



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 09:41 pm GMT

PDB ID : 6F9D
EMDB ID: : EMD-4199
Title : Model of the Rift Valley fever virus glycoprotein hexamer type 2
Authors : Halldorsson, S.; Bowden, T.A.; Huiskonen, J.T.
Deposited on : 2017-12-14
Resolution : 13.30 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

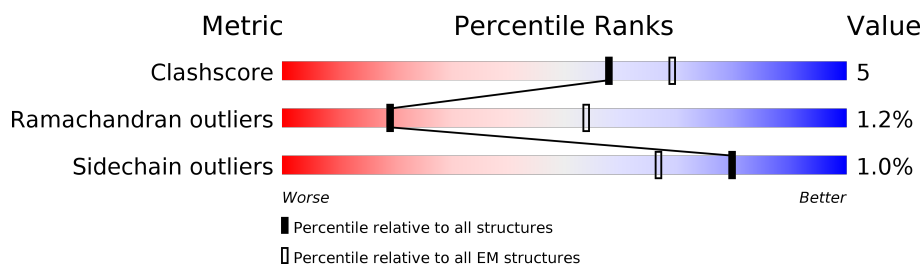
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.30 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	79% 15% • 5%
1	C	316	83% 12% 5%
1	E	316	80% 15% 5%
1	G	316	80% 15% • 5%
1	I	316	79% 16% 5%
1	K	316	80% 16% 5%
2	B	431	83% 16%
2	D	431	84% 16%
2	F	431	81% 18%

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Mol	Chain	Length	Quality of chain
2	H	431	<div><div></div><div>87%13%</div></div>
2	J	431	<div><div></div><div>84%16%</div></div>
2	L	431	<div><div></div><div>85%14%</div></div>

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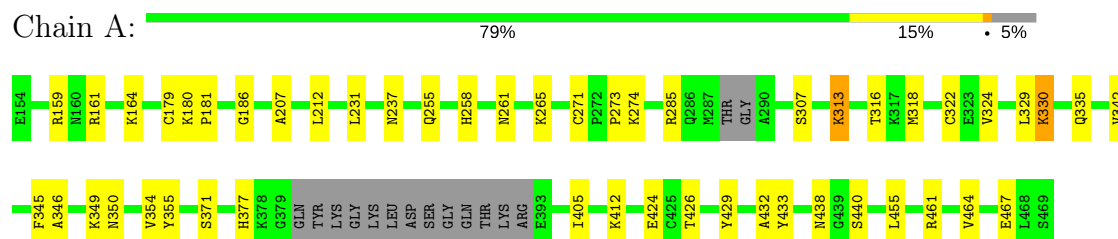
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Chain	Residue	Modelled	Actual	Comment	Reference
B	690	GLY	-	expression tag	UNP A2T072
D	688	ASP	-	expression tag	UNP A2T072
D	689	PRO	-	expression tag	UNP A2T072
D	690	GLY	-	expression tag	UNP A2T072
F	688	ASP	-	expression tag	UNP A2T072
F	689	PRO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

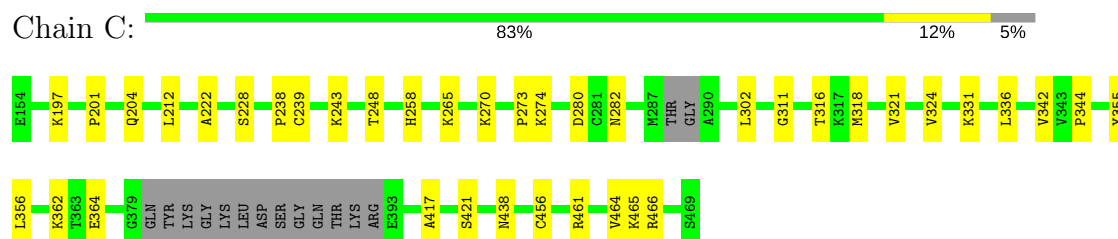
3 Residue-property plots [i](#)

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.

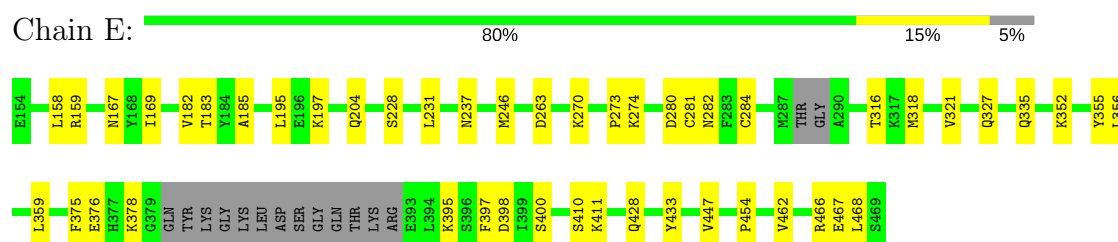
- Molecule 1: Glycoprotein



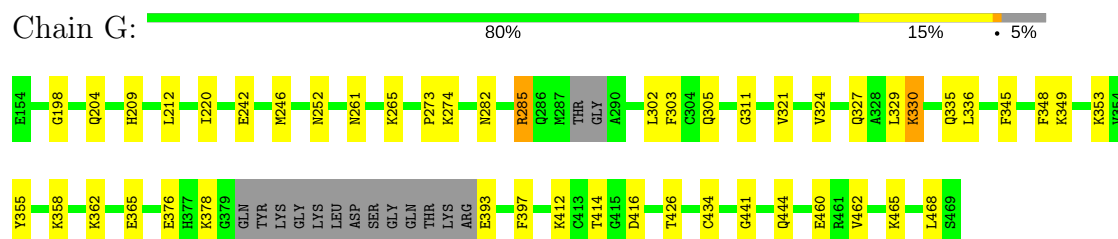
- Molecule 1: Glycoprotein



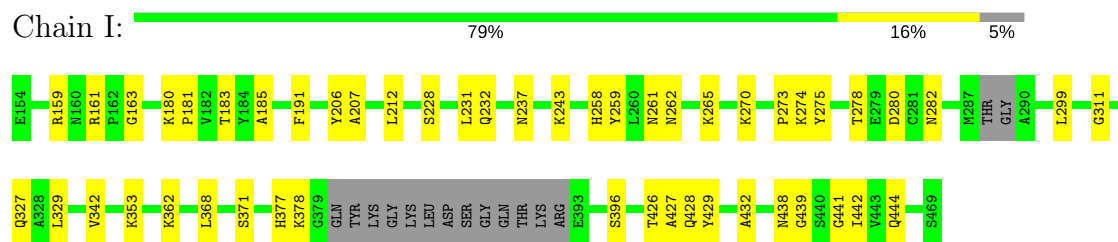
- Molecule 1: Glycoprotein



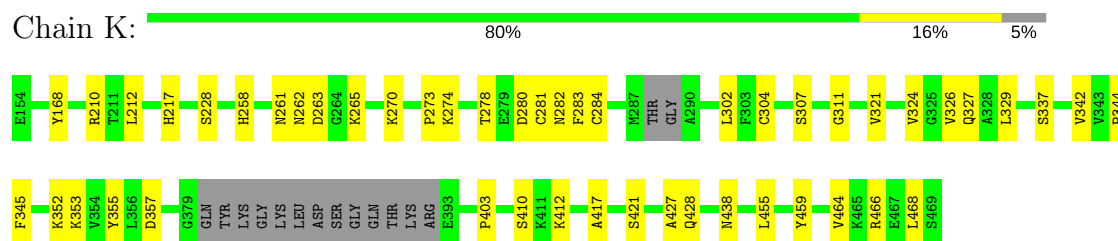
- Molecule 1: Glycoprotein



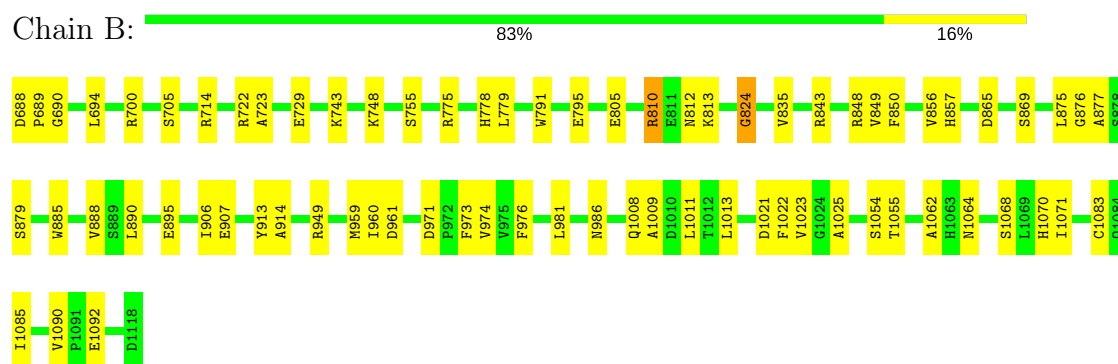
- Molecule 1: Glycoprotein



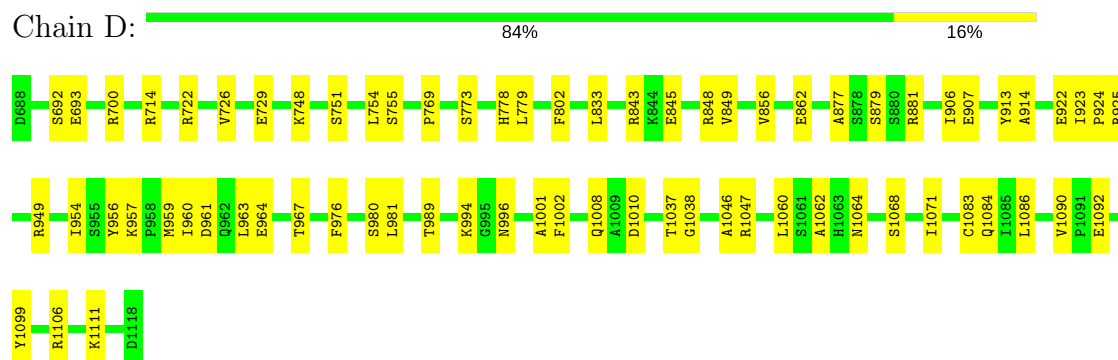
- Molecule 1: Glycoprotein



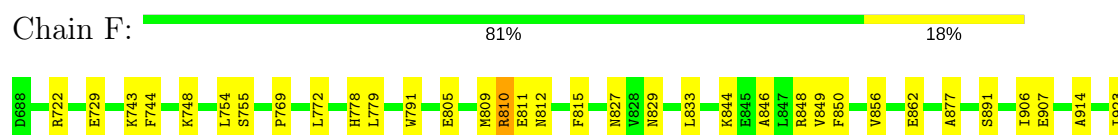
- Molecule 2: Glycoprotein

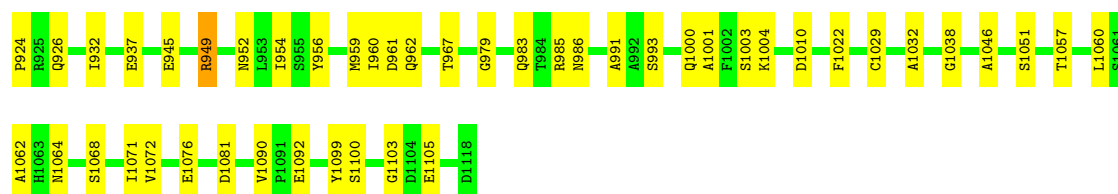


- Molecule 2: Glycoprotein



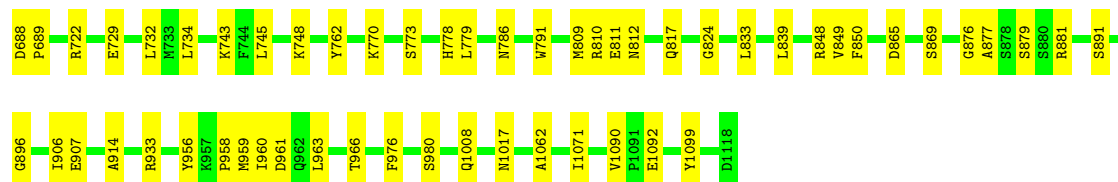
- Molecule 2: Glycoprotein





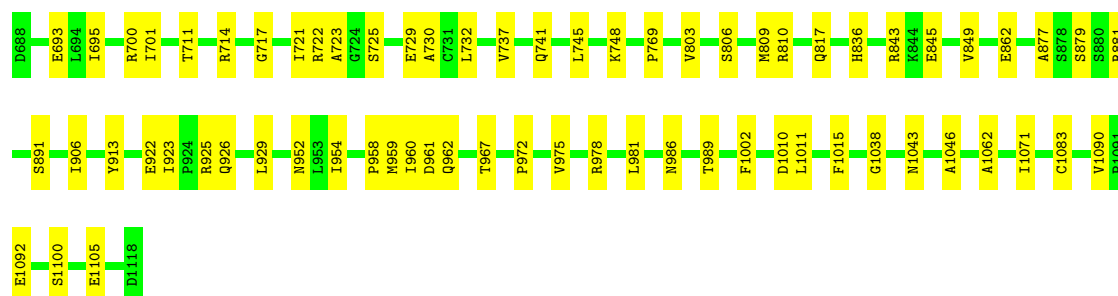
• Molecule 2: Glycoprotein

Chain H: 87% 13%



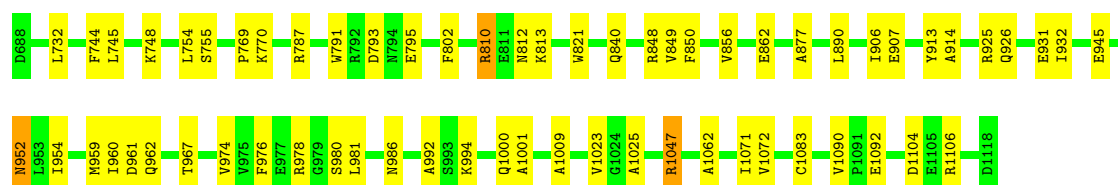
• Molecule 2: Glycoprotein

Chain J: 84% 16%



• Molecule 2: Glycoprotein

Chain L: 85% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	2995	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	0.40	0/3136
1	E	0.24	0/2333	0.42	0/3136
1	G	0.24	0/2333	0.41	0/3136
1	I	0.24	0/2333	0.41	0/3136
1	K	0.24	0/2333	0.40	0/3136
2	B	0.24	0/3284	0.41	0/4431
2	D	0.24	0/3284	0.42	0/4431
2	F	0.24	0/3284	0.42	0/4431
2	H	0.24	0/3284	0.42	0/4431
2	J	0.24	0/3284	0.43	0/4431
2	L	0.24	0/3284	0.43	0/4431
All	All	0.24	0/33702	0.42	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	26	0
1	C	2284	0	2205	19	0
1	E	2284	0	2205	27	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	26	0
1	K	2284	0	2205	26	0
2	B	3224	0	3071	38	0
2	D	3224	0	3071	35	0
2	F	3224	0	3071	43	0
2	H	3224	0	3071	28	0
2	J	3224	0	3071	36	0
2	L	3224	0	3071	34	0
All	All	33048	0	31656	348	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 (348) 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:K:212:LEU:HB2	1:K:302:LEU:HD11	1.77	0.66
2:D:748:LYS:HB3	2:D:862:GLU:HB3	1.79	0.65
2:B:1062:ALA:HB3	2:B:1071:ILE:HB	1.79	0.64
2:F:805:GLU:OE2	2:F:810:ARG:NH2	2.30	0.64
2:H:1062:ALA:HB3	2:H:1071:ILE:HB	1.78	0.64
2:F:791:TRP:HE1	2:F:812:ASN:HB3	1.62	0.63
2:L:748:LYS:HB3	2:L:862:GLU:HB3	1.81	0.63
2:D:729:GLU:HG2	2:D:748:LYS:HA	1.81	0.62
2:B:805:GLU:OE2	2:B:810:ARG:NH2	2.32	0.62
2:J:729:GLU:HG2	2:J:748:LYS:HA	1.81	0.62
2:L:1104:ASP:OD2	2:L:1106:ARG:NH1	2.33	0.62
1:E:321:VAL:HG22	1:E:466:ARG:HG2	1.82	0.61
1:E:316:THR:HG23	1:E:355:TYR:HB2	1.82	0.61
2:L:1062:ALA:HB3	2:L:1071:ILE:HB	1.83	0.61
1:E:197:LYS:HA	1:E:204:GLN:HE22	1.66	0.60
2:F:748:LYS:HB3	2:F:862:GLU:HB3	1.83	0.60
2:H:732:LEU:HB3	2:H:745:LEU:HB3	1.82	0.60
1:I:261:ASN:HD21	1:I:265:LYS:HB2	1.65	0.60
2:J:732:LEU:HB3	2:J:745:LEU:HB3	1.85	0.59
1:E:359:LEU:H	2:F:772:LEU:HG	1.68	0.58
1:G:376:GLU:HB2	1:G:397:PHE:HB2	1.85	0.58
1:K:403:PRO:HG2	1:K:412:LYS:HD3	1.86	0.58
1:C:212:LEU:HD13	1:C:302:LEU:HD11	1.86	0.58
1:E:375:PHE:HB2	1:E:433:TYR:HB3	1.84	0.58
1:E:280:ASP:OD2	1:E:282:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:HE22	2:L:821:TRP:HB2	1.70	0.57
1:C:197:LYS:HA	1:C:204:GLN:HE22	1.69	0.57
2:D:849:VAL:HG22	2:D:906:ILE:HG12	1.87	0.57
1:C:316:THR:HG23	1:C:355:TYR:HB2	1.86	0.57
2:D:906:ILE:HB	2:D:914:ALA:HB3	1.87	0.57
2:F:849:VAL:HG22	2:F:906:ILE:HG12	1.87	0.57
2:H:966:THR:HG1	2:J:879:SER:HG	1.51	0.57
1:G:336:LEU:HD11	1:G:465:LYS:HB3	1.86	0.56
2:F:1032:ALA:HB3	2:F:1051:SER:HB3	1.87	0.56
1:E:158:LEU:HD12	1:E:159:ARG:HG3	1.86	0.56
2:L:974:VAL:O	2:L:978:ARG:HB2	2.05	0.56
2:B:1064:ASN:HD21	2:B:1068:SER:H	1.51	0.56
2:F:1060:LEU:HD21	2:F:1099:TYR:HB2	1.88	0.56
1:I:262:ASN:OD1	1:I:327:GLN:NE2	2.40	0.55
2:J:849:VAL:HG22	2:J:906:ILE:HG12	1.88	0.55
2:L:732:LEU:HB3	2:L:745:LEU:HB3	1.88	0.55
1:C:212:LEU:HD23	1:C:258:HIS:HD2	1.71	0.55
1:G:198:GLY:H	1:G:204:GLN:HE22	1.54	0.55
2:J:891:SER:HB3	2:J:1010:ASP:HB2	1.88	0.55
2:F:959:MET:HB2	2:F:962:GLN:HB2	1.87	0.55
1:I:371:SER:HA	1:I:441:GLY:HA2	1.88	0.54
2:J:922:GLU:HG2	2:J:923:ILE:HG12	1.88	0.54
2:B:848:ARG:NH2	2:B:907:GLU:OE1	2.39	0.54
2:D:769:PRO:HG3	2:D:967:THR:HG23	1.89	0.54
2:J:748:LYS:HB3	2:J:862:GLU:HB3	1.88	0.54
1:K:321:VAL:HG22	1:K:466:ARG:HG2	1.88	0.54
2:H:849:VAL:HG22	2:H:906:ILE:HG12	1.89	0.54
2:H:906:ILE:HB	2:H:914:ALA:HB3	1.90	0.54
1:E:263:ASP:OD1	1:E:352:LYS:NZ	2.41	0.54
1:I:212:LEU:HD23	1:I:258:HIS:HD2	1.72	0.54
1:K:280:ASP:OD2	1:K:282:ASN:ND2	2.41	0.54
2:D:913:TYR:HB2	2:D:981:LEU:HD12	1.89	0.53
2:B:890:LEU:HD11	2:B:1009:ALA:HB1	1.89	0.53
2:J:711:THR:HB	2:J:741:GLN:HE22	1.73	0.53
2:J:989:THR:HB	2:J:1002:PHE:HB2	1.91	0.53
1:C:201:PRO:HG2	2:D:802:PHE:HB3	1.89	0.53
1:K:261:ASN:HD21	1:K:265:LYS:HB2	1.72	0.53
2:J:1062:ALA:HB3	2:J:1071:ILE:HB	1.89	0.53
2:J:879:SER:OG	2:J:881:ARG:NH1	2.41	0.53
1:A:342:VAL:HG22	1:A:461:ARG:HG2	1.91	0.53
2:H:773:SER:HB2	2:H:833:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:983:GLN:OE1	2:F:985:ARG:NH2	2.42	0.53
1:A:426:THR:HB	1:A:429:TYR:HB2	1.89	0.52
2:B:690:GLY:H	2:B:1085:ILE:HG12	1.74	0.52
1:E:376:GLU:OE1	1:E:395:LYS:NZ	2.37	0.52
2:F:906:ILE:HB	2:F:914:ALA:HB3	1.92	0.52
1:E:467:GLU:OE1	2:H:1017:ASN:ND2	2.42	0.52
1:A:330:LYS:NZ	1:A:467:GLU:OE2	2.42	0.52
2:H:876:GLY:H	2:H:879:SER:HB3	1.74	0.52
1:K:357:ASP:OD2	2:L:770:LYS:NZ	2.40	0.52
2:F:1064:ASN:HD21	2:F:1068:SER:H	1.57	0.52
2:D:773:SER:HB2	2:D:833:LEU:HD11	1.90	0.52
1:C:228:SER:HB2	1:C:270:LYS:HB2	1.92	0.52
2:F:926:GLN:NE2	2:F:952:ASN:O	2.43	0.52
2:H:734:LEU:HB3	2:H:743:LYS:HB2	1.92	0.52
2:J:693:GLU:OE2	2:J:722:ARG:NH2	2.43	0.52
2:B:791:TRP:HE1	2:B:812:ASN:HB3	1.75	0.52
1:C:243:LYS:NZ	1:C:282:ASN:OD1	2.41	0.52
2:D:1064:ASN:HD21	2:D:1068:SER:H	1.58	0.52
1:E:231:LEU:HD23	1:E:237:ASN:HD21	1.74	0.52
1:I:362:LYS:HD2	1:I:444:GLN:HB2	1.92	0.52
2:L:754:LEU:HB2	2:L:1001:ALA:HB3	1.92	0.52
2:B:722:ARG:NH2	2:B:1008:GLN:OE1	2.43	0.52
2:F:1090:VAL:HG22	2:F:1092:GLU:H	1.74	0.52
2:F:1062:ALA:HB3	2:F:1071:ILE:HB	1.92	0.51
2:J:954:ILE:HA	2:J:967:THR:HG22	1.91	0.51
1:G:412:LYS:HD2	1:G:426:THR:HG21	1.91	0.51
1:C:342:VAL:HG22	1:C:461:ARG:HG2	1.93	0.51
2:J:806:SER:O	2:J:810:ARG:NH1	2.44	0.51
2:F:744:PHE:HZ	2:F:1072:VAL:HG13	1.76	0.51
1:A:161:ARG:NH1	1:A:207:ALA:O	2.43	0.51
2:D:879:SER:OG	2:D:881:ARG:NH1	2.41	0.51
2:H:879:SER:OG	2:H:881:ARG:NH1	2.44	0.51
1:K:337:SER:HB2	1:K:468:LEU:HD22	1.93	0.51
1:E:183:THR:HG23	1:E:185:ALA:H	1.76	0.51
1:I:426:THR:HB	1:I:429:TYR:HB2	1.91	0.51
1:A:237:ASN:HD22	1:K:428:GLN:HG3	1.76	0.51
2:D:722:ARG:NH1	2:D:1010:ASP:OD1	2.43	0.51
1:G:345:PHE:HA	1:G:355:TYR:HA	1.93	0.50
1:K:263:ASP:OD1	1:K:352:LYS:NZ	2.40	0.50
1:E:428:GLN:NE2	1:G:282:ASN:O	2.44	0.50
1:I:161:ARG:NH1	1:I:207:ALA:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:721:ILE:HD13	2:J:730:ALA:HB1	1.94	0.50
2:B:795:GLU:O	2:B:812:ASN:ND2	2.44	0.50
1:I:342:VAL:HB	2:J:803:VAL:HG13	1.93	0.50
2:F:815:PHE:HB2	2:F:833:LEU:HB3	1.91	0.50
2:J:1090:VAL:HG22	2:J:1092:GLU:H	1.76	0.50
1:A:349:LYS:NZ	1:A:350:ASN:OD1	2.41	0.50
2:B:775:ARG:HH22	2:B:824:GLY:HA3	1.77	0.50
2:D:1038:GLY:HA3	2:D:1046:ALA:HA	1.92	0.50
2:L:1090:VAL:HG22	2:L:1092:GLU:H	1.76	0.50
2:L:926:GLN:NE2	2:L:952:ASN:O	2.44	0.50
2:F:1057:THR:HA	2:F:1076:GLU:HA	1.94	0.50
2:D:1062:ALA:HB3	2:D:1071:ILE:HB	1.94	0.50
1:I:428:GLN:NE2	1:K:284:CYS:O	2.45	0.50
2:B:1090:VAL:HG22	2:B:1092:GLU:H	1.77	0.49
1:I:280:ASP:OD2	1:I:282:ASN:ND2	2.45	0.49
2:J:700:ARG:HG3	2:J:701:ILE:HG23	1.94	0.49
1:A:377:HIS:NE2	1:A:432:ALA:O	2.46	0.49
2:B:875:LEU:HD21	2:B:888:VAL:HG23	1.93	0.49
1:I:206:TYR:HA	1:I:439:GLY:HA2	1.95	0.49
1:K:278:THR:OG1	1:K:280:ASP:OD1	2.30	0.49
2:L:1062:ALA:N	2:L:1071:ILE:O	2.45	0.49
2:D:726:VAL:HG22	2:D:751:SER:HA	1.95	0.49
2:D:923:ILE:HD12	2:D:924:PRO:HD2	1.95	0.49
1:I:273:PRO:HA	1:I:274:LYS:HA	1.54	0.49
2:J:1038:GLY:HA3	2:J:1046:ALA:HA	1.95	0.49
2:D:1060:LEU:HD21	2:D:1099:TYR:HB2	1.93	0.49
1:I:327:GLN:HE21	1:I:353:LYS:HB3	1.78	0.49
2:L:769:PRO:HG3	2:L:967:THR:HG23	1.94	0.49
1:A:212:LEU:HD23	1:A:258:HIS:HD2	1.78	0.48
1:E:228:SER:HB2	1:E:270:LYS:HB2	1.95	0.48
2:F:923:ILE:HD12	2:F:924:PRO:HD2	1.96	0.48
1:K:307:SER:HB3	1:K:455:LEU:HD23	1.95	0.48
1:G:378:LYS:O	1:G:393:GLU:N	2.45	0.48
2:D:843:ARG:HG3	2:D:845:GLU:H	1.79	0.48
2:B:729:GLU:HG2	2:B:748:LYS:HA	1.95	0.48
2:D:1046:ALA:N	2:D:1086:LEU:O	2.46	0.48
2:D:954:ILE:HA	2:D:967:THR:HG22	1.94	0.48
2:D:957:LYS:HD3	2:D:964:GLU:HB2	1.96	0.48
2:H:722:ARG:NH2	2:H:1008:GLN:OE1	2.46	0.48
2:F:846:ALA:HB3	2:F:937:GLU:HG3	1.94	0.48
2:B:1064:ASN:ND2	2:B:1068:SER:OG	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASP:OD2	1:C:282:ASN:ND2	2.47	0.47
1:G:273:PRO:HA	1:G:274:LYS:HA	1.55	0.47
2:H:791:TRP:HE1	2:H:812:ASN:HB3	1.79	0.47
1:I:243:LYS:NZ	1:I:282:ASN:OD1	2.38	0.47
1:K:342:VAL:HG11	2:L:802:PHE:HB2	1.96	0.47
1:G:355:TYR:HE1	1:G:460:GLU:HG3	1.79	0.47
2:B:694:LEU:HD22	2:B:1070:HIS:HB3	1.96	0.47
1:C:344:PRO:HG2	1:C:356:LEU:HB2	1.97	0.47
1:C:417:ALA:O	1:C:421:SER:HB3	2.13	0.47
2:F:811:GLU:OE2	2:F:956:TYR:OH	2.27	0.47
2:H:848:ARG:NH2	2:H:907:GLU:OE1	2.40	0.47
2:L:906:ILE:HB	2:L:914:ALA:HB3	1.95	0.47
1:K:210:ARG:O	1:K:304:CYS:N	2.48	0.47
1:A:255:GLN:NE2	1:A:271:CYS:O	2.42	0.47
1:G:362:LYS:HB3	1:G:444:GLN:HB2	1.97	0.47
2:H:811:GLU:OE2	2:H:956:TYR:OH	2.29	0.47
1:K:212:LEU:HD23	1:K:258:HIS:HD2	1.80	0.47
1:A:307:SER:HB3	1:A:455:LEU:HD23	1.96	0.47
2:D:959:MET:O	2:D:961:ASP:N	2.47	0.47
2:L:959:MET:O	2:L:961:ASP:N	2.48	0.47
2:D:989:THR:HB	2:D:1002:PHE:HB2	1.97	0.47
2:B:906:ILE:HB	2:B:914:ALA:HB3	1.96	0.47
1:K:273:PRO:HA	1:K:274:LYS:HA	1.46	0.47
1:G:220:ILE:O	1:G:349:LYS:NZ	2.46	0.47
1:A:261:ASN:HD21	1:A:265:LYS:HB2	1.80	0.46
2:D:1037:THR:O	2:D:1047:ARG:N	2.48	0.46
1:K:168:TYR:O	1:K:217:HIS:NE2	2.41	0.46
1:A:345:PHE:HA	1:A:355:TYR:HA	1.97	0.46
2:J:975:VAL:HA	2:J:978:ARG:HG2	1.97	0.46
1:K:417:ALA:O	1:K:421:SER:HB2	2.15	0.46
2:L:1023:VAL:HG22	2:L:1025:ALA:H	1.80	0.46
1:E:316:THR:OG1	1:E:327:GLN:OE1	2.32	0.46
1:I:278:THR:OG1	1:I:280:ASP:OD1	2.32	0.46
1:A:324:VAL:HG23	1:A:464:VAL:HG22	1.96	0.46
2:B:1023:VAL:HG22	2:B:1025:ALA:H	1.80	0.46
1:K:344:PRO:HA	1:K:459:TYR:HA	1.97	0.46
2:B:743:LYS:NZ	2:B:1021:ASP:O	2.45	0.46
2:B:723:ALA:HB2	2:B:1011:LEU:HG	1.97	0.46
2:J:695:ILE:HD13	2:J:721:ILE:HB	1.97	0.46
2:B:849:VAL:HG22	2:B:906:ILE:HG12	1.97	0.46
2:F:754:LEU:HB2	2:F:1001:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:HIS:HD2	1:G:303:PHE:HB2	1.79	0.46
1:I:428:GLN:HE22	1:K:283:PHE:HB3	1.80	0.46
2:D:722:ARG:NH2	2:D:1008:GLN:OE1	2.49	0.46
2:B:885:TRP:HH2	2:B:1013:LEU:HD22	1.81	0.46
1:E:316:THR:HG22	1:E:318:MET:H	1.81	0.46
2:F:959:MET:O	2:F:961:ASP:N	2.48	0.46
2:J:769:PRO:HG3	2:J:967:THR:HG23	1.98	0.46
1:G:246:MET:HA	1:G:462:VAL:HA	1.98	0.46
2:B:850:PHE:HE1	2:B:907:GLU:HB2	1.82	0.45
1:C:248:THR:OG1	1:C:280:ASP:O	2.32	0.45
1:E:335:GLN:HG3	1:E:468:LEU:HB3	1.98	0.45
1:K:228:SER:HB2	1:K:270:LYS:HB3	1.97	0.45
2:L:850:PHE:HE1	2:L:907:GLU:HB2	1.81	0.45
2:L:848:ARG:NH2	2:L:907:GLU:OE1	2.38	0.45
1:E:376:GLU:HB2	1:E:397:PHE:HB2	1.99	0.45
2:J:959:MET:O	2:J:961:ASP:N	2.48	0.45
1:A:405:ILE:HA	1:A:424:GLU:HB2	1.98	0.45
1:A:412:LYS:HD2	1:A:426:THR:HG21	1.98	0.45
2:B:843:ARG:NH2	2:B:971:ASP:OD2	2.49	0.45
1:G:330:LYS:HB2	2:J:714:ARG:HH21	1.82	0.45
1:C:222:ALA:HB3	1:C:265:LYS:HG2	1.98	0.45
1:C:324:VAL:HG23	1:C:464:VAL:HG22	1.98	0.45
2:J:817:GLN:HE22	2:J:958:PRO:HB2	1.81	0.45
1:A:231:LEU:O	1:K:428:GLN:NE2	2.50	0.45
2:F:979:GLY:HA2	2:F:983:GLN:HE22	1.82	0.45
1:K:262:ASN:OD1	1:K:327:GLN:NE2	2.49	0.45
1:A:313:LYS:HD2	1:A:313:LYS:H	1.80	0.45
2:L:793:ASP:OD1	2:L:813:LYS:NZ	2.50	0.45
2:F:891:SER:HB3	2:F:1010:ASP:HB2	1.99	0.45
1:G:311:GLY:HA3	1:G:348:PHE:HD2	1.81	0.45
2:H:959:MET:O	2:H:961:ASP:N	2.50	0.45
1:E:273:PRO:HA	1:E:274:LYS:HA	1.53	0.45
1:E:398:ASP:OD2	1:E:400:SER:OG	2.27	0.45
1:K:345:PHE:HA	1:K:355:TYR:HA	1.99	0.45
2:D:1090:VAL:HG22	2:D:1092:GLU:H	1.81	0.45
1:I:183:THR:HG23	1:I:185:ALA:H	1.82	0.45
1:E:468:LEU:HD12	2:F:844:LYS:HG2	1.98	0.45
2:H:850:PHE:HE1	2:H:907:GLU:HB2	1.81	0.44
2:L:954:ILE:HA	2:L:967:THR:HG22	1.98	0.44
2:L:959:MET:HB2	2:L:962:GLN:HB2	1.98	0.44
1:G:242:GLU:OE2	1:G:353:LYS:NZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:377:HIS:H	1:I:432:ALA:HA	1.82	0.44
1:I:163:GLY:H	1:I:396:SER:HB3	1.82	0.44
2:F:991:ALA:HB3	2:F:1000:GLN:HE21	1.81	0.44
2:F:810:ARG:NH1	2:F:945:GLU:OE1	2.47	0.44
2:H:809:MET:HB2	2:H:839:LEU:HB2	1.98	0.44
2:L:1047:ARG:HD2	2:L:1047:ARG:H	1.82	0.44
2:J:1100:SER:HB3	2:J:1105:GLU:HG3	1.98	0.44
1:A:346:ALA:N	1:A:354:VAL:O	2.50	0.44
2:B:876:GLY:H	2:B:879:SER:HB3	1.83	0.44
1:G:261:ASN:HD21	1:G:265:LYS:HB2	1.83	0.44
1:E:410:SER:OG	1:E:411:LYS:N	2.49	0.44
2:J:913:TYR:HB2	2:J:981:LEU:HD12	2.00	0.44
1:K:327:GLN:HE22	1:K:353:LYS:HB3	1.82	0.44
2:L:913:TYR:HB2	2:L:981:LEU:HD12	2.00	0.44
2:B:813:LYS:HB2	2:B:835:VAL:HB	1.99	0.43
2:B:865:ASP:OD2	2:B:869:SER:OG	2.36	0.43
2:B:973:PHE:HA	2:B:976:PHE:HB3	1.99	0.43
2:H:1062:ALA:HA	2:H:1099:TYR:HA	2.00	0.43
2:L:992:ALA:O	2:L:1000:GLN:NE2	2.51	0.43
2:B:959:MET:O	2:B:961:ASP:N	2.51	0.43
2:J:723:ALA:HB2	2:J:1011:LEU:HG	2.00	0.43
2:L:849:VAL:HG22	2:L:906:ILE:HG12	1.99	0.43
1:A:316:THR:HG22	1:A:318:MET:H	1.83	0.43
2:F:810:ARG:H	2:F:810:ARG:HD3	1.82	0.43
2:L:787:ARG:NH2	2:L:795:GLU:OE2	2.44	0.43
2:F:827:ASN:HD21	2:F:829:ASN:HD22	1.65	0.43
1:G:252:ASN:HD21	1:G:285:ARG:HH11	1.67	0.43
1:G:365:GLU:HG2	1:G:441:GLY:HA3	2.00	0.43
1:A:377:HIS:CE1	1:A:433:TYR:HB2	2.53	0.43
2:D:778:HIS:ND1	2:D:779:LEU:HG	2.34	0.43
1:E:158:LEU:HD13	1:E:195:LEU:HD22	2.01	0.43
2:F:778:HIS:ND1	2:F:779:LEU:HG	2.33	0.43
1:G:209:HIS:CE1	1:G:305:GLN:HB3	2.54	0.43
2:H:729:GLU:HA	2:H:748:LYS:HA	2.01	0.43
2:F:729:GLU:OE2	2:F:748:LYS:NZ	2.40	0.43
2:H:976:PHE:O	2:H:980:SER:OG	2.32	0.43
2:D:692:SER:OG	2:D:693:GLU:OE1	2.30	0.43
2:J:711:THR:HG21	2:J:737:VAL:HG22	2.00	0.43
2:L:770:LYS:HG3	2:L:840:GLN:HE22	1.83	0.43
1:A:273:PRO:HA	1:A:274:LYS:HA	1.48	0.42
2:D:754:LEU:HB2	2:D:1001:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1100:SER:HB3	2:F:1105:GLU:HG2	2.00	0.42
1:G:327:GLN:NE2	1:G:353:LYS:O	2.52	0.42
1:I:259:TYR:HB3	1:I:299:LEU:HB2	2.01	0.42
1:C:321:VAL:HG22	1:C:466:ARG:HG2	2.00	0.42
1:I:228:SER:HB2	1:I:270:LYS:HB2	2.00	0.42
2:D:848:ARG:NH2	2:D:907:GLU:OE1	2.36	0.42
2:F:932:ILE:HG12	2:F:949:ARG:HB2	2.01	0.42
2:J:959:MET:HB2	2:J:962:GLN:HB2	2.01	0.42
1:K:324:VAL:HG23	1:K:464:VAL:HG22	2.01	0.42
2:B:755:SER:O	2:B:856:VAL:N	2.52	0.42
2:H:762:TYR:HB2	2:H:933:ARG:HB2	2.02	0.42
2:H:778:HIS:ND1	2:H:779:LEU:HG	2.34	0.42
2:J:717:GLY:H	2:J:1015:PHE:HB2	1.84	0.42
1:G:335:GLN:HB3	1:G:468:LEU:HB2	2.00	0.42
1:I:231:LEU:HD23	1:I:237:ASN:HD21	1.84	0.42
2:J:929:LEU:HD11	2:J:972:PRO:HB3	1.99	0.42
1:A:180:LYS:HA	1:A:181:PRO:HA	1.87	0.42
2:H:817:GLN:HE22	2:H:958:PRO:HB2	1.84	0.42
2:B:1054:SER:OG	2:B:1055:THR:N	2.53	0.42
2:B:743:LYS:HE3	2:B:1022:PHE:HB2	2.02	0.42
1:C:336:LEU:HD13	1:C:465:LYS:HB3	2.01	0.42
1:E:167:ASN:HD22	1:E:182:VAL:HG21	1.84	0.42
2:J:725:SER:OG	2:J:1043:ASN:ND2	2.51	0.42
1:E:246:MET:HG2	1:E:462:VAL:HG12	2.01	0.42
2:F:1081:ASP:N	2:F:1081:ASP:OD1	2.53	0.42
2:H:773:SER:HB3	2:H:963:LEU:HB2	2.01	0.42
2:F:954:ILE:HA	2:F:967:THR:HG22	2.02	0.42
2:B:688:ASP:HB2	2:B:689:PRO:HD3	2.01	0.42
2:D:1071:ILE:HG12	2:D:1084:GLN:HE21	1.85	0.42
2:J:926:GLN:NE2	2:J:952:ASN:O	2.52	0.42
1:C:316:THR:HG22	1:C:318:MET:H	1.85	0.41
1:C:362:LYS:NZ	1:C:364:GLU:OE2	2.52	0.41
1:I:368:LEU:HD13	1:I:442:ILE:HD12	2.02	0.41
2:D:755:SER:N	2:D:856:VAL:O	2.52	0.41
2:L:744:PHE:HZ	2:L:1072:VAL:HG23	1.85	0.41
2:H:865:ASP:OD2	2:H:869:SER:OG	2.39	0.41
1:C:273:PRO:HA	1:C:274:LYS:HA	1.50	0.41
2:F:1003:SER:OG	2:F:1004:LYS:N	2.53	0.41
2:F:1038:GLY:HA3	2:F:1046:ALA:HA	2.02	0.41
2:F:848:ARG:NH2	2:F:907:GLU:OE1	2.42	0.41
2:B:913:TYR:HB2	2:B:981:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:GLN:HE22	1:I:275:TYR:HE2	1.68	0.41
2:L:931:GLU:HG3	2:L:932:ILE:HG13	2.01	0.41
2:H:688:ASP:HB2	2:H:689:PRO:HD3	2.02	0.41
2:B:755:SER:N	2:B:856:VAL:O	2.54	0.41
2:B:971:ASP:HB3	2:B:974:VAL:HG23	2.03	0.41
2:D:956:TYR:HD1	2:D:963:LEU:HD21	1.85	0.41
2:F:993:SER:HB2	2:F:1000:GLN:HB3	2.01	0.41
2:L:755:SER:O	2:L:856:VAL:N	2.44	0.41
2:L:791:TRP:HE1	2:L:812:ASN:HB3	1.86	0.41
1:E:169:ILE:HD12	1:E:169:ILE:HA	1.95	0.41
1:A:371:SER:OG	1:A:440:SER:OG	2.31	0.41
2:B:778:HIS:ND1	2:B:779:LEU:HG	2.35	0.41
2:D:755:SER:O	2:D:856:VAL:N	2.53	0.41
1:E:356:LEU:HD21	1:E:447:VAL:HG23	2.03	0.41
2:F:755:SER:O	2:F:856:VAL:N	2.44	0.41
1:G:212:LEU:HD22	1:G:302:LEU:HD11	2.03	0.41
1:G:321:VAL:HG11	1:G:324:VAL:HB	2.03	0.41
1:G:414:THR:O	1:G:434:CYS:N	2.43	0.41
1:I:180:LYS:HA	1:I:181:PRO:HA	1.92	0.41
2:B:705:SER:HB2	2:B:714:ARG:HH12	1.86	0.40
2:D:907:GLU:HG3	2:D:913:TYR:CE1	2.56	0.40
2:H:1090:VAL:HG22	2:H:1092:GLU:H	1.86	0.40
1:I:159:ARG:HG2	1:I:191:PHE:HE2	1.86	0.40
2:J:843:ARG:HG3	2:J:845:GLU:HG2	2.03	0.40
2:F:769:PRO:HG3	2:F:967:THR:HG23	2.02	0.40
2:F:743:LYS:HD3	2:F:1022:PHE:HD1	1.85	0.40
2:L:890:LEU:HD11	2:L:1009:ALA:HB1	2.02	0.40
2:L:976:PHE:O	2:L:980:SER:OG	2.35	0.40
1:A:159:ARG:NH2	1:A:186:GLY:O	2.54	0.40
2:B:857:HIS:CD2	2:B:895:GLU:HB2	2.56	0.40
2:D:976:PHE:O	2:D:980:SER:OG	2.31	0.40
2:F:850:PHE:HE1	2:F:907:GLU:HB2	1.86	0.40
1:G:358:LYS:HD2	2:H:770:LYS:HD2	2.03	0.40
2:J:810:ARG:HD2	2:J:836:HIS:CE1	2.56	0.40
2:L:810:ARG:NH1	2:L:945:GLU:OE1	2.47	0.40
1:A:316:THR:HG23	1:A:355:TYR:HB2	2.04	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	295/316 (93%)	254 (86%)	37 (12%)	4 (1%)	12	52
1	C	295/316 (93%)	250 (85%)	41 (14%)	4 (1%)	12	52
1	E	295/316 (93%)	260 (88%)	32 (11%)	3 (1%)	17	60
1	G	295/316 (93%)	254 (86%)	39 (13%)	2 (1%)	24	67
1	I	295/316 (93%)	256 (87%)	36 (12%)	3 (1%)	17	60
1	K	295/316 (93%)	261 (88%)	28 (10%)	6 (2%)	8	45
2	B	429/431 (100%)	380 (89%)	44 (10%)	5 (1%)	14	56
2	D	429/431 (100%)	378 (88%)	47 (11%)	4 (1%)	19	61
2	F	429/431 (100%)	380 (89%)	43 (10%)	6 (1%)	12	52
2	H	429/431 (100%)	382 (89%)	42 (10%)	5 (1%)	14	56
2	J	429/431 (100%)	376 (88%)	48 (11%)	5 (1%)	14	56
2	L	429/431 (100%)	382 (89%)	43 (10%)	4 (1%)	19	61
All	All	4344/4482 (97%)	3813 (88%)	480 (11%)	51 (1%)	19	56

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1083	CYS
1	C	239	CYS
2	D	1083	CYS
1	E	281	CYS
1	E	284	CYS
1	A	179	CYS
2	B	824	GLY
2	B	877	ALA
2	B	986	ASN
1	C	456	CYS
2	F	1029	CYS
2	J	877	ALA

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Mol	Chain	Res	Type
1	K	281	CYS
2	L	1083	CYS
1	A	164	LYS
1	A	329	LEU
2	B	960	ILE
2	D	922	GLU
2	F	877	ALA
2	F	986	ASN
2	H	824	GLY
2	H	960	ILE
1	I	329	LEU
1	I	427	ALA
2	J	809	MET
1	K	329	LEU
1	K	410	SER
1	K	427	ALA
2	D	877	ALA
2	D	960	ILE
2	F	809	MET
2	F	960	ILE
1	G	329	LEU
1	G	416	ASP
2	H	877	ALA
2	H	891	SER
1	I	311	GLY
2	J	960	ILE
2	L	877	ALA
2	L	960	ILE
2	L	986	ASN
2	F	1103	GLY
2	J	986	ASN
2	J	1083	CYS
1	K	311	GLY
1	A	322	CYS
1	K	326	VAL
1	C	238	PRO
1	C	311	GLY
1	E	454	PRO
2	H	896	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%)	237 (98%)	4 (2%)	63	83
1	C	241/271 (89%)	239 (99%)	2 (1%)	83	92
1	E	241/271 (89%)	240 (100%)	1 (0%)	92	95
1	G	241/271 (89%)	239 (99%)	2 (1%)	83	92
1	I	241/271 (89%)	239 (99%)	2 (1%)	83	92
1	K	241/271 (89%)	240 (100%)	1 (0%)	92	95
2	B	347/371 (94%)	344 (99%)	3 (1%)	81	90
2	D	347/371 (94%)	339 (98%)	8 (2%)	53	76
2	F	347/371 (94%)	344 (99%)	3 (1%)	81	90
2	H	347/371 (94%)	345 (99%)	2 (1%)	87	93
2	J	347/371 (94%)	346 (100%)	1 (0%)	93	96
2	L	347/371 (94%)	342 (99%)	5 (1%)	69	85
All	All	3528/3852 (92%)	3494 (99%)	34 (1%)	80	89

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	ARG
1	A	313	LYS
1	A	330	LYS
1	A	438	ASN
2	B	700	ARG
2	B	810	ARG
2	B	949	ARG
1	C	331	LYS
1	C	438	ASN
2	D	700	ARG
2	D	714	ARG
2	D	925	ARG
2	D	949	ARG
2	D	994	LYS

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Mol	Chain	Res	Type
2	D	996	ASN
2	D	1106	ARG
2	D	1111	LYS
1	E	378	LYS
2	F	722	ARG
2	F	810	ARG
2	F	949	ARG
1	G	285	ARG
1	G	330	LYS
2	H	786	ASN
2	H	810	ARG
1	I	378	LYS
1	I	438	ASN
2	J	925	ARG
1	K	438	ASN
2	L	810	ARG
2	L	925	ARG
2	L	952	ASN
2	L	994	LYS
2	L	1047	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	335	GLN
1	A	431	ASN
2	B	1064	ASN
1	C	166	HIS
1	C	204	GLN
1	C	438	ASN
2	D	1000	GLN
2	D	1084	GLN
1	E	160	ASN
1	E	166	HIS
2	F	829	ASN
2	F	901	ASN
2	F	1000	GLN
1	G	157	HIS
1	G	204	GLN
1	G	252	ASN
2	H	784	HIS

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Mol	Chain	Res	Type
2	H	786	ASN
2	H	944	HIS
2	H	1043	ASN
1	I	166	HIS
1	I	232	GLN
1	I	327	GLN
1	I	436	HIS
1	I	438	ASN
2	J	741	GLN
2	J	817	GLN
2	J	1000	GLN
2	J	1043	ASN
2	J	1063	HIS
2	J	1084	GLN
1	K	166	HIS
1	K	258	HIS
1	K	327	GLN
1	K	428	GLN
1	K	438	ASN
2	L	952	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.