



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 09:41 pm GMT

PDB ID : 6F9C
EMDB ID: : EMD-4198
Title : Model of the Rift Valley fever virus glycoprotein hexamer type 1
Authors : Halldorsson, S.; Bowden, T.A.; Huiskonen, J.T.
Deposited on : 2017-12-14
Resolution : 8.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

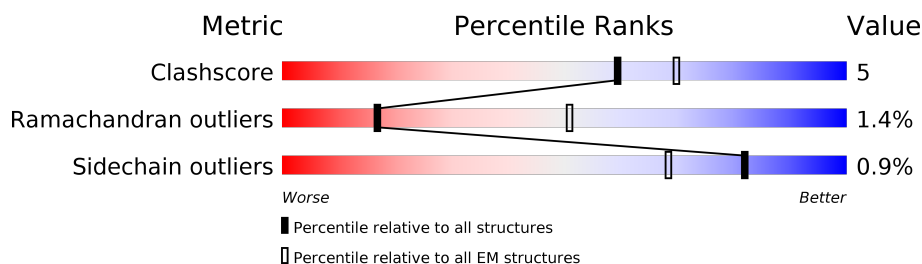
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	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	316	81% 14% 5%
1	C	316	81% 14% • 5%
1	E	316	82% 13% • 5%
1	G	316	82% 13% • 5%
1	I	316	78% 16% • 5%
1	K	316	83% 12% 5%
2	B	431	86% 14%
2	D	431	82% 18%
2	F	431	83% 17%

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Mol	Chain	Length	Quality of chain	
2	H	431		16%
2	J	431		16%
2	L	431		17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33048 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 Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	C	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	E	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	G	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	I	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	K	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		

- Molecule 2 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	D	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	F	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	H	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	J	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	L	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	688	ASP	-	expression tag	UNP A2T072
B	689	PRO	-	expression tag	UNP A2T072

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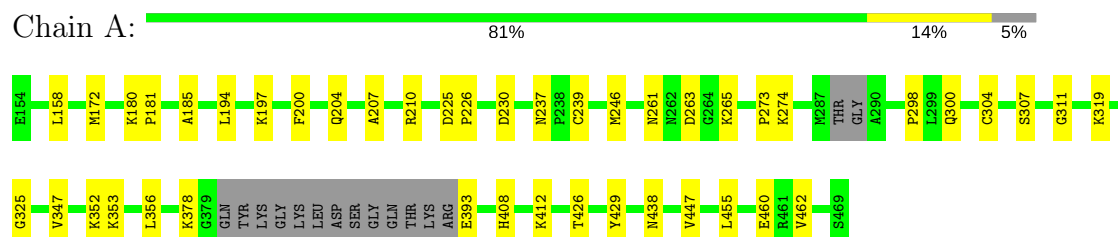
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Chain	Residue	Modelled	Actual	Comment	Reference
B	690	GLY	-	expression tag	UNP A2T072
D	688	ASP	-	expression tag	UNP A2T072
D	689	PRO	-	expression tag	UNP A2T072
D	690	GLY	-	expression tag	UNP A2T072
F	688	ASP	-	expression tag	UNP A2T072
F	689	PRO	-	expression tag	UNP A2T072
F	690	GLY	-	expression tag	UNP A2T072
H	688	ASP	-	expression tag	UNP A2T072
H	689	PRO	-	expression tag	UNP A2T072
H	690	GLY	-	expression tag	UNP A2T072
J	688	ASP	-	expression tag	UNP A2T072
J	689	PRO	-	expression tag	UNP A2T072
J	690	GLY	-	expression tag	UNP A2T072
L	688	ASP	-	expression tag	UNP A2T072
L	689	PRO	-	expression tag	UNP A2T072
L	690	GLY	-	expression tag	UNP A2T072

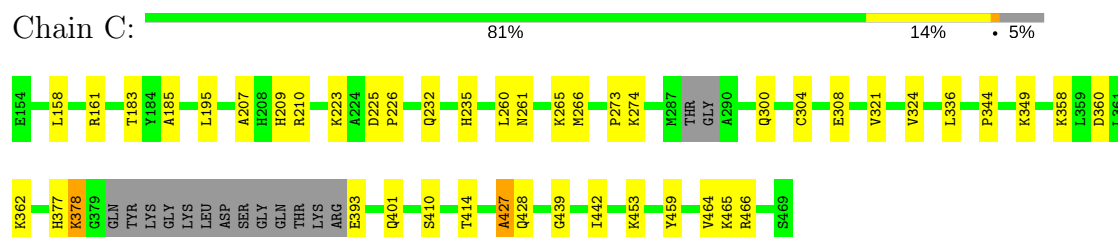
3 Residue-property plots [i](#)

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.

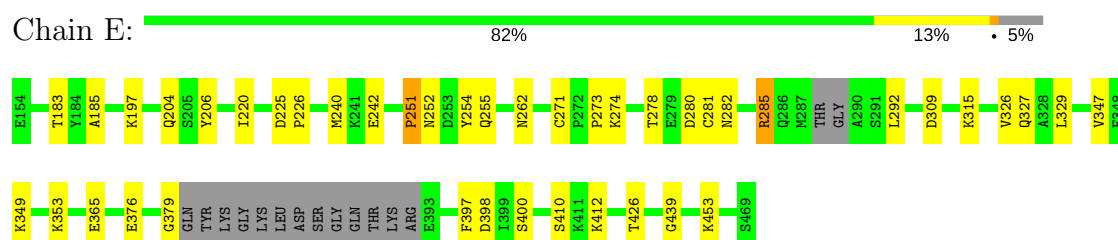
- Molecule 1: Glycoprotein



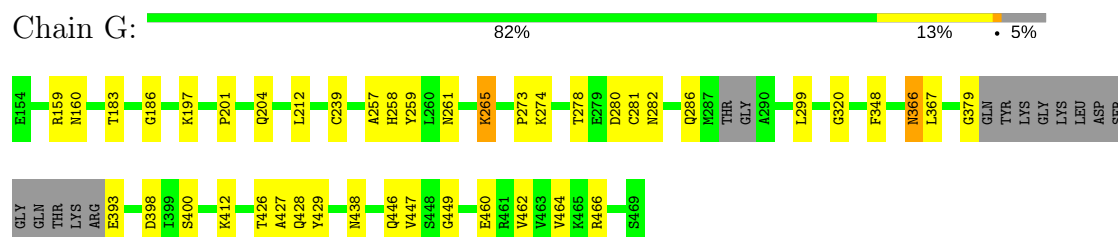
- Molecule 1: Glycoprotein



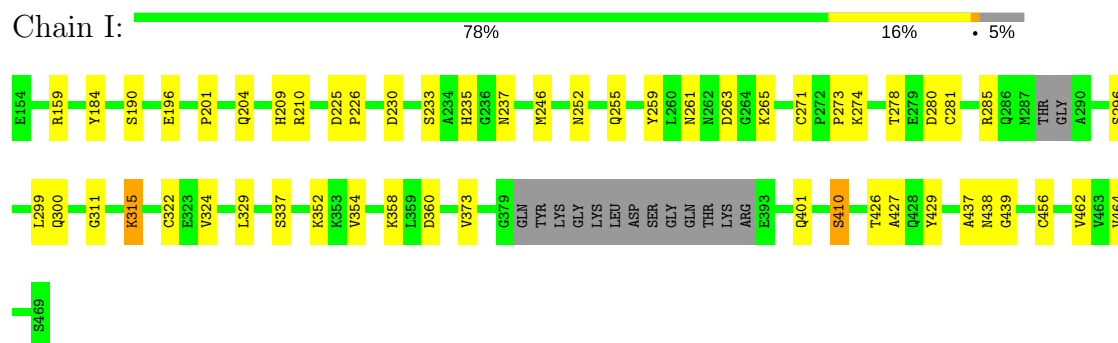
- Molecule 1: Glycoprotein



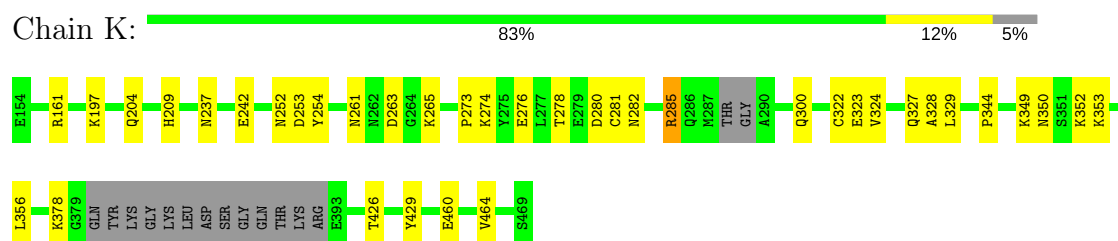
- Molecule 1: Glycoprotein



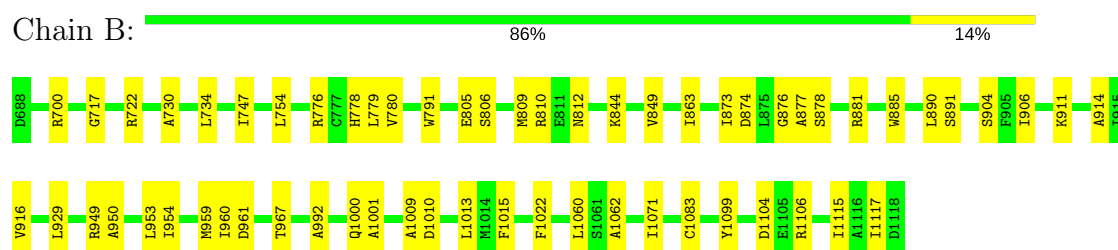
- Molecule 1: Glycoprotein



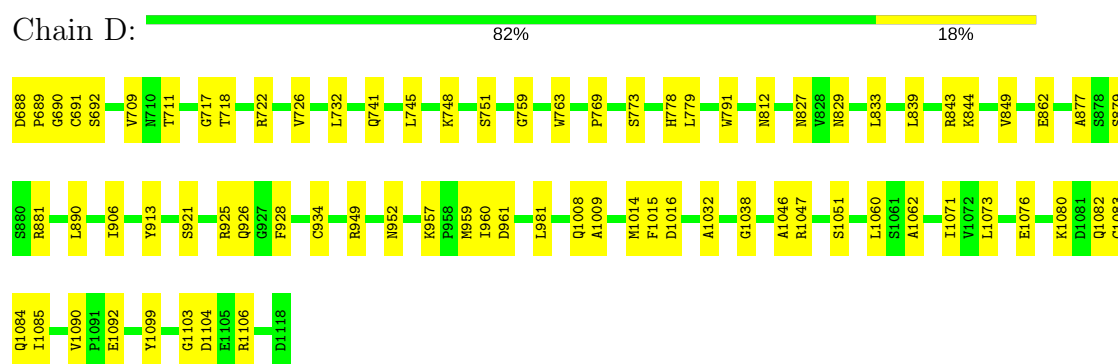
- Molecule 1: Glycoprotein



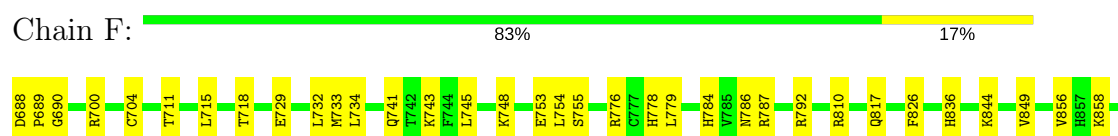
- Molecule 2: Glycoprotein

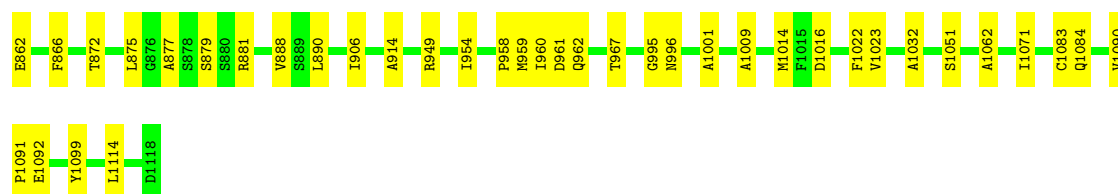


- Molecule 2: Glycoprotein



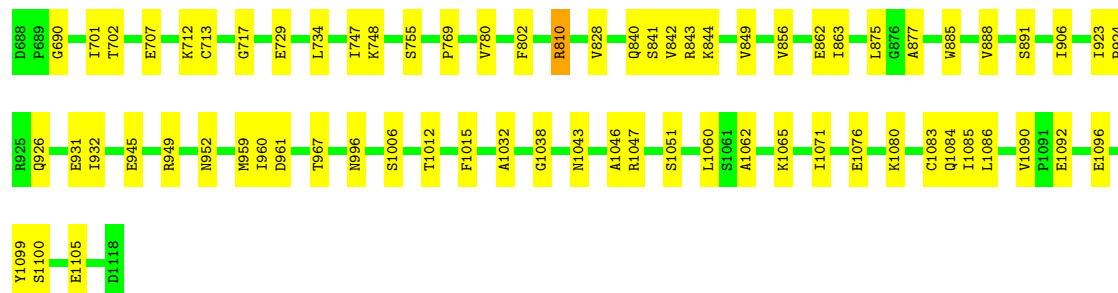
- Molecule 2: Glycoprotein





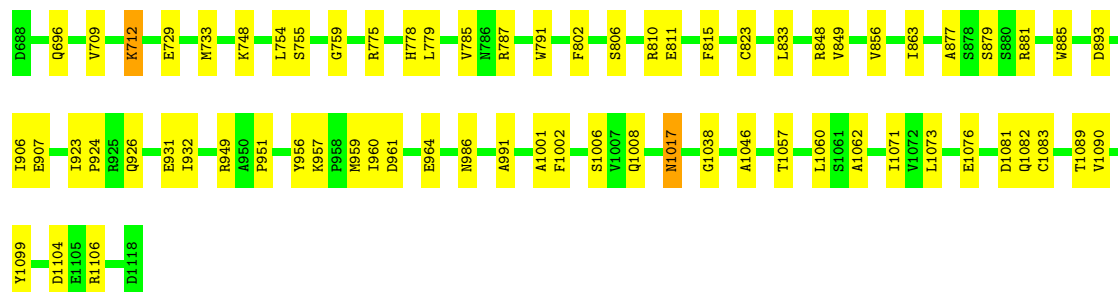
• Molecule 2: Glycoprotein

Chain H: 84% 16%



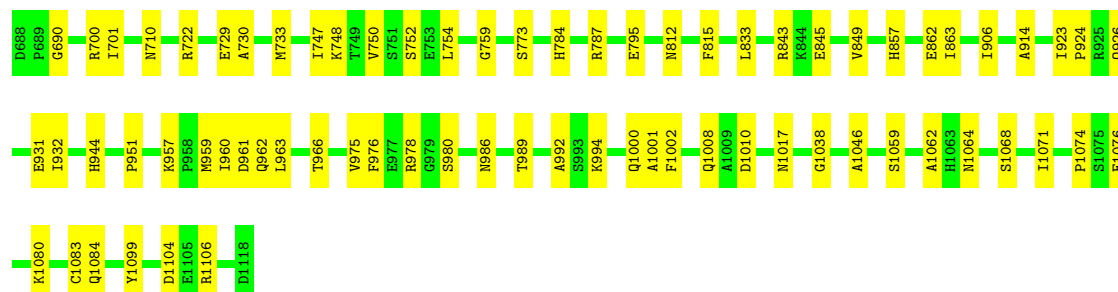
• Molecule 2: Glycoprotein

Chain J: 84% 16%



• Molecule 2: Glycoprotein

Chain L: 83% 17%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	55710	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	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 [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/2333	0.41	0/3136
1	C	0.24	0/2333	0.41	0/3136
1	E	0.24	0/2333	0.40	0/3136
1	G	0.24	0/2333	0.40	0/3136
1	I	0.24	0/2333	0.40	0/3136
1	K	0.24	0/2333	0.40	0/3136
2	B	0.24	0/3284	0.42	0/4431
2	D	0.24	0/3284	0.43	0/4431
2	F	0.24	0/3284	0.43	0/4431
2	H	0.24	0/3284	0.42	0/4431
2	J	0.24	0/3284	0.42	0/4431
2	L	0.24	0/3284	0.42	0/4431
All	All	0.24	0/33702	0.41	0/45402

There are no bond length outliers.

There are no bond angle outliers.

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	A	2284	0	2205	24	0
1	C	2284	0	2205	25	0
1	E	2284	0	2205	24	0
1	G	2284	0	2205	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2284	0	2205	25	0
1	K	2284	0	2205	17	0
2	B	3224	0	3071	29	0
2	D	3224	0	3071	37	0
2	F	3224	0	3071	39	0
2	H	3224	0	3071	38	0
2	J	3224	0	3071	34	0
2	L	3224	0	3071	35	0
All	All	33048	0	31656	334	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 5.

All (334) 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)
1:A:412:LYS:HD2	1:A:426:THR:HG21	1.76	0.68
1:A:261:ASN:HD21	1:A:265:LYS:HB2	1.60	0.66
2:L:843:ARG:HG3	2:L:845:GLU:H	1.61	0.65
1:E:262:ASN:HD22	1:E:326:VAL:HG22	1.60	0.65
2:L:1064:ASN:HD21	2:L:1068:SER:H	1.44	0.65
2:H:1062:ALA:HB3	2:H:1071:ILE:HB	1.80	0.63
2:D:1032:ALA:HB3	2:D:1051:SER:HB2	1.81	0.62
2:J:1062:ALA:HB3	2:J:1071:ILE:HB	1.81	0.62
1:C:377:HIS:HB3	1:E:285:ARG:HH21	1.65	0.62
2:F:1062:ALA:HB3	2:F:1071:ILE:HB	1.81	0.62
2:J:1104:ASP:OD2	2:J:1106:ARG:NH1	2.33	0.62
2:L:752:SER:HG	2:L:857:HIS:HE2	1.48	0.61
2:B:890:LEU:HD11	2:B:1009:ALA:HB1	1.81	0.61
2:D:1062:ALA:HB3	2:D:1071:ILE:HB	1.82	0.61
2:D:1104:ASP:OD2	2:D:1106:ARG:NH1	2.33	0.61
1:G:426:THR:HB	1:G:429:TYR:HB2	1.83	0.61
2:F:1032:ALA:HB3	2:F:1051:SER:HB2	1.82	0.61
2:L:1104:ASP:OD2	2:L:1106:ARG:NH1	2.35	0.60
2:B:1104:ASP:OD2	2:B:1106:ARG:NH1	2.34	0.60
2:J:1038:GLY:HA3	2:J:1046:ALA:HA	1.83	0.59
1:K:280:ASP:OD2	1:K:282:ASN:ND2	2.36	0.59
2:H:828:VAL:HG11	1:I:337:SER:HA	1.84	0.59
2:D:849:VAL:HG22	2:D:906:ILE:HG12	1.85	0.59
2:L:989:THR:HB	2:L:1002:PHE:HB2	1.85	0.58
2:B:722:ARG:NH1	2:B:1010:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:849:VAL:HG22	2:F:906:ILE:HG12	1.86	0.58
2:L:849:VAL:HG22	2:L:906:ILE:HG12	1.85	0.58
1:E:280:ASP:OD2	1:E:282:ASN:ND2	2.36	0.58
1:K:426:THR:HB	1:K:429:TYR:HB2	1.86	0.58
1:A:197:LYS:HA	1:A:204:GLN:HE22	1.69	0.57
2:D:890:LEU:HD11	2:D:1009:ALA:HB1	1.86	0.57
1:I:255:GLN:NE2	1:I:271:CYS:O	2.36	0.57
2:L:1062:ALA:HB3	2:L:1071:ILE:HB	1.85	0.57
1:G:197:LYS:HA	1:G:204:GLN:HE22	1.70	0.57
2:H:1038:GLY:HA3	2:H:1046:ALA:HA	1.86	0.57
2:D:769:PRO:HB3	2:D:839:LEU:HD23	1.86	0.57
2:L:690:GLY:H	2:L:1084:GLN:HA	1.69	0.57
2:F:754:LEU:HB2	2:F:1001:ALA:HB3	1.86	0.57
2:J:849:VAL:HG22	2:J:906:ILE:HG12	1.87	0.57
2:F:718:THR:HG22	2:F:1014:MET:HG2	1.86	0.56
1:I:358:LYS:NZ	1:I:360:ASP:OD2	2.39	0.56
1:E:255:GLN:NE2	1:E:271:CYS:O	2.37	0.56
2:J:785:VAL:HG21	2:L:944:HIS:HE1	1.70	0.56
1:C:161:ARG:NH2	1:C:209:HIS:O	2.37	0.56
2:L:923:ILE:HD12	2:L:924:PRO:HD2	1.88	0.56
2:F:690:GLY:HA3	2:F:1084:GLN:HA	1.89	0.55
2:L:748:LYS:HB3	2:L:862:GLU:HB3	1.89	0.55
1:G:201:PRO:HG2	2:H:802:PHE:HB3	1.88	0.55
2:B:730:ALA:HB3	2:B:747:ILE:HB	1.88	0.55
1:I:252:ASN:OD1	1:I:285:ARG:NH1	2.40	0.55
1:A:300:GLN:NE2	1:A:460:GLU:OE1	2.40	0.55
2:F:1090:VAL:HG22	2:F:1092:GLU:H	1.72	0.55
2:H:701:ILE:HD12	2:H:717:GLY:HA3	1.87	0.55
1:C:261:ASN:HD21	1:C:265:LYS:HB2	1.72	0.54
2:F:906:ILE:HB	2:F:914:ALA:HB3	1.89	0.54
2:J:926:GLN:NE2	2:J:951:PRO:O	2.40	0.54
1:G:212:LEU:HD23	1:G:258:HIS:HD2	1.72	0.54
2:B:885:TRP:HH2	2:B:1013:LEU:HD22	1.71	0.54
2:B:805:GLU:OE1	2:B:810:ARG:NH2	2.40	0.54
1:E:309:ASP:HB2	1:E:453:LYS:HE3	1.90	0.54
2:F:741:GLN:NE2	2:F:1023:VAL:O	2.40	0.54
1:G:446:GLN:HE21	1:G:449:GLY:HA2	1.73	0.54
2:L:959:MET:HB2	2:L:962:GLN:HB2	1.89	0.54
2:L:975:VAL:HA	2:L:978:ARG:HG2	1.90	0.54
1:C:442:ILE:HG23	1:C:453:LYS:HD2	1.89	0.54
2:D:843:ARG:NH1	2:F:1014:MET:SD	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:696:GLN:NE2	2:J:733:MET:SD	2.81	0.54
2:J:879:SER:OG	2:J:881:ARG:NH1	2.40	0.54
1:E:347:VAL:HG22	1:E:353:LYS:HA	1.90	0.53
2:F:711:THR:HB	2:F:1022:PHE:HB2	1.89	0.53
2:B:906:ILE:HB	2:B:914:ALA:HB3	1.90	0.53
2:J:923:ILE:HD12	2:J:924:PRO:HD2	1.90	0.53
2:H:1032:ALA:HB3	2:H:1051:SER:HB3	1.90	0.53
2:J:957:LYS:HB2	2:J:964:GLU:HB3	1.91	0.53
1:K:300:GLN:NE2	1:K:460:GLU:OE1	2.41	0.53
2:H:690:GLY:HA3	2:H:1085:ILE:H	1.72	0.53
2:B:1062:ALA:HB3	2:B:1071:ILE:HB	1.91	0.53
2:H:842:VAL:HG23	2:H:843:ARG:HD2	1.89	0.53
2:J:806:SER:O	2:J:810:ARG:NH1	2.42	0.53
2:B:754:LEU:HB2	2:B:1001:ALA:HB3	1.91	0.53
2:H:1060:LEU:HD21	2:H:1099:TYR:HB2	1.91	0.53
1:E:274:LYS:HG2	1:E:292:LEU:HD11	1.91	0.53
2:H:748:LYS:HB3	2:H:862:GLU:HB3	1.91	0.53
2:D:879:SER:OG	2:D:881:ARG:NH1	2.39	0.52
2:H:1065:LYS:HE2	2:H:1096:GLU:HB3	1.91	0.52
2:B:992:ALA:O	2:B:1000:GLN:NE2	2.42	0.52
2:H:717:GLY:H	2:H:1015:PHE:HB2	1.74	0.52
2:L:926:GLN:NE2	2:L:951:PRO:O	2.42	0.52
2:L:992:ALA:O	2:L:1000:GLN:NE2	2.43	0.52
1:K:252:ASN:O	1:K:254:TYR:N	2.42	0.52
1:I:246:MET:SD	1:I:300:GLN:NE2	2.83	0.51
1:K:161:ARG:NH2	1:K:209:HIS:O	2.42	0.51
2:F:890:LEU:HD11	2:F:1009:ALA:HB1	1.91	0.51
2:F:959:MET:HB2	2:F:962:GLN:HB2	1.91	0.51
2:D:844:LYS:NZ	2:F:1016:ASP:OD1	2.44	0.51
1:I:263:ASP:OD1	1:I:352:LYS:NZ	2.39	0.51
2:B:849:VAL:HG22	2:B:906:ILE:HG12	1.93	0.51
2:L:976:PHE:O	2:L:980:SER:OG	2.29	0.50
1:E:262:ASN:O	1:E:327:GLN:NE2	2.43	0.50
2:H:1071:ILE:HD11	2:H:1086:LEU:HD11	1.93	0.50
2:D:791:TRP:HE1	2:D:812:ASN:HB3	1.77	0.50
2:F:778:HIS:HD1	2:F:779:LEU:HG	1.76	0.50
2:H:1006:SER:OG	2:H:1043:ASN:ND2	2.37	0.50
1:G:366:ASN:HD22	1:G:367:LEU:H	1.60	0.50
1:K:263:ASP:OD1	1:K:352:LYS:NZ	2.40	0.50
2:B:891:SER:HB2	2:B:1010:ASP:HB2	1.93	0.50
2:F:879:SER:OG	2:F:881:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:324:VAL:HG23	1:K:464:VAL:HG22	1.94	0.49
1:K:327:GLN:NE2	1:K:353:LYS:O	2.45	0.49
2:H:840:GLN:NE2	2:H:841:SER:O	2.45	0.49
2:J:1060:LEU:HD21	2:J:1099:TYR:HB2	1.94	0.49
1:G:280:ASP:OD2	1:G:282:ASN:ND2	2.43	0.49
2:H:729:GLU:HG2	2:H:748:LYS:HA	1.94	0.49
1:I:196:GLU:O	1:I:204:GLN:NE2	2.41	0.49
2:H:926:GLN:NE2	2:H:952:ASN:O	2.45	0.49
2:J:1057:THR:HA	2:J:1076:GLU:HA	1.92	0.49
1:K:197:LYS:HA	1:K:204:GLN:HE22	1.78	0.49
2:B:904:SER:HB2	2:B:916:VAL:HB	1.95	0.49
1:A:426:THR:HB	1:A:429:TYR:HB2	1.94	0.49
2:D:711:THR:O	2:D:741:GLN:NE2	2.45	0.49
2:J:815:PHE:HB2	2:J:833:LEU:HB3	1.95	0.49
1:C:428:GLN:HB3	1:E:240:MET:HG3	1.94	0.49
1:A:408:HIS:HD2	1:A:426:THR:HG22	1.78	0.48
1:E:278:THR:HG22	1:E:285:ARG:HG2	1.96	0.48
2:H:849:VAL:HG22	2:H:906:ILE:HG12	1.95	0.48
1:I:426:THR:HB	1:I:429:TYR:HB2	1.94	0.48
2:F:729:GLU:HG2	2:F:748:LYS:HA	1.95	0.48
2:L:729:GLU:HG2	2:L:748:LYS:HA	1.95	0.48
2:D:722:ARG:NH2	2:D:1008:GLN:OE1	2.46	0.48
2:D:957:LYS:HG2	2:F:996:ASN:HD21	1.77	0.48
1:I:261:ASN:HD21	1:I:265:LYS:HB2	1.78	0.48
1:A:307:SER:HB3	1:A:455:LEU:HD23	1.94	0.48
2:D:732:LEU:HB3	2:D:745:LEU:HB3	1.96	0.48
1:A:230:ASP:O	1:A:237:ASN:ND2	2.47	0.48
2:B:791:TRP:HE1	2:B:812:ASN:HB3	1.78	0.47
1:C:336:LEU:HD11	1:C:465:LYS:HB3	1.95	0.47
1:A:185:ALA:HB2	1:A:393:GLU:HG2	1.94	0.47
1:A:319:LYS:NZ	2:D:1016:ASP:OD2	2.47	0.47
2:H:891:SER:HB2	2:H:1012:THR:HG23	1.97	0.47
2:L:784:HIS:HB2	2:L:787:ARG:HB2	1.97	0.47
1:A:246:MET:HG2	1:A:462:VAL:HG12	1.96	0.47
2:L:747:ILE:HG23	2:L:863:ILE:HG12	1.96	0.47
2:F:954:ILE:HA	2:F:967:THR:HG22	1.97	0.47
1:G:159:ARG:HH21	1:G:186:GLY:H	1.61	0.47
2:H:1100:SER:HB3	2:H:1105:GLU:HG3	1.97	0.47
1:G:460:GLU:HG2	1:G:462:VAL:HG13	1.97	0.47
1:K:242:GLU:OE2	1:K:353:LYS:NZ	2.45	0.47
2:L:1062:ALA:HA	2:L:1099:TYR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ALA:HB3	2:B:953:LEU:HD11	1.97	0.47
1:E:273:PRO:HA	1:E:274:LYS:HA	1.56	0.47
2:F:817:GLN:HE22	2:F:958:PRO:HB2	1.80	0.47
1:I:324:VAL:HG23	1:I:464:VAL:HG22	1.96	0.47
1:I:201:PRO:HG2	2:J:802:PHE:HB3	1.95	0.47
2:H:810:ARG:NH1	2:H:945:GLU:OE1	2.46	0.47
2:L:1076:GLU:HB3	2:L:1080:LYS:HG3	1.96	0.47
2:B:959:MET:O	2:B:961:ASP:N	2.48	0.47
2:H:755:SER:O	2:H:856:VAL:N	2.48	0.47
2:L:957:LYS:NZ	2:L:966:THR:OG1	2.47	0.47
2:H:923:ILE:HD12	2:H:924:PRO:HD2	1.95	0.47
2:F:784:HIS:ND1	2:F:786:ASN:OD1	2.48	0.46
1:I:273:PRO:HA	1:I:274:LYS:HA	1.57	0.46
2:L:730:ALA:HB3	2:L:747:ILE:HB	1.96	0.46
1:A:273:PRO:HA	1:A:274:LYS:HA	1.56	0.46
2:J:1006:SER:HB3	2:J:1008:GLN:HE22	1.80	0.46
2:L:931:GLU:HG3	2:L:932:ILE:HG13	1.98	0.46
2:H:959:MET:O	2:H:961:ASP:N	2.49	0.46
2:J:1073:LEU:HD22	2:J:1082:GLN:HB3	1.98	0.46
1:E:242:GLU:HG2	1:E:326:VAL:HG21	1.96	0.46
1:E:365:GLU:HG3	2:F:826:PHE:HD1	1.80	0.46
1:G:261:ASN:HD21	1:G:265:LYS:HB2	1.79	0.46
1:G:379:GLY:HA3	1:G:393:GLU:HB3	1.97	0.46
1:C:362:LYS:NZ	2:D:961:ASP:OD2	2.48	0.46
1:K:344:PRO:HG2	1:K:356:LEU:HB2	1.97	0.46
2:J:848:ARG:NH2	2:J:907:GLU:OE1	2.38	0.46
2:B:906:ILE:HD11	2:B:929:LEU:HD21	1.97	0.46
2:F:875:LEU:HD21	2:F:888:VAL:HG13	1.96	0.46
1:I:401:GLN:HB3	1:I:410:SER:HB2	1.98	0.46
2:L:959:MET:O	2:L:961:ASP:N	2.49	0.46
2:H:702:THR:HG21	2:H:734:LEU:HD11	1.98	0.46
1:C:273:PRO:HA	1:C:274:LYS:HA	1.48	0.46
2:H:1047:ARG:HG2	2:H:1085:ILE:HG12	1.97	0.46
2:J:712:LYS:H	2:J:712:LYS:HD2	1.81	0.46
2:J:775:ARG:NH2	2:J:823:CYS:O	2.49	0.46
1:K:278:THR:OG1	1:K:280:ASP:OD1	2.33	0.46
2:D:1038:GLY:HA3	2:D:1046:ALA:HA	1.98	0.45
2:D:1073:LEU:HD22	2:D:1082:GLN:HB3	1.98	0.45
2:F:732:LEU:HD23	2:F:745:LEU:HD23	1.97	0.45
2:J:863:ILE:HG21	2:J:885:TRP:HE1	1.81	0.45
1:E:376:GLU:HB3	1:E:397:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:863:ILE:HG21	2:H:885:TRP:HE1	1.81	0.45
2:D:690:GLY:H	2:D:1047:ARG:HG2	1.80	0.45
2:D:726:VAL:HG13	2:D:751:SER:HA	1.98	0.45
1:I:278:THR:OG1	1:I:280:ASP:OD1	2.32	0.45
2:L:1059:SER:HA	2:L:1074:PRO:HA	1.97	0.45
2:D:763:TRP:O	2:D:934:CYS:N	2.50	0.45
1:G:428:GLN:HB2	1:I:237:ASN:H	1.81	0.45
2:L:754:LEU:HB2	2:L:1001:ALA:HB3	1.98	0.45
2:B:873:ILE:HB	2:B:881:ARG:HG3	1.99	0.45
2:D:959:MET:O	2:D:961:ASP:N	2.49	0.45
1:K:273:PRO:HA	1:K:274:LYS:HA	1.48	0.45
1:K:323:GLU:HG2	1:K:328:ALA:HA	1.98	0.45
1:E:398:ASP:OD2	1:E:400:SER:OG	2.27	0.45
2:L:773:SER:HB3	2:L:963:LEU:HD22	1.97	0.45
2:L:722:ARG:NH1	2:L:1010:ASP:OD1	2.45	0.45
1:E:412:LYS:HD2	1:E:426:THR:HG21	1.97	0.45
2:F:784:HIS:HD1	2:F:786:ASN:H	1.64	0.45
1:C:321:VAL:HG11	1:C:324:VAL:HB	1.98	0.45
2:D:1090:VAL:HG22	2:D:1092:GLU:H	1.81	0.45
2:H:1090:VAL:HG22	2:H:1092:GLU:H	1.81	0.45
2:J:755:SER:N	2:J:856:VAL:O	2.49	0.45
1:A:356:LEU:HD21	1:A:447:VAL:HG23	1.99	0.45
1:E:251:PRO:HB2	1:E:252:ASN:H	1.59	0.45
1:E:252:ASN:O	1:E:254:TYR:N	2.43	0.45
2:F:715:LEU:HD11	2:F:734:LEU:HD22	1.99	0.45
2:H:747:ILE:HD12	2:H:863:ILE:HG12	1.99	0.45
1:C:344:PRO:HB3	1:C:459:TYR:HD1	1.82	0.44
2:D:692:SER:HA	2:D:1085:ILE:HB	1.99	0.44
1:E:206:TYR:HE1	2:F:776:ARG:HH22	1.65	0.44
1:G:259:TYR:HB3	1:G:299:LEU:HD12	1.99	0.44
2:D:1060:LEU:HD21	2:D:1099:TYR:HB2	1.98	0.44
2:D:926:GLN:NE2	2:D:952:ASN:O	2.50	0.44
2:L:700:ARG:HG3	2:L:701:ILE:HG23	1.98	0.44
1:C:183:THR:HG23	1:C:185:ALA:H	1.83	0.44
2:H:931:GLU:HG3	2:H:932:ILE:HG13	1.99	0.44
1:E:379:GLY:HA2	1:G:286:GLN:H	1.83	0.44
1:G:273:PRO:HA	1:G:274:LYS:HA	1.46	0.44
1:K:349:LYS:NZ	1:K:350:ASN:OD1	2.44	0.44
1:C:414:THR:HB	1:C:427:ALA:H	1.83	0.44
2:D:778:HIS:ND1	2:D:779:LEU:HG	2.33	0.44
1:C:324:VAL:HG23	1:C:464:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:959:MET:O	2:F:961:ASP:N	2.51	0.44
2:F:1062:ALA:HA	2:F:1099:TYR:HA	2.00	0.44
1:K:261:ASN:HD21	1:K:265:LYS:HB2	1.83	0.44
1:A:325:GLY:HA2	1:A:462:VAL:HG21	2.00	0.44
2:D:1076:GLU:OE1	2:D:1080:LYS:NZ	2.51	0.44
2:B:954:ILE:HA	2:B:967:THR:HG22	1.99	0.43
2:H:1076:GLU:OE1	2:H:1080:LYS:NZ	2.51	0.43
2:L:815:PHE:HB2	2:L:833:LEU:HB3	2.00	0.43
1:C:358:LYS:NZ	1:C:360:ASP:OD2	2.44	0.43
1:G:398:ASP:OD2	1:G:400:SER:OG	2.30	0.43
1:I:315:LYS:HA	1:I:354:VAL:HG22	2.00	0.43
2:B:874:ASP:N	2:B:874:ASP:OD1	2.51	0.43
1:E:220:ILE:O	1:E:349:LYS:NZ	2.51	0.43
2:F:778:HIS:ND1	2:F:779:LEU:HG	2.32	0.43
2:B:778:HIS:ND1	2:B:779:LEU:HG	2.34	0.43
2:B:734:LEU:HD22	2:B:1022:PHE:HZ	1.84	0.43
1:G:320:GLY:O	1:G:466:ARG:NH1	2.52	0.43
1:I:190:SER:HG	1:I:296:SER:H	1.66	0.43
2:B:1060:LEU:HD21	2:B:1099:TYR:HB2	2.01	0.43
1:C:260:LEU:HB3	1:C:300:GLN:HE22	1.83	0.43
1:I:259:TYR:HB3	1:I:299:LEU:HD12	2.00	0.43
2:J:729:GLU:HA	2:J:748:LYS:HA	2.01	0.43
1:C:158:LEU:HD22	1:C:195:LEU:HD22	2.00	0.43
1:E:225:ASP:HA	1:E:226:PRO:HA	1.89	0.43
2:F:753:GLU:OE2	2:F:858:LYS:NZ	2.44	0.43
1:G:160:ASN:OD1	1:G:183:THR:OG1	2.36	0.43
2:J:778:HIS:ND1	2:J:779:LEU:HG	2.34	0.43
1:K:276:GLU:HG3	1:K:285:ARG:HE	1.84	0.43
1:A:194:LEU:HA	1:A:200:PHE:HD2	1.83	0.42
2:F:787:ARG:HH22	2:F:792:ARG:HH22	1.67	0.42
2:J:754:LEU:HB2	2:J:1001:ALA:HB3	2.00	0.42
2:J:991:ALA:HB3	2:J:1002:PHE:HE2	1.84	0.42
2:J:1081:ASP:OD1	2:J:1081:ASP:N	2.51	0.42
2:B:776:ARG:HD2	2:B:780:VAL:HG11	2.02	0.42
2:J:931:GLU:HG3	2:J:932:ILE:HG13	2.01	0.42
2:D:717:GLY:H	2:D:1015:PHE:HB2	1.84	0.42
2:D:748:LYS:HB3	2:D:862:GLU:HB3	2.00	0.42
2:L:722:ARG:NH2	2:L:1008:GLN:OE1	2.52	0.42
2:J:787:ARG:HH21	2:J:791:TRP:HZ3	1.67	0.42
2:F:1091:PRO:HA	2:F:1114:LEU:HB2	2.01	0.42
2:F:755:SER:O	2:F:856:VAL:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:VAL:HG22	1:C:466:ARG:HG2	2.02	0.42
1:G:348:PHE:HZ	1:G:447:VAL:HG21	1.84	0.42
2:H:1071:ILE:HG12	2:H:1084:GLN:HE21	1.83	0.42
2:B:876:GLY:O	2:B:878:SER:N	2.53	0.42
1:C:308:GLU:OE1	1:C:349:LYS:NZ	2.43	0.42
1:G:412:LYS:HD2	1:G:426:THR:HG21	2.02	0.42
1:I:225:ASP:HA	1:I:226:PRO:HA	1.93	0.42
1:A:273:PRO:HB3	1:A:274:LYS:HD3	2.01	0.42
2:F:688:ASP:HB2	2:F:689:PRO:HD3	2.02	0.42
1:I:159:ARG:NE	1:I:184:TYR:O	2.53	0.42
1:I:373:VAL:HG13	1:I:437:ALA:HB2	2.01	0.42
2:D:913:TYR:HB2	2:D:981:LEU:HD12	2.01	0.42
1:I:230:ASP:HB3	1:I:233:SER:HB2	2.01	0.42
2:D:773:SER:HB2	2:D:833:LEU:HD11	2.02	0.41
2:B:1115:ILE:HG13	2:B:1117:ILE:HG12	2.02	0.41
2:B:806:SER:O	2:B:810:ARG:NH1	2.52	0.41
2:F:875:LEU:HD11	2:F:888:VAL:HG22	2.01	0.41
2:L:1038:GLY:HA3	2:L:1046:ALA:HA	2.00	0.41
1:C:210:ARG:O	1:C:304:CYS:N	2.53	0.41
1:C:401:GLN:HB3	1:C:410:SER:HB2	2.02	0.41
2:L:906:ILE:HB	2:L:914:ALA:HB3	2.03	0.41
1:A:194:LEU:HD21	1:A:298:PRO:HG2	2.02	0.41
1:G:278:THR:OG1	1:G:280:ASP:OD1	2.30	0.41
1:G:320:GLY:HA2	2:J:1017:ASN:HD21	1.85	0.41
2:H:707:GLU:O	2:H:712:LYS:NZ	2.53	0.41
2:H:875:LEU:HD11	2:H:888:VAL:HG13	2.02	0.41
1:A:263:ASP:OD1	1:A:352:LYS:NZ	2.45	0.41
2:B:747:ILE:HG23	2:B:863:ILE:HG12	2.03	0.41
1:G:257:ALA:HB1	1:G:299:LEU:HD11	2.02	0.41
1:I:209:HIS:CD2	1:I:210:ARG:H	2.39	0.41
2:J:959:MET:O	2:J:961:ASP:N	2.53	0.41
2:B:717:GLY:H	2:B:1015:PHE:HB2	1.85	0.41
1:C:223:LYS:HA	1:C:266:MET:HB3	2.02	0.41
1:G:464:VAL:HG12	1:G:466:ARG:HG3	2.03	0.41
1:A:158:LEU:HB2	1:A:207:ALA:HB1	2.02	0.41
2:H:690:GLY:HA3	2:H:1084:GLN:HB2	2.02	0.41
1:C:161:ARG:NH1	1:C:207:ALA:O	2.53	0.41
2:D:691:CYS:H	2:D:1084:GLN:HA	1.86	0.41
1:G:429:TYR:HH	1:I:235:HIS:CE1	2.38	0.41
1:G:438:ASN:HD22	2:H:780:VAL:HG22	1.86	0.41
1:I:246:MET:HG3	1:I:462:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:795:GLU:O	2:L:812:ASN:ND2	2.54	0.41
2:D:827:ASN:ND2	2:D:829:ASN:OD1	2.54	0.41
1:A:429:TYR:OH	1:C:235:HIS:N	2.54	0.40
2:D:718:THR:OG1	2:D:1014:MET:SD	2.67	0.40
1:E:183:THR:HG23	1:E:185:ALA:H	1.86	0.40
2:F:862:GLU:HA	2:F:872:THR:HA	2.02	0.40
2:F:743:LYS:HD3	2:F:866:PHE:HB3	2.02	0.40
1:A:225:ASP:HA	1:A:226:PRO:HA	1.89	0.40
1:E:197:LYS:HD2	1:E:204:GLN:HE22	1.86	0.40
1:A:347:VAL:HG22	1:A:353:LYS:HA	2.03	0.40
1:C:378:LYS:NZ	1:C:393:GLU:OE2	2.43	0.40
2:D:921:SER:HB2	2:D:928:PHE:HE2	1.86	0.40
2:H:1062:ALA:HA	2:H:1099:TYR:HA	2.04	0.40
2:H:769:PRO:HG3	2:H:967:THR:HG23	2.03	0.40
2:F:810:ARG:HD2	2:F:836:HIS:CE1	2.56	0.40
1:A:180:LYS:HA	1:A:181:PRO:HA	1.88	0.40
1:A:210:ARG:O	1:A:304:CYS:N	2.55	0.40
1:C:225:ASP:HA	1:C:226:PRO:HA	1.89	0.40
2:D:688:ASP:HB2	2:D:689:PRO:HD3	2.02	0.40
2:J:1089:THR:HG23	2:J:1090:VAL:HG13	2.04	0.40
2:J:811:GLU:OE2	2:J:956:TYR:OH	2.34	0.40
2:J:893:ASP:OD1	2:J:893:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/316 (93%)	250 (85%)	43 (15%)	2 (1%)	24	67
1	C	295/316 (93%)	259 (88%)	33 (11%)	3 (1%)	17	60
1	E	295/316 (93%)	258 (88%)	32 (11%)	5 (2%)	10	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	295/316 (93%)	255 (86%)	36 (12%)	4 (1%)	12	52
1	I	295/316 (93%)	246 (83%)	41 (14%)	8 (3%)	5	38
1	K	295/316 (93%)	255 (86%)	35 (12%)	5 (2%)	10	49
2	B	429/431 (100%)	375 (87%)	49 (11%)	5 (1%)	14	56
2	D	429/431 (100%)	384 (90%)	39 (9%)	6 (1%)	12	52
2	F	429/431 (100%)	370 (86%)	54 (13%)	5 (1%)	14	56
2	H	429/431 (100%)	376 (88%)	49 (11%)	4 (1%)	19	61
2	J	429/431 (100%)	380 (89%)	42 (10%)	7 (2%)	11	50
2	L	429/431 (100%)	377 (88%)	47 (11%)	5 (1%)	14	56
All	All	4344/4482 (97%)	3785 (87%)	500 (12%)	59 (1%)	17	52

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1083	CYS
1	E	281	CYS
2	F	1083	CYS
1	G	239	CYS
1	I	456	CYS
2	J	1083	CYS
1	K	281	CYS
2	L	1083	CYS
2	B	877	ALA
2	D	759	GLY
2	D	877	ALA
2	D	1083	CYS
1	E	251	PRO
1	E	439	GLY
2	F	704	CYS
2	F	877	ALA
2	H	1083	CYS
1	I	281	CYS
1	I	427	ALA
2	J	877	ALA
2	J	960	ILE
2	J	1017	ASN
2	B	911	LYS
1	C	427	ALA
1	E	329	LEU

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Mol	Chain	Res	Type
2	F	960	ILE
1	G	265	LYS
1	G	281	CYS
1	G	427	ALA
2	H	713	CYS
1	I	311	GLY
1	I	329	LEU
1	I	439	GLY
2	J	709	VAL
1	K	253	ASP
1	K	322	CYS
1	K	329	LEU
1	A	239	CYS
2	B	960	ILE
2	D	960	ILE
1	E	410	SER
2	H	877	ALA
2	H	960	ILE
2	L	759	GLY
2	L	960	ILE
2	L	986	ASN
2	B	809	MET
1	I	410	SER
2	J	986	ASN
1	K	237	ASN
1	C	232	GLN
2	D	709	VAL
1	I	322	CYS
2	L	750	VAL
1	A	311	GLY
2	D	1103	GLY
2	J	759	GLY
2	F	995	GLY
1	C	439	GLY

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	241/271 (89%)	238 (99%)	3 (1%)	74	87
1	C	241/271 (89%)	240 (100%)	1 (0%)	92	95
1	E	241/271 (89%)	239 (99%)	2 (1%)	83	92
1	G	241/271 (89%)	240 (100%)	1 (0%)	92	95
1	I	241/271 (89%)	239 (99%)	2 (1%)	83	92
1	K	241/271 (89%)	239 (99%)	2 (1%)	83	92
2	B	347/371 (94%)	344 (99%)	3 (1%)	81	90
2	D	347/371 (94%)	345 (99%)	2 (1%)	87	93
2	F	347/371 (94%)	343 (99%)	4 (1%)	74	87
2	H	347/371 (94%)	343 (99%)	4 (1%)	74	87
2	J	347/371 (94%)	345 (99%)	2 (1%)	87	93
2	L	347/371 (94%)	343 (99%)	4 (1%)	74	87
All	All	3528/3852 (92%)	3498 (99%)	30 (1%)	82	90

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	MET
1	A	378	LYS
1	A	438	ASN
2	B	700	ARG
2	B	844	LYS
2	B	949	ARG
1	C	378	LYS
2	D	925	ARG
2	D	949	ARG
1	E	285	ARG
1	E	315	LYS
2	F	700	ARG
2	F	733	MET
2	F	844	LYS
2	F	949	ARG
1	G	366	ASN
2	H	810	ARG
2	H	844	LYS
2	H	949	ARG
2	H	996	ASN
1	I	315	LYS
1	I	438	ASN

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Mol	Chain	Res	Type
2	J	712	LYS
2	J	949	ARG
1	K	285	ARG
1	K	378	LYS
2	L	710	ASN
2	L	733	MET
2	L	994	LYS
2	L	1017	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	408	HIS
1	A	438	ASN
2	B	840	GLN
1	C	166	HIS
1	E	167	ASN
1	E	204	GLN
1	E	327	GLN
1	G	174	GLN
1	G	204	GLN
1	G	209	HIS
1	G	235	HIS
1	G	366	ASN
1	G	377	HIS
1	G	438	ASN
1	G	446	GLN
2	H	829	ASN
2	H	996	ASN
2	H	1000	GLN
2	H	1084	GLN
1	I	209	HIS
2	J	1008	GLN
1	K	204	GLN
2	L	710	ASN
2	L	812	ASN
2	L	836	HIS
2	L	944	HIS
2	L	1017	ASN
2	L	1084	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.