



Full wwPDB EM Validation Report ⓘ

Oct 2, 2024 – 12:13 PM JST

PDB ID : 8WQG
EMDB ID : EMD-37744
Title : cryo-EM structure of neddylated CUL2-RBX1-ELOB-ELOC-FEM1B bound with the C-degron of CCDC89 (conformation 1)
Authors : Chen, X.; Zhang, K.; Xu, C.
Deposited on : 2023-10-11
Resolution : 4.09 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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

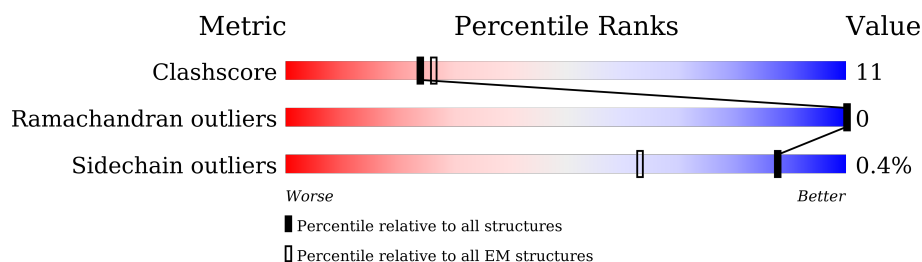
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.09 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	D	118	57% 22% 21%
1	I	118	50% 28% 21%
2	F	96	53% 35% 11%
2	J	96	60% 27% 12%
3	B	96	75% 25%
3	H	96	68% 32%
4	C	750	73% 23% .
4	E	750	69% 27% .
5	K	76	82% 18%

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Mol	Chain	Length	Quality of chain
5	N	76	 95%5%
6	A	627	 79%21%
6	G	627	 68%31%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26832 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 Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	93	Total	C	N	O	S	0	0
			735	467	126	139	3		
1	I	93	Total	C	N	O	S	0	0
			735	467	126	139	3		

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	85	Total	C	N	O	S	0	0
			693	438	127	119	9		
2	J	84	Total	C	N	O	S	0	0
			679	431	122	117	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	13	SER	-	expression tag	UNP P62877
F	14	HIS	-	expression tag	UNP P62877
F	15	MET	-	expression tag	UNP P62877
J	13	SER	-	expression tag	UNP P62877
J	14	HIS	-	expression tag	UNP P62877
J	15	MET	-	expression tag	UNP P62877

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	96	Total	C	N	O	S	0	0
			760	487	122	145	6		
3	H	96	Total	C	N	O	S	0	0
			760	487	122	145	6		

- Molecule 4 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	720	Total	C	N	O	S	0	0
			5902	3751	1003	1105	43		
4	E	720	Total	C	N	O	S	0	0
			5902	3751	1003	1105	43		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	SER	-	expression tag	UNP Q13617
C	-18	ALA	-	expression tag	UNP Q13617
C	-17	SER	-	expression tag	UNP Q13617
C	-16	TRP	-	expression tag	UNP Q13617
C	-15	SER	-	expression tag	UNP Q13617
C	-14	HIS	-	expression tag	UNP Q13617
C	-13	PRO	-	expression tag	UNP Q13617
C	-12	GLN	-	expression tag	UNP Q13617
C	-11	PHE	-	expression tag	UNP Q13617
C	-10	GLU	-	expression tag	UNP Q13617
C	-9	LYS	-	expression tag	UNP Q13617
C	-8	GLY	-	expression tag	UNP Q13617
C	-7	GLY	-	expression tag	UNP Q13617
C	-6	GLY	-	expression tag	UNP Q13617
C	-5	SER	-	expression tag	UNP Q13617
C	-4	GLY	-	expression tag	UNP Q13617
C	-3	GLY	-	expression tag	UNP Q13617
C	-2	GLY	-	expression tag	UNP Q13617
C	-1	SER	-	expression tag	UNP Q13617
C	0	GLY	-	expression tag	UNP Q13617
C	1	THR	-	expression tag	UNP Q13617
C	?	-	LYS	deletion	UNP Q13617
C	?	-	LEU	deletion	UNP Q13617
C	?	-	THR	deletion	UNP Q13617
C	?	-	GLU	deletion	UNP Q13617
C	?	-	ALA	deletion	UNP Q13617
C	?	-	ASP	deletion	UNP Q13617
C	?	-	LEU	deletion	UNP Q13617
C	?	-	GLN	deletion	UNP Q13617
C	?	-	TYR	deletion	UNP Q13617
C	?	-	GLY	deletion	UNP Q13617
C	?	-	TYR	deletion	UNP Q13617
C	?	-	GLY	deletion	UNP Q13617
C	?	-	GLY	deletion	UNP Q13617
C	?	-	VAL	deletion	UNP Q13617

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP Q13617
C	132	GLY	MET	conflict	UNP Q13617
C	133	GLY	ASN	conflict	UNP Q13617
C	134	GLY	GLU	conflict	UNP Q13617
E	-19	SER	-	expression tag	UNP Q13617
E	-18	ALA	-	expression tag	UNP Q13617
E	-17	SER	-	expression tag	UNP Q13617
E	-16	TRP	-	expression tag	UNP Q13617
E	-15	SER	-	expression tag	UNP Q13617
E	-14	HIS	-	expression tag	UNP Q13617
E	-13	PRO	-	expression tag	UNP Q13617
E	-12	GLN	-	expression tag	UNP Q13617
E	-11	PHE	-	expression tag	UNP Q13617
E	-10	GLU	-	expression tag	UNP Q13617
E	-9	LYS	-	expression tag	UNP Q13617
E	-8	GLY	-	expression tag	UNP Q13617
E	-7	GLY	-	expression tag	UNP Q13617
E	-6	GLY	-	expression tag	UNP Q13617
E	-5	SER	-	expression tag	UNP Q13617
E	-4	GLY	-	expression tag	UNP Q13617
E	-3	GLY	-	expression tag	UNP Q13617
E	-2	GLY	-	expression tag	UNP Q13617
E	-1	SER	-	expression tag	UNP Q13617
E	0	GLY	-	expression tag	UNP Q13617
E	1	THR	-	expression tag	UNP Q13617
E	?	-	LYS	deletion	UNP Q13617
E	?	-	LEU	deletion	UNP Q13617
E	?	-	THR	deletion	UNP Q13617
E	?	-	GLU	deletion	UNP Q13617
E	?	-	ALA	deletion	UNP Q13617
E	?	-	ASP	deletion	UNP Q13617
E	?	-	LEU	deletion	UNP Q13617
E	?	-	GLN	deletion	UNP Q13617
E	?	-	TYR	deletion	UNP Q13617
E	?	-	GLY	deletion	UNP Q13617
E	?	-	TYR	deletion	UNP Q13617
E	?	-	GLY	deletion	UNP Q13617
E	?	-	GLY	deletion	UNP Q13617
E	?	-	VAL	deletion	UNP Q13617
E	?	-	ASP	deletion	UNP Q13617
E	132	GLY	MET	conflict	UNP Q13617
E	133	GLY	ASN	conflict	UNP Q13617

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Chain	Residue	Modelled	Actual	Comment	Reference
E	134	GLY	GLU	conflict	UNP Q13617

- Molecule 5 is a protein called NEDD8.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	76	Total	C	N	O	0	0
			402	245	81	76		
5	K	76	Total	C	N	O	0	0
			400	243	81	76		

- Molecule 6 is a protein called Protein fem-1 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	627	Total	C	N	O	S	0	0
			4929	3091	882	927	29		
6	G	627	Total	C	N	O	S	0	0
			4929	3091	882	927	29		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	F	3	Total	Zn	0
			3	3	
7	J	3	Total	Zn	0
			3	3	

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.

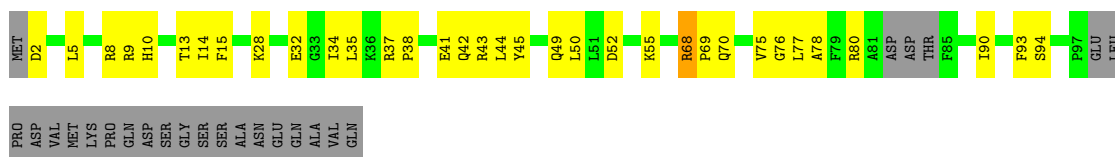
- Molecule 1: Elongin-B

Chain D: 



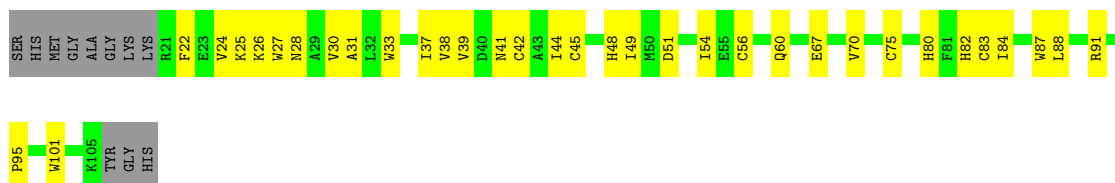
- Molecule 1: Elongin-B

Chain I: 



- Molecule 2: E3 ubiquitin-protein ligase RBX1, N-terminally processed

Chain F: 



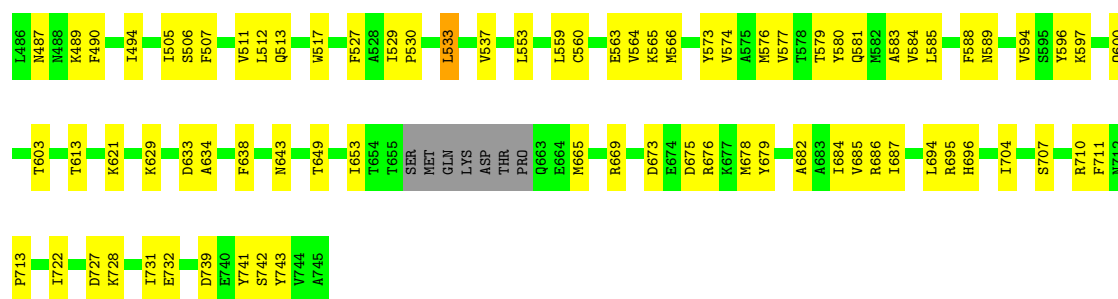
- Molecule 2: E3 ubiquitin-protein ligase RBX1, N-terminally processed

Chain J: 



- Molecule 3: Elongin-C

Chain B: 



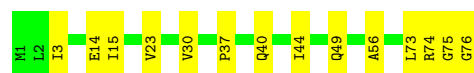
• Molecule 5: NEDD8

Chain N: 95% 5%



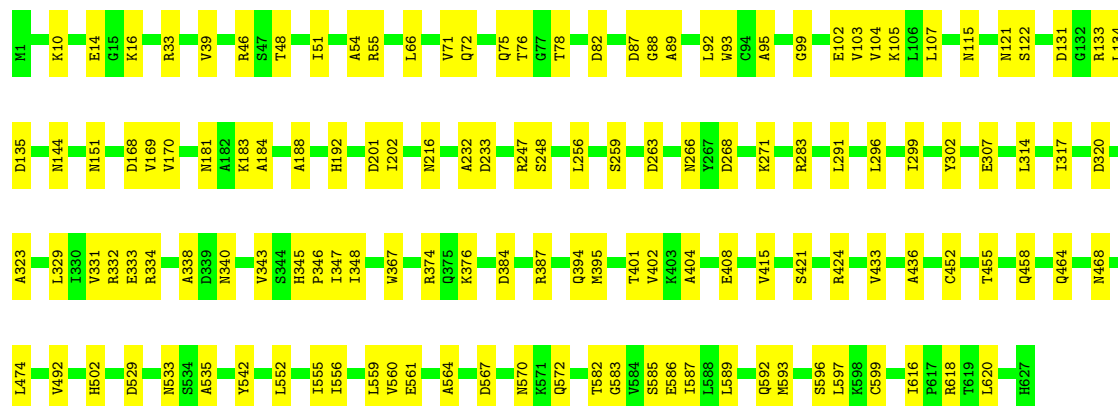
• Molecule 5: NEDD8

Chain K: 82% 18%



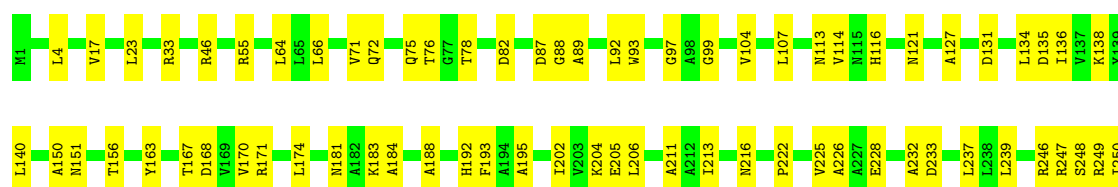
• Molecule 6: Protein fem-1 homolog B

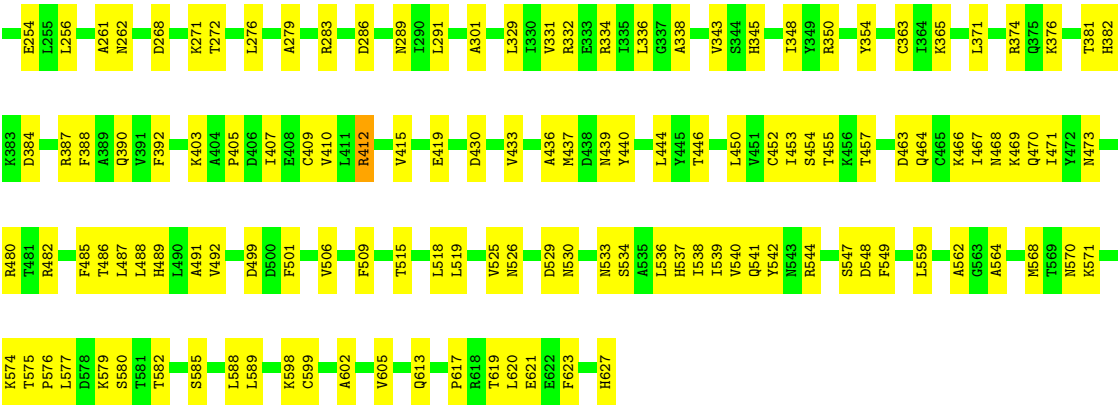
Chain A: 79% 21%



• Molecule 6: Protein fem-1 homolog B

Chain G: 68% 31%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102432	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 ($e^-/\text{\AA}^2$)	57.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 > 5$	RMSZ	# $ Z > 5$
1	D	0.25	0/749	0.53	0/1010
1	I	0.26	0/749	0.57	0/1010
2	F	0.27	0/713	0.50	0/971
2	J	0.26	0/699	0.48	0/953
3	B	0.25	0/777	0.45	0/1050
3	H	0.30	0/777	0.51	0/1050
4	C	0.26	0/6016	0.48	1/8100 (0.0%)
4	E	0.30	0/6016	0.51	1/8100 (0.0%)
5	K	0.24	0/401	0.49	0/554
5	N	0.25	0/404	0.50	0/559
6	A	0.24	0/5015	0.46	1/6799 (0.0%)
6	G	0.24	0/5015	0.47	0/6799
All	All	0.26	0/27331	0.49	3/36955 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	122	SER	C-N-CA	6.37	137.62	121.70
4	C	498	ASP	CB-CG-OD1	6.24	123.92	118.30
4	E	533	LEU	CA-CB-CG	5.83	128.71	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	D	735	0	737	20	0
1	I	735	0	737	25	0
2	F	693	0	640	33	0
2	J	679	0	622	26	0
3	B	760	0	749	18	0
3	H	760	0	749	29	0
4	C	5902	0	5893	114	0
4	E	5902	0	5893	141	0
5	K	400	0	232	10	0
5	N	402	0	238	3	0
6	A	4929	0	4910	79	0
6	G	4929	0	4910	126	0
7	F	3	0	0	0	0
7	J	3	0	0	0	0
All	All	26832	0	26310	565	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 (565) 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)
2:F:45:CYS:SG	2:F:80:HIS:CE1	2.61	0.94
6:A:263:ASP:OD2	6:A:266:ASN:ND2	2.16	0.79
2:J:48:HIS:HB2	2:J:51:ASP:HB2	1.65	0.78
6:G:384:ASP:OD1	6:G:387:ARG:NH2	2.18	0.77
2:F:42:CYS:HB3	2:F:45:CYS:SG	2.25	0.77
2:F:30:VAL:HG11	4:E:444:ILE:HD11	1.68	0.76
2:J:45:CYS:HB3	2:J:83:CYS:SG	2.27	0.75
3:H:91:PRO:HD2	1:I:68:ARG:HH21	1.52	0.73
6:G:374:ARG:NE	6:G:384:ASP:OD2	2.21	0.73
6:A:384:ASP:OD1	6:A:387:ARG:NH1	2.22	0.72
6:G:480:ARG:HH22	6:G:486:THR:HG22	1.54	0.72
6:A:492:VAL:HG12	6:A:555:ILE:HD11	1.71	0.71
4:E:316:GLN:HG3	4:E:371:ALA:HB2	1.72	0.71
4:C:484:ALA:O	4:C:487:ASN:HB2	1.91	0.70
3:B:22:ILE:HB	3:B:61:ASN:HA	1.74	0.69
2:F:33:TRP:HE1	4:E:513:GLN:HG2	1.57	0.69
6:A:66:LEU:HD11	6:A:107:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:228:GLU:OE2	6:G:332:ARG:NH1	2.20	0.68
6:G:544:ARG:HD3	6:G:547:SER:HB3	1.76	0.68
6:G:466:LYS:HG3	6:G:470:GLN:HE22	1.59	0.68
4:C:16:LYS:NZ	4:C:41:ASP:OD2	2.27	0.68
4:E:72:LEU:HD21	4:E:90:TYR:HB3	1.76	0.67
6:G:261:ALA:O	6:G:350:ARG:NH2	2.28	0.67
4:C:664:GLU:HB3	4:C:667:GLN:HE22	1.59	0.67
4:C:480:MET:SD	4:C:510:TYR:OH	2.49	0.66
2:J:45:CYS:SG	2:J:80:HIS:CE1	2.89	0.66
1:I:68:ARG:HG2	1:I:69:PRO:HD2	1.78	0.66
1:I:43:ARG:HH12	1:I:80:ARG:HH21	1.43	0.66
4:C:455:GLU:OE1	4:C:459:ASN:ND2	2.29	0.65
4:C:511:VAL:HG22	2:J:31:ALA:HB3	1.77	0.65
2:J:75:CYS:SG	2:J:94:CYS:HB2	2.36	0.65
3:B:56:GLU:HG2	3:B:57:THR:HG23	1.77	0.65
1:I:9:ARG:HB2	1:I:77:LEU:HB3	1.78	0.65
4:C:185:ILE:HG21	4:C:254:LEU:HA	1.77	0.65
2:F:48:HIS:HB3	2:F:51:ASP:HB2	1.79	0.64
6:G:76:THR:HB	6:G:88:GLY:HA2	1.78	0.64
1:D:23:THR:HA	1:D:56:THR:HA	1.78	0.64
4:E:483:SER:O	4:E:487:ASN:ND2	2.29	0.64
2:F:22:PHE:HD2	4:E:589:ASN:HB2	1.62	0.64
2:J:55:GLU:HG2	2:J:86:ARG:HH22	1.63	0.64
6:G:541:GLN:OE1	6:G:579:LYS:NZ	2.30	0.63
6:G:430:ASP:HA	6:G:433:VAL:HG12	1.80	0.63
2:F:25:LYS:HE2	4:E:565:LYS:HB2	1.79	0.63
6:G:466:LYS:O	6:G:470:GLN:NE2	2.31	0.63
2:F:31:ALA:HB3	4:E:511:VAL:HG12	1.80	0.63
6:A:14:GLU:OE1	6:A:16:LYS:NZ	2.32	0.63
2:F:25:LYS:HB2	4:E:563:GLU:HG3	1.81	0.63
6:A:72:GLN:O	6:A:75:GLN:NE2	2.32	0.63
6:G:171:ARG:HG2	6:G:205:GLU:HG3	1.81	0.63
2:J:75:CYS:SG	2:J:94:CYS:CB	2.86	0.62
4:C:391:LEU:HD22	4:C:425:ILE:HD11	1.81	0.62
6:G:599:CYS:SG	6:G:627:HIS:NE2	2.67	0.62
4:C:298:TYR:OH	4:C:302:ARG:NH1	2.32	0.62
3:B:79:TYR:OH	3:B:91:PRO:O	2.15	0.62
6:G:577:LEU:HD21	6:G:589:LEU:HB3	1.81	0.61
4:E:391:LEU:HD22	4:E:425:ILE:HD11	1.81	0.61
6:G:570:ASN:HD21	6:G:574:LYS:HB2	1.66	0.61
2:F:39:VAL:O	2:F:41:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:72:GLN:O	6:G:75:GLN:NE2	2.34	0.60
2:J:37:ILE:HG13	2:J:38:VAL:HG13	1.83	0.60
4:E:485:ASP:OD2	4:E:489:LYS:NZ	2.35	0.60
6:G:575:THR:HG22	6:G:577:LEU:H	1.67	0.60
1:I:68:ARG:HD3	1:I:70:GLN:HB3	1.83	0.60
6:G:542:TYR:OH	6:G:548:ASP:OD2	2.12	0.60
4:C:491:ASN:O	4:C:494:ILE:HB	2.02	0.59
3:H:104:LEU:HG	6:G:620:LEU:HD21	1.84	0.59
4:E:512:LEU:HB3	4:E:517:TRP:CD1	2.37	0.59
4:C:428:LYS:NZ	4:E:463:GLN:O	2.35	0.59
6:A:582:THR:HG22	6:A:585:SER:H	1.67	0.59
6:G:4:LEU:HD11	6:G:23:LEU:HD22	1.84	0.59
2:F:31:ALA:HB1	4:E:553:LEU:HD22	1.83	0.59
4:E:710:ARG:NH2	5:N:32:GLU:O	2.35	0.59
6:G:403:LYS:HG3	6:G:405:PRO:HD2	1.84	0.59
1:D:2:ASP:N	1:D:18:ALA:O	2.35	0.59
2:F:38:VAL:HG21	2:J:95:PRO:HB2	1.84	0.59
4:E:565:LYS:HZ2	4:E:566:MET:H	1.50	0.59
6:G:121:ASN:HB3	6:G:151:ASN:HA	1.84	0.59
4:C:369:ASP:HA	4:C:424:TYR:HE1	1.68	0.58
4:C:94:TYR:O	4:C:98:ALA:N	2.35	0.58
1:D:34:ILE:HG13	1:D:35:LEU:HG	1.86	0.58
2:J:52:LEU:HD11	2:J:65:SER:HB2	1.86	0.58
4:E:563:GLU:HA	4:E:576:MET:HA	1.84	0.58
4:E:171:ARG:NH2	4:E:215:THR:OG1	2.37	0.58
2:F:26:LYS:NZ	2:F:28:ASN:OD1	2.35	0.57
5:K:40:GLN:HA	5:K:75:GLY:HA3	1.86	0.57
1:D:28:LYS:NZ	1:D:42:GLN:O	2.37	0.57
4:E:444:ILE:HD13	4:E:559:LEU:HD23	1.85	0.57
4:C:330:LEU:O	4:C:332:GLN:NE2	2.38	0.57
4:E:389:GLU:OE2	4:E:393:LYS:NZ	2.30	0.57
4:C:633:ASP:H	4:C:636:SER:HB3	1.69	0.57
4:E:372:LEU:HA	4:E:375:VAL:HG12	1.86	0.57
6:G:301:ALA:HA	6:G:365:LYS:HB3	1.86	0.57
6:G:170:VAL:HG11	6:G:202:ILE:HG23	1.86	0.57
4:E:268:GLN:O	4:E:269:ARG:NE	2.37	0.57
2:J:44:ILE:HB	2:J:83:CYS:HB3	1.86	0.57
4:C:178:GLN:NE2	4:C:252:LYS:O	2.37	0.57
4:C:249:ARG:HA	4:C:252:LYS:HE3	1.87	0.57
4:C:466:GLY:HA2	4:E:428:LYS:HB2	1.87	0.56
4:E:47:VAL:HG11	6:G:617:PRO:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:530:PRO:HG3	4:E:583:ALA:HB2	1.86	0.56
4:C:671:ALA:HA	4:C:674:GLU:HB3	1.88	0.56
3:H:32:LYS:HB2	3:H:35:HIS:CD2	2.41	0.56
1:I:43:ARG:HB2	1:I:78:ALA:HB3	1.87	0.56
6:G:33:ARG:HH12	6:G:71:VAL:HA	1.70	0.56
1:D:42:GLN:HB2	1:D:77:LEU:HD12	1.86	0.56
4:E:732:GLU:OE2	4:E:742:SER:OG	2.23	0.56
4:C:556:LEU:HB2	2:J:30:VAL:HG23	1.86	0.56
4:E:32:ARG:NH2	3:H:49:PRO:O	2.38	0.56
4:C:245:ASP:OD2	4:C:249:ARG:NH2	2.38	0.56
6:A:296:LEU:HG	6:A:334:ARG:HG3	1.88	0.56
4:C:514:ALA:HA	2:J:32:LEU:HG	1.88	0.56
4:C:567:ASN:ND2	4:C:589:ASN:OD1	2.38	0.56
4:C:274:HIS:HB3	4:C:277:PHE:HB3	1.88	0.56
4:C:566:MET:HA	2:J:22:PHE:HD2	1.71	0.56
4:C:584:VAL:HG12	4:C:603:THR:HG21	1.88	0.56
4:C:2:SER:OG	4:C:3:LEU:N	2.38	0.55
1:I:49:GLN:NE2	1:I:50:LEU:O	2.39	0.55
4:E:224:SER:O	4:E:228:GLN:NE2	2.39	0.55
4:E:682:ALA:O	4:E:686:ARG:NE	2.39	0.55
4:E:354:ILE:HD12	4:E:368:LEU:HD12	1.87	0.55
6:A:529:ASP:OD1	6:A:533:ASN:N	2.39	0.55
6:G:488:LEU:HD11	6:G:515:THR:HG23	1.87	0.55
4:C:79:SER:HB2	4:C:82:GLN:HG2	1.87	0.55
4:C:486:LEU:HA	4:C:489:LYS:HB2	1.89	0.55
3:H:63:ARG:O	3:H:63:ARG:NH1	2.40	0.55
5:K:73:LEU:HD23	5:K:74:ARG:HG3	1.88	0.55
6:A:452:CYS:O	6:A:455:THR:OG1	2.23	0.55
6:G:134:LEU:HD22	6:G:168:ASP:HB2	1.88	0.55
4:C:38:ARG:NE	4:C:41:ASP:OD2	2.36	0.55
4:C:695:ARG:HG3	4:C:697:ASN:H	1.72	0.55
4:E:268:GLN:HA	4:E:272:ALA:HB3	1.89	0.55
2:F:67:GLU:HG3	2:F:82:HIS:HE1	1.72	0.55
4:C:711:PHE:HD1	4:C:713:PRO:HD3	1.71	0.55
4:C:586:LEU:HD23	2:J:22:PHE:HB2	1.88	0.54
6:G:222:PRO:HA	6:G:225:VAL:HB	1.88	0.54
4:C:329:ASN:ND2	4:C:329:ASN:O	2.37	0.54
4:E:105:TYR:HB2	4:E:139:ILE:HG21	1.89	0.54
6:A:76:THR:HB	6:A:88:GLY:HA2	1.88	0.54
4:E:696:HIS:ND1	4:E:741:TYR:OH	2.33	0.54
6:G:436:ALA:O	6:G:440:TYR:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:512:LEU:HD13	4:E:517:TRP:CD2	2.43	0.54
6:G:331:VAL:HG23	6:G:334:ARG:HE	1.72	0.54
4:C:695:ARG:O	4:C:699:LEU:N	2.37	0.54
3:H:100:ALA:HB1	6:G:605:VAL:HG22	1.89	0.54
6:A:134:LEU:HD22	6:A:168:ASP:HB2	1.90	0.54
6:A:567:ASP:OD2	6:A:599:CYS:HB3	2.08	0.54
6:G:536:LEU:HD21	6:G:589:LEU:HD11	1.89	0.54
4:E:338:LEU:HD11	4:E:711:PHE:HA	1.90	0.54
6:A:464:GLN:NE2	6:A:468:ASN:OD1	2.40	0.54
6:G:104:VAL:HG11	6:G:136:ILE:HG23	1.88	0.54
4:E:271:VAL:HG21	4:E:300:LEU:HB3	1.91	0.53
4:E:594:VAL:HB	4:E:638:PHE:HB2	1.90	0.53
6:A:133:ARG:NH2	6:A:135:ASP:OD2	2.38	0.53
3:H:68:HIS:ND1	1:I:94:SER:OG	2.36	0.53
4:E:25:VAL:HA	4:E:97:GLY:HA3	1.89	0.53
6:G:247:ARG:NH2	6:G:248:SER:OG	2.41	0.53
4:C:226:LEU:HA	4:C:229:GLU:HB3	1.89	0.53
6:G:409:CYS:HA	6:G:412:ARG:HE	1.73	0.53
2:F:75:CYS:HB3	2:F:101:TRP:HZ3	1.73	0.53
4:C:565:LYS:NZ	4:C:566:MET:O	2.41	0.53
3:B:40:GLY:HA3	3:B:111:ASP:HB2	1.89	0.53
3:B:62:PHE:HB3	3:B:65:ILE:HG12	1.89	0.53
4:C:731:ILE:HD12	4:C:743:TYR:HB3	1.91	0.53
6:A:329:LEU:HD22	6:A:347:ILE:HG12	1.90	0.53
6:G:213:ILE:HD11	6:G:222:PRO:HG2	1.91	0.53
6:G:338:ALA:HA	6:G:343:VAL:HG21	1.91	0.53
2:F:56:CYS:HA	2:F:60:GLN:HG2	1.91	0.53
6:A:78:THR:OG1	6:A:87:ASP:OD1	2.27	0.53
4:C:14:TRP:NE1	4:C:60:GLU:OE1	2.42	0.52
2:J:90:THR:HG23	2:J:91:ARG:HD3	1.91	0.52
6:A:102:GLU:HA	6:A:105:LYS:HE3	1.90	0.52
6:G:89:ALA:HB1	6:G:93:TRP:HB3	1.91	0.52
6:G:204:LYS:HG2	6:G:237:LEU:HD11	1.92	0.52
6:G:409:CYS:HA	6:G:412:ARG:HH21	1.75	0.52
1:D:9:ARG:HH21	1:D:79:PHE:HB2	1.74	0.52
1:I:14:ILE:HD13	1:I:34:ILE:HD11	1.92	0.52
4:E:223:ALA:HB2	4:E:270:MET:HG3	1.91	0.52
4:C:316:GLN:HG3	4:C:371:ALA:HB2	1.92	0.52
6:A:54:ALA:HB1	6:A:95:ALA:HB2	1.91	0.52
4:C:148:ARG:HB3	4:C:191:VAL:HG11	1.92	0.52
4:E:728:LYS:HA	6:A:561:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:LEU:HD12	1:I:75:VAL:HG13	1.92	0.51
6:A:401:THR:OG1	6:A:458:GLN:OE1	2.27	0.51
6:A:421:SER:HA	6:A:424:ARG:HD2	1.92	0.51
6:A:570:ASN:HD21	6:A:572:GLN:HB2	1.75	0.51
6:G:469:LYS:HE3	6:G:473:ASN:HD21	1.75	0.51
4:C:688:MET:HA	4:C:691:ARG:HG2	1.92	0.51
6:A:89:ALA:HB1	6:A:93:TRP:HB3	1.92	0.51
3:B:72:LYS:HD2	3:B:93:PHE:HE1	1.75	0.51
4:E:404:LYS:HG3	4:E:669:ARG:HE	1.76	0.51
6:A:232:ALA:HA	6:A:256:LEU:HD21	1.92	0.51
6:A:394:GLN:OE1	6:A:502:HIS:ND1	2.44	0.51
6:G:99:GLY:HA3	6:G:131:ASP:OD2	2.11	0.51
4:E:396:ASP:OD2	4:E:400:LYS:NZ	2.34	0.51
6:G:433:VAL:O	6:G:437:MET:N	2.36	0.51
6:G:453:ILE:HD13	6:G:506:VAL:HG11	1.92	0.51
1:D:80:ARG:HG2	1:D:85:PHE:HA	1.93	0.51
6:A:583:GLY:HA2	6:A:586:GLU:OE2	2.11	0.51
4:E:178:GLN:HG2	4:E:253:TYR:HE1	1.76	0.51
4:E:372:LEU:HD23	4:E:424:TYR:HE2	1.75	0.51
4:E:597:LYS:HA	4:E:600:GLN:HG2	1.93	0.51
4:E:731:ILE:HA	4:E:743:TYR:HA	1.93	0.51
4:C:407:THR:HG23	4:C:410:GLU:H	1.76	0.51
6:A:39:VAL:HB	6:A:46:ARG:HG2	1.93	0.51
6:A:348:ILE:HD11	6:A:387:ARG:HD2	1.92	0.51
5:N:22:LYS:HA	5:N:55:THR:HA	1.92	0.50
6:A:247:ARG:NH2	6:A:248:SER:OG	2.44	0.50
6:A:345:HIS:HA	6:A:348:ILE:HG22	1.93	0.50
4:E:574:VAL:N	4:E:649:THR:O	2.44	0.50
6:A:259:SER:OG	6:A:332:ARG:NH2	2.42	0.50
6:G:246:ARG:HH21	6:G:283:ARG:HA	1.76	0.50
2:F:49:ILE:HD11	2:F:70:VAL:HG13	1.93	0.50
6:A:404:ALA:O	6:A:408:GLU:N	2.38	0.50
4:C:148:ARG:HA	4:C:152:VAL:HB	1.94	0.50
4:C:153:GLU:OE1	4:C:156:GLN:NE2	2.44	0.50
6:A:340:ASN:HB2	6:A:343:VAL:HB	1.94	0.50
2:F:26:LYS:HB2	4:E:506:SER:HB2	1.94	0.50
4:C:34:THR:HG23	4:C:38:ARG:NH1	2.27	0.50
4:C:510:TYR:HD2	2:J:30:VAL:HG12	1.77	0.50
4:C:730:TYR:HA	5:K:74:ARG:HH21	1.77	0.50
4:E:178:GLN:HE21	4:E:252:LYS:HG2	1.77	0.50
1:I:10:HIS:H	1:I:90:ILE:HG12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:33:ARG:HH12	6:A:71:VAL:HA	1.76	0.50
6:A:555:ILE:O	6:A:559:LEU:N	2.40	0.50
4:C:472:LYS:NZ	4:C:515:GLY:O	2.37	0.50
1:I:8:ARG:HG2	1:I:13:THR:HG23	1.93	0.50
6:G:195:ALA:HB1	6:G:226:ALA:HB2	1.94	0.50
4:E:36:ASN:ND2	3:H:61:ASN:H	2.10	0.50
4:E:533:LEU:HD23	4:E:537:VAL:HG23	1.93	0.50
6:A:348:ILE:HD12	6:A:367:TRP:CD1	2.47	0.50
6:A:556:ILE:HA	6:A:559:LEU:HD12	1.94	0.50
6:G:519:LEU:HD21	6:G:562:ALA:HB2	1.94	0.50
6:G:525:VAL:HG22	6:G:564:ALA:HB2	1.93	0.50
3:B:25:ASP:OD1	3:B:25:ASP:N	2.45	0.50
4:C:21:ILE:HA	4:C:24:VAL:HB	1.93	0.50
4:C:577:VAL:HB	4:C:581:GLN:HG3	1.94	0.50
4:E:684:ILE:HD13	4:E:722:ILE:HG13	1.94	0.50
2:F:87:TRP:CE2	2:F:91:ARG:HD2	2.46	0.49
4:C:483:SER:HA	4:C:486:LEU:HB3	1.93	0.49
4:E:4:LYS:HD2	4:E:5:PRO:HD2	1.94	0.49
4:E:11:ASP:N	4:E:11:ASP:OD1	2.42	0.49
1:I:52:ASP:OD1	1:I:55:LYS:N	2.45	0.49
6:G:71:VAL:HG22	6:G:75:GLN:HE22	1.76	0.49
6:G:464:GLN:HA	6:G:467:ILE:HB	1.94	0.49
4:C:359:ASN:O	4:C:359:ASN:ND2	2.45	0.49
4:C:472:LYS:HZ2	4:C:516:ALA:HA	1.77	0.49
6:A:395:MET:HE1	6:A:402:VAL:HG22	1.93	0.49
6:G:466:LYS:HA	6:G:469:LYS:HB3	1.94	0.49
4:C:476:MET:HG2	4:C:517:TRP:CE2	2.48	0.49
3:H:25:ASP:N	3:H:25:ASP:OD1	2.43	0.49
6:G:371:LEU:HD11	6:G:381:THR:HB	1.94	0.49
4:C:9:ASP:OD1	4:C:9:ASP:N	2.45	0.49
6:G:382:HIS:CD2	6:G:439:ASN:HD21	2.30	0.49
6:G:239:LEU:HD13	6:G:249:ARG:HG3	1.93	0.49
6:G:354:TYR:HB2	6:G:363:CYS:HB3	1.93	0.49
2:F:67:GLU:HG3	2:F:82:HIS:CE1	2.48	0.49
6:G:492:VAL:HB	6:G:539:ILE:HD11	1.94	0.49
4:C:680:LEU:O	4:C:684:ILE:N	2.46	0.49
6:G:97:GLY:HA2	6:G:127:ALA:HB1	1.95	0.49
1:D:9:ARG:NH2	1:D:79:PHE:HB2	2.28	0.48
4:E:102:ASP:OD1	4:E:109:ASN:ND2	2.46	0.48
4:E:323:GLY:O	4:E:327:THR:OG1	2.23	0.48
1:D:8:ARG:NH2	1:D:91:GLU:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:37:LEU:HD22	3:B:43:LYS:HG3	1.94	0.48
4:C:331:THR:HG21	4:C:672:VAL:HG22	1.94	0.48
6:A:283:ARG:NH1	6:A:291:LEU:O	2.42	0.48
6:G:613:GLN:HA	6:G:621:GLU:OE2	2.14	0.48
1:D:15:PHE:HE2	3:B:75:MET:HG3	1.79	0.48
4:C:350:PHE:O	4:C:354:ILE:HG12	2.13	0.48
2:J:47:ASN:ND2	2:J:52:LEU:O	2.44	0.48
4:E:222:GLU:OE2	4:E:242:ARG:NE	2.33	0.48
4:E:250:CYS:HB2	4:E:254:LEU:HD12	1.95	0.48
4:C:686:ARG:HH11	5:K:37:PRO:HG3	1.79	0.48
6:G:206:LEU:HB3	6:G:211:ALA:HB2	1.95	0.48
4:E:189:VAL:HG11	4:E:255:HIS:CD2	2.49	0.48
2:F:27:TRP:CZ3	4:E:533:LEU:HD21	2.49	0.48
4:C:109:ASN:HA	4:C:113:ILE:HB	1.94	0.48
4:E:23:ALA:HB1	4:E:28:GLU:HB3	1.95	0.48
6:G:66:LEU:HD11	6:G:107:LEU:HD23	1.94	0.48
6:G:181:ASN:O	6:G:183:LYS:NZ	2.46	0.48
1:I:32:GLU:HA	1:I:37:ARG:H	1.78	0.48
6:G:283:ARG:NH1	6:G:291:LEU:O	2.41	0.48
6:G:537:HIS:HA	6:G:576:PRO:HB3	1.96	0.48
4:C:544:TYR:OH	4:C:551:ARG:NH1	2.46	0.48
4:E:403:ALA:HB2	4:E:665:MET:HG2	1.95	0.48
4:E:596:TYR:HD2	4:E:634:ALA:HA	1.79	0.48
6:A:10:LYS:NZ	6:A:14:GLU:OE2	2.46	0.48
2:F:42:CYS:SG	2:F:80:HIS:N	2.82	0.47
6:A:121:ASN:HB3	6:A:151:ASN:HA	1.95	0.47
2:F:37:ILE:HG13	2:F:38:VAL:HG23	1.96	0.47
4:C:223:ALA:HB1	4:C:274:HIS:HE1	1.80	0.47
4:E:490:PHE:O	4:E:494:ILE:HG13	2.14	0.47
4:E:182:HIS:O	4:E:182:HIS:ND1	2.48	0.47
4:E:560:CYS:SG	4:E:579:THR:OG1	2.50	0.47
6:G:250:ILE:HG23	6:G:279:ALA:HB1	1.95	0.47
2:F:45:CYS:HB2	2:F:54:ILE:HB	1.95	0.47
4:C:469:PHE:HD2	4:C:470:THR:HG23	1.80	0.47
4:E:673:ASP:HA	4:E:676:ARG:HD2	1.97	0.47
1:D:7:ILE:HG23	1:D:77:LEU:HD23	1.97	0.47
1:D:68:ARG:HG3	1:D:71:ALA:H	1.80	0.47
4:C:548:PHE:HB3	4:C:551:ARG:HD2	1.96	0.47
4:C:556:LEU:HD11	2:J:32:LEU:HD13	1.97	0.47
4:E:183:GLY:O	4:E:187:SER:OG	2.32	0.47
6:A:201:ASP:OD1	6:A:201:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:150:ALA:HB2	6:G:156:THR:HG22	1.97	0.47
6:G:407:ILE:HA	6:G:410:VAL:HG12	1.96	0.47
4:E:629:LYS:HZ1	4:E:633:ASP:HB3	1.80	0.47
6:G:113:ASN:HB3	6:G:116:HIS:HB2	1.95	0.47
2:F:44:ILE:HB	2:F:83:CYS:HB3	1.96	0.47
4:C:521:GLN:NE2	4:C:522:ALA:O	2.43	0.47
3:H:28:GLU:OE1	3:H:28:GLU:N	2.41	0.47
6:G:489:HIS:CE1	6:G:538:ILE:HG13	2.50	0.47
4:E:111:GLN:HG3	6:G:619:THR:HG21	1.96	0.47
4:E:245:ASP:OD2	4:E:249:ARG:NH2	2.48	0.47
3:H:46:LEU:HA	3:H:52:PHE:HE1	1.78	0.47
4:E:283:HIS:CE1	4:E:287:ARG:HH21	2.33	0.46
3:H:105:MET:HG2	6:G:617:PRO:HD2	1.97	0.46
6:A:192:HIS:HD2	6:A:216:ASN:HD22	1.62	0.46
6:A:492:VAL:HG11	6:A:535:ALA:HB1	1.97	0.46
4:E:105:TYR:CD2	4:E:139:ILE:HG12	2.51	0.46
1:I:42:GLN:HB2	1:I:77:LEU:HD11	1.96	0.46
6:A:314:LEU:HD12	6:A:317:ILE:HD11	1.96	0.46
6:G:82:ASP:OD1	6:G:82:ASP:N	2.44	0.46
2:F:87:TRP:CE2	2:F:95:PRO:HB3	2.50	0.46
1:I:28:LYS:HB3	1:I:42:GLN:HE21	1.80	0.46
1:I:45:TYR:O	1:I:76:GLY:N	2.32	0.46
6:A:115:ASN:ND2	6:A:144:ASN:O	2.48	0.46
6:G:392:PHE:HE2	6:G:410:VAL:HG11	1.80	0.46
4:C:171:ARG:NH1	4:C:246:GLU:OE1	2.48	0.46
4:C:355:ASN:HD21	4:E:355:ASN:ND2	2.14	0.46
4:E:584:VAL:HG22	4:E:603:THR:HG21	1.97	0.46
6:A:268:ASP:N	6:A:268:ASP:OD1	2.48	0.46
6:G:184:ALA:N	6:G:188:ALA:O	2.41	0.46
1:D:31:VAL:HB	1:D:35:LEU:HD12	1.96	0.46
4:C:377:ASN:ND2	4:C:425:ILE:O	2.35	0.46
1:D:12:THR:HA	3:B:28:GLU:HB3	1.97	0.46
4:C:230:SER:HB2	4:C:234:GLN:HB2	1.97	0.46
4:E:694:LEU:HD12	4:E:694:LEU:HA	1.82	0.46
6:G:163:TYR:HB2	6:G:193:PHE:HB3	1.97	0.46
6:G:167:THR:HG22	6:G:171:ARG:HG3	1.97	0.46
6:G:233:ASP:N	6:G:233:ASP:OD1	2.48	0.46
6:G:446:THR:O	6:G:450:LEU:N	2.48	0.46
2:J:45:CYS:HB2	2:J:54:ILE:H	1.80	0.46
3:H:45:MET:SD	3:H:62:PHE:HE1	2.39	0.46
4:C:223:ALA:HB1	4:C:274:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:203:TYR:O	4:E:208:GLU:HB2	2.16	0.45
6:A:596:SER:OG	6:A:599:CYS:SG	2.70	0.45
6:G:529:ASP:OD1	6:G:533:ASN:N	2.31	0.45
3:B:21:LEU:HD22	3:B:70:LEU:HD11	1.97	0.45
2:J:39:VAL:HG11	2:J:48:HIS:CE1	2.51	0.45
4:E:289:GLU:OE2	4:E:349:LYS:NZ	2.47	0.45
4:E:455:GLU:HB2	4:E:477:TYR:CZ	2.52	0.45
4:E:685:VAL:HG21	5:N:73:LEU:HB3	1.97	0.45
6:A:184:ALA:N	6:A:188:ALA:O	2.43	0.45
3:B:103:LEU:HD21	6:A:597:LEU:HD11	1.98	0.45
6:G:286:ASP:HB3	6:G:289:ASN:HB2	1.98	0.45
2:F:27:TRP:HB2	4:E:505:ILE:HD11	1.99	0.45
4:C:304:VAL:HG12	4:C:306:THR:H	1.82	0.45
4:E:236:MET:HB3	4:E:296:ASN:HB3	1.98	0.45
4:C:530:PRO:HD2	4:C:533:LEU:HD21	1.98	0.45
4:E:203:TYR:CE2	4:E:255:HIS:HB3	2.52	0.45
4:E:403:ALA:HB3	4:E:669:ARG:HG3	1.98	0.45
4:E:13:THR:OG1	4:E:41:ASP:OD1	2.35	0.45
4:E:695:ARG:HG3	4:E:739:ASP:HB3	1.99	0.45
5:K:23:VAL:HA	5:K:56:ALA:HB2	1.98	0.45
6:G:382:HIS:CG	6:G:439:ASN:HD21	2.35	0.45
4:C:595:SER:HA	4:C:637:SER:HA	1.98	0.45
3:B:19:VAL:HG11	3:B:46:LEU:HD21	1.98	0.45
4:E:72:LEU:HD11	4:E:90:TYR:CG	2.52	0.45
6:A:299:ILE:HB	6:A:302:TYR:HD2	1.81	0.45
6:G:549:PHE:HE1	6:G:588:LEU:HD11	1.81	0.45
4:C:512:LEU:HB3	4:C:517:TRP:NE1	2.32	0.44
4:E:135:PRO:HB2	4:E:136:LEU:H	1.54	0.44
1:I:2:ASP:N	1:I:2:ASP:OD1	2.50	0.44
6:G:46:ARG:NH1	6:G:78:THR:OG1	2.49	0.44
6:G:390:GLN:HB3	6:G:501:PHE:HD2	1.82	0.44
1:D:7:ILE:HA	1:D:75:VAL:HG13	1.99	0.44
4:C:340:VAL:HG21	4:C:394:TYR:CG	2.53	0.44
4:C:414:ARG:O	4:C:418:PHE:N	2.50	0.44
4:E:565:LYS:NZ	4:E:573:TYR:O	2.48	0.44
6:A:135:ASP:OD1	6:A:135:ASP:N	2.45	0.44
6:G:454:SER:O	6:G:457:THR:OG1	2.34	0.44
4:E:282:CYS:HA	4:E:285:ILE:HG22	1.99	0.44
4:E:458:ILE:HD12	4:E:473:LEU:HB3	2.00	0.44
4:E:704:ILE:HG12	4:E:713:PRO:HG2	1.99	0.44
6:A:170:VAL:HG11	6:A:202:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ILE:HD11	1:D:35:LEU:HD21	1.99	0.44
4:C:685:VAL:HG11	5:K:73:LEU:HG	1.99	0.44
1:I:28:LYS:HE3	1:I:44:LEU:HG	2.00	0.44
6:G:114:VAL:HG13	6:G:140:LEU:HD22	1.99	0.44
4:C:428:LYS:HB2	4:E:466:GLY:HA2	1.99	0.44
4:E:527:PHE:HE2	4:E:530:PRO:HD3	1.81	0.44
4:E:529:ILE:HD13	4:E:537:VAL:HG11	1.99	0.44
4:E:687:ILE:HG21	4:E:694:LEU:HD22	1.99	0.44
3:H:94:PRO:HD3	1:I:70:GLN:HE21	1.82	0.44
3:H:88:THR:OG1	3:H:89:GLU:N	2.49	0.44
1:D:2:ASP:HB3	1:D:20:GLU:HG2	2.00	0.44
2:F:75:CYS:HB3	2:F:101:TRP:CZ3	2.53	0.44
4:E:679:TYR:HE2	4:E:707:SER:HB3	1.82	0.44
3:H:27:HIS:HB3	3:H:29:PHE:HE1	1.83	0.44
6:A:82:ASP:OD1	6:A:82:ASP:N	2.50	0.44
6:G:192:HIS:CE1	6:G:222:PRO:HG3	2.53	0.44
6:G:540:VAL:HB	6:G:580:SER:HA	2.00	0.44
4:E:675:ASP:HA	4:E:678:MET:HB3	2.00	0.44
6:A:54:ALA:HA	6:A:103:VAL:HG11	2.00	0.44
6:A:168:ASP:OD1	6:A:169:VAL:N	2.50	0.44
6:A:542:TYR:HD2	6:A:552:LEU:HD12	1.81	0.44
6:G:452:CYS:O	6:G:455:THR:OG1	2.34	0.44
4:C:84:LEU:HG	4:C:162:MET:SD	2.58	0.43
4:C:315:LEU:HD23	4:C:364:PHE:HD1	1.83	0.43
4:E:354:ILE:HG22	4:E:360:GLY:HA2	1.99	0.43
6:G:135:ASP:HA	6:G:138:LYS:HE2	2.00	0.43
4:E:45:LEU:HD23	4:E:45:LEU:HA	1.82	0.43
3:H:68:HIS:HA	1:I:93:PHE:HB3	2.00	0.43
5:K:44:ILE:HA	5:K:49:GLN:HA	1.99	0.43
4:E:380:GLU:HB2	4:E:383:SER:HB3	2.00	0.43
3:H:56:GLU:HG2	3:H:57:THR:HG23	1.99	0.43
2:F:24:VAL:HA	4:E:564:VAL:HA	1.99	0.43
4:C:18:LEU:HA	4:C:21:ILE:HG12	2.01	0.43
4:E:32:ARG:NH2	3:H:52:PHE:H	2.17	0.43
6:A:374:ARG:NE	6:A:384:ASP:OD2	2.52	0.43
6:G:530:ASN:O	6:G:571:LYS:NZ	2.47	0.43
6:A:560:VAL:HG11	6:A:592:GLN:HB3	2.00	0.43
6:G:463:ASP:O	6:G:467:ILE:N	2.41	0.43
6:G:526:ASN:ND2	6:G:568:MET:SD	2.92	0.43
4:C:494:ILE:HD11	4:C:503:LEU:HD11	2.00	0.43
4:E:219:TYR:OH	4:E:246:GLU:OE1	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:696:HIS:HB2	4:E:739:ASP:HA	2.00	0.43
4:C:441:LYS:HA	4:C:441:LYS:HD3	1.92	0.43
4:C:593:THR:HA	4:C:639:SER:HA	2.01	0.43
4:C:700:ILE:HG13	4:C:715:ILE:HG13	2.00	0.43
4:E:324:LEU:HD12	4:E:375:VAL:HG23	2.01	0.43
3:H:31:VAL:HG12	1:I:15:PHE:HB2	2.01	0.43
6:A:92:LEU:HD11	6:A:104:VAL:HG13	2.00	0.43
6:A:433:VAL:HA	6:A:436:ALA:HB3	2.00	0.43
4:E:577:VAL:HG12	4:E:653:ILE:HG13	2.01	0.43
4:E:621:LYS:HD3	4:E:621:LYS:HA	1.80	0.43
4:E:665:MET:SD	4:E:665:MET:N	2.90	0.43
6:A:616:ILE:HD12	6:A:620:LEU:HB3	1.99	0.43
3:B:37:LEU:HD21	3:B:46:LEU:HD22	2.01	0.43
3:B:72:LYS:HA	3:B:72:LYS:HD3	1.91	0.43
4:C:559:LEU:HD22	2:J:30:VAL:HG21	2.01	0.43
4:E:18:LEU:HA	4:E:21:ILE:HG22	2.01	0.43
6:A:560:VAL:HA	6:A:564:ALA:HB3	2.01	0.43
6:A:616:ILE:HB	6:A:620:LEU:HD23	2.00	0.43
6:G:491:ALA:HA	6:G:509:PHE:HE1	1.84	0.43
6:G:579:LYS:HD2	6:G:579:LYS:O	2.18	0.43
4:E:27:LEU:HD23	4:E:93:GLU:HA	2.01	0.43
4:E:251:ARG:HA	4:E:259:TYR:CZ	2.54	0.43
4:E:643:ASN:OD1	4:E:643:ASN:N	2.51	0.43
3:H:74:CYS:HA	3:H:77:PHE:CD2	2.54	0.43
6:A:332:ARG:CZ	6:A:346:PRO:HG2	2.49	0.43
6:G:390:GLN:HG2	6:G:499:ASP:OD2	2.18	0.43
2:F:44:ILE:HA	2:J:37:ILE:HD12	2.01	0.42
4:C:541:GLU:OE2	4:C:555:TRP:NE1	2.42	0.42
4:E:596:TYR:CD2	4:E:634:ALA:HA	2.54	0.42
6:A:320:ASP:HB3	6:A:323:ALA:HB3	2.01	0.42
6:G:268:ASP:OD1	6:G:268:ASP:N	2.50	0.42
4:C:509:ILE:HG12	4:C:540:PHE:CZ	2.54	0.42
4:E:386:LYS:O	4:E:390:LEU:HD13	2.19	0.42
6:A:181:ASN:O	6:A:183:LYS:NZ	2.52	0.42
6:A:268:ASP:OD2	6:A:271:LYS:HB2	2.18	0.42
6:G:371:LEU:HD22	6:G:388:PHE:HE2	1.84	0.42
3:B:48:GLY:HA3	4:C:32:ARG:HH22	1.83	0.42
6:A:307:GLU:OE2	6:A:331:VAL:HA	2.19	0.42
4:E:585:LEU:HA	4:E:588:PHE:HB3	2.01	0.42
3:H:38:THR:OG1	3:H:80:LYS:NZ	2.35	0.42
5:K:3:ILE:H	5:K:14:GLU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:333:GLU:HG3	6:A:338:ALA:HB2	2.00	0.42
6:G:433:VAL:HA	6:G:436:ALA:HB3	2.01	0.42
6:G:534:SER:H	6:G:537:HIS:HB3	1.83	0.42
1:D:2:ASP:HB2	1:D:19:LYS:HD3	2.01	0.42
4:E:66:GLU:OE2	4:E:70:ARG:NH1	2.52	0.42
6:G:262:ASN:HA	6:G:350:ARG:HH21	1.83	0.42
6:G:192:HIS:CD2	6:G:216:ASN:HB3	2.54	0.42
6:G:582:THR:HB	6:G:585:SER:HB3	2.01	0.42
2:F:84:ILE:HG13	2:F:88:LEU:HD23	2.02	0.42
2:J:105:LYS:HE2	2:J:105:LYS:HB2	1.92	0.42
4:E:144:LEU:HD23	4:E:144:LEU:HA	1.90	0.42
4:E:580:TYR:HB3	4:E:613:THR:HG21	2.02	0.42
3:H:37:LEU:HD12	3:H:37:LEU:HA	1.84	0.42
6:G:348:ILE:HD11	6:G:387:ARG:HH12	1.85	0.42
4:C:292:ASN:O	4:C:296:ASN:ND2	2.53	0.42
4:C:395:CYS:HG	4:C:435:TYR:HE2	1.68	0.42
4:C:689:LYS:NZ	5:K:76:GLY:O	2.51	0.42
4:E:413:ASP:O	4:E:416:THR:OG1	2.32	0.42
4:E:418:PHE:HD2	4:E:457:MET:HE1	1.83	0.42
4:E:577:VAL:HB	4:E:581:GLN:HB2	2.02	0.42
3:H:91:PRO:HD2	1:I:68:ARG:NH2	2.29	0.42
6:A:233:ASP:OD1	6:A:233:ASP:N	2.49	0.42
6:G:254:GLU:HG2	6:G:276:LEU:HD13	2.02	0.42
4:C:614:ILE:HG21	4:C:638:PHE:CZ	2.55	0.42
6:G:254:GLU:HG3	6:G:279:ALA:HB3	2.02	0.42
4:C:562:GLY:O	4:C:577:VAL:N	2.32	0.41
4:C:713:PRO:HG2	4:C:718:ILE:HD11	2.02	0.41
6:A:99:GLY:HA3	6:A:131:ASP:OD2	2.20	0.41
4:C:50:PRO:O	6:A:618:ARG:NH1	2.53	0.41
4:C:571:LYS:HB3	4:C:573:TYR:CZ	2.56	0.41
4:E:178:GLN:HG2	4:E:253:TYR:CE1	2.55	0.41
4:E:512:LEU:HD22	4:E:517:TRP:CE2	2.55	0.41
6:A:48:THR:HG23	6:A:51:ILE:HD12	2.02	0.41
4:E:105:TYR:HD2	4:E:139:ILE:HG12	1.84	0.41
1:I:34:ILE:HG13	1:I:35:LEU:HD12	2.01	0.41
5:K:15:ILE:HA	5:K:30:VAL:HA	2.02	0.41
6:A:415:VAL:HG12	6:A:474:LEU:HB2	2.01	0.41
6:G:17:VAL:HG13	6:G:64:LEU:HD22	2.03	0.41
6:G:268:ASP:OD2	6:G:271:LYS:HD2	2.20	0.41
4:C:192:GLU:HG3	4:C:202:PHE:HB2	2.03	0.41
4:C:423:LYS:O	4:C:428:LYS:NZ	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:587:ILE:HD12	6:A:587:ILE:HA	1.94	0.41
6:G:371:LEU:HD12	6:G:371:LEU:HA	1.88	0.41
4:C:354:ILE:HG22	4:C:360:GLY:HA2	2.02	0.41
4:C:601:ASP:OD1	4:C:601:ASP:N	2.44	0.41
4:E:286:ILE:HD11	4:E:315:LEU:HD13	2.02	0.41
6:G:92:LEU:HD13	6:G:107:LEU:HB2	2.03	0.41
6:G:174:LEU:HD21	6:G:206:LEU:HD23	2.02	0.41
6:G:536:LEU:HD13	6:G:559:LEU:HB2	2.01	0.41
4:C:533:LEU:HD12	2:J:27:TRP:CE2	2.56	0.41
4:C:670:SER:O	4:C:674:GLU:N	2.48	0.41
4:E:167:ILE:HG12	4:E:211:PHE:HE1	1.85	0.41
6:G:468:ASN:HA	6:G:471:ILE:HD12	2.03	0.41
6:G:518:LEU:HD23	6:G:518:LEU:HA	1.91	0.41
6:G:620:LEU:HD12	6:G:623:PHE:HB3	2.03	0.41
1:D:14:ILE:HG13	3:B:30:ILE:HB	2.02	0.41
3:H:31:VAL:HG11	3:H:74:CYS:HB2	2.03	0.41
6:A:78:THR:HA	6:A:87:ASP:HA	2.03	0.41
6:G:345:HIS:O	6:G:348:ILE:HG22	2.21	0.41
6:G:485:PHE:HB3	6:G:489:HIS:HB3	2.02	0.41
4:E:10:PHE:HB2	4:E:53:LEU:HD13	2.01	0.41
4:E:286:ILE:HG13	4:E:294:MET:HE1	2.01	0.41
6:A:589:LEU:O	6:A:593:MET:N	2.54	0.41
6:G:78:THR:OG1	6:G:87:ASP:OD1	2.30	0.41
3:B:40:GLY:N	3:B:111:ASP:O	2.46	0.41
4:C:87:TYR:HD2	4:C:184:VAL:HG22	1.86	0.41
4:C:209:SER:OG	4:C:210:PRO:HD3	2.21	0.41
4:C:218:TYR:O	4:C:221:GLN:HG3	2.20	0.41
4:E:35:TRP:CD2	3:H:49:PRO:HD3	2.55	0.41
4:E:443:LEU:HB3	4:E:480:MET:HG3	2.02	0.41
3:H:52:PHE:CD2	3:H:58:ASN:HA	2.55	0.41
6:G:329:LEU:HA	6:G:329:LEU:HD23	1.83	0.41
6:G:444:LEU:HD22	6:G:487:LEU:HD12	2.02	0.41
4:C:74:LYS:HA	4:C:77:LEU:HD12	2.03	0.41
6:G:232:ALA:HA	6:G:256:LEU:HD21	2.03	0.41
4:E:408:GLU:O	4:E:412:GLU:HG2	2.21	0.40
6:G:415:VAL:O	6:G:419:GLU:N	2.44	0.40
4:C:509:ILE:HD12	4:C:509:ILE:HA	1.91	0.40
4:E:21:ILE:HD11	4:E:101:MET:SD	2.61	0.40
6:G:228:GLU:HG3	6:G:336:LEU:HD21	2.04	0.40
4:C:519:LEU:HD11	2:J:32:LEU:HD11	2.03	0.40
4:C:625:HIS:HA	4:C:638:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:3:LEU:HD12	3:H:105:MET:SD	2.62	0.40
6:G:598:LYS:HG2	6:G:623:PHE:CE2	2.56	0.40
6:G:602:ALA:HA	6:G:605:VAL:HB	2.02	0.40
2:F:26:LYS:HG2	4:E:563:GLU:HG2	2.02	0.40
4:E:32:ARG:HD2	3:H:52:PHE:CZ	2.57	0.40
4:E:505:ILE:HG23	4:E:507:PHE:HB2	2.04	0.40
1:I:38:PRO:HD2	1:I:41:GLU:HG3	2.02	0.40
1:D:42:GLN:HA	1:D:78:ALA:O	2.22	0.40
2:F:22:PHE:CD2	4:E:589:ASN:HB2	2.50	0.40
4:C:155:LEU:HG	4:C:159:LEU:HD23	2.02	0.40
4:C:275:LEU:HD21	4:C:304:VAL:HG11	2.04	0.40
4:E:148:ARG:HB3	4:E:191:VAL:HG11	2.03	0.40
4:E:291:LYS:HE2	4:E:357:VAL:HG21	2.03	0.40
4:E:727:ASP:N	4:E:727:ASP:OD1	2.54	0.40
6:G:261:ALA:HB2	6:G:272:THR:HG21	2.03	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	D	89/118 (75%)	85 (96%)	4 (4%)	0	100	100
1	I	89/118 (75%)	82 (92%)	7 (8%)	0	100	100
2	F	83/96 (86%)	71 (86%)	12 (14%)	0	100	100
2	J	82/96 (85%)	79 (96%)	3 (4%)	0	100	100
3	B	94/96 (98%)	87 (93%)	7 (7%)	0	100	100
3	H	94/96 (98%)	77 (82%)	17 (18%)	0	100	100
4	C	714/750 (95%)	666 (93%)	48 (7%)	0	100	100
4	E	714/750 (95%)	673 (94%)	41 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	74/76 (97%)	64 (86%)	10 (14%)	0	100	100
5	N	74/76 (97%)	63 (85%)	11 (15%)	0	100	100
6	A	625/627 (100%)	597 (96%)	28 (4%)	0	100	100
6	G	625/627 (100%)	590 (94%)	35 (6%)	0	100	100
All	All	3357/3526 (95%)	3134 (93%)	223 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	D	81/103 (79%)	81 (100%)	0	100	100
1	I	81/103 (79%)	80 (99%)	1 (1%)	67	79
2	F	73/82 (89%)	73 (100%)	0	100	100
2	J	71/82 (87%)	71 (100%)	0	100	100
3	B	85/85 (100%)	85 (100%)	0	100	100
3	H	85/85 (100%)	84 (99%)	1 (1%)	67	79
4	C	658/679 (97%)	655 (100%)	3 (0%)	86	90
4	E	658/679 (97%)	657 (100%)	1 (0%)	92	94
5	K	8/66 (12%)	8 (100%)	0	100	100
5	N	9/66 (14%)	9 (100%)	0	100	100
6	A	535/536 (100%)	533 (100%)	2 (0%)	89	91
6	G	535/536 (100%)	531 (99%)	4 (1%)	81	86
All	All	2879/3102 (93%)	2867 (100%)	12 (0%)	88	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	329	ASN

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Mol	Chain	Res	Type
4	C	359	ASN
4	C	720	LYS
4	E	386	LYS
3	H	82	ARG
1	I	68	ARG
6	A	55	ARG
6	A	376	LYS
6	G	55	ARG
6	G	376	LYS
6	G	412	ARG
6	G	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	329	ASN
4	C	667	GLN
4	E	36	ASN
4	E	355	ASN
1	I	42	GLN
6	G	382	HIS
6	G	470	GLN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.