



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 10, 2019 – 05:27 PM EST

PDB ID : 6C23
EMDB ID: : EMD-7334
Title : Cryo-EM structure of PRC2 bound to cofactors AEBP2 and JARID2 in the Compact Active State
Authors : Kasinath, V.; Faini, M.; Poepsel, S.; Reif, D.; Feng, A.; Stjepanovic, G.; Aebersold, R.; Nogales, E.
Deposited on : 2018-01-05
Resolution : 3.90 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.

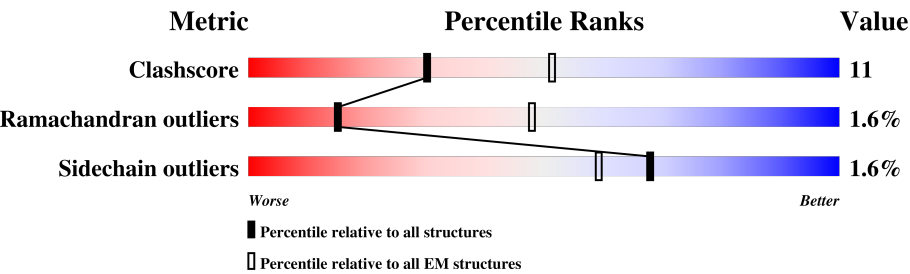
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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	A	739	14% .. 83%
1	M	739	14% . 83%
1	Q	739	7% . 91%
2	E	348	6% .. 92%
3	C	746	22% . 74%
3	K	746	36% 8% 56%
4	L	441	61% 20% . 18%
5	N	425	71% 19% . 9%
6	O	7	100%

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Mol	Chain	Length	Quality of chain
7	P	295	<div><div></div><div>19% .. 78%</div></div>
8	Z	135	<div><div></div><div>93% 7%</div></div>
9	B	345	<div><div></div><div>.. 96%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13440 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 Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	123	Total	C	N	O	S	0	0
			860	549	157	148	6		
1	M	122	Total	C	N	O	S	0	0
			962	609	169	175	9		
1	Q	66	Total	C	N	O	S	0	0
			496	315	94	85	2		

- Molecule 2 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	27	Total	C	N	O	S	0	0
			181	111	32	37	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	SER	-	expression tag	UNP Q92833
E	104	ASN	-	expression tag	UNP Q92833
E	105	ALA	-	expression tag	UNP Q92833

- Molecule 3 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	325	Total	C	N	O	S	0	0
			2406	1514	426	436	30		
3	C	193	Total	C	N	O	S	0	0
			1307	820	230	253	4		

- Molecule 4 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	362	Total	C	N	O	S	0	0
			2877	1826	505	526	20		

- Molecule 5 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	386	Total	C	N	O	S	0	0
			3058	1931	524	593	10		

- Molecule 6 is a protein called JARID2-substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	7	Total	C	N	O	0	0
			51	33	11	7		

- Molecule 7 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	64	Total	C	N	O	S	0	0
			484	304	91	87	2		

- Molecule 8 is a protein called SUZ12.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Z	135	Total	C	N	O	0	0
			674	404	135	135		

- Molecule 9 is a protein called Protein Jumonji.

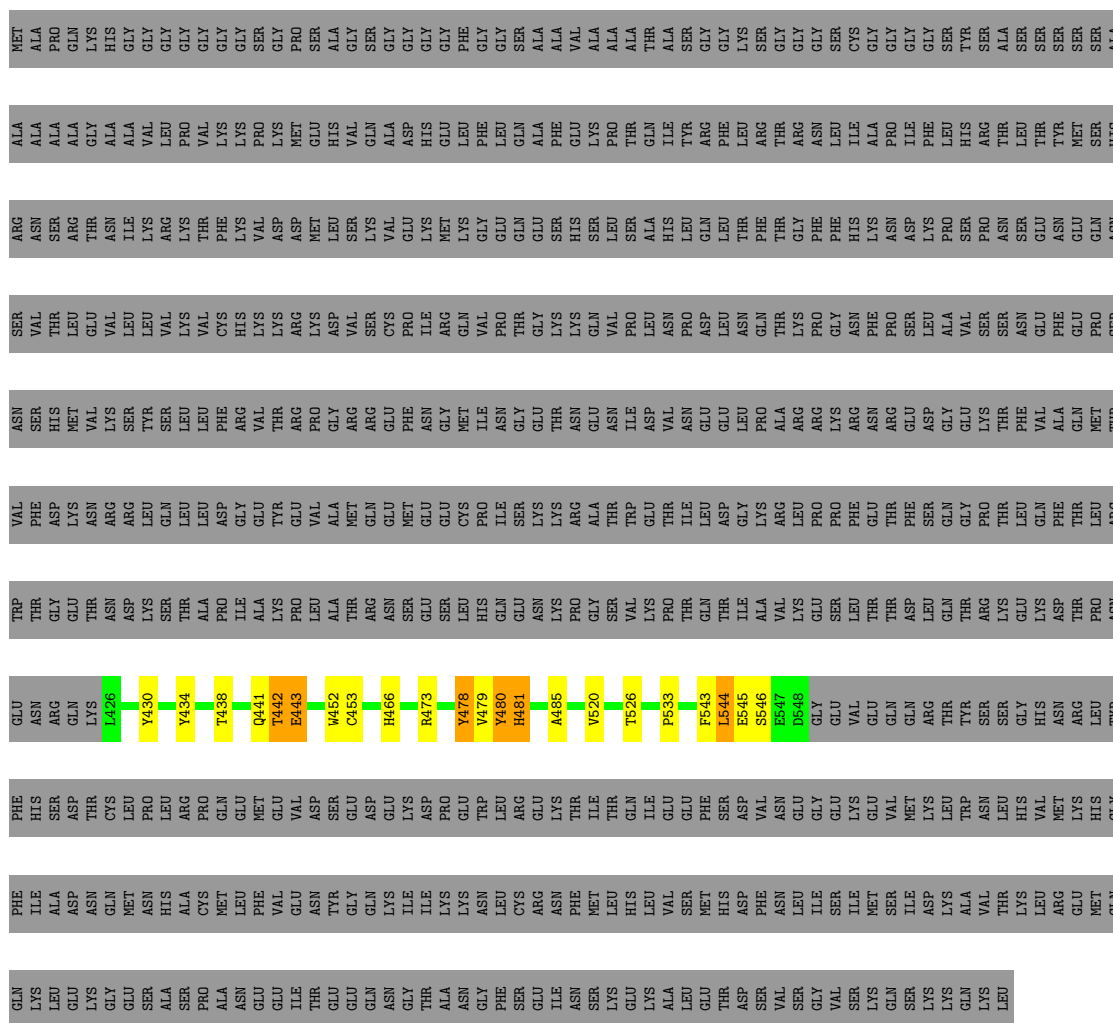
Mol	Chain	Residues	Atoms				AltConf	Trace
9	B	13	Total	C	N	O	0	0
			84	55	15	14		

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.

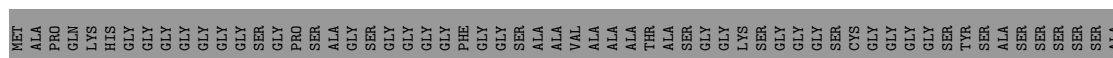
- Molecule 1: Polycomb protein SUZ12

Chain A:  14% .. 83%



- Molecule 1: Polycomb protein SUZ12

Chain M:  14% 1% 83%



● Molecule 1: Polycomb protein SUZ12

Chain Q: 7% . 91%

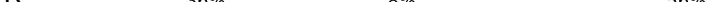
[illegible]

- Molecule 2: Protein Jumonji

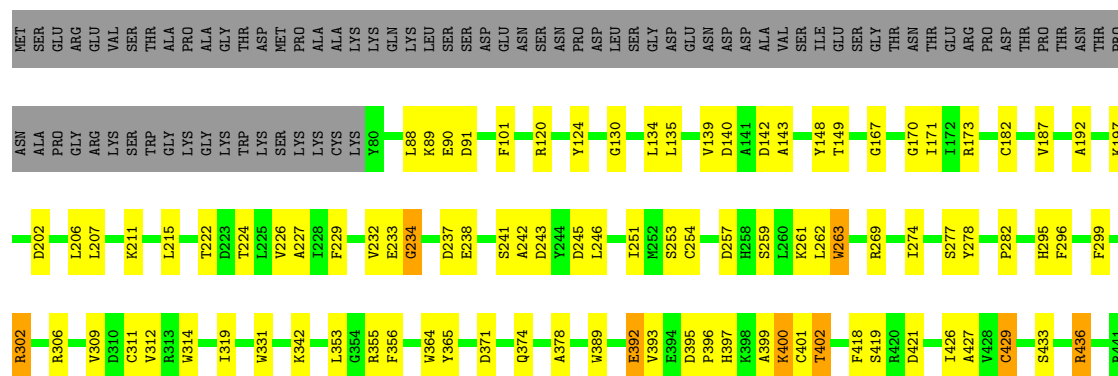
Chain E: 6% .. 92%

[illegible]

- Molecule 3: Histone-lysine N-methyltransferase EZH2

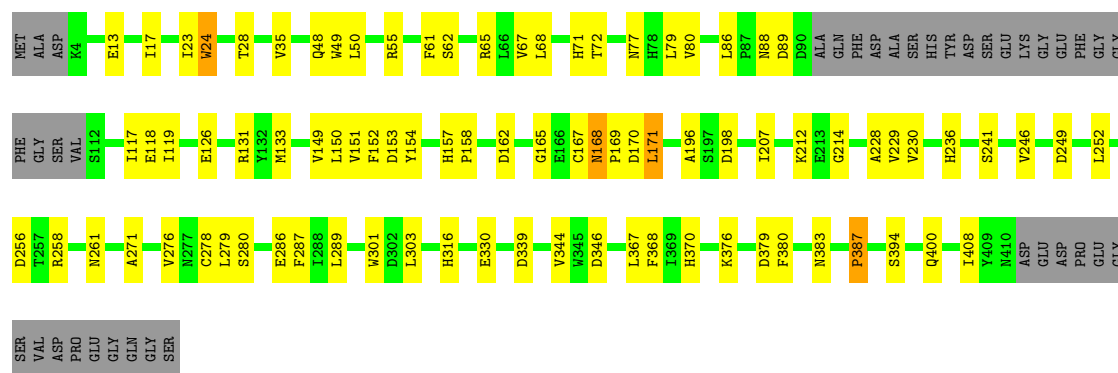
Chain K:  36% 8% 56%

[illegible]



• Molecule 5: Histone-binding protein RBBP4

Chain N: 71% 19% 9%



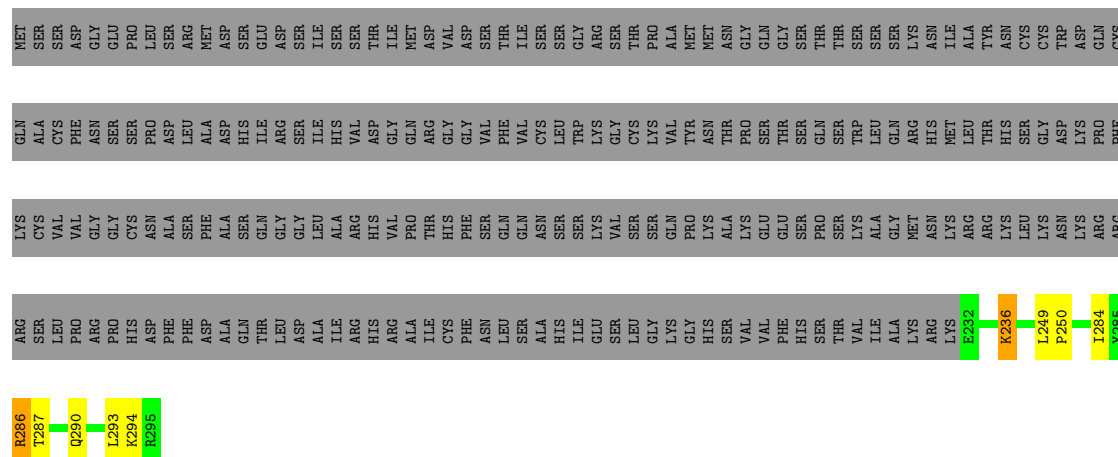
• Molecule 6: JARID2-substrate

Chain O: 100%

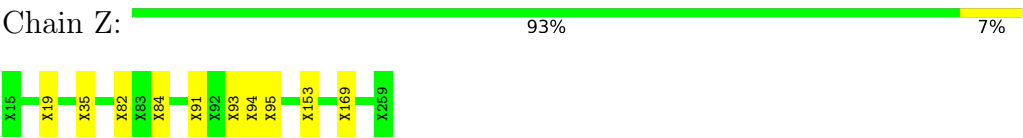
There are no outlier residues recorded for this chain.

• Molecule 7: Zinc finger protein AEBP2

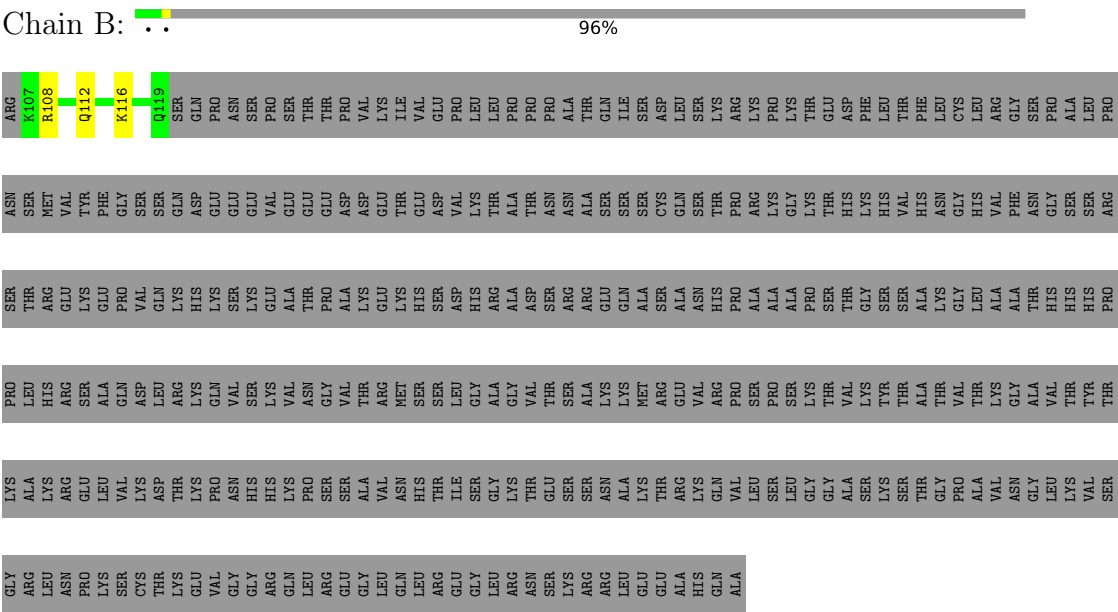
Chain P: 19% 78%



● Molecule 8: SUZ12



● Molecule 9: Protein Jumonji



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145592	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: M3L

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	0.58	0/882	0.82	1/1208 (0.1%)
1	M	0.58	0/983	0.75	0/1328
1	Q	0.61	0/506	0.86	0/687
2	E	0.40	0/182	0.75	0/246
3	C	0.49	0/1328	0.66	0/1815
3	K	0.49	0/2466	0.66	2/3352 (0.1%)
4	L	0.84	1/2952 (0.0%)	0.92	7/4008 (0.2%)
5	N	0.58	1/3142 (0.0%)	0.73	0/4286
6	O	0.54	0/51	0.74	0/66
7	P	0.53	0/492	0.81	0/666
9	B	0.44	0/73	0.43	0/100
All	All	0.62	2/13057 (0.0%)	0.77	10/17762 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	M	0	1
1	Q	0	1
3	C	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	234	GLY	CA-C	-22.83	1.15	1.51
5	N	24	TRP	CB-CG	-6.19	1.39	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	234	GLY	CA-C-O	-12.45	98.19	120.60
4	L	234	GLY	CA-C-N	9.64	138.40	117.20
4	L	234	GLY	N-CA-C	8.16	133.51	113.10
4	L	302	ARG	NE-CZ-NH2	-7.22	116.69	120.30
3	K	685	ARG	NE-CZ-NH2	5.79	123.20	120.30
4	L	302	ARG	NE-CZ-NH1	5.76	123.18	120.30
4	L	429	CYS	CA-CB-SG	5.59	124.07	114.00
3	K	581	ASP	CB-CG-OD1	5.14	122.93	118.30
4	L	173	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	473	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	441	GLN	Peptide
1	A	478	TYR	Peptide
1	A	480	TYR	Peptide
3	C	129	HIS	Peptide
1	M	579	MET	Peptide
1	Q	129	ARG	Peptide

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	860	0	729	20	0
1	M	962	0	898	13	0
1	Q	496	0	450	11	0
2	E	181	0	170	3	0
3	C	1307	0	1048	23	0
3	K	2406	0	2122	65	0
4	L	2877	0	2749	68	0
5	N	3058	0	2904	81	0
6	O	51	0	54	0	0
7	P	484	0	476	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Z	674	0	167	5	0
9	B	84	0	65	3	0
All	All	13440	0	11832	274	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:152:PHE:CD1	5:N:170:ASP:OD2	1.71	1.43
3:K:443:LEU:HB3	3:K:447:TYR:CE2	1.61	1.36
3:K:443:LEU:CB	3:K:447:TYR:CE2	2.09	1.34
3:K:443:LEU:CB	3:K:447:TYR:HE2	1.41	1.32
3:K:662:MET:SD	3:K:732:ASP:OD1	1.92	1.28
3:K:729:SER:C	3:K:730:GLN:OE1	1.69	1.28
5:N:157:HIS:ND1	5:N:168:ASN:ND2	1.78	1.27
5:N:152:PHE:HA	5:N:170:ASP:CG	1.60	1.21
3:K:443:LEU:CD2	3:K:447:TYR:OH	1.91	1.17
5:N:152:PHE:CG	5:N:170:ASP:OD2	2.01	1.14
4:L:233:GLU:HB2	4:L:295:HIS:O	1.48	1.13
3:K:443:LEU:HD23	3:K:447:TYR:OH	1.54	1.05
3:K:443:LEU:CG	3:K:447:TYR:CE2	2.41	1.03
3:K:443:LEU:HD23	3:K:447:TYR:CZ	1.96	1.00
5:N:157:HIS:CG	5:N:168:ASN:HD22	1.78	1.00
5:N:152:PHE:CD1	5:N:170:ASP:CG	2.36	0.98
5:N:152:PHE:HD1	5:N:170:ASP:CG	1.68	0.97
1:A:543:PHE:O	1:A:546:SER:N	1.97	0.95
3:K:443:LEU:CA	3:K:447:TYR:HE2	1.79	0.95
3:K:443:LEU:CG	3:K:447:TYR:HE2	1.76	0.95
5:N:152:PHE:HD1	5:N:170:ASP:OD1	1.52	0.92
3:K:443:LEU:CA	3:K:447:TYR:CE2	2.51	0.91
4:L:395:ASP:N	4:L:396:PRO:HA	1.87	0.89
3:K:443:LEU:HG	3:K:447:TYR:CE2	2.08	0.88
4:L:401:CYS:O	4:L:402:THR:OG1	1.93	0.85
4:L:389:TRP:HD1	4:L:400:LYS:CB	1.89	0.85
5:N:167:CYS:O	5:N:169:PRO:HD3	1.77	0.84
3:K:440:PHE:O	3:K:444:ILE:HG12	1.78	0.84
4:L:140:ASP:OD1	3:C:101:LEU:HB2	1.76	0.84
4:L:429:CYS:SG	4:L:433:SER:OG	2.35	0.83
3:K:729:SER:CA	3:K:730:GLN:OE1	2.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:157:HIS:CE1	5:N:168:ASN:HB3	2.15	0.82
5:N:62:SER:OG	5:N:88:ASN:ND2	2.12	0.81
4:L:356:PHE:CE1	4:L:396:PRO:HB2	2.18	0.79
5:N:170:ASP:O	5:N:171:LEU:CB	2.30	0.79
5:N:152:PHE:CA	5:N:170:ASP:CG	2.47	0.78
3:K:443:LEU:CG	3:K:447:TYR:OH	2.31	0.78
4:L:233:GLU:HG3	4:L:296:PHE:CD1	2.19	0.77
3:K:730:GLN:OE1	3:K:730:GLN:N	2.16	0.77
8:Z:91:UNK:HA	8:Z:95:UNK:O	1.84	0.76
3:K:443:LEU:CG	3:K:447:TYR:CZ	2.70	0.75
5:N:346:ASP:HB2	5:N:367:LEU:HD12	1.67	0.74
1:M:580:GLU:O	1:M:582:ASP:N	2.21	0.74
3:K:530:CYS:N	3:K:549:CYS:SG	2.60	0.74
1:A:533:PRO:HD2	5:N:35:VAL:HG22	1.69	0.74
5:N:152:PHE:CB	5:N:170:ASP:OD2	2.36	0.73
1:A:453:CYS:SG	1:A:466:HIS:NE2	2.62	0.72
4:L:306:ARG:HG3	3:C:159:GLY:O	1.89	0.72
4:L:90:GLU:OE2	4:L:124:TYR:OH	2.08	0.71
5:N:152:PHE:HA	5:N:170:ASP:OD2	1.89	0.70
1:A:434:TYR:O	1:A:438:THR:OG1	2.08	0.70
3:K:443:LEU:CD2	3:K:447:TYR:CZ	2.63	0.70
5:N:86:LEU:HD23	5:N:86:LEU:N	2.06	0.69
3:K:592:ASP:O	3:K:593:HIS:HB2	1.92	0.69
4:L:234:GLY:HA3	4:L:261:LYS:HE3	1.73	0.69
3:K:729:SER:O	3:K:730:GLN:OE1	2.11	0.68
3:K:443:LEU:HB3	3:K:447:TYR:CD2	2.24	0.68
3:K:604:CYS:SG	3:K:608:ARG:NH1	2.67	0.68
4:L:262:LEU:HD12	4:L:299:PHE:HB3	1.76	0.67
3:K:443:LEU:HG	3:K:447:TYR:OH	1.94	0.67
5:N:170:ASP:O	5:N:171:LEU:HB2	1.93	0.67
5:N:50:LEU:HD21	5:N:67:VAL:HG23	1.75	0.67
3:C:153:TYR:HB3	3:C:156:LYS:O	1.95	0.67
1:A:452:TRP:CZ3	1:Q:94:THR:HG22	2.30	0.67
3:K:677:ALA:O	3:K:685:ARG:NH2	2.28	0.66
3:K:443:LEU:HG	3:K:447:TYR:CZ	2.30	0.66
5:N:86:LEU:HD23	5:N:86:LEU:H	1.62	0.65
3:K:443:LEU:HG	3:K:447:TYR:HE2	1.49	0.65
5:N:65:ARG:NH1	5:N:118:GLU:OE2	2.29	0.65
4:L:274:ILE:O	4:L:277:SER:OG	2.11	0.65
5:N:278:CYS:SG	5:N:279:LEU:N	2.67	0.65
3:K:272:VAL:O	3:K:441:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PHE:O	1:A:544:LEU:C	2.35	0.64
3:K:443:LEU:HA	3:K:447:TYR:HE2	1.63	0.64
1:A:543:PHE:O	1:A:545:GLU:N	2.31	0.64
5:N:152:PHE:CA	5:N:170:ASP:OD2	2.46	0.63
4:L:356:PHE:HE1	4:L:396:PRO:CG	2.11	0.63
3:K:443:LEU:HD21	3:K:447:TYR:OH	1.92	0.62
1:Q:115:LEU:HD21	1:Q:117:TYR:CE2	2.34	0.62
3:K:662:MET:CE	3:K:732:ASP:OD1	2.47	0.61
5:N:241:SER:OG	5:N:256:ASP:OD1	2.16	0.61
4:L:254:CYS:SG	4:L:309:VAL:HG12	2.40	0.61
3:K:592:ASP:N	3:K:592:ASP:OD1	2.34	0.61
3:K:443:LEU:HA	3:K:447:TYR:CE2	2.35	0.61
3:C:142:ASP:O	3:C:145:PHE:N	2.30	0.60
5:N:154:TYR:HA	5:N:157:HIS:HD2	1.66	0.60
5:N:62:SER:OG	5:N:88:ASN:CG	2.40	0.59
1:A:533:PRO:CD	5:N:35:VAL:HG22	2.31	0.59
3:K:582:PRO:O	3:K:591:ALA:HB2	2.02	0.59
5:N:271:ALA:HB1	5:N:301:TRP:CH2	2.37	0.59
1:A:452:TRP:CH2	2:E:147:LEU:HD22	2.37	0.59
5:N:152:PHE:HA	5:N:170:ASP:OD1	1.92	0.59
4:L:356:PHE:CE1	4:L:396:PRO:CB	2.86	0.58
1:M:656:PHE:CE2	1:M:660:LEU:HD11	2.38	0.58
4:L:419:SER:OG	4:L:421:ASP:OD1	2.17	0.58
4:L:88:LEU:HD23	4:L:89:LYS:N	2.19	0.58
8:Z:93:UNK:O	8:Z:94:UNK:CB	2.50	0.58
4:L:389:TRP:CD1	4:L:400:LYS:CB	2.79	0.57
9:B:108:ARG:O	9:B:112:GLN:N	2.36	0.57
3:K:283:THR:HG23	3:K:284:LEU:HD22	1.86	0.57
5:N:198:ASP:HA	5:N:229:VAL:HG23	1.87	0.57
4:L:262:LEU:HD12	4:L:299:PHE:CB	2.34	0.57
1:A:480:TYR:O	1:A:485:ALA:N	2.38	0.56
5:N:67:VAL:O	5:N:68:LEU:HD12	2.04	0.56
3:K:593:HIS:HB3	3:K:596:SER:O	2.06	0.56
2:E:151:LYS:CB	2:E:152:PRO:HD3	2.37	0.55
1:A:520:VAL:HA	7:P:290:GLN:HE22	1.71	0.55
4:L:364:TRP:CZ3	9:B:116:M3L:HM22	2.41	0.55
4:L:356:PHE:HE1	4:L:396:PRO:CB	2.19	0.55
1:M:647:ILE:O	1:M:651:ASN:N	2.39	0.55
3:K:582:PRO:CB	3:K:591:ALA:HA	2.37	0.54
5:N:344:VAL:CG2	5:N:368:PHE:HB3	2.37	0.54
2:E:154:THR:O	2:E:155:GLU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:355:ARG:O	4:L:397:HIS:HA	2.08	0.54
4:L:182:CYS:HB2	3:C:101:LEU:HD22	1.88	0.54
5:N:246:VAL:HG21	5:N:279:LEU:HB2	1.90	0.54
4:L:365:TYR:CD2	9:B:116:M3L:HM23	2.42	0.53
5:N:88:ASN:O	5:N:89:ASP:HB3	2.08	0.53
1:A:452:TRP:CH2	1:Q:94:THR:HG22	2.42	0.53
4:L:378:ALA:HB2	4:L:418:PHE:CE1	2.43	0.53
5:N:80:VAL:HG13	5:N:117:ILE:HG23	1.90	0.53
7:P:293:LEU:HD23	7:P:294:LYS:N	2.22	0.53
1:Q:127:ILE:O	1:Q:129:ARG:NH1	2.41	0.53
5:N:170:ASP:O	5:N:171:LEU:HB3	2.09	0.53
4:L:233:GLU:CB	4:L:295:HIS:O	2.40	0.53
5:N:379:ASP:OD1	5:N:380:PHE:N	2.42	0.53
1:Q:92:LYS:CB	1:Q:93:PRO:HD3	2.38	0.53
5:N:154:TYR:HA	5:N:157:HIS:CD2	2.44	0.52
4:L:226:VAL:HG12	4:L:227:ALA:HB2	1.91	0.52
5:N:72:THR:HG22	5:N:77:ASN:OD1	2.10	0.52
4:L:207:LEU:HD11	4:L:215:LEU:HD23	1.92	0.52
3:K:462:THR:O	3:K:466:VAL:HG23	2.10	0.52
5:N:61:PHE:HA	5:N:88:ASN:OD1	2.10	0.52
1:A:430:TYR:HB2	1:A:443:GLU:CB	2.40	0.51
3:K:635:ASN:OD1	3:K:696:TYR:OH	2.22	0.51
3:K:729:SER:O	3:K:730:GLN:HB2	2.08	0.51
4:L:139:VAL:HG12	4:L:140:ASP:N	2.26	0.51
3:C:153:TYR:CB	3:C:156:LYS:O	2.59	0.50
3:K:296:LEU:H	3:K:296:LEU:HD23	1.76	0.50
3:K:589:GLY:HA2	3:K:592:ASP:CG	2.32	0.50
5:N:330:GLU:OE1	5:N:330:GLU:N	2.43	0.50
4:L:282:PRO:O	1:M:575:ARG:NH1	2.45	0.50
1:A:479:VAL:HG13	1:A:481:HIS:HA	1.92	0.50
3:C:126:THR:O	3:C:128:LEU:N	2.45	0.50
5:N:86:LEU:N	5:N:86:LEU:CD2	2.73	0.50
4:L:241:SER:OG	4:L:242:ALA:N	2.44	0.49
4:L:306:ARG:NH1	3:C:159:GLY:O	2.45	0.49
4:L:253:SER:HG	4:L:263:TRP:HZ3	1.60	0.49
5:N:196:ALA:HB1	5:N:230:VAL:HG13	1.93	0.49
7:P:284:ILE:HG22	7:P:287:THR:HG23	1.93	0.49
4:L:356:PHE:HE1	4:L:396:PRO:HG2	1.75	0.49
5:N:339:ASP:HA	7:P:286:ARG:NH2	2.28	0.49
1:A:452:TRP:HZ3	1:Q:94:THR:HG22	1.74	0.49
3:K:617:ALA:HB1	3:K:618:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:157:HIS:ND1	5:N:168:ASN:CG	2.61	0.48
5:N:246:VAL:CG1	5:N:276:VAL:HG12	2.43	0.48
1:Q:115:LEU:HD21	1:Q:117:TYR:CZ	2.48	0.48
1:M:630:ASN:OD1	1:M:631:GLN:N	2.46	0.48
5:N:151:VAL:O	5:N:170:ASP:O	2.32	0.48
5:N:370:HIS:NE2	5:N:400:GLN:OE1	2.46	0.48
1:A:520:VAL:HA	7:P:290:GLN:NE2	2.29	0.48
3:K:647:SER:OG	3:K:649:ASP:OD1	2.24	0.47
4:L:215:LEU:HB2	4:L:229:PHE:HB2	1.95	0.47
5:N:133:MET:CE	5:N:207:ILE:HD11	2.45	0.47
5:N:118:GLU:HG2	5:N:119:ILE:HG22	1.96	0.47
5:N:152:PHE:CA	5:N:170:ASP:OD1	2.57	0.47
3:K:617:ALA:HB2	1:M:565:TYR:HA	1.97	0.47
5:N:48:GLN:OE1	5:N:131:ARG:NH1	2.47	0.47
3:C:106:SER:OG	3:C:107:VAL:N	2.47	0.46
3:K:716:ILE:HG23	3:K:720:GLU:OE1	2.14	0.46
4:L:211:LYS:HA	4:L:238:GLU:HB2	1.97	0.46
7:P:286:ARG:NH1	7:P:287:THR:O	2.47	0.46
5:N:157:HIS:ND1	5:N:168:ASN:HB3	2.28	0.46
3:C:49:ILE:O	3:C:53:THR:HG22	2.16	0.46
4:L:88:LEU:HD21	3:C:85:VAL:CB	2.45	0.46
3:K:440:PHE:O	3:K:444:ILE:CG1	2.58	0.46
4:L:331:TRP:HA	4:L:353:LEU:CD2	2.45	0.46
3:K:662:MET:SD	3:K:732:ASP:CG	2.86	0.46
4:L:254:CYS:SG	4:L:309:VAL:CG1	3.03	0.46
5:N:80:VAL:CG1	5:N:117:ILE:HG23	2.46	0.46
1:A:442:THR:O	1:A:443:GLU:CB	2.65	0.45
8:Z:153:UNK:O	8:Z:169:UNK:CB	2.63	0.45
4:L:140:ASP:OD1	3:C:101:LEU:CB	2.59	0.45
5:N:149:VAL:C	5:N:150:LEU:HD12	2.37	0.45
5:N:157:HIS:CB	5:N:168:ASN:ND2	2.80	0.45
5:N:23:ILE:HD13	5:N:23:ILE:HG21	1.79	0.45
3:K:279:HIS:O	3:K:283:THR:HG22	2.17	0.45
4:L:237:ASP:OD1	4:L:238:GLU:N	2.45	0.45
4:L:246:LEU:HD21	4:L:374:GLN:NE2	2.32	0.45
4:L:392:GLU:HG2	4:L:392:GLU:H	1.47	0.45
5:N:157:HIS:HB3	5:N:158:PRO:HD2	1.99	0.45
4:L:319:ILE:HG21	4:L:331:TRP:CZ2	2.52	0.45
4:L:130:GLY:HA2	4:L:436:ARG:NH1	2.32	0.45
3:K:432:TRP:HH2	3:K:466:VAL:HG22	1.80	0.44
4:L:142:ASP:OD1	4:L:143:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:376:LYS:O	5:N:394:SER:OG	2.18	0.44
3:K:639:SER:OG	3:K:640:GLU:N	2.51	0.44
4:L:426:ILE:HG22	4:L:427:ALA:N	2.33	0.44
3:C:226:ALA:O	3:C:229:SER:OG	2.19	0.44
4:L:232:VAL:HG13	4:L:233:GLU:HG2	1.99	0.44
1:M:671:ILE:HA	1:M:674:ILE:HD13	1.99	0.44
3:C:107:VAL:HG13	3:C:108:PRO:HD2	1.99	0.44
5:N:157:HIS:CG	5:N:168:ASN:ND2	2.57	0.43
5:N:61:PHE:CA	5:N:88:ASN:OD1	2.66	0.43
4:L:311:CYS:SG	4:L:312:VAL:N	2.90	0.43
1:Q:115:LEU:HD23	1:Q:115:LEU:C	2.38	0.43
4:L:134:LEU:HD12	4:L:135:LEU:N	2.33	0.43
4:L:371:ASP:OD1	4:L:374:GLN:N	2.52	0.43
5:N:49:TRP:CD2	5:N:383:ASN:HB3	2.53	0.43
3:K:582:PRO:HB2	3:K:591:ALA:HA	2.00	0.43
7:P:249:LEU:HB2	7:P:250:PRO:HD3	2.00	0.43
1:Q:115:LEU:HD21	1:Q:117:TYR:CD2	2.53	0.43
4:L:167:GLY:O	4:L:170:GLY:N	2.48	0.43
3:K:281:PHE:CE1	1:M:610:GLU:HG3	2.54	0.43
3:K:278:LEU:HD23	1:M:658:LEU:HD21	2.01	0.43
4:L:302:ARG:HH22	3:C:129:HIS:CB	2.32	0.43
4:L:197:LYS:O	4:L:206:LEU:HD12	2.19	0.43
5:N:246:VAL:HG13	5:N:276:VAL:HG12	2.01	0.43
3:K:283:THR:HG23	3:K:284:LEU:CD2	2.49	0.42
3:C:31:ARG:O	3:C:35:ALA:HB2	2.19	0.42
4:L:251:ILE:HD13	4:L:251:ILE:HG21	1.86	0.42
4:L:426:ILE:CG2	4:L:427:ALA:N	2.83	0.42
5:N:71:HIS:ND1	5:N:126:GLU:OE1	2.44	0.42
1:A:526:THR:HG22	1:M:579:MET:CE	2.49	0.42
5:N:228:ALA:N	5:N:249:ASP:OD1	2.48	0.42
5:N:316:HIS:ND1	5:N:339:ASP:OD2	2.52	0.42
5:N:246:VAL:HG13	5:N:276:VAL:CG1	2.49	0.42
8:Z:82:UNK:O	8:Z:84:UNK:N	2.52	0.42
3:K:619:SER:OG	3:K:620:ASP:N	2.51	0.42
1:M:571:CYS:SG	3:C:110:MET:SD	3.17	0.42
5:N:157:HIS:ND1	5:N:168:ASN:CB	2.83	0.42
5:N:162:ASP:OD1	5:N:165:GLY:HA3	2.20	0.42
1:A:478:TYR:OH	1:A:545:GLU:O	2.37	0.42
3:C:142:ASP:O	3:C:143:GLY:C	2.58	0.42
4:L:171:ILE:HG12	4:L:187:VAL:HG22	2.01	0.42
5:N:367:LEU:HD21	5:N:408:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:24:TRP:O	5:N:28:THR:HG23	2.19	0.42
4:L:257:ASP:OD1	4:L:259:SER:OG	2.19	0.42
4:L:91:ASP:OD1	4:L:120:ARG:NH1	2.47	0.42
5:N:157:HIS:CB	5:N:168:ASN:HD22	2.29	0.42
5:N:279:LEU:HD13	5:N:280:SER:N	2.35	0.42
3:K:446:THR:HG23	3:K:447:TYR:N	2.34	0.42
4:L:202:ASP:OD2	4:L:278:TYR:OH	2.23	0.41
1:M:607:ASN:OD1	1:M:608:GLU:N	2.53	0.41
1:M:674:ILE:O	1:M:678:VAL:HG23	2.19	0.41
5:N:162:ASP:CG	5:N:165:GLY:H	2.24	0.41
4:L:148:TYR:O	4:L:149:THR:HG23	2.19	0.41
5:N:152:PHE:HA	5:N:170:ASP:CB	2.46	0.41
5:N:252:LEU:HD21	5:N:289:LEU:HD21	2.01	0.41
3:K:582:PRO:HB3	3:K:591:ALA:HA	2.02	0.41
3:K:649:ASP:OD1	3:K:650:GLU:N	2.52	0.41
3:K:729:SER:HA	3:K:730:GLN:OE1	2.15	0.41
5:N:13:GLU:O	5:N:17:ILE:HG12	2.20	0.41
4:L:139:VAL:O	3:C:101:LEU:N	2.54	0.41
3:K:687:ALA:O	3:K:726:TYR:OH	2.38	0.41
1:Q:110:PHE:HE2	1:Q:115:LEU:HD12	1.85	0.41
3:K:588:CYS:SG	3:K:590:ALA:HB2	2.61	0.41
4:L:243:ASP:OD2	4:L:312:VAL:HG13	2.21	0.41
3:C:133:TYR:O	3:C:135:GLY:N	2.54	0.41
5:N:236:HIS:NE2	5:N:286:GLU:O	2.51	0.41
1:Q:116:THR:O	1:Q:119:SER:N	2.54	0.41
7:P:236:LYS:HE3	3:C:105:ALA:HB2	2.02	0.41
1:A:479:VAL:HG13	1:A:481:HIS:CA	2.51	0.41
3:C:137:GLU:N	3:C:137:GLU:OE1	2.54	0.41
3:K:565:GLN:OE1	3:K:567:ASN:ND2	2.54	0.41
4:L:245:ASP:HA	4:L:314:TRP:CD1	2.55	0.41
8:Z:19:UNK:O	8:Z:35:UNK:N	2.54	0.41
4:L:399:ALA:O	4:L:400:LYS:CB	2.70	0.40
5:N:153:ASP:O	5:N:157:HIS:CD2	2.74	0.40
3:K:695:CYS:SG	3:K:722:LEU:HD22	2.62	0.40
4:L:101:PHE:CZ	4:L:426:ILE:CD1	3.04	0.40
5:N:287:PHE:HA	5:N:303:LEU:HD12	2.04	0.40
3:C:136:ASP:N	3:C:137:GLU:OE1	2.54	0.40
4:L:222:THR:HG23	4:L:224:THR:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	121/739 (16%)	89 (74%)	28 (23%)	4 (3%)	4	36
1	M	120/739 (16%)	105 (88%)	13 (11%)	2 (2%)	10	48
1	Q	64/739 (9%)	48 (75%)	15 (23%)	1 (2%)	11	49
2	E	25/348 (7%)	15 (60%)	8 (32%)	2 (8%)	1	16
3	C	189/746 (25%)	160 (85%)	24 (13%)	5 (3%)	6	40
3	K	319/746 (43%)	270 (85%)	46 (14%)	3 (1%)	19	59
4	L	360/441 (82%)	305 (85%)	51 (14%)	4 (1%)	16	56
5	N	382/425 (90%)	335 (88%)	42 (11%)	5 (1%)	13	53
6	O	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
7	P	62/295 (21%)	48 (77%)	14 (23%)	0	100	100
9	B	10/345 (3%)	9 (90%)	1 (10%)	0	100	100
All	All	1657/5570 (30%)	1388 (84%)	243 (15%)	26 (2%)	15	49

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	HIS
4	L	400	LYS
1	M	581	VAL
5	N	171	LEU
3	C	127	VAL
1	A	443	GLU
1	A	544	LEU
4	L	393	VAL
4	L	402	THR
3	C	126	THR
2	E	158	LEU
3	K	593	HIS
1	Q	131	THR

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Mol	Chain	Res	Type
3	C	134	MET
3	C	141	GLN
1	A	442	THR
2	E	155	GLU
4	L	192	ALA
1	M	580	GLU
5	N	387	PRO
3	K	305	THR
5	N	212	LYS
3	C	130	ASN
5	N	168	ASN
5	N	214	GLY
3	K	262	PRO

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	A	72/646 (11%)	72 (100%)	0	100	100
1	M	101/646 (16%)	100 (99%)	1 (1%)	78	89
1	Q	45/646 (7%)	45 (100%)	0	100	100
2	E	18/297 (6%)	17 (94%)	1 (6%)	23	58
3	C	100/667 (15%)	99 (99%)	1 (1%)	78	89
3	K	233/667 (35%)	227 (97%)	6 (3%)	49	75
4	L	310/392 (79%)	305 (98%)	5 (2%)	65	84
5	N	340/375 (91%)	335 (98%)	5 (2%)	67	85
6	O	3/3 (100%)	3 (100%)	0	100	100
7	P	50/263 (19%)	48 (96%)	2 (4%)	34	65
9	B	3/294 (1%)	3 (100%)	0	100	100
All	All	1275/4896 (26%)	1254 (98%)	21 (2%)	68	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	158	LEU
3	K	547	CYS
3	K	555	ASN
3	K	592	ASP
3	K	653	ARG
3	K	668	ASN
3	K	685	ARG
4	L	263	TRP
4	L	269	ARG
4	L	342	LYS
4	L	392	GLU
4	L	436	ARG
1	M	563	ARG
5	N	55	ARG
5	N	79	LEU
5	N	258	ARG
5	N	261	ASN
5	N	387	PRO
7	P	236	LYS
7	P	286	ARG
3	C	45	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	668	ASN
4	L	204	ASN
4	L	213	HIS
5	N	168	ASN
5	N	188	ASN
5	N	226	HIS
5	N	261	ASN
7	P	290	GLN
1	Q	83	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	M3L	B	116	9,3	11,11,12	0.62	0	10,14,16	0.85	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	M3L	B	116	9,3	-	1/8/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	116	M3L	O-C-CA	-2.06	119.46	124.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	116	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	116	M3L	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	Z	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	182:UNK	C	247:UNK	N	39.79
1	Z	45:UNK	C	55:UNK	N	32.97
1	Z	67:UNK	C	77:UNK	N	29.83
1	Z	138:UNK	C	143:UNK	N	25.66
1	Z	99:UNK	C	120:UNK	N	10.57
1	Z	25:UNK	C	30:UNK	N	5.09