Full wwPDB EM Validation Report ⓘ

Oct 8, 2023 – 12:37 AM JST

PDB ID	:	8KC7
EMDB ID	:	EMD-37096
Title	:	Rpd3S histone deacetylase complex
Authors	:	Dong, S.; Li, H.; Wang, M.; Rasheed, N.; Zou, B.; Gao, X.; Guan, J.; Li, W.; Zhang, J.; Wang, C.; Zhou, N.; Shi, X.; Li, M.; Zhou, M.; Huang, J.; Li, H.; Zhang, Y.; Wong, K.H.; Zhang, X.; Chao, W.C.H.; He, J.
Deposited on	:	2023-08-06
Resolution	:	3.46 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

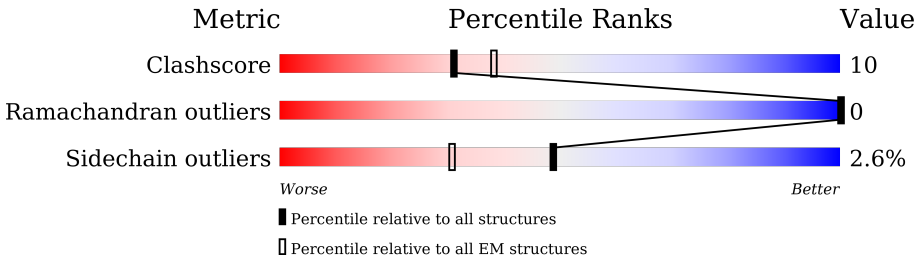
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.46 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	433	75% 18% 6%
2	B	1371	31% 8% • 61%
3	D	401	36% 9% 55%
3	F	401	28% 9% 62%
4	E	733	34% 11% • 54%
4	G	733	14% • 82%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14326 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 deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	406	3216	2040	542	608	26	0	0

- Molecule 2 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	539	4520	2910	759	837	14	0	0

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	166	MET	-	initiating methionine	UNP P22579
B	167	HIS	-	expression tag	UNP P22579
B	168	HIS	-	expression tag	UNP P22579
B	169	HIS	-	expression tag	UNP P22579
B	170	HIS	-	expression tag	UNP P22579
B	171	HIS	-	expression tag	UNP P22579
B	172	HIS	-	expression tag	UNP P22579
B	173	HIS	-	expression tag	UNP P22579
B	174	HIS	-	expression tag	UNP P22579
B	175	PRO	-	expression tag	UNP P22579
B	176	GLN	-	expression tag	UNP P22579
B	177	LEU	-	expression tag	UNP P22579
B	178	ALA	-	expression tag	UNP P22579
B	179	MET	-	expression tag	UNP P22579
B	180	TRP	-	expression tag	UNP P22579
B	181	SER	-	expression tag	UNP P22579
B	182	HIS	-	expression tag	UNP P22579
B	183	PRO	-	expression tag	UNP P22579
B	184	GLN	-	expression tag	UNP P22579
B	185	PHE	-	expression tag	UNP P22579
B	186	GLU	-	expression tag	UNP P22579

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Chain	Residue	Modelled	Actual	Comment	Reference
B	187	LYS	-	expression tag	UNP P22579
B	188	GLY	-	expression tag	UNP P22579
B	189	GLY	-	expression tag	UNP P22579
B	190	GLY	-	expression tag	UNP P22579
B	191	SER	-	expression tag	UNP P22579
B	192	GLY	-	expression tag	UNP P22579
B	193	GLY	-	expression tag	UNP P22579
B	194	GLY	-	expression tag	UNP P22579
B	195	SER	-	expression tag	UNP P22579
B	196	GLY	-	expression tag	UNP P22579
B	197	GLY	-	expression tag	UNP P22579
B	198	GLY	-	expression tag	UNP P22579
B	199	SER	-	expression tag	UNP P22579
B	200	TRP	-	expression tag	UNP P22579
B	201	SER	-	expression tag	UNP P22579
B	202	HIS	-	expression tag	UNP P22579
B	203	PRO	-	expression tag	UNP P22579
B	204	GLN	-	expression tag	UNP P22579
B	205	PHE	-	expression tag	UNP P22579
B	206	GLU	-	expression tag	UNP P22579
B	207	LYS	-	expression tag	UNP P22579
B	208	GLU	-	expression tag	UNP P22579
B	209	ASN	-	expression tag	UNP P22579
B	210	LEU	-	expression tag	UNP P22579
B	211	TYR	-	expression tag	UNP P22579
B	212	PHE	-	expression tag	UNP P22579
B	213	GLN	-	expression tag	UNP P22579
B	214	SER	-	expression tag	UNP P22579

- Molecule 3 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	182	Total	C	N	O	S	0	0
			1474	944	237	284	9		
3	F	152	Total	C	N	O	S	0	0
			1242	803	199	232	8		

- Molecule 4 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	334	Total	C	N	O	S	0	0
			2762	1759	481	505	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	135	Total	C	N	O	S	0	0
			1112	717	184	201	10		

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	685	MET	-	expression tag	UNP Q04779
E	686	HIS	-	expression tag	UNP Q04779
E	687	HIS	-	expression tag	UNP Q04779
E	688	HIS	-	expression tag	UNP Q04779
E	689	HIS	-	expression tag	UNP Q04779
E	690	HIS	-	expression tag	UNP Q04779
E	691	HIS	-	expression tag	UNP Q04779
E	692	HIS	-	expression tag	UNP Q04779
E	693	HIS	-	expression tag	UNP Q04779
E	694	PRO	-	expression tag	UNP Q04779
E	695	GLN	-	expression tag	UNP Q04779
E	696	LEU	-	expression tag	UNP Q04779
E	697	ALA	-	expression tag	UNP Q04779
E	698	MET	-	expression tag	UNP Q04779
E	699	TRP	-	expression tag	UNP Q04779
E	700	SER	-	expression tag	UNP Q04779
E	701	HIS	-	expression tag	UNP Q04779
E	702	PRO	-	expression tag	UNP Q04779
E	703	GLN	-	expression tag	UNP Q04779
E	704	PHE	-	expression tag	UNP Q04779
E	705	GLU	-	expression tag	UNP Q04779
E	706	LYS	-	expression tag	UNP Q04779
E	707	GLY	-	expression tag	UNP Q04779
E	708	GLY	-	expression tag	UNP Q04779
E	709	GLY	-	expression tag	UNP Q04779
E	710	SER	-	expression tag	UNP Q04779
E	711	GLY	-	expression tag	UNP Q04779
E	712	GLY	-	expression tag	UNP Q04779
E	713	GLY	-	expression tag	UNP Q04779
E	714	SER	-	expression tag	UNP Q04779
E	715	GLY	-	expression tag	UNP Q04779
E	716	GLY	-	expression tag	UNP Q04779
E	717	GLY	-	expression tag	UNP Q04779
E	718	SER	-	expression tag	UNP Q04779
E	719	TRP	-	expression tag	UNP Q04779
E	720	SER	-	expression tag	UNP Q04779

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Chain	Residue	Modelled	Actual	Comment	Reference
E	721	HIS	-	expression tag	UNP Q04779
E	722	PRO	-	expression tag	UNP Q04779
E	723	GLN	-	expression tag	UNP Q04779
E	724	PHE	-	expression tag	UNP Q04779
E	725	GLU	-	expression tag	UNP Q04779
E	726	LYS	-	expression tag	UNP Q04779
E	727	GLU	-	expression tag	UNP Q04779
E	728	ASN	-	expression tag	UNP Q04779
E	729	LEU	-	expression tag	UNP Q04779
E	730	TYR	-	expression tag	UNP Q04779
E	731	PHE	-	expression tag	UNP Q04779
E	732	GLN	-	expression tag	UNP Q04779
E	733	SER	-	expression tag	UNP Q04779
G	685	MET	-	expression tag	UNP Q04779
G	686	HIS	-	expression tag	UNP Q04779
G	687	HIS	-	expression tag	UNP Q04779
G	688	HIS	-	expression tag	UNP Q04779
G	689	HIS	-	expression tag	UNP Q04779
G	690	HIS	-	expression tag	UNP Q04779
G	691	HIS	-	expression tag	UNP Q04779
G	692	HIS	-	expression tag	UNP Q04779
G	693	HIS	-	expression tag	UNP Q04779
G	694	PRO	-	expression tag	UNP Q04779
G	695	GLN	-	expression tag	UNP Q04779
G	696	LEU	-	expression tag	UNP Q04779
G	697	ALA	-	expression tag	UNP Q04779
G	698	MET	-	expression tag	UNP Q04779
G	699	TRP	-	expression tag	UNP Q04779
G	700	SER	-	expression tag	UNP Q04779
G	701	HIS	-	expression tag	UNP Q04779
G	702	PRO	-	expression tag	UNP Q04779
G	703	GLN	-	expression tag	UNP Q04779
G	704	PHE	-	expression tag	UNP Q04779
G	705	GLU	-	expression tag	UNP Q04779
G	706	LYS	-	expression tag	UNP Q04779
G	707	GLY	-	expression tag	UNP Q04779
G	708	GLY	-	expression tag	UNP Q04779
G	709	GLY	-	expression tag	UNP Q04779
G	710	SER	-	expression tag	UNP Q04779
G	711	GLY	-	expression tag	UNP Q04779
G	712	GLY	-	expression tag	UNP Q04779
G	713	GLY	-	expression tag	UNP Q04779

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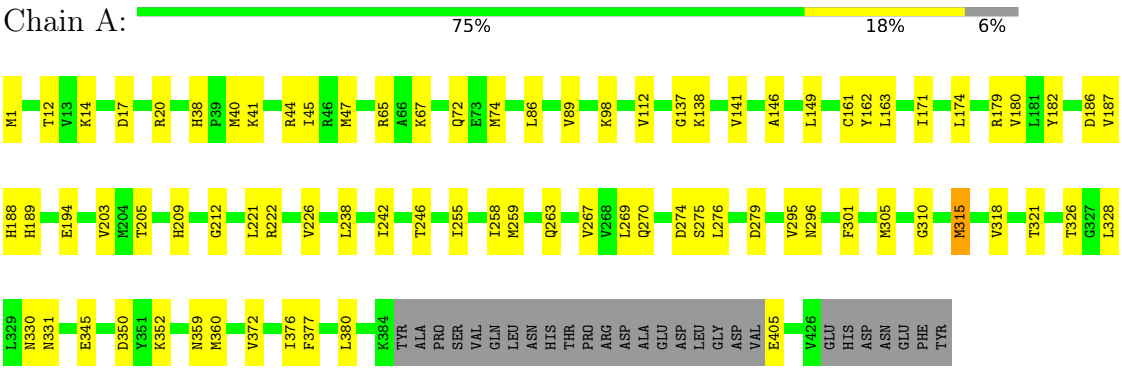
Chain	Residue	Modelled	Actual	Comment	Reference
G	714	SER	-	expression tag	UNP Q04779
G	715	GLY	-	expression tag	UNP Q04779
G	716	GLY	-	expression tag	UNP Q04779
G	717	GLY	-	expression tag	UNP Q04779
G	718	SER	-	expression tag	UNP Q04779
G	719	TRP	-	expression tag	UNP Q04779
G	720	SER	-	expression tag	UNP Q04779
G	721	HIS	-	expression tag	UNP Q04779
G	722	PRO	-	expression tag	UNP Q04779
G	723	GLN	-	expression tag	UNP Q04779
G	724	PHE	-	expression tag	UNP Q04779
G	725	GLU	-	expression tag	UNP Q04779
G	726	LYS	-	expression tag	UNP Q04779
G	727	GLU	-	expression tag	UNP Q04779
G	728	ASN	-	expression tag	UNP Q04779
G	729	LEU	-	expression tag	UNP Q04779
G	730	TYR	-	expression tag	UNP Q04779
G	731	PHE	-	expression tag	UNP Q04779
G	732	GLN	-	expression tag	UNP Q04779
G	733	SER	-	expression tag	UNP Q04779

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.

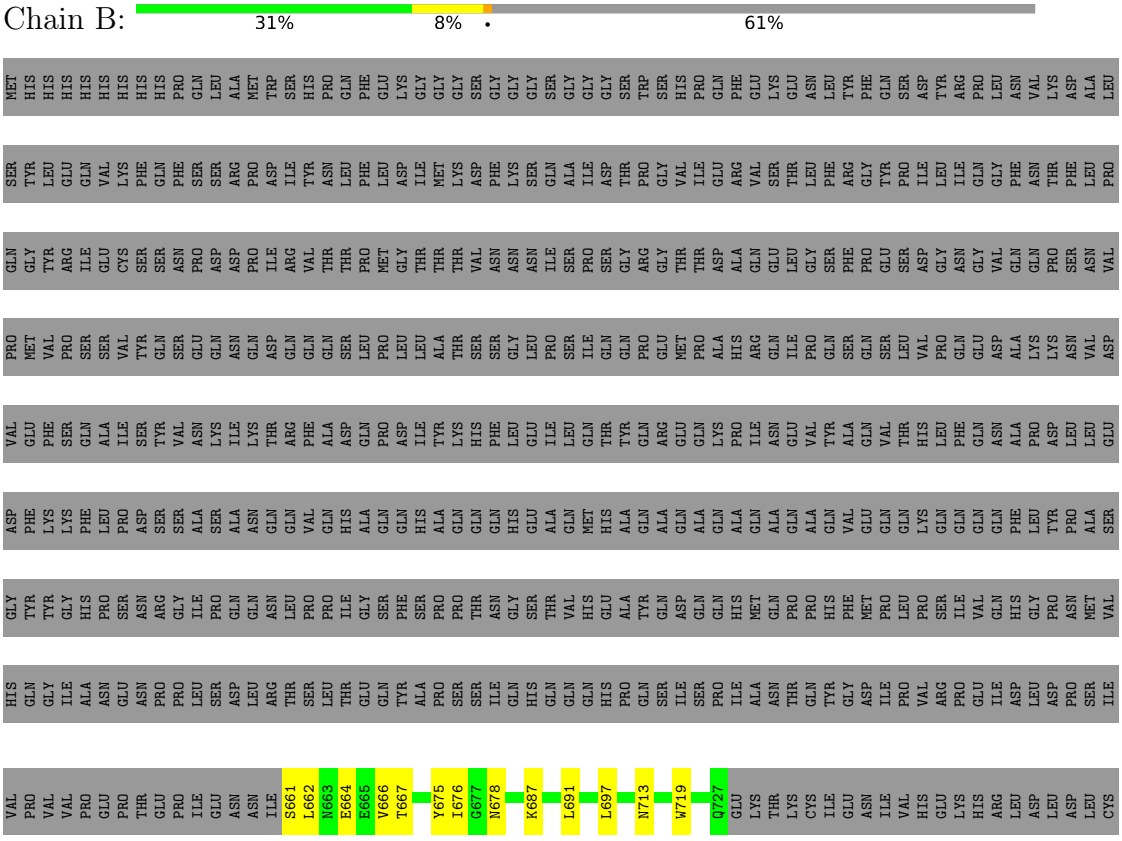
- Molecule 1: Histone deacetylase RPD3

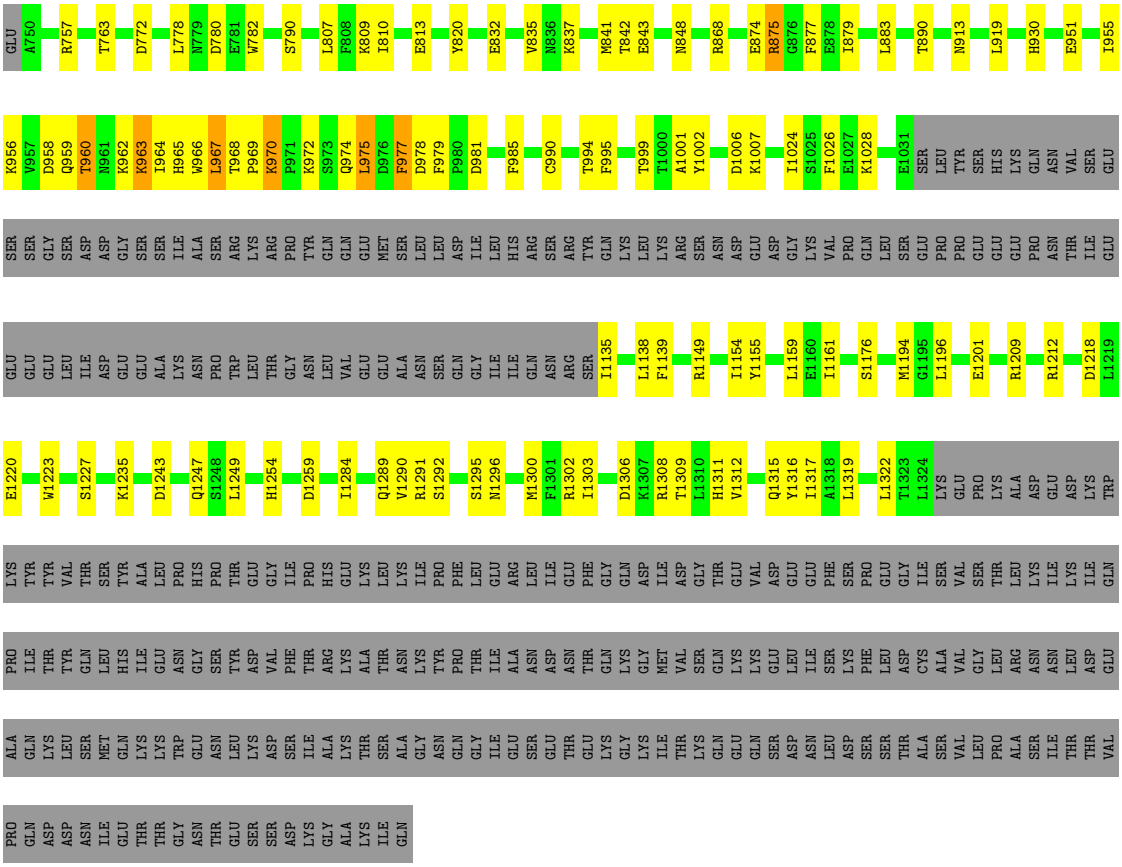
Chain A:



- Molecule 2: Transcriptional regulatory protein SIN3

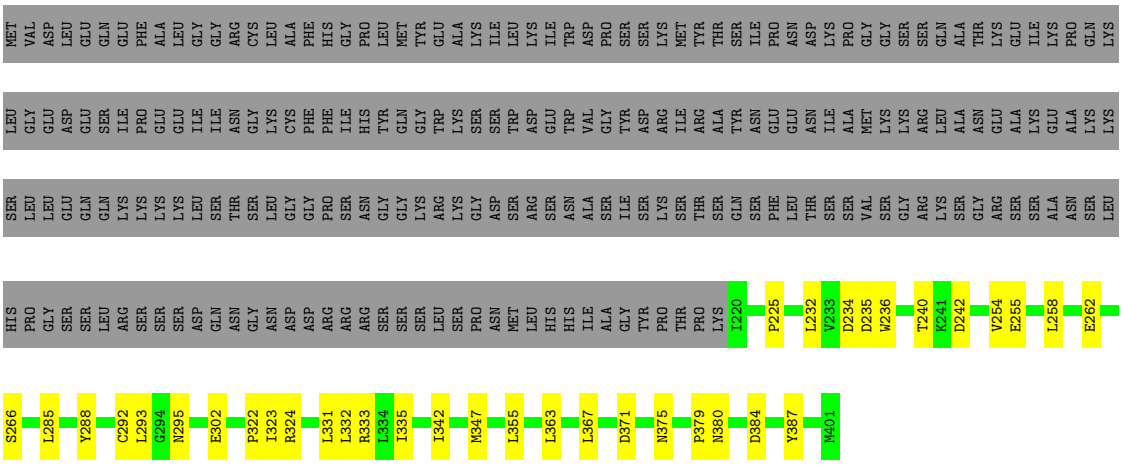
Chain B:





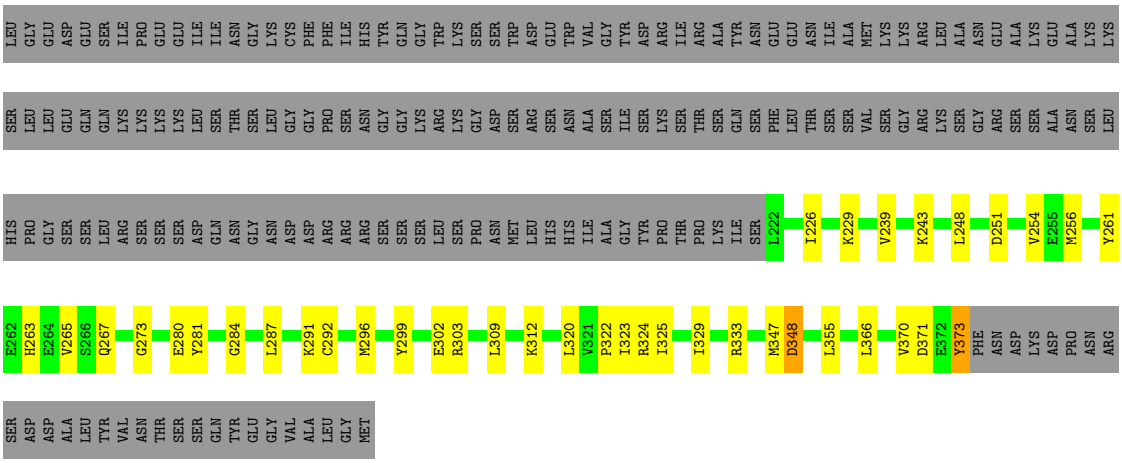
• Molecule 3: Chromatin modification-related protein EAF3

Chain D:



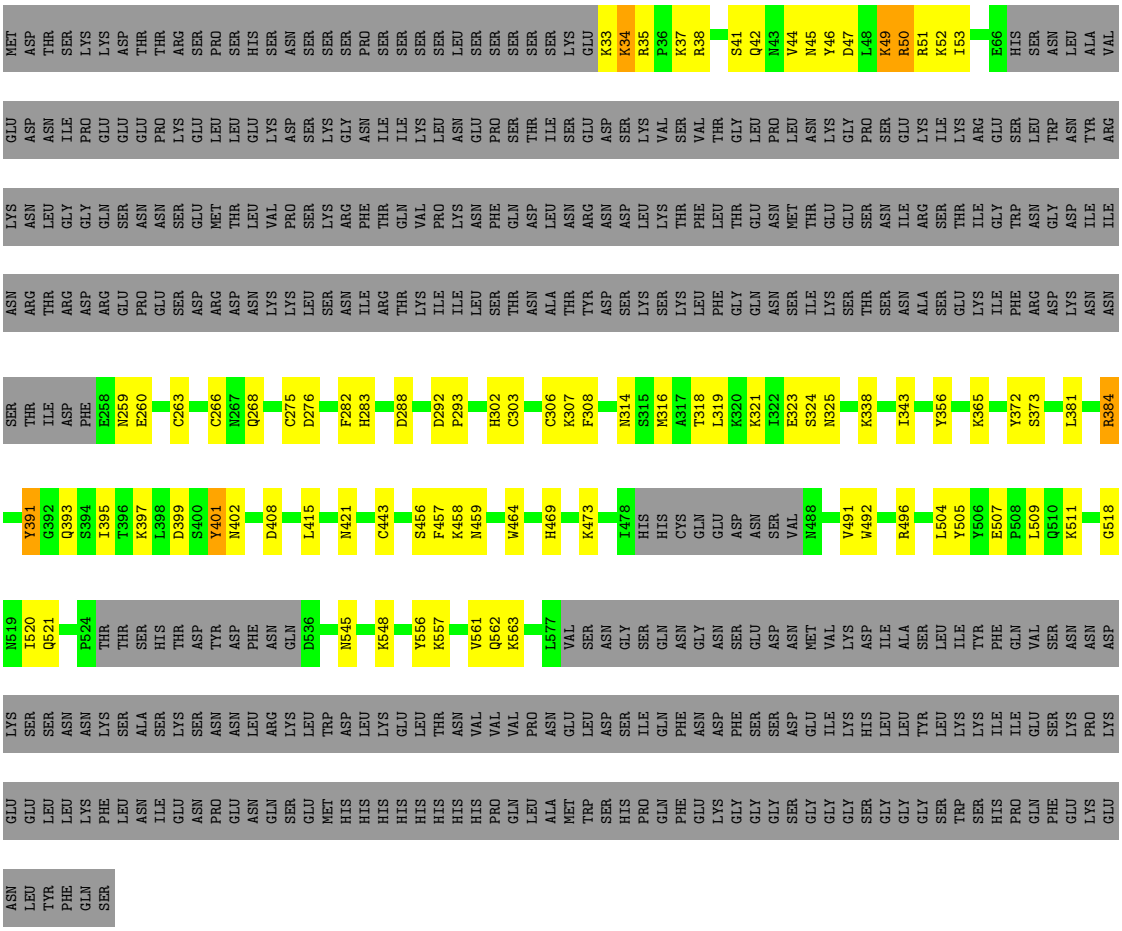
• Molecule 3: Chromatin modification-related protein EAF3

Chain F:



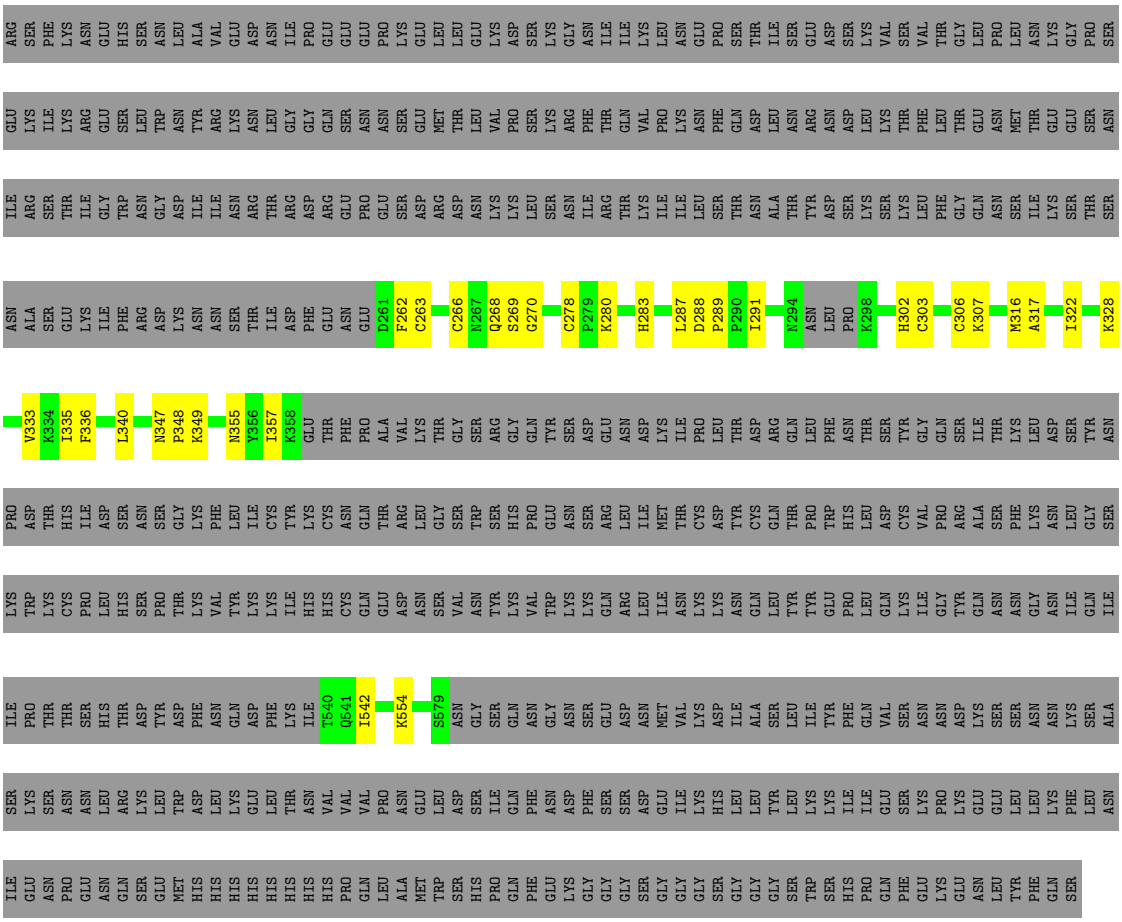
• Molecule 4: Transcriptional regulatory protein RCO1

Chain E:



• Molecule 4: Transcriptional regulatory protein RCO1

Chain G:


ARG SER PHE LYS ASN GLU HIS SER ASN LEU ALA VAL GLU ASP ASN ILE PRO GLU GLU GLU PRO LYS GLU LEU LEU GLU LYS ASP SER LYS GLY ASN ILE ILE LYS LEU ASN GLU PRO SER THR ILE SER GLU ASP SER LYS VAL SER VAL THR GLY LEU PRO LEU ASN LYS GLY PRO SER
GLU LYS ILE LYS ARG GLU SER LEU TRP ASN TYR ARG LYS ASN LEU GLY GLY GLN SER ASN ASN SER GLU MET THR LEU VAL PRO SER LYS ARG PHE THR GLN VAL PRO LYS ASN PHE GLN ASP LEU ASN ARG ASP LEU LYS THR PHE LEU THR GLU GLN ASN MET THR GLU GLU SER ASN
ILE ARG SER THR ILE GLY TRP ASN GLY ASP ILE ILE ASN ARG THR ARG ASP ARG GLU PRO GLU SER ASP ARG ASP ASN LYS LYS LEU SER ASN ILE ILE LEU SER THR ASN ALA THR TYR ASP SER LYS SER LYS LEU PHE GLY GLN ASN SER ILE LYS SER THR SER
ASN ALA SER GLU LYS ILE PHE ARG ASP LYS ASP PHE GLU ASN GLU D261 F262 C263 C266 N267 Q268 S269 G270 C278 P279 K280 H283 L287 D288 P289 P290 I291 N294 ASN LEU PRO K298 H302 C303 C306 K307 M316 A317 I322 K328
V333 K334 I335 F336 L340 N347 P348 K349 N355 Y356 I357 K358 GLU THR PHE PRO ALA VAL LYS THR GLY SER ARG GLY GLN TYR SER ASP GLU ASN ASP LYS ILE PRO LEU THR ASP ARG GLN LEU PHE ASN THR SER TYR GLY GLN SER ILE THR LYS LEU ASP SER TYR ASN
PRO ASP THR HIS ILE ASP SER ASN SER GLY LYS PHE LEU ILE CYS TYR LYS CYS ASN GLN THR ARG LEU GLY SER TRP SER HIS PRO GLU ASN SER ARG LEU ILE MET THR CYS ASP TYR CYS GLN THR PRO TRP HIS LEU ASP CYS VAL PRO ARG GLU SER PHE LYS ASN LEU LEU GLY SER
LYS TRP LYS CYS PRO LEU HIS SER PRO THR LYS VAL TYR LYS LYS ILE HIS HIS CYS GLN GLU GLU ASP SER VAL ASN TYR LYS VAL TRP LYS LYS GLN ARG LEU ILE ASN LYS LYS ASN GLN LEU TYR TYR GLU PRO LEU GLN LYS ILE GLY TYR GLN ASN ASN GLY ASN ILE GLN ILE
ILE PRO THR THR SER HIS THR ASP TYR ASP PHE ASN GLN ASP PHE LYS ILE T540 Q541 I542 K554 S579 ASN GLY SER GLN ASN GLY ASN SER GLU ASP ASN MET VAL LYS ASP ILE ALA SER LEU ILE TYR PHE GLN VAL SER ASN ASN ASP LYS SER SER ASN ASN LYS SER ALA
SER LYS SER ASN ASN LEU ARG LYS LEU TRP ASP LEU LYS GLU LEU THR ASN VAL VAL VAL PRO ASN GLU GLU LEU ASP SER ILE GLN PHE ASN ASP PHE SER SER ASP GLU ILE LYS HIS LEU LEU TYR LEU LYS LYS ILE ILE GLU SER LYS PRO LYS GLU GLU LEU LEU LYS PHE LEU ASN
ILE GLU ASN PRO GLU ASN GLN SER GLU MET HIS HIS HIS HIS HIS HIS HIS PRO GLN LEU ALA MET TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY GLY SER GLY GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS GLU GLU ASN LEU TYR PHE GLN SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/3296	0.50	0/4456
2	B	0.25	0/4622	0.47	0/6232
3	D	0.24	0/1500	0.47	0/2028
3	F	0.24	0/1264	0.50	0/1709
4	E	0.26	0/2827	0.55	1/3801 (0.0%)
4	G	0.26	0/1137	0.49	0/1523
All	All	0.25	0/14646	0.50	1/19749 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	47	ASP	CB-CG-OD2	5.17	122.95	118.30

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	A	3216	0	3082	54	0
2	B	4520	0	4488	80	0
3	D	1474	0	1497	23	0
3	F	1242	0	1286	27	0
4	E	2762	0	2748	95	0
4	G	1112	0	1100	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14326	0	14201	276	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (276) 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)
4:G:263:CYS:SG	4:G:266:CYS:HB2	1.65	1.35
4:E:263:CYS:SG	4:E:283:HIS:CD2	2.22	1.33
4:E:42:GLN:HB3	4:E:46:TYR:CE1	1.82	1.15
4:E:263:CYS:SG	4:E:283:HIS:NE2	2.21	1.11
4:E:263:CYS:SG	4:E:283:HIS:CE1	2.43	1.11
4:E:263:CYS:SG	4:E:283:HIS:CG	2.44	1.11
4:E:42:GLN:HB2	4:E:46:TYR:CE2	1.87	1.10
4:E:42:GLN:CB	4:E:46:TYR:CZ	2.42	1.03
4:E:42:GLN:HB3	4:E:46:TYR:CD1	1.97	1.00
4:E:42:GLN:HG2	4:E:46:TYR:CZ	1.96	1.00
4:E:42:GLN:HB2	4:E:46:TYR:CD2	1.98	0.99
4:E:42:GLN:CG	4:E:46:TYR:CZ	2.47	0.97
4:G:263:CYS:SG	4:G:266:CYS:CB	2.54	0.95
4:G:303:CYS:HB2	4:G:306:CYS:SG	2.08	0.94
4:E:42:GLN:CB	4:E:46:TYR:CE2	2.53	0.92
4:E:303:CYS:HB2	4:E:306:CYS:SG	2.12	0.90
4:E:42:GLN:HG2	4:E:46:TYR:OH	1.73	0.88
2:B:959:GLN:HB2	2:B:970:LYS:HE3	1.62	0.81
2:B:883:LEU:HD23	2:B:890:THR:OG1	1.81	0.81
4:E:42:GLN:CB	4:E:46:TYR:CE1	2.56	0.80
3:D:288:TYR:O	3:D:292:CYS:HB2	1.79	0.80
4:E:263:CYS:SG	4:E:283:HIS:ND1	2.55	0.78
2:B:972:LYS:HB3	2:B:975:LEU:HD23	1.66	0.78
2:B:1302:ARG:HB3	2:B:1315:GLN:HB3	1.69	0.73
1:A:186:ASP:HA	1:A:275:SER:HB3	1.73	0.71
2:B:1138:LEU:HB3	2:B:1303:ILE:HB	1.76	0.67
4:E:42:GLN:CB	4:E:46:TYR:CD2	2.76	0.67
1:A:270:GLN:HE22	1:A:310:GLY:HA3	1.60	0.66
1:A:38:HIS:O	1:A:41:LYS:NZ	2.23	0.65
2:B:956:LYS:NZ	2:B:1316:TYR:O	2.29	0.64
4:E:46:TYR:H	4:E:51:ARG:HH12	1.45	0.64
3:D:347:MET:HG3	4:E:338:LYS:HD2	1.80	0.64
4:E:263:CYS:HB2	4:E:266:CYS:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:O	1:A:331:ASN:ND2	2.31	0.62
2:B:965:HIS:HB2	2:B:969:PRO:HG3	1.83	0.61
2:B:1291:ARG:HE	2:B:1322:LEU:HD13	1.65	0.61
4:E:42:GLN:CB	4:E:46:TYR:CD1	2.79	0.61
4:E:391:TYR:HD1	4:E:393:GLN:H	1.48	0.61
4:G:302:HIS:O	4:G:307:LYS:HE3	2.01	0.61
3:D:254:VAL:HG13	3:D:331:LEU:HD22	1.83	0.60
4:E:42:GLN:OE1	4:E:46:TYR:CE2	2.55	0.59
3:F:371:ASP:N	3:F:371:ASP:OD2	2.36	0.59
1:A:44:ARG:NH2	1:A:310:GLY:O	2.35	0.59
4:G:263:CYS:HB2	4:G:266:CYS:SG	2.43	0.59
4:E:399:ASP:OD1	4:E:402:ASN:ND2	2.31	0.58
2:B:813:GLU:HA	4:E:49:LYS:HE2	1.86	0.58
2:B:820:TYR:CE2	4:E:50:ARG:HG2	2.38	0.58
1:A:186:ASP:HB2	1:A:274:ASP:HB2	1.85	0.58
1:A:221:LEU:HD11	1:A:372:VAL:HG22	1.87	0.57
4:E:266:CYS:SG	4:E:283:HIS:ND1	2.77	0.57
1:A:171:ILE:HD11	2:B:778:LEU:HD11	1.86	0.57
2:B:1291:ARG:NH1	2:B:1295:SER:O	2.37	0.57
3:D:235:ASP:OD1	3:D:387:TYR:OH	2.23	0.56
4:E:266:CYS:HG	4:E:283:HIS:HD1	1.53	0.56
2:B:1284:ILE:HD12	2:B:1284:ILE:H	1.70	0.56
1:A:350:ASP:OD1	1:A:350:ASP:N	2.39	0.56
4:E:44:VAL:HG13	4:E:45:ASN:H	1.71	0.56
2:B:883:LEU:CD2	2:B:890:THR:OG1	2.53	0.56
4:E:318:THR:HG22	4:E:319:LEU:H	1.71	0.56
1:A:194:GLU:HA	1:A:205:THR:HG21	1.88	0.56
4:E:505:TYR:CE2	4:E:507:GLU:HB3	2.40	0.56
4:E:35:ARG:HE	4:E:38:ARG:NH2	2.04	0.55
4:E:42:GLN:CB	4:E:46:TYR:CG	2.90	0.55
4:E:511:LYS:NZ	3:F:280:GLU:OE1	2.40	0.55
3:D:225:PRO:HB3	3:D:367:LEU:HD22	1.88	0.55
2:B:772:ASP:OD1	2:B:772:ASP:N	2.39	0.55
2:B:675:TYR:CZ	2:B:962:LYS:HD3	2.42	0.55
4:E:381:LEU:HB3	4:E:384:ARG:HB2	1.87	0.55
3:F:281:TYR:HA	4:G:335:ILE:HG21	1.87	0.55
4:G:303:CYS:O	4:G:307:LYS:HG3	2.06	0.55
2:B:981:ASP:N	2:B:1155:TYR:OH	2.40	0.54
4:G:263:CYS:SG	4:G:268:GLN:O	2.65	0.54
1:A:345:GLU:OE1	2:B:913:ASN:ND2	2.37	0.54
3:F:329:ILE:HG13	3:F:333:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:977:PHE:HZ	2:B:1149:ARG:HD2	1.71	0.54
2:B:960:THR:HG23	2:B:970:LYS:HE2	1.90	0.54
2:B:1135:ILE:HA	2:B:1306:ASP:HA	1.89	0.54
2:B:974:GLN:C	2:B:975:LEU:HG	2.28	0.53
4:E:321:LYS:O	4:E:325:ASN:ND2	2.41	0.53
1:A:187:VAL:HG22	1:A:274:ASP:HB3	1.91	0.53
4:G:288:ASP:HB3	4:G:348:PRO:HD2	1.90	0.53
1:A:98:LYS:HE3	4:E:293:PRO:HB2	1.90	0.53
4:E:46:TYR:N	4:E:51:ARG:HH12	2.06	0.53
4:E:443:CYS:SG	4:E:469:HIS:NE2	2.79	0.53
4:G:317:ALA:HB1	4:G:322:ILE:HD11	1.91	0.53
4:E:456:SER:OG	4:E:457:PHE:N	2.41	0.53
3:F:320:LEU:HD11	3:F:325:ILE:HD13	1.91	0.52
4:G:262:PHE:HA	4:G:269:SER:HA	1.91	0.52
4:E:282:PHE:HE2	4:E:303:CYS:SG	2.32	0.52
2:B:979:PHE:HD2	2:B:985:PHE:HE1	1.58	0.52
1:A:179:ARG:NH1	1:A:263:GLN:O	2.43	0.52
4:E:263:CYS:HB3	4:E:266:CYS:SG	2.50	0.52
4:E:372:TYR:OH	4:E:496:ARG:NH2	2.43	0.52
3:F:299:TYR:HB2	3:F:302:GLU:HG2	1.92	0.52
2:B:675:TYR:CE1	2:B:962:LYS:HD3	2.45	0.52
1:A:221:LEU:HD21	1:A:372:VAL:HG13	1.92	0.51
1:A:238:LEU:HD13	1:A:242:ILE:HD13	1.91	0.51
2:B:842:THR:OG1	2:B:843:GLU:N	2.43	0.51
3:F:254:VAL:HB	3:F:323:ILE:HG23	1.92	0.51
2:B:995:PHE:O	2:B:999:THR:OG1	2.23	0.51
1:A:360:MET:HB3	2:B:930:HIS:HB2	1.91	0.51
3:D:302:GLU:OE2	3:D:333:ARG:NH1	2.41	0.51
2:B:1243:ASP:N	2:B:1243:ASP:OD1	2.43	0.51
3:F:248:LEU:HB3	3:F:309:LEU:HD21	1.93	0.50
2:B:964:ILE:HB	2:B:966:TRP:NE1	2.26	0.50
4:E:45:ASN:OD1	4:E:51:ARG:HB3	2.11	0.50
4:E:45:ASN:OD1	4:E:53:ILE:HG22	2.11	0.50
2:B:1154:ILE:HD12	2:B:1249:LEU:HD13	1.92	0.50
3:F:309:LEU:HD22	3:F:312:LYS:HZ3	1.75	0.50
3:D:293:LEU:HD13	3:D:322:PRO:HB2	1.92	0.50
3:F:303:ARG:NH1	4:G:287:LEU:O	2.40	0.50
3:F:263:HIS:O	3:F:267:GLN:NE2	2.45	0.50
1:A:352:LYS:NZ	2:B:1176:SER:O	2.39	0.50
1:A:326:THR:O	1:A:330:ASN:ND2	2.45	0.50
2:B:832:GLU:HA	2:B:835:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:239:VAL:HA	3:F:243:LYS:HA	1.94	0.49
3:F:322:PRO:HA	3:F:325:ILE:HG12	1.94	0.49
2:B:1002:TYR:O	2:B:1007:LYS:NZ	2.44	0.49
1:A:20:ARG:NE	1:A:138:LYS:O	2.45	0.49
4:E:408:ASP:HB3	4:E:415:LEU:HD21	1.94	0.49
2:B:675:TYR:CZ	2:B:713:ASN:HB2	2.47	0.49
2:B:963:LYS:HG2	4:E:421:ASN:HB2	1.94	0.49
3:F:261:TYR:O	3:F:265:VAL:HG12	2.13	0.49
2:B:1201:GLU:OE1	2:B:1209:ARG:NH2	2.46	0.49
4:E:46:TYR:HB2	4:E:51:ARG:HH12	1.77	0.49
3:D:232:LEU:HD21	3:D:332:LEU:HB3	1.95	0.48
1:A:279:ASP:OD1	1:A:279:ASP:N	2.46	0.48
2:B:978:ASP:HB2	2:B:1311:HIS:ND1	2.27	0.48
2:B:874:GLU:HG2	2:B:875:ARG:HG2	1.94	0.48
4:E:42:GLN:CG	4:E:46:TYR:CE2	2.93	0.48
4:G:303:CYS:O	4:G:307:LYS:N	2.43	0.48
2:B:1024:ILE:HG22	2:B:1026:PHE:H	1.78	0.48
3:F:226:ILE:HG23	3:F:229:LYS:HG3	1.95	0.48
1:A:296:ASN:HB2	1:A:328:LEU:HD13	1.96	0.48
1:A:149:LEU:HB3	1:A:161:CYS:HB3	1.96	0.48
1:A:276:LEU:HD21	1:A:321:THR:HG21	1.96	0.48
2:B:757:ARG:NH1	3:D:379:PRO:O	2.46	0.47
4:E:33:LYS:N	4:E:34:LYS:HZ3	2.13	0.47
2:B:1291:ARG:NH2	2:B:1296:ASN:OD1	2.46	0.47
3:F:347:MET:CE	3:F:355:LEU:HD12	2.44	0.47
2:B:990:CYS:SG	2:B:1212:ARG:NH2	2.87	0.47
1:A:189:HIS:HB2	1:A:209:HIS:CG	2.50	0.47
2:B:879:ILE:O	2:B:883:LEU:HG	2.15	0.47
1:A:72:GLN:HB3	1:A:405:GLU:HA	1.97	0.47
2:B:837:LYS:HE3	2:B:837:LYS:HB3	1.78	0.47
4:E:35:ARG:HE	4:E:38:ARG:HH22	1.62	0.47
3:D:236:TRP:O	3:D:240:THR:OG1	2.33	0.47
4:E:302:HIS:HB3	4:E:306:CYS:HB2	1.95	0.47
3:F:287:LEU:HD12	4:G:333:VAL:HG21	1.97	0.46
2:B:820:TYR:HE2	4:E:50:ARG:HG2	1.80	0.46
2:B:1259:ASP:OD1	2:B:1259:ASP:N	2.47	0.46
4:G:263:CYS:SG	4:G:266:CYS:SG	3.13	0.46
1:A:226:VAL:HG21	2:B:782:TRP:CD2	2.51	0.46
4:E:303:CYS:O	4:E:307:LYS:N	2.49	0.46
1:A:359:ASN:HD21	2:B:1235:LYS:HD3	1.81	0.46
2:B:661:SER:OG	2:B:662:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:262:GLU:O	3:D:266:SER:HB2	2.16	0.46
4:E:321:LYS:HD2	4:E:323:GLU:HB3	1.98	0.46
4:E:42:GLN:HG2	4:E:46:TYR:CE1	2.49	0.46
4:E:509:LEU:HG	3:F:348:ASP:HB3	1.97	0.46
4:E:562:GLN:HE22	4:E:563:LYS:HD2	1.81	0.46
4:E:263:CYS:CB	4:E:266:CYS:SG	3.03	0.46
4:G:347:ASN:O	4:G:349:LYS:NZ	2.39	0.46
4:G:278:CYS:O	4:G:280:LYS:NZ	2.46	0.46
1:A:180:VAL:HB	1:A:203:VAL:HG22	1.97	0.45
1:A:212:GLY:HA3	4:E:456:SER:HB3	1.96	0.45
2:B:809:LYS:O	2:B:813:GLU:HG3	2.16	0.45
1:A:45:ILE:HD13	1:A:146:ALA:HA	1.99	0.45
1:A:89:VAL:HG22	1:A:112:VAL:HG11	1.97	0.45
2:B:676:ILE:HG22	2:B:678:ASN:H	1.81	0.45
2:B:1006:ASP:OD2	2:B:1254:HIS:NE2	2.50	0.45
2:B:967:LEU:O	2:B:968:THR:C	2.54	0.45
4:E:545:ASN:HA	4:E:548:LYS:HG2	1.98	0.45
2:B:868:ARG:HD3	2:B:877:PHE:HE2	1.81	0.45
4:E:282:PHE:HE2	4:E:303:CYS:HG	1.60	0.45
2:B:810:ILE:HD11	2:B:919:LEU:HD23	1.98	0.45
3:D:288:TYR:O	3:D:292:CYS:CB	2.56	0.45
4:E:473:LYS:HE3	4:E:491:VAL:HG13	1.99	0.45
2:B:691:LEU:HD12	2:B:697:LEU:HB2	1.99	0.44
2:B:1196:LEU:HD23	2:B:1227:SER:HB3	1.99	0.44
2:B:1309:THR:HG23	2:B:1311:HIS:HB2	1.98	0.44
3:D:323:ILE:H	3:D:323:ILE:HG13	1.64	0.44
2:B:1220:GLU:HG3	2:B:1223:TRP:H	1.83	0.44
4:E:557:LYS:O	4:E:561:VAL:HG12	2.17	0.44
4:G:542:ILE:HD12	4:G:542:ILE:HA	1.90	0.44
2:B:807:LEU:HD23	2:B:807:LEU:HA	1.89	0.44
2:B:1300:MET:HB3	2:B:1317:ILE:HB	1.98	0.44
3:D:234:ASP:OD1	4:E:496:ARG:NH1	2.50	0.44
2:B:1161:ILE:HD13	2:B:1161:ILE:HA	1.84	0.44
4:G:554:LYS:HA	4:G:554:LYS:HD3	1.79	0.44
3:D:335:ILE:HG21	3:D:363:LEU:HD21	2.00	0.44
4:E:492:TRP:HZ2	4:E:518:GLY:HA3	1.82	0.44
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.89	0.44
2:B:964:ILE:H	2:B:964:ILE:HG12	1.63	0.43
4:G:263:CYS:CB	4:G:266:CYS:SG	3.06	0.43
1:A:269:LEU:HD21	1:A:295:VAL:HG22	2.00	0.43
2:B:1317:ILE:HG22	2:B:1319:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:342:ILE:HD11	3:D:355:LEU:HD23	2.01	0.43
4:E:268:GLN:HB2	4:E:283:HIS:HE1	1.82	0.43
3:D:371:ASP:OD1	3:D:371:ASP:N	2.49	0.43
4:E:504:LEU:O	4:E:505:TYR:HB3	2.19	0.43
4:E:458:LYS:HB3	4:E:464:TRP:HB2	2.00	0.43
4:G:270:GLY:HA3	4:G:283:HIS:NE2	2.34	0.43
4:E:308:PHE:O	4:E:314:ASN:HB2	2.19	0.43
2:B:1139:PHE:HB3	2:B:1290:VAL:HG21	2.01	0.43
3:D:258:LEU:HD21	3:D:285:LEU:HD23	2.01	0.43
4:E:263:CYS:HB2	4:E:266:CYS:CB	2.49	0.43
1:A:12:THR:O	1:A:296:ASN:ND2	2.43	0.43
1:A:242:ILE:HG13	1:A:246:THR:HB	2.00	0.43
3:D:255:GLU:OE1	3:D:324:ARG:NE	2.44	0.43
1:A:267:VAL:HB	1:A:305:MET:HB2	2.01	0.42
2:B:981:ASP:HB2	2:B:1159:LEU:HD13	2.01	0.42
4:E:49:LYS:HD2	4:E:49:LYS:HA	1.73	0.42
4:E:259:ASN:ND2	4:E:260:GLU:O	2.52	0.42
1:A:259:MET:HE1	1:A:301:PHE:CD2	2.54	0.42
2:B:790:SER:OG	2:B:790:SER:O	2.36	0.42
2:B:1220:GLU:HB3	2:B:1223:TRP:HD1	1.84	0.42
4:E:397:LYS:HA	4:E:397:LYS:HD3	1.87	0.42
3:F:370:VAL:HA	3:F:373:TYR:HB2	2.01	0.42
4:E:46:TYR:HB2	4:E:51:ARG:NH1	2.34	0.42
4:G:289:PRO:HB2	4:G:291:ILE:HG23	2.01	0.42
3:D:384:ASP:OD1	3:D:384:ASP:N	2.43	0.42
1:A:377:PHE:HA	1:A:380:LEU:HB2	2.02	0.42
4:E:37:LYS:H	4:E:37:LYS:HD2	1.85	0.42
3:F:355:LEU:HD23	3:F:355:LEU:HA	1.93	0.42
2:B:757:ARG:HB3	3:D:380:ASN:HA	2.02	0.42
2:B:763:THR:HG23	2:B:780:ASP:HB2	2.02	0.42
4:E:391:TYR:N	4:E:401:TYR:OH	2.53	0.42
4:E:509:LEU:CD1	3:F:348:ASP:HB3	2.50	0.42
1:A:20:ARG:NH2	1:A:137:GLY:O	2.53	0.42
1:A:376:ILE:HD13	1:A:376:ILE:HA	1.94	0.42
3:D:295:ASN:HD22	4:E:343:ILE:HG13	1.85	0.42
1:A:141:VAL:HG22	1:A:305:MET:HG2	2.01	0.42
1:A:179:ARG:HH12	1:A:263:GLN:HB2	1.85	0.42
2:B:666:VAL:HG23	2:B:667:THR:HG23	2.01	0.41
4:E:321:LYS:HG3	4:E:324:SER:H	1.85	0.41
3:F:291:LYS:HD3	4:G:340:LEU:HD22	2.02	0.41
1:A:47:MET:H	1:A:47:MET:HG2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:556:TYR:HD2	3:F:273:GLY:HA2	1.86	0.41
4:E:562:GLN:NE2	4:E:563:LYS:HD2	2.35	0.41
1:A:255:ILE:HD13	1:A:255:ILE:HA	1.88	0.41
1:A:149:LEU:HD13	1:A:162:TYR:H	1.85	0.41
4:E:276:ASP:OD1	4:E:276:ASP:N	2.49	0.41
3:F:229:LYS:HD2	4:G:357:ILE:HG12	2.03	0.41
1:A:315:MET:HA	1:A:318:VAL:HG12	2.01	0.41
4:E:365:LYS:N	4:E:373:SER:O	2.54	0.41
4:E:393:GLN:HB3	4:E:459:ASN:ND2	2.36	0.41
4:E:509:LEU:CG	3:F:348:ASP:HB3	2.51	0.41
2:B:951:GLU:O	2:B:955:ILE:HG22	2.21	0.41
2:B:977:PHE:HB3	2:B:1312:VAL:O	2.21	0.41
2:B:1289:GLN:O	2:B:1292:SER:OG	2.34	0.41
3:F:284:GLY:HA2	4:G:333:VAL:HG13	2.03	0.41
1:A:67:LYS:HE3	1:A:67:LYS:HB3	1.89	0.41
1:A:74:MET:HB2	1:A:163:LEU:HD11	2.02	0.41
1:A:187:VAL:HG23	1:A:188:HIS:CD2	2.56	0.41
2:B:999:THR:HG22	2:B:1001:ALA:H	1.86	0.41
4:E:51:ARG:HG2	4:E:52:LYS:H	1.86	0.41
2:B:664:GLU:OE1	2:B:719:TRP:NE1	2.54	0.41
2:B:1291:ARG:HD2	2:B:1291:ARG:HA	1.91	0.41
1:A:174:LEU:HD21	1:A:203:VAL:HG23	2.02	0.40
4:E:49:LYS:HB3	4:E:50:ARG:H	1.64	0.40
4:E:275:CYS:SG	4:E:276:ASP:N	2.93	0.40
4:G:355:ASN:OD1	4:G:355:ASN:N	2.51	0.40
4:E:51:ARG:HG2	4:E:52:LYS:N	2.36	0.40
1:A:182:TYR:HD2	1:A:205:THR:HB	1.86	0.40
1:A:258:ILE:HG13	1:A:380:LEU:HD11	2.03	0.40
2:B:687:LYS:HA	4:E:520:ILE:HD11	2.04	0.40
2:B:1194:MET:HG3	2:B:1196:LEU:HD13	2.04	0.40
4:E:42:GLN:CG	4:E:46:TYR:OH	2.53	0.40
4:E:292:ASP:OD1	4:E:292:ASP:N	2.54	0.40
2:B:994:THR:HG21	2:B:1212:ARG:HG3	2.04	0.40
4:E:395:ILE:HG23	4:E:401:TYR:HD2	1.85	0.40
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.89	0.40
3:D:375:ASN:OD1	3:D:375:ASN:N	2.54	0.40
4:E:44:VAL:HG13	4:E:45:ASN:N	2.35	0.40
3:F:366:LEU:HD23	3:F:366:LEU:HA	1.94	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	402/433 (93%)	381 (95%)	21 (5%)	0	100	100
2	B	533/1371 (39%)	505 (95%)	28 (5%)	0	100	100
3	D	180/401 (45%)	174 (97%)	6 (3%)	0	100	100
3	F	150/401 (37%)	140 (93%)	10 (7%)	0	100	100
4	E	326/733 (44%)	286 (88%)	40 (12%)	0	100	100
4	G	129/733 (18%)	121 (94%)	8 (6%)	0	100	100
All	All	1720/4072 (42%)	1607 (93%)	113 (7%)	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	343/367 (94%)	337 (98%)	6 (2%)	60	82
2	B	501/1247 (40%)	487 (97%)	14 (3%)	43	72
3	D	171/359 (48%)	170 (99%)	1 (1%)	86	95
3	F	145/359 (40%)	138 (95%)	7 (5%)	25	58
4	E	318/692 (46%)	307 (96%)	11 (4%)	36	67
4	G	130/692 (19%)	127 (98%)	3 (2%)	50	76
All	All	1608/3716 (43%)	1566 (97%)	42 (3%)	49	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	LYS
1	A	40	MET
1	A	65	ARG
1	A	222	ARG
1	A	315	MET
2	B	841	MET
2	B	848	ASN
2	B	875	ARG
2	B	958	ASP
2	B	960	THR
2	B	963	LYS
2	B	967	LEU
2	B	970	LYS
2	B	975	LEU
2	B	977	PHE
2	B	1028	LYS
2	B	1218	ASP
2	B	1247	GLN
2	B	1308	ARG
3	D	242	ASP
4	E	34	LYS
4	E	41	SER
4	E	49	LYS
4	E	50	ARG
4	E	288	ASP
4	E	316	MET
4	E	356	TYR
4	E	384	ARG
4	E	391	TYR
4	E	401	TYR
4	E	521	GLN
3	F	251	ASP
3	F	256	MET
3	F	292	CYS
3	F	296	MET
3	F	324	ARG
3	F	348	ASP
3	F	373	TYR
4	G	316	MET
4	G	328	LYS
4	G	336	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
2	B	961	ASN
4	G	313	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.