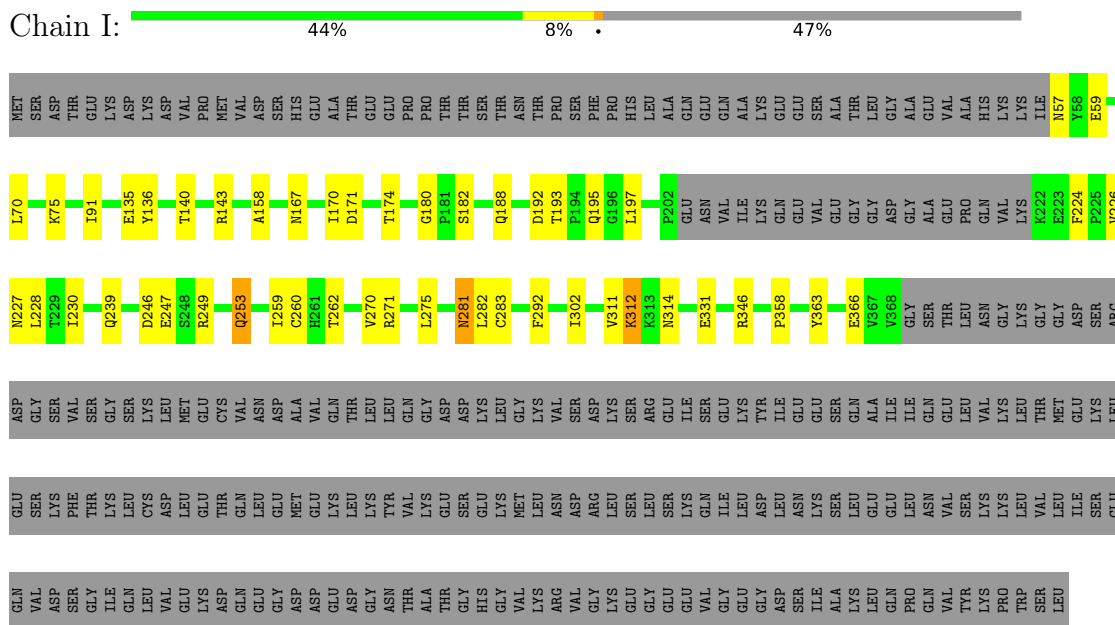
- Molecule 5: Chromatin structure-remodeling complex protein RSC3

Chain G: 5% . 94%

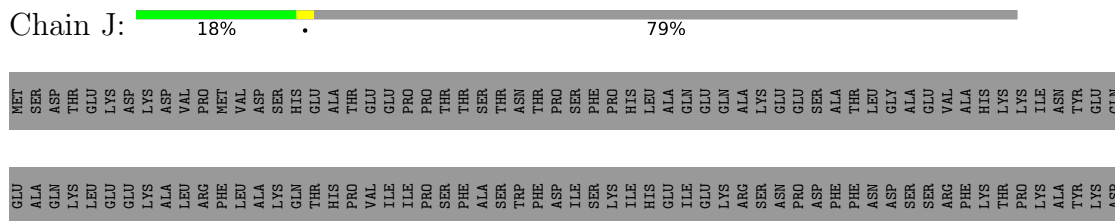


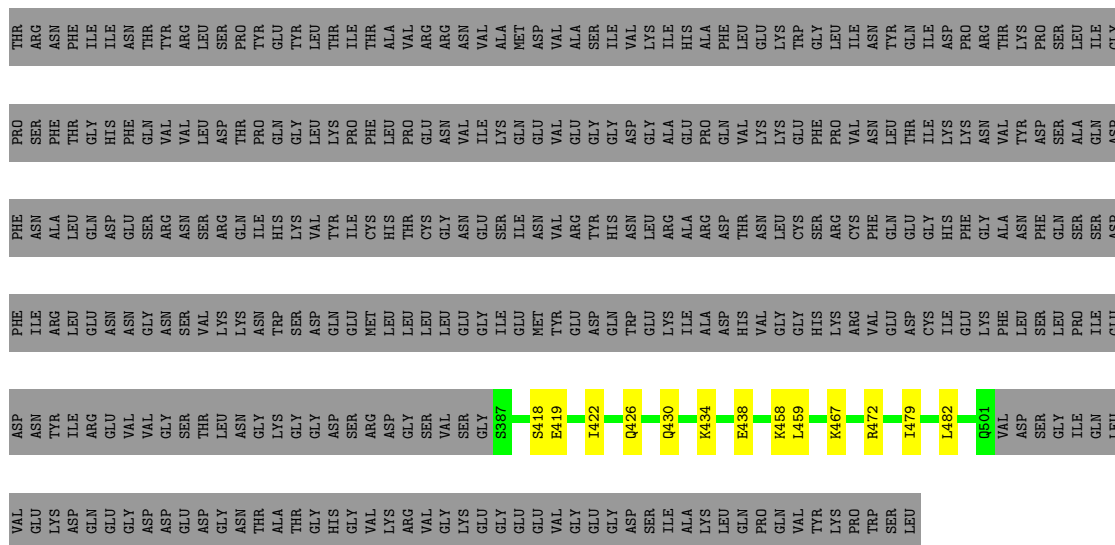


- Molecule 7: Chromatin structure-remodeling complex protein RSC8



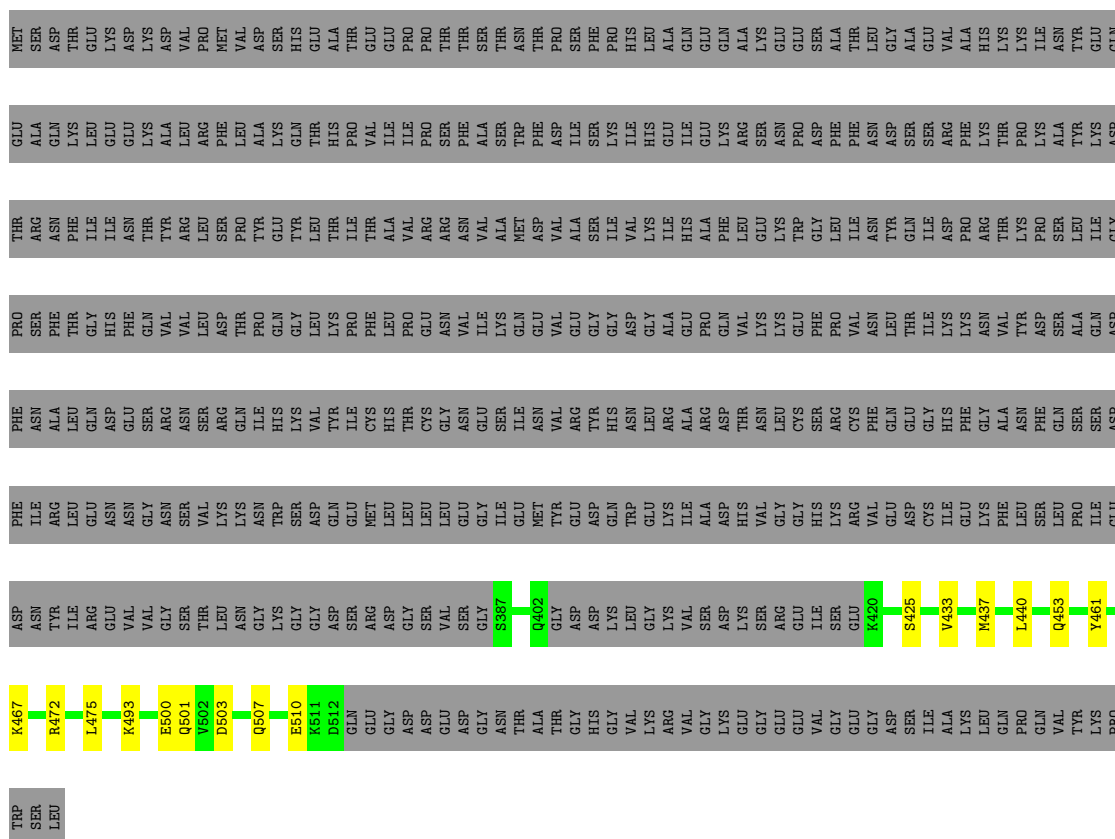
- Molecule 7: Chromatin structure-remodeling complex protein RSC8





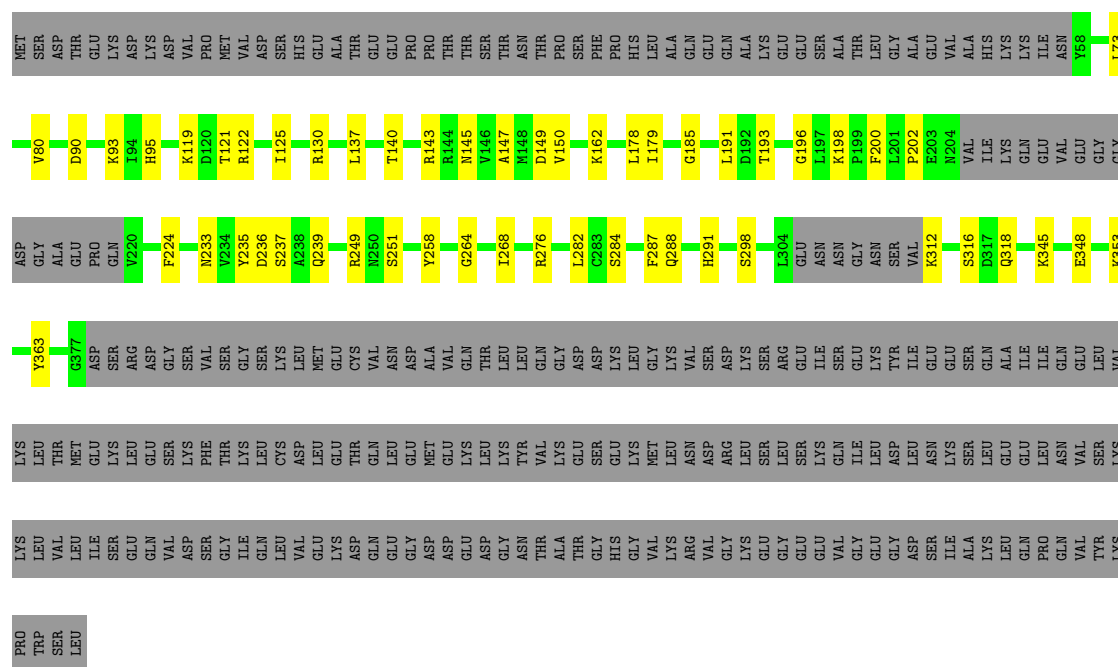
- Molecule 7: Chromatin structure-remodeling complex protein RSC8

Chain K: 17% 3% 80%

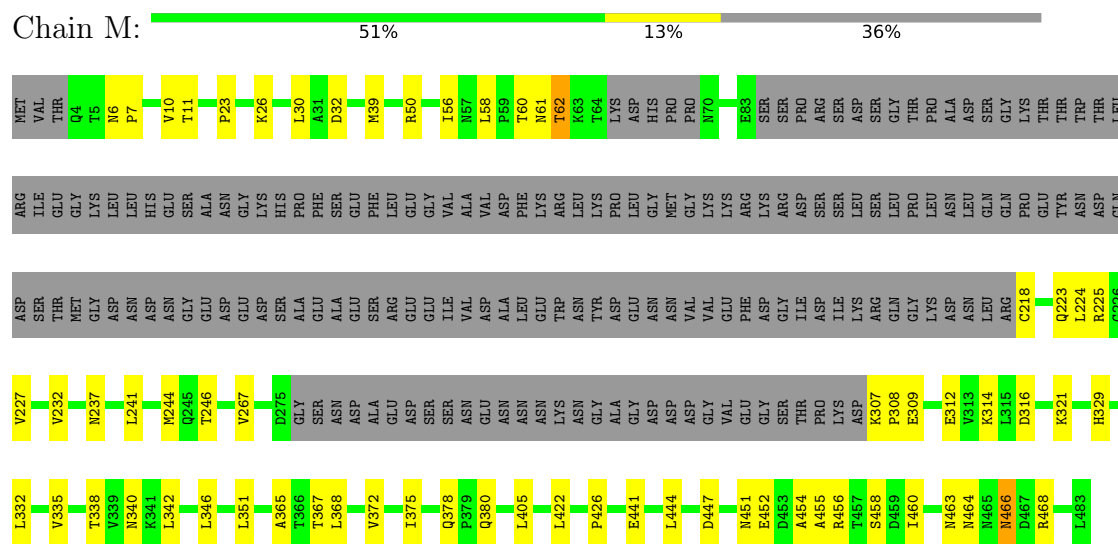


- Molecule 7: Chromatin structure-remodeling complex protein RSC8

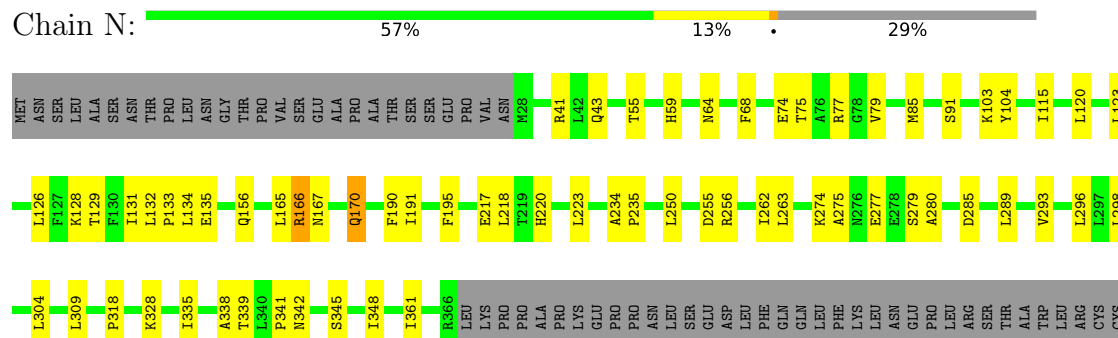
Chain L:  44% 9% 46%

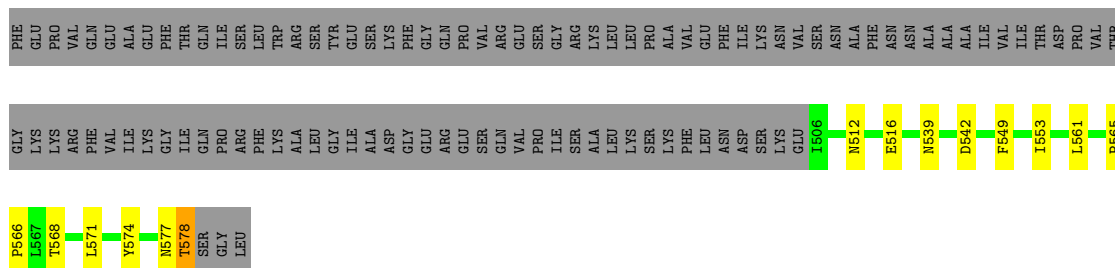


• Molecule 8: Chromatin structure-remodeling complex protein RSC6



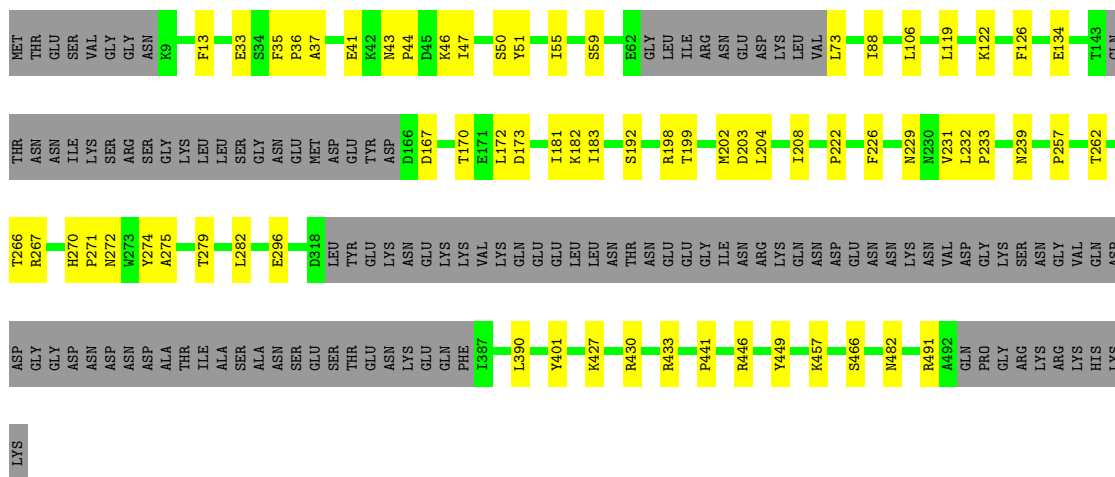
• Molecule 9: Chromatin structure-remodeling complex subunit RSC9





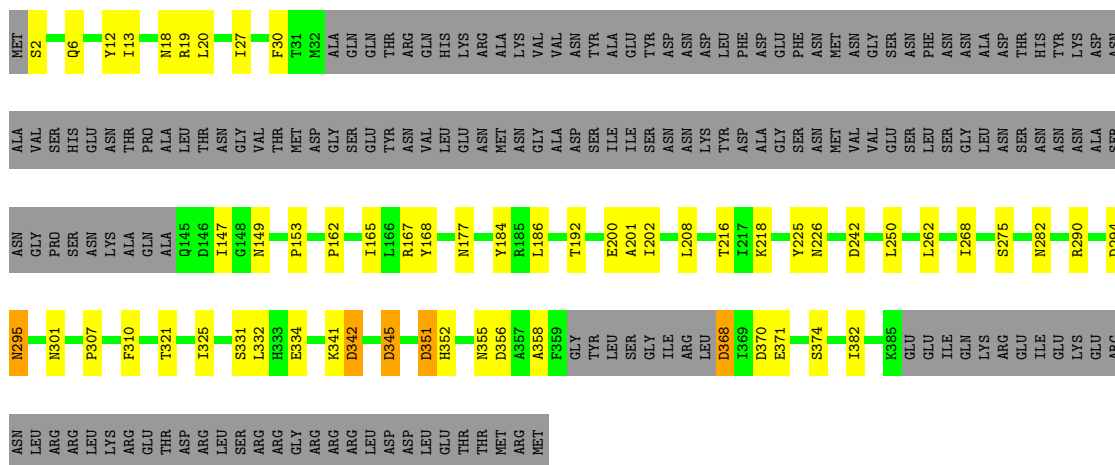
• Molecule 10: Chromatin structure-remodeling complex protein RSC58

Chain O: 63% 13% 24%



• Molecule 11: Chromatin structure-remodeling complex subunit SFH1

Chain Q: 48% 12% 38%



• Molecule 12: Nuclear protein STH1/NPS1

Chain R: 16% 81%




GLU	VAL	ASP	SER	HIS	PRO	ARG	THR	SER	ILE	PHE	GLU	LYS	LEU	PRO	SER	LYS	ARG	ASP	TYR	PRO	ASP	TYR	LYS	VAL	ILE	GLU	LYS	PRO	MET	ALA	ALA	ILE	ILE	ILE	LEU	LYS	ASN	CYS	CYS	LYS	ASN	GLY	THR	TYR	LYS	THR	THR	LEU	GLU	GLU	VAL	VAL	ARG	GLN	GLN	ALA	ALA	LEU	GLN	THR	MET	PHE	GLN
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ASN ALA ARG PHE TYR ASN GLU GLU GLY SER TRP VAL TYR VAL ASP ALA ASP LYS LEU ASN GLU PHE THR ASP GLU TRP PHE LYS GLU HIS SER SER

- Molecule 13: Chromatin structure-remodeling complex protein RSC30

Chain S:  96%

MET	MET	ASP	MET	GLN	VAL	ARG	LYS	VAL	ARG	ARG	LYS	PRO	PRO	ALA	ALA	CYS	THR	GLN	CYS	ARG	LYS	ARG	ALA	LYS	ILE	GLY	CYS	ASP	ARG	ASN	ALA	LYS	PRO	PRO	ILE	CYS	GLY	GLY	ASN	CYS	VAL	VAL	LYS	TYR	TYR	PRO	PRO	ASP	GLY	GLY	PRO	GLY	LYS	MET	VAL	ALA	ALA	VAL	PRO	PRO	SER	SER	TYR
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MET	THR	GLY	ASN	GLN	GLY	SER	ASN	HIS	PHE	SER	GLN	GLY	ASN	VAL	ASN	LYS	ASN	VAL	MET	ILE	GLN	THR	GLN	TYR	PRO	ILE	MET	GLN	THR	SER	ILE	GLU	ALA	PHE	ASN	PHE	SER	PHE	ASN	PRO	SER	VAL	ASP	ALA	THR	ALA	MET	GLN	TRP	THR	LYS	ALA	ALA	ALA	SER	THR
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[illegible]

ASN	PRO	TYR	SER	PHE	ASN	VAL	GLY	ILE	ASN	GLN	ASP	SER	L194	L198	F203	V208 L209	G226 L227	LEU	SYS	SER	LEU	LVS	GLU	LVS	LVS	LVS	THR	ALA	ASN	ASP	ASN	ASN	ASN	LYS	THR	THR	ALA	ASN	LYS	ILE	ASN	LVS	LYS	LYS	GLY	GLU	ASN	SER	SER	LVS	LVS	GLY	LVS	VAL	ASP	GLY	LVS	PC
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[illegible]

ILE	LEU	HIS	HIS	ASP	ILE	CYS	HIS	ILE	ASN	GLN	ASN	PHE	LYS	VAL	SER	PRO	PRO	ASN	ASN	ASN	LYS	HIS	GLN	GLN	TYR	MET	GLU	VAL	CYS	LYS	VAL	ASN	ASN	PHE	PRO	PRO	LYS	ALA	ILE	ILE	ILE	THR	GLU	LEU	ASN	SER	GLU	SER	LEU	LEU	ASN	ASN	ASN	ILE	ILE	GLU	GLU	PHE	PRO	PRO	ILE	PHE	SER
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[illegible]

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ASP
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THR
LEU
PHE
LYS
ALA
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PHE
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GLU
SER
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GLU
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LEU
SER
CYS
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LEU
SER
PHE
TYR

ILE LYS ASP LYS ASP LYS PHE PHE LYS LYS LEU PHE HIS HIS PHE LEU LEU LYS LYS MET TYR TYR SER SER ARG SER HIS SER LEU LEU GLY GLY GLN SER SER PHE MET MET VAL VAL PRO PRO ALA ALA ALA GLU GLU ASN ASN LEU LEU SER SER PRO PRO ILE ILE PRO PRO ALA ALA SER SER ILE ILE ASP ASP THR THR ASN ASN ASP ASP ILE ILE LEU LEU PRO PRO LEU LEU ILE ILE LEU LEU ALA ALA ASN ASN ASP ASP LEU LEU LYS LYS LEU LEU LEU LEU GLU GLU THR THR GLN GLN ALA ALA

LYS LEU LEU ASN ASN LEU GLN GLY VAL PRO TYR LEU LEU VAL ASN THR LYS ILE GLU SER THR THR MET GLY VAL SER ASP LEU PHE THR HIS ASP ASN GLU VAL ARG LYS LYS TRP THR LYS ASP THR THR LEU LEU ASN PHE ILE ASN THR ILE VAL THR

THR ASN PHE PHE LEU PHE VAL GLN ASN ASN SER SER LEU SER SER HIS SER SER ASN ASN ASN LYS THR SER SER SER SER GLU ARG CYS ALA LYS ASP LEU LEU MET LYS ILE ILE SER SER MET HIS PHE PHE TYR SER ILE THR PHE ASN ASN PHE ILE PHE PRO ILE LYS SER THR

LYS SER PHE SER SER GLY ASN ASN PHE ARG PHE HIS SER SER ASN GLY LYS LYS PHE PHE LEU LEU PHE PHE LEU ALA ALA HIS HIS PHE PHE ILE ILE GLU ILE LEU LEU GLN ASN ASN PHE PHE ILE ILE ALA ALA THR THR PHE PHE ALA ALA PHE PHE GLN GLN ARG ARG CYS GLU VAL ILE ILE LEU LEU TYR TYR ASP ASP GLU PHE TYR LYS ASN ASN LEU LEU SER SER ASN ASN ILE ILE LYS LYS

GLN LEU LEU LEU LEU HIS ASP LYS ILE LEU LEU GLU ILE LEU LEU LYS LYS LYS ILE GLU ILE ILE VAL SER PHE ARG LEU ASP GLU MET ASN SER SER ASN ASN GLY SER PHE LYS LYS LYS LYS LYS TYR MET MET LEU LEU LEU ILE ILE LYS PHE ARG PHE SER LYS LYS LYS LYS LYS LYS LYS LYS LYS LYS

ARG ASN SER ASP ASN ASN ASN VAL THR TYR SER GLN SER ALA LYS ASN LYS ASN VAL VAL LEU LEU LYS PHE PRO VAL SER SER GLU LEU LEU LYS ARG ARG ILE TYR TYR LEU LEU LYS LYS LEU LEU PHE PHE LEU MET MET GLU GLU ARG ARG GLU VAL VAL GLN ARG ARG SER SER ILE ILE ILE ILE ILE ASP LYS ASP ASP LEU LEU

SER
ASP
ASN
LEU
GLY
ILE
THR
THR
ALA
ASN
PHE
ASN
ASP
PHE
TYR
ASP
ALA
PHE
TYR
ASN

- Molecule 14: Unknown protein

Chain 2:  96%



- Molecule 15: Unknown Protein

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Unknown Protein

Chain 4:  95%



- Molecule 16: Unknown protein

Chain 5:  100%

There are no outlier residues recorded for this chain.

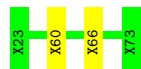
- Molecule 17: Unknown Protein

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Unknown Protein

Chain 7:  96%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1920066	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
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

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	C	0.24	0/495	0.36	0/662
10	O	0.30	0/3216	0.42	1/4358 (0.0%)
11	Q	0.27	0/2181	0.45	0/2964
12	R	0.27	0/2154	0.40	0/2897
13	S	0.26	0/281	0.35	0/378
2	D	0.27	0/786	0.38	0/1062
3	E	0.28	0/997	0.44	0/1356
4	F	0.27	0/551	0.41	0/748
5	G	0.26	0/431	0.43	0/584
6	H	0.29	0/1108	0.48	0/1497
7	I	0.32	0/2474	0.41	0/3343
7	J	0.30	0/926	0.40	0/1233
7	K	0.27	0/879	0.39	0/1172
7	L	0.29	0/2502	0.40	0/3376
8	M	0.28	0/2515	0.42	0/3423
9	N	0.30	0/3334	0.42	0/4515
All	All	0.29	0/24830	0.42	1/33568 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	231	VAL	C-N-CA	5.36	135.09	121.70

There are no chirality outliers.

There are no planarity outliers.

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	C	493	0	507	6	0
2	D	772	0	754	11	0
3	E	978	0	935	24	0
4	F	536	0	533	14	0
5	G	422	0	423	10	0
6	H	1083	0	1062	22	0
7	I	2416	0	2358	35	0
7	J	924	0	976	10	0
7	K	878	0	930	14	0
7	L	2445	0	2402	47	0
8	M	2474	0	2465	51	0
9	N	3275	0	3373	51	0
10	O	3145	0	3168	50	0
11	Q	2137	0	2069	39	0
12	R	2126	0	2205	34	0
13	S	278	0	287	6	0
14	2	140	0	34	1	0
15	3	95	0	21	0	0
15	4	95	0	21	1	0
16	5	70	0	16	0	0
17	6	75	0	17	0	0
18	7	245	0	63	2	0
19	I	1	0	0	0	0
All	All	25103	0	24619	323	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 6.

All (323) 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)
11:Q:282:ASN:OD1	11:Q:295:ASN:ND2	2.20	0.75
9:N:217:GLU:OE1	12:R:287:ARG:NH1	2.21	0.74
2:D:96:GLN:NE2	15:4:15:UNK:O	2.22	0.72
4:F:813:LEU:HD11	10:O:183:ILE:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:268:ILE:HD11	10:O:232:LEU:HD22	1.73	0.70
7:I:136:TYR:O	7:I:167:ASN:ND2	2.26	0.69
9:N:345:SER:HA	9:N:348:ILE:HD11	1.75	0.68
10:O:35:PHE:O	10:O:73:LEU:N	2.26	0.68
12:R:231:SER:HB3	12:R:234:MET:HG2	1.75	0.68
9:N:220:HIS:NE2	10:O:296:GLU:O	2.27	0.68
7:I:135:GLU:OE2	11:Q:19:ARG:NH2	2.27	0.68
1:C:20:THR:HG22	10:O:275:ALA:H	1.58	0.68
3:E:376:ASN:ND2	3:E:381:ASP:O	2.27	0.67
7:L:178:LEU:HD21	11:Q:325:ILE:HD11	1.76	0.67
8:M:218:CYS:SG	18:7:60:UNK:N	2.68	0.67
8:M:456:ARG:NH2	10:O:262:THR:O	2.28	0.66
10:O:126:PHE:HB2	12:R:226:THR:HG22	1.78	0.66
11:Q:18:ASN:ND2	11:Q:177:ASN:O	2.29	0.66
6:H:527:THR:C	6:H:529:ASN:H	1.97	0.66
9:N:55:THR:O	9:N:64:ASN:ND2	2.28	0.65
7:L:363:TYR:OH	12:R:116:ASN:ND2	2.29	0.65
10:O:401:TYR:OH	12:R:48:LYS:NZ	2.21	0.65
10:O:33:GLU:HG3	10:O:106:LEU:HD11	1.79	0.65
4:F:813:LEU:HD22	7:L:276:ARG:HH21	1.62	0.65
7:J:426:GLN:NE2	8:M:26:LYS:O	2.30	0.64
11:Q:184:TYR:OH	11:Q:242:ASP:OD1	2.15	0.64
3:E:392:ASP:HB3	7:I:226:VAL:HB	1.80	0.64
7:K:501:GLN:HG2	8:M:244:MET:HB3	1.79	0.63
10:O:430:ARG:NH2	12:R:130:ASP:OD1	2.31	0.63
10:O:41:GLU:OE2	10:O:50:SER:OG	2.16	0.62
4:F:875:THR:HG22	12:R:221:CYS:HB3	1.81	0.62
6:H:449:LYS:O	6:H:516:THR:OG1	2.16	0.61
7:I:260:CYS:HB2	7:I:283:CYS:SG	2.40	0.61
3:E:405:ILE:HD11	7:L:162:LYS:HD3	1.82	0.61
9:N:296:LEU:HD21	9:N:309:LEU:HG	1.83	0.61
7:I:282:LEU:HD21	7:I:292:PHE:HB3	1.83	0.61
7:L:95:HIS:ND1	7:L:95:HIS:O	2.34	0.61
2:D:64:HIS:HD2	2:D:66:TYR:H	1.47	0.60
8:M:463:ASN:HA	8:M:468:ARG:HH21	1.66	0.60
7:L:237:SER:OG	7:L:249:ARG:NH1	2.35	0.60
7:I:312:LYS:H	7:I:312:LYS:HD3	1.66	0.60
7:L:288:GLN:HB2	7:L:291:HIS:CE1	2.37	0.60
11:Q:368:ASP:N	11:Q:368:ASP:OD1	2.35	0.59
11:Q:351:ASP:N	11:Q:351:ASP:OD1	2.35	0.59
9:N:75:THR:HG1	11:Q:12:TYR:HH	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:239:GLN:OE1	7:I:346:ARG:NH1	2.35	0.59
8:M:378:GLN:OE1	8:M:380:GLN:NE2	2.36	0.59
10:O:170:THR:HG22	10:O:172:LEU:H	1.68	0.59
11:Q:2:SER:N	11:Q:6:GLN:OE1	2.35	0.58
3:E:408:GLU:OE1	3:E:408:GLU:N	2.35	0.58
10:O:167:ASP:OD2	10:O:182:LYS:NZ	2.36	0.58
4:F:852:ASP:OD1	4:F:853:VAL:N	2.36	0.57
7:J:434:LYS:NZ	7:J:438:GLU:OE2	2.37	0.57
9:N:574:TYR:O	9:N:578:THR:OG1	2.21	0.57
7:I:271:ARG:HD2	7:I:281:ASN:HD22	1.68	0.57
1:C:33:ARG:NH2	8:M:441:GLU:OE2	2.36	0.56
3:E:380:SER:HB2	8:M:464:ASN:HA	1.85	0.56
7:I:57:ASN:N	7:I:59:GLU:OE1	2.38	0.56
10:O:266:THR:HG23	10:O:267:ARG:HG3	1.87	0.56
6:H:527:THR:O	6:H:529:ASN:N	2.33	0.56
9:N:156:GLN:OE1	12:R:287:ARG:NH2	2.38	0.56
8:M:227:VAL:HG12	9:N:361:ILE:HD12	1.88	0.55
6:H:489:ASN:O	6:H:490:GLU:HG2	2.06	0.55
7:I:226:VAL:HG13	7:I:228:LEU:HG	1.88	0.55
4:F:814:PRO:O	7:L:276:ARG:NH2	2.39	0.55
6:H:513:SER:O	6:H:588:THR:HA	2.07	0.55
3:E:372:ARG:HB2	7:I:188:GLN:HB2	1.89	0.55
11:Q:202:ILE:HG12	11:Q:226:ASN:HB2	1.87	0.55
7:L:179:ILE:HD11	11:Q:321:THR:HA	1.89	0.55
12:R:111:ASP:N	12:R:111:ASP:OD1	2.38	0.55
4:F:813:LEU:HD23	4:F:814:PRO:HD2	1.90	0.54
10:O:198:ARG:NH2	10:O:199:THR:O	2.41	0.54
7:L:268:ILE:HD12	10:O:233:PRO:HD2	1.88	0.54
7:L:251:SER:OG	12:R:57:GLN:NE2	2.41	0.54
12:R:105:ASP:OD1	12:R:106:LYS:N	2.40	0.54
12:R:253:LYS:HE3	12:R:257:ILE:HD11	1.90	0.54
6:H:448:TYR:HA	6:H:493:GLN:HE21	1.73	0.54
7:I:302:ILE:HD11	12:R:239:ILE:HG12	1.89	0.54
10:O:35:PHE:HB2	10:O:36:PRO:HD2	1.89	0.54
7:L:193:THR:OG1	7:L:196:GLY:O	2.26	0.54
2:D:98:GLU:OE2	9:N:41:ARG:NH2	2.29	0.54
7:L:191:LEU:HG	7:L:200:PHE:HB2	1.90	0.54
7:I:363:TYR:HA	7:I:366:GLU:HG2	1.91	0.53
10:O:167:ASP:HB3	10:O:173:ASP:HB3	1.89	0.53
7:J:430:GLN:NE2	7:K:425:SER:OG	2.41	0.53
7:J:458:LYS:NZ	7:K:453:GLN:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:80:VAL:HG21	7:L:130:ARG:HG2	1.91	0.53
3:E:431:CYS:HA	3:E:434:TYR:HD2	1.72	0.53
8:M:451:ASN:N	8:M:451:ASN:OD1	2.42	0.53
9:N:170:GLN:HG3	12:R:295:VAL:HG12	1.90	0.53
8:M:225:ARG:HB3	18:7:66:UNK:HA	1.90	0.53
8:M:267:VAL:HG22	8:M:314:LYS:HE3	1.89	0.53
3:E:327:CYS:SG	7:L:145:ASN:ND2	2.82	0.52
5:G:159:VAL:HG11	13:S:208:VAL:HG21	1.91	0.52
6:H:453:GLN:HA	6:H:486:PHE:O	2.09	0.52
7:I:70:LEU:O	7:I:75:LYS:NZ	2.39	0.52
7:L:233:ASN:ND2	12:R:126:GLU:OE2	2.42	0.52
8:M:456:ARG:NH1	12:R:192:GLU:OE2	2.42	0.52
11:Q:342:ASP:N	11:Q:342:ASP:OD1	2.42	0.52
10:O:491:ARG:HG2	14:2:358:UNK:HA	1.91	0.52
4:F:798:ILE:HD11	10:O:192:SER:HB2	1.92	0.52
7:I:91:ILE:HD12	7:L:185:GLY:HA2	1.91	0.52
3:E:402:LEU:HD12	3:E:405:ILE:HD13	1.92	0.52
7:L:235:TYR:O	10:O:446:ARG:NH1	2.41	0.52
11:Q:147:ILE:HD11	11:Q:167:ARG:HB3	1.90	0.52
8:M:351:LEU:HD11	8:M:368:LEU:HD11	1.90	0.52
3:E:380:SER:OG	8:M:463:ASN:ND2	2.43	0.52
6:H:497:ALA:HB3	10:O:229:ASN:HA	1.92	0.52
7:K:433:VAL:HG21	8:M:32:ASP:HB3	1.90	0.52
8:M:466:ASN:OD1	8:M:466:ASN:N	2.42	0.52
9:N:250:LEU:HB2	9:N:262:ILE:HG21	1.92	0.51
11:Q:358:ALA:H	11:Q:371:GLU:HB2	1.75	0.51
12:R:62:TYR:HB2	12:R:79:ILE:HG21	1.91	0.51
11:Q:268:ILE:HD13	11:Q:341:LYS:HG2	1.93	0.51
3:E:417:ASP:N	3:E:417:ASP:OD1	2.42	0.51
11:Q:200:GLU:HG3	11:Q:201:ALA:H	1.76	0.51
10:O:122:LYS:HG3	12:R:226:THR:HG21	1.93	0.51
9:N:255:ASP:OD1	9:N:256:ARG:N	2.44	0.51
8:M:60:THR:O	8:M:61:ASN:ND2	2.44	0.51
9:N:285:ASP:OD1	9:N:285:ASP:N	2.36	0.51
11:Q:345:ASP:OD1	11:Q:345:ASP:N	2.43	0.50
7:L:348:GLU:HB3	10:O:457:LYS:HE3	1.92	0.50
5:G:175:ASP:N	5:G:175:ASP:OD1	2.43	0.50
10:O:270:HIS:HD2	10:O:272:ASN:HB2	1.77	0.50
7:I:249:ARG:NH2	7:I:253:GLN:HE21	2.09	0.50
11:Q:275:SER:O	11:Q:301:ASN:ND2	2.41	0.50
6:H:511:LEU:HD23	6:H:525:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:147:ALA:HB1	11:Q:355:ASN:HD22	1.76	0.49
7:I:358:PRO:HB2	7:L:224:PHE:HB2	1.95	0.49
4:F:869:ARG:H	7:L:318:GLN:NE2	2.09	0.49
11:Q:153:PRO:HB3	11:Q:168:TYR:CE1	2.47	0.49
5:G:163:ALA:HB1	13:S:194:ALA:HB1	1.94	0.49
2:D:66:TYR:OH	7:I:331:GLU:OE2	2.20	0.49
7:L:236:ASP:OD2	7:L:239:GLN:NE2	2.45	0.49
7:L:284:SER:HB2	10:O:181:ILE:HD11	1.95	0.49
7:K:440:LEU:HD13	8:M:39:MET:HE2	1.93	0.49
7:I:192:ASP:OD1	7:I:193:THR:N	2.45	0.49
8:M:454:ALA:HB1	8:M:460:ILE:HG21	1.93	0.49
9:N:75:THR:OG1	11:Q:12:TYR:OH	2.20	0.49
11:Q:208:LEU:O	11:Q:218:LYS:HA	2.13	0.49
7:L:282:LEU:HD22	7:L:291:HIS:CD2	2.48	0.49
7:J:419:GLU:O	7:J:422:ILE:HG12	2.13	0.49
3:E:345:ASP:O	11:Q:149:ASN:ND2	2.45	0.49
11:Q:30:PHE:HA	11:Q:216:THR:O	2.11	0.49
11:Q:294:ASP:OD1	11:Q:295:ASN:N	2.46	0.49
2:D:62:ALA:HB3	2:D:71:VAL:HG23	1.94	0.48
7:I:249:ARG:HH21	7:I:253:GLN:HE21	1.61	0.48
8:M:308:PRO:HB3	8:M:329:HIS:CD2	2.48	0.48
12:R:217:SER:OG	12:R:220:ASP:OD1	2.32	0.48
5:G:167:MET:HE1	5:G:177:ILE:HA	1.95	0.48
3:E:331:ASN:HD21	7:L:137:LEU:HA	1.78	0.48
7:L:140:THR:HG22	7:L:143:ARG:HH22	1.79	0.48
7:J:467:LYS:NZ	8:M:62:THR:O	2.42	0.48
11:Q:202:ILE:HB	11:Q:225:TYR:HB3	1.96	0.48
9:N:191:ILE:HD12	9:N:218:LEU:HD21	1.96	0.47
8:M:237:ASN:ND2	8:M:321:LYS:O	2.47	0.47
8:M:23:PRO:HB2	8:M:26:LYS:HG2	1.97	0.47
9:N:115:ILE:HA	9:N:120:LEU:HD12	1.96	0.47
11:Q:307:PRO:HB3	11:Q:332:LEU:HD23	1.97	0.47
9:N:341:PRO:HD3	9:N:553:ILE:HD11	1.95	0.47
9:N:68:PHE:CZ	11:Q:13:ILE:HD11	2.49	0.47
10:O:198:ARG:HD3	10:O:203:ASP:OD1	2.14	0.47
2:D:64:HIS:CD2	2:D:66:TYR:H	2.29	0.47
7:L:258:TYR:OH	10:O:173:ASP:OD1	2.33	0.47
6:H:444:GLU:HG2	6:H:445:TYR:H	1.80	0.47
10:O:427:LYS:HZ1	12:R:133:ASP:HA	1.80	0.47
5:G:175:ASP:O	5:G:178:ILE:HG22	2.15	0.47
7:L:147:ALA:HB3	11:Q:371:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:298:SER:HB3	10:O:390:LEU:HG	1.98	0.46
3:E:372:ARG:HH12	7:I:227:ASN:HD21	1.62	0.46
7:K:493:LYS:HE2	7:K:510:GLU:HG2	1.97	0.46
12:R:215:THR:HG21	12:R:237:PHE:H	1.79	0.46
2:D:64:HIS:HD2	2:D:66:TYR:HB2	1.81	0.46
3:E:331:ASN:ND2	7:L:137:LEU:HA	2.31	0.46
9:N:279:SER:OG	9:N:280:ALA:N	2.48	0.46
7:I:311:VAL:HB	7:I:314:ASN:HD22	1.79	0.46
11:Q:331:SER:O	11:Q:334:GLU:HB2	2.15	0.46
8:M:444:LEU:HD13	12:R:177:LYS:HG2	1.98	0.46
6:H:524:THR:HG23	6:H:605:ARG:HB3	1.97	0.46
8:M:335:VAL:O	8:M:338:THR:OG1	2.31	0.46
1:C:44:GLU:HB2	12:R:157:LYS:HD3	1.98	0.46
5:G:192:LEU:HD11	13:S:209:LEU:HD22	1.97	0.46
7:I:246:ASP:OD1	7:I:247:GLU:N	2.49	0.46
7:J:472:ARG:HH22	7:K:467:LYS:HB2	1.81	0.46
10:O:55:ILE:O	10:O:59:SER:N	2.48	0.46
11:Q:162:PRO:O	11:Q:165:ILE:HB	2.16	0.46
4:F:818:TRP:HA	7:L:287:PHE:CD2	2.51	0.45
6:H:527:THR:C	6:H:529:ASN:N	2.68	0.45
9:N:561:LEU:HD21	9:N:571:LEU:HD12	1.98	0.45
6:H:490:GLU:HG3	7:L:264:GLY:O	2.15	0.45
8:M:309:GLU:N	8:M:312:GLU:OE1	2.47	0.45
3:E:414:VAL:HG22	3:E:418:VAL:HB	1.98	0.45
7:J:482:LEU:HD11	7:K:507:GLN:HA	1.99	0.45
8:M:452:GLU:HA	8:M:455:ALA:HB3	1.98	0.45
7:L:150:VAL:HG11	11:Q:310:PHE:CE1	2.51	0.45
2:D:123:ASP:OD2	6:H:474:ARG:NH2	2.50	0.45
8:M:227:VAL:HG13	8:M:346:LEU:HD12	1.99	0.45
10:O:466:SER:OG	12:R:112:GLU:OE2	2.29	0.45
7:I:171:ASP:O	7:I:174:THR:HG22	2.17	0.45
8:M:372:VAL:HG12	8:M:375:ILE:HB	1.98	0.45
9:N:234:ALA:HB3	9:N:235:PRO:HD3	1.99	0.45
9:N:59:HIS:O	9:N:59:HIS:ND1	2.49	0.45
11:Q:20:LEU:HA	11:Q:27:ILE:HD12	1.99	0.45
2:D:85:HIS:O	12:R:208:ARG:NH1	2.48	0.45
6:H:525:LEU:O	6:H:532:PRO:HD2	2.16	0.45
7:L:353:LYS:HA	7:L:353:LYS:HD2	1.86	0.44
10:O:173:ASP:N	10:O:173:ASP:OD1	2.48	0.44
9:N:77:ARG:NH1	13:S:198:LEU:H	2.15	0.44
3:E:392:ASP:OD2	3:E:395:LEU:HD13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:500:GLU:OE1	8:M:246:THR:OG1	2.33	0.44
8:M:447:ASP:HB3	10:O:270:HIS:CD2	2.52	0.44
10:O:257:PRO:HG2	12:R:248:LEU:O	2.18	0.44
8:M:30:LEU:HD23	8:M:30:LEU:HA	1.85	0.44
6:H:608:ASP:O	6:H:609:LYS:HG2	2.16	0.44
7:I:180:GLY:HA3	7:L:198:LYS:HE3	2.00	0.44
8:M:372:VAL:HG13	8:M:375:ILE:HD12	1.99	0.44
2:D:64:HIS:CD2	2:D:66:TYR:HB2	2.52	0.44
3:E:388:THR:HG23	7:I:230:ILE:HB	1.99	0.44
3:E:372:ARG:HH22	7:I:227:ASN:HD21	1.64	0.44
7:K:433:VAL:O	7:K:437:MET:HG2	2.17	0.44
3:E:371:TRP:CD2	7:L:202:PRO:HG3	2.53	0.44
10:O:202:MET:HG3	10:O:204:LEU:HD11	2.00	0.44
7:I:281:ASN:N	7:I:281:ASN:OD1	2.50	0.43
8:M:50:ARG:HA	8:M:50:ARG:HD3	1.78	0.43
3:E:394:ASP:HB2	3:E:428:PHE:HE1	1.84	0.43
8:M:458:SER:OG	8:M:458:SER:O	2.35	0.43
1:C:36:ILE:HA	1:C:36:ILE:HD13	1.89	0.43
9:N:542:ASP:N	9:N:542:ASP:OD1	2.50	0.43
9:N:539:ASN:OD1	9:N:577:ASN:ND2	2.51	0.43
5:G:158:TRP:CD1	9:N:74:GLU:HG3	2.54	0.43
9:N:338:ALA:O	9:N:342:ASN:ND2	2.52	0.43
7:I:135:GLU:HG2	7:I:136:TYR:H	1.84	0.43
7:I:140:THR:HG23	7:I:143:ARG:HH21	1.83	0.43
6:H:491:LEU:HA	6:H:491:LEU:HD23	1.90	0.43
7:J:479:ILE:HD11	7:K:475:LEU:HD21	2.01	0.43
8:M:378:GLN:HG2	8:M:380:GLN:HG3	2.00	0.43
8:M:332:LEU:HD23	9:N:565:PRO:HB3	2.00	0.43
10:O:51:TYR:CE2	10:O:55:ILE:HD11	2.53	0.43
6:H:523:GLU:HG2	6:H:606:CYS:SG	2.59	0.43
9:N:132:LEU:N	9:N:133:PRO:HD2	2.33	0.43
9:N:85:MET:SD	9:N:103:LYS:HB3	2.59	0.42
10:O:44:PRO:HA	10:O:47:ILE:HG13	2.00	0.42
11:Q:356:ASP:O	11:Q:374:SER:N	2.37	0.42
5:G:178:ILE:HD12	13:S:226:LEU:HD23	2.01	0.42
9:N:166:ARG:HG3	9:N:167:ASN:N	2.34	0.42
10:O:433:ARG:NH1	10:O:441:PRO:HB3	2.34	0.42
3:E:320:LEU:HB3	7:L:73:LEU:HD11	2.02	0.42
7:L:121:THR:O	7:L:125:ILE:HG13	2.20	0.42
9:N:328:LYS:HE2	9:N:328:LYS:HB3	1.87	0.42
7:I:158:ALA:HB2	11:Q:186:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:10:VAL:HG22	8:M:11:THR:H	1.84	0.42
9:N:126:LEU:O	9:N:129:THR:OG1	2.26	0.42
11:Q:20:LEU:HD23	11:Q:27:ILE:HG21	2.01	0.42
11:Q:358:ALA:H	11:Q:371:GLU:CB	2.32	0.42
5:G:168:LEU:HD23	5:G:168:LEU:HA	1.93	0.42
7:I:260:CYS:SG	7:I:262:THR:OG1	2.76	0.42
10:O:427:LYS:NZ	12:R:133:ASP:HA	2.34	0.42
12:R:212:ASN:OD1	12:R:212:ASN:N	2.48	0.42
7:L:119:LYS:HG3	7:L:122:ARG:NH2	2.34	0.42
8:M:7:PRO:HB2	10:O:282:LEU:HB3	2.02	0.42
10:O:13:PHE:CE1	10:O:134:GLU:HB3	2.55	0.42
3:E:407:LYS:HA	3:E:410:TYR:CZ	2.55	0.42
4:F:808:ASP:OD1	4:F:809:PRO:HD2	2.19	0.42
7:I:195:GLN:C	7:I:197:LEU:H	2.23	0.42
10:O:119:LEU:HA	10:O:119:LEU:HD23	1.91	0.42
1:C:61:SER:O	1:C:65:MET:HG2	2.20	0.41
4:F:818:TRP:HA	7:L:287:PHE:HD2	1.85	0.41
9:N:165:LEU:HD23	9:N:165:LEU:HA	1.79	0.41
2:D:110:HIS:NE2	2:D:115:CYS:SG	2.93	0.41
9:N:298:LEU:HD12	9:N:304:LEU:HD23	2.01	0.41
7:L:287:PHE:HA	12:R:63:ARG:HH21	1.85	0.41
4:F:862:GLY:HA3	4:F:864:PHE:CE2	2.56	0.41
7:K:472:ARG:NH2	7:K:503:ASP:OD2	2.37	0.41
10:O:222:PRO:HG2	10:O:226:PHE:CE2	2.55	0.41
10:O:270:HIS:ND1	10:O:271:PRO:HD2	2.34	0.41
12:R:136:LEU:C	12:R:139:PRO:HD2	2.40	0.41
12:R:248:LEU:HD23	12:R:248:LEU:HA	1.85	0.41
8:M:405:LEU:HA	8:M:405:LEU:HD12	1.92	0.41
8:M:340:ASN:HD21	9:N:516:GLU:HG3	1.86	0.41
9:N:275:ALA:HB2	9:N:318:PRO:O	2.20	0.41
9:N:335:ILE:O	9:N:339:THR:OG1	2.24	0.41
9:N:361:ILE:HA	9:N:512:ASN:HD21	1.85	0.41
10:O:37:ALA:HB3	10:O:73:LEU:HB2	2.02	0.41
9:N:561:LEU:HD22	9:N:568:THR:HA	2.03	0.41
9:N:274:LYS:HB2	9:N:277:GLU:HB3	2.02	0.41
10:O:239:ASN:ND2	10:O:482:ASN:O	2.53	0.41
1:C:52:ILE:O	1:C:57:ARG:NH2	2.54	0.41
8:M:223:GLN:HG3	8:M:224:LEU:H	1.86	0.41
8:M:422:LEU:HD12	8:M:426:PRO:HA	2.03	0.41
9:N:289:LEU:O	9:N:293:VAL:HG23	2.21	0.41
9:N:549:PHE:CZ	9:N:553:ILE:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:455:TYR:CD2	6:H:485:ILE:HG12	2.56	0.41
6:H:502:LEU:HD11	6:H:509:LEU:HD11	2.03	0.41
7:K:493:LYS:HG3	7:K:510:GLU:HG2	2.02	0.41
8:M:451:ASN:O	12:R:184:THR:HG21	2.21	0.41
7:K:461:TYR:HE2	8:M:56:ILE:HG22	1.86	0.41
10:O:449:TYR:HH	12:R:126:GLU:CD	2.24	0.41
10:O:43:ASN:HD21	10:O:46:LYS:HD2	1.86	0.41
11:Q:356:ASP:N	11:Q:374:SER:HA	2.35	0.41
5:G:157:ASN:ND2	13:S:203:PHE:O	2.46	0.41
3:E:373:ARG:HH22	7:I:182:SER:HA	1.86	0.41
9:N:131:ILE:O	9:N:134:LEU:HB3	2.21	0.41
9:N:128:LYS:O	9:N:132:LEU:HG	2.22	0.41
8:M:6:ASN:HA	8:M:7:PRO:HD3	1.86	0.40
9:N:565:PRO:N	9:N:566:PRO:HD2	2.36	0.40
4:F:868:LEU:HD23	4:F:868:LEU:HA	1.94	0.40
6:H:489:ASN:OD1	6:H:489:ASN:N	2.54	0.40
6:H:487:ASN:ND2	6:H:490:GLU:OE2	2.43	0.40
7:J:418:SER:O	7:J:422:ILE:HG23	2.21	0.40
7:L:90:ASP:HB3	7:L:93:LYS:HB2	2.02	0.40
8:M:338:THR:O	8:M:342:LEU:HG	2.21	0.40
8:M:365:ALA:O	8:M:367:THR:HG23	2.21	0.40
11:Q:290:ARG:HG2	11:Q:382:ILE:HG12	2.04	0.40
7:L:149:ASP:N	7:L:149:ASP:OD1	2.54	0.40
4:F:807:GLY:O	7:L:316:SER:HB2	2.21	0.40
8:M:307:LYS:HA	8:M:308:PRO:HD3	1.96	0.40
7:I:259:ILE:HD12	9:N:43:GLN:HG2	2.03	0.40
7:L:312:LYS:N	7:L:345:LYS:HZ2	2.19	0.40
8:M:316:ASP:OD1	8:M:316:ASP:N	2.53	0.40
9:N:135:GLU:HG3	9:N:190:PHE:CD1	2.57	0.40
9:N:223:LEU:HA	9:N:223:LEU:HD23	1.82	0.40
9:N:263:LEU:HD23	9:N:263:LEU:HA	1.88	0.40
10:O:427:LYS:NZ	12:R:131:VAL:O	2.52	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	C	58/78 (74%)	56 (97%)	2 (3%)	0	100	100
2	D	96/180 (53%)	90 (94%)	6 (6%)	0	100	100
3	E	118/435 (27%)	108 (92%)	10 (8%)	0	100	100
4	F	63/889 (7%)	56 (89%)	7 (11%)	0	100	100
5	G	51/885 (6%)	49 (96%)	2 (4%)	0	100	100
6	H	127/625 (20%)	114 (90%)	10 (8%)	3 (2%)	6	29
7	I	289/557 (52%)	274 (95%)	15 (5%)	0	100	100
7	J	113/557 (20%)	109 (96%)	4 (4%)	0	100	100
7	K	105/557 (19%)	101 (96%)	4 (4%)	0	100	100
7	L	292/557 (52%)	278 (95%)	14 (5%)	0	100	100
8	M	302/483 (62%)	281 (93%)	21 (7%)	0	100	100
9	N	408/581 (70%)	380 (93%)	28 (7%)	0	100	100
10	O	376/502 (75%)	352 (94%)	24 (6%)	0	100	100
11	Q	258/426 (61%)	224 (87%)	34 (13%)	0	100	100
12	R	258/1359 (19%)	236 (92%)	22 (8%)	0	100	100
13	S	32/883 (4%)	32 (100%)	0	0	100	100
All	All	2946/9554 (31%)	2740 (93%)	203 (7%)	3 (0%)	56	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	528	ILE
6	H	529	ASN
6	H	527	THR

5.3.2 Protein sidechains ⓘ

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	C	58/75 (77%)	58 (100%)	0	100	100
2	D	82/151 (54%)	82 (100%)	0	100	100
3	E	113/388 (29%)	105 (93%)	8 (7%)	16	48
4	F	60/810 (7%)	60 (100%)	0	100	100
5	G	48/832 (6%)	47 (98%)	1 (2%)	56	81
6	H	126/578 (22%)	124 (98%)	2 (2%)	65	86
7	I	268/500 (54%)	261 (97%)	7 (3%)	49	77
7	J	111/500 (22%)	110 (99%)	1 (1%)	81	91
7	K	106/500 (21%)	106 (100%)	0	100	100
7	L	270/500 (54%)	270 (100%)	0	100	100
8	M	286/435 (66%)	281 (98%)	5 (2%)	63	85
9	N	374/521 (72%)	366 (98%)	8 (2%)	56	81
10	O	358/462 (78%)	354 (99%)	4 (1%)	76	89
11	Q	243/384 (63%)	233 (96%)	10 (4%)	33	68
12	R	240/1228 (20%)	237 (99%)	3 (1%)	71	88
13	S	33/824 (4%)	32 (97%)	1 (3%)	44	74
All	All	2776/8688 (32%)	2726 (98%)	50 (2%)	64	84

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	327	CYS
3	E	351	ASP
3	E	356	ILE
3	E	359	ILE
3	E	384	ILE
3	E	413	VAL
3	E	414	VAL
3	E	417	ASP
5	G	175	ASP
6	H	510	THR
6	H	527	THR
7	I	170	ILE
7	I	224	PHE
7	I	253	GLN
7	I	270	VAL
7	I	275	LEU

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Mol	Chain	Res	Type
7	I	281	ASN
7	I	312	LYS
7	J	459	LEU
8	M	58	LEU
8	M	62	THR
8	M	232	VAL
8	M	241	LEU
8	M	466	ASN
9	N	79	VAL
9	N	91	SER
9	N	104	TYR
9	N	123	LEU
9	N	166	ARG
9	N	170	GLN
9	N	195	PHE
9	N	578	THR
10	O	88	ILE
10	O	208	ILE
10	O	274	TYR
10	O	279	THR
11	Q	192	THR
11	Q	250	LEU
11	Q	262	LEU
11	Q	295	ASN
11	Q	342	ASP
11	Q	345	ASP
11	Q	351	ASP
11	Q	352	HIS
11	Q	368	ASP
11	Q	370	ASP
12	R	215	THR
12	R	265	VAL
12	R	297	VAL
13	S	198	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	64	HIS
2	D	108	HIS
3	E	331	ASN
3	E	432	ASN

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Mol	Chain	Res	Type
5	G	180	HIS
6	H	493	GLN
6	H	506	GLN
6	H	601	HIS
7	I	60	GLN
7	I	63	GLN
7	I	227	ASN
7	I	314	ASN
7	K	426	GLN
7	K	501	GLN
7	L	145	ASN
7	L	291	HIS
7	L	318	GLN
8	M	61	ASN
8	M	233	GLN
8	M	340	ASN
8	M	378	GLN
8	M	380	GLN
9	N	43	GLN
9	N	512	ASN
9	N	559	HIS
9	N	577	ASN
10	O	18	GLN
10	O	22	ASN
10	O	97	HIS
10	O	270	HIS
10	O	484	ASN
11	Q	3	HIS
11	Q	15	ASN
11	Q	158	GLN
11	Q	164	ASN
11	Q	261	GLN
12	R	57	GLN
12	R	72	ASN
12	R	116	ASN
12	R	123	GLN
12	R	270	HIS
12	R	290	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	57:UNK	C	60:UNK	N	4.98