



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 09:44 pm GMT

PDB ID : 6F9B
EMDB ID: : EMD-4197
Title : Asymmetric unit of Rift Valley fever virus glycoprotein shell
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.

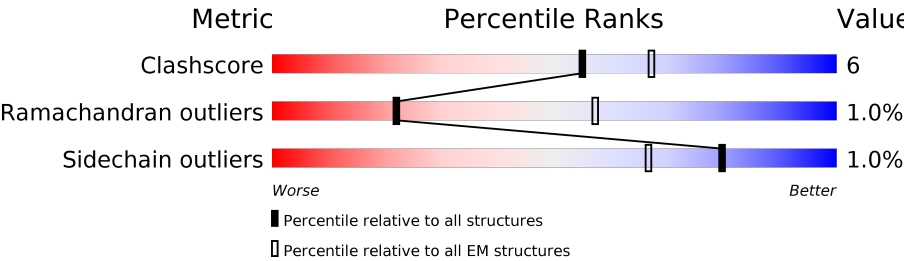
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

1 Overall quality at a glance i

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	80% 15% 5%
1	C	316	83% 12% 5%
1	E	316	83% 11% • 5%
1	G	316	82% 14% 5%
1	I	316	79% 15% • 5%
1	K	316	82% 13% • 5%
1	M	316	80% 16% 5%
1	O	316	79% 16% • 5%
1	Q	316	82% 13% 5%

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Mol	Chain	Length	Quality of chain
1	S	316	 80%15%5%
1	U	316	 76%18%5%
1	X	316	 76%19%5%
2	B	431	 83%17%
2	D	431	 80%19%•
2	F	431	 82%18%
2	H	431	 79%20%
2	J	431	 85%15%
2	L	431	 83%17%
2	N	431	 82%17%
2	P	431	 83%17%
2	R	431	 82%18%
2	T	431	 81%19%
2	V	431	 78%22%
2	Y	431	 83%17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 67152 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
			2324	1455	400	445	24		
1	C	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	E	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	G	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	I	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	K	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	M	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	O	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	Q	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	S	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	U	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		
1	X	301	Total	C	N	O	S	0	0
			2324	1455	400	445	24		

- Molecule 2 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	D	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	F	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	J	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	L	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	N	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	P	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	R	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	T	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	V	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		
2	Y	431	Total	C	N	O	S	0	0
			3272	2030	561	652	29		

There are 36 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
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
N	688	ASP	-	expression tag	UNP A2T072
N	689	PRO	-	expression tag	UNP A2T072
N	690	GLY	-	expression tag	UNP A2T072

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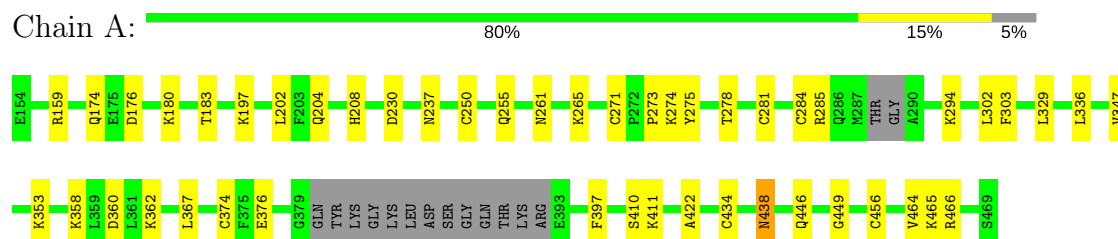
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Chain	Residue	Modelled	Actual	Comment	Reference
P	688	ASP	-	expression tag	UNP A2T072
P	689	PRO	-	expression tag	UNP A2T072
P	690	GLY	-	expression tag	UNP A2T072
R	688	ASP	-	expression tag	UNP A2T072
R	689	PRO	-	expression tag	UNP A2T072
R	690	GLY	-	expression tag	UNP A2T072
T	688	ASP	-	expression tag	UNP A2T072
T	689	PRO	-	expression tag	UNP A2T072
T	690	GLY	-	expression tag	UNP A2T072
V	688	ASP	-	expression tag	UNP A2T072
V	689	PRO	-	expression tag	UNP A2T072
V	690	GLY	-	expression tag	UNP A2T072
Y	688	ASP	-	expression tag	UNP A2T072
Y	689	PRO	-	expression tag	UNP A2T072
Y	690	GLY	-	expression tag	UNP A2T072

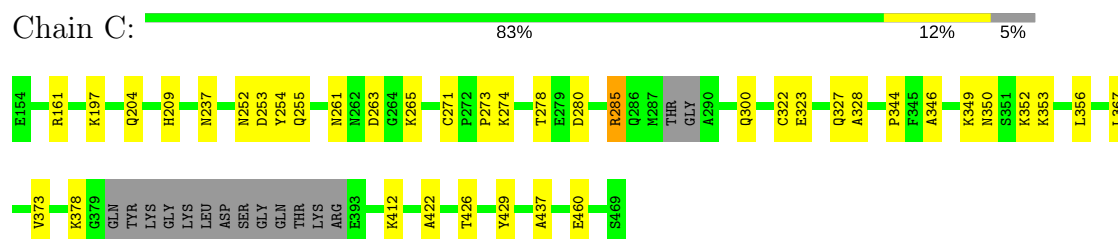
3 Residue-property plots [i](#)

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.

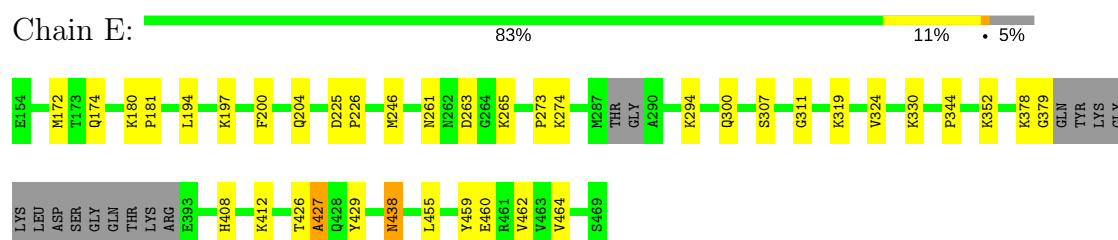
- Molecule 1: Glycoprotein



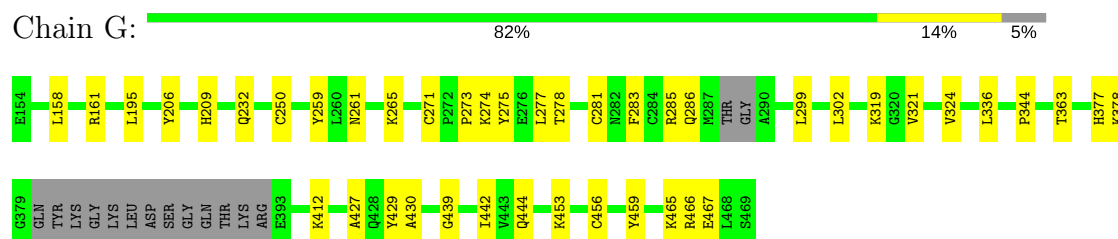
- Molecule 1: Glycoprotein



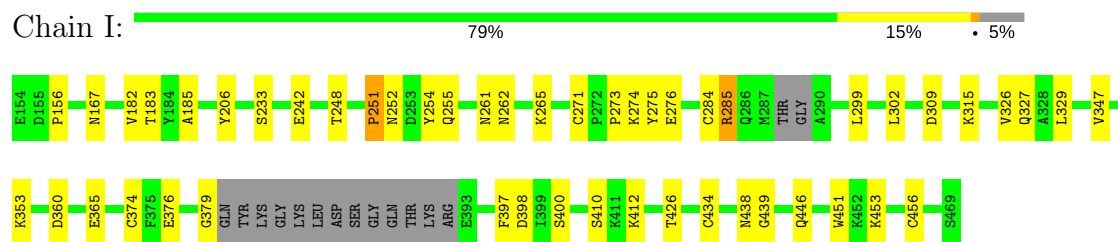
- Molecule 1: Glycoprotein



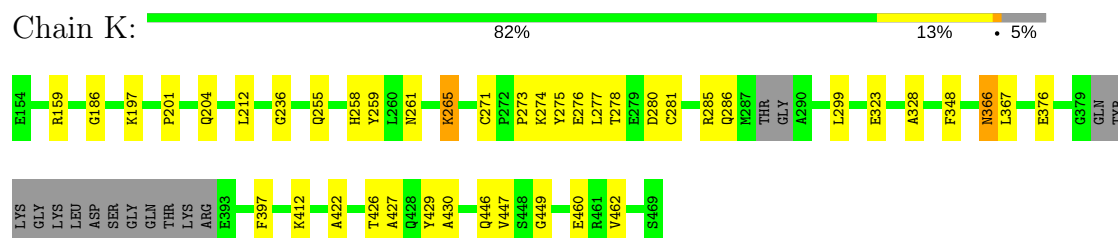
- Molecule 1: Glycoprotein



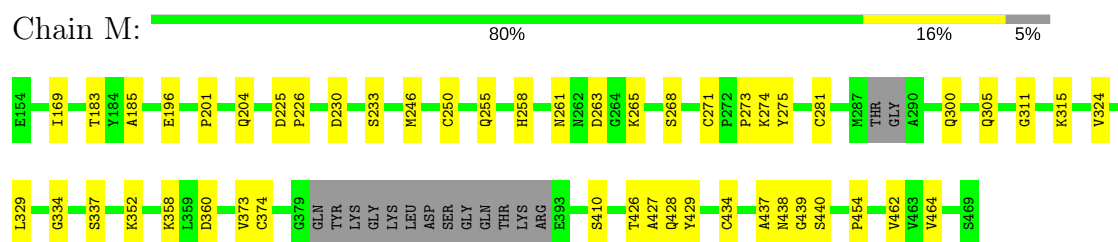
- Molecule 1: Glycoprotein



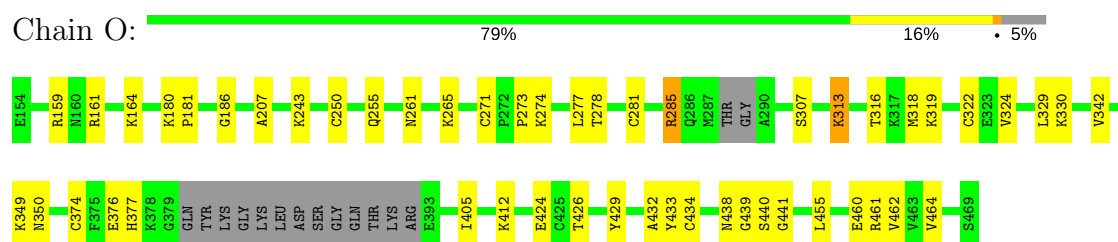
- Molecule 1: Glycoprotein



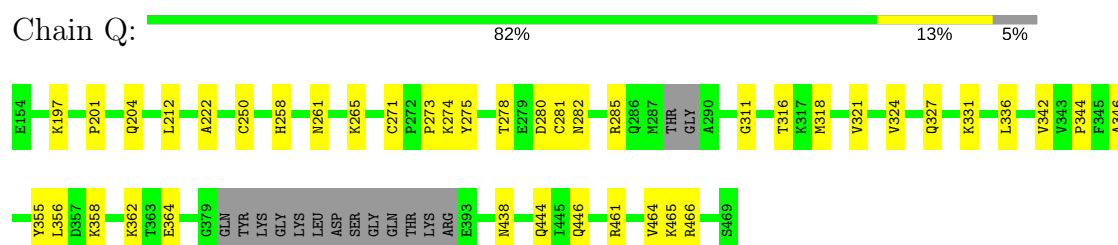
- Molecule 1: Glycoprotein



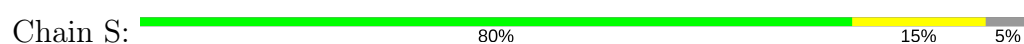
- Molecule 1: Glycoprotein

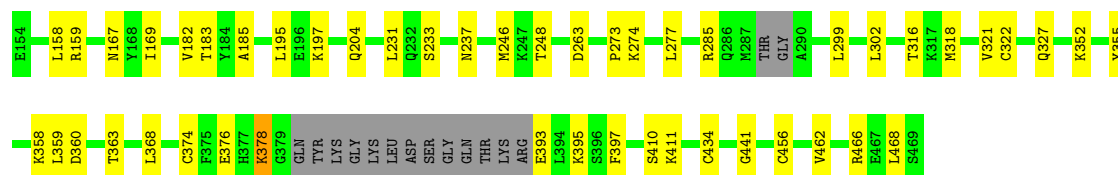


- Molecule 1: Glycoprotein



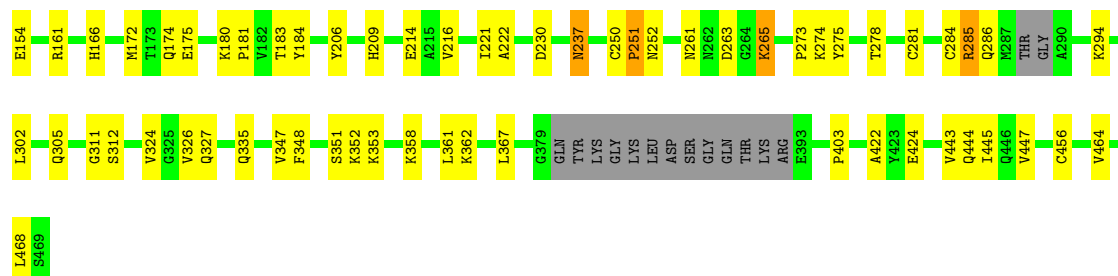
- Molecule 1: Glycoprotein





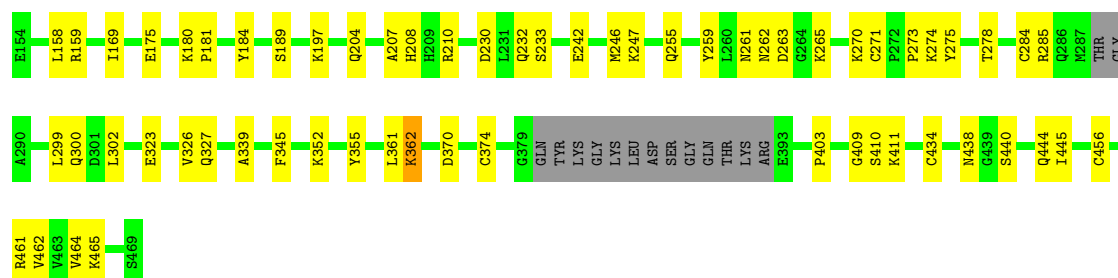
• Molecule 1: Glycoprotein

Chain U: 76% 18% 5%



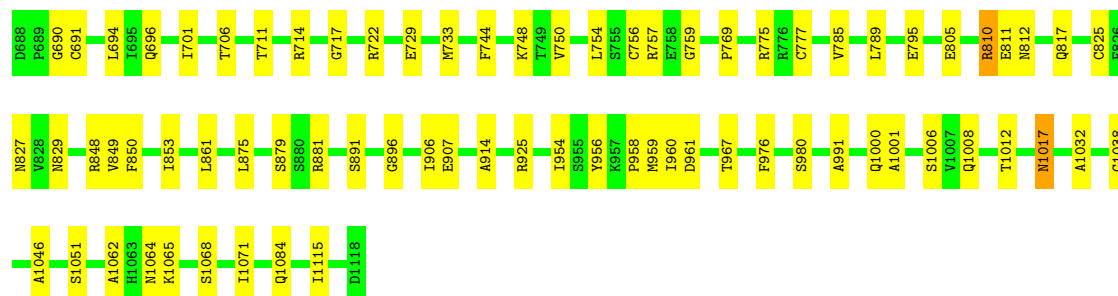
• Molecule 1: Glycoprotein

Chain X: 76% 19% 5%



• Molecule 2: Glycoprotein

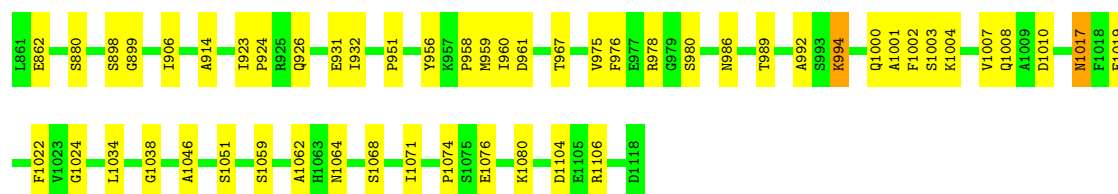
Chain B: 83% 17%



• Molecule 2: Glycoprotein

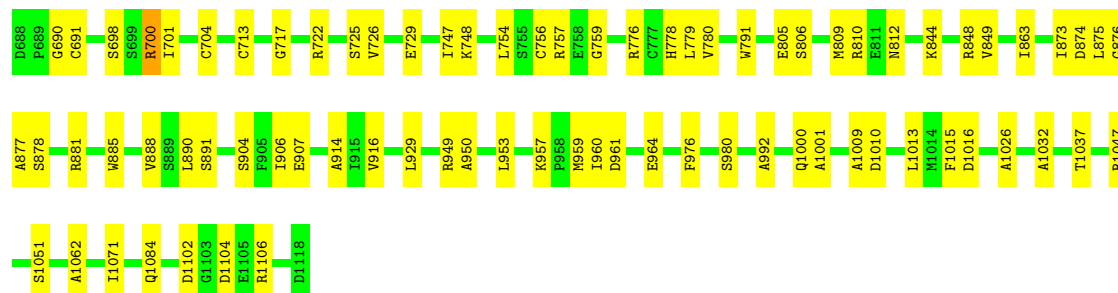
Chain D: 80% 19%





• Molecule 2: Glycoprotein

Chain F: 82% 18%



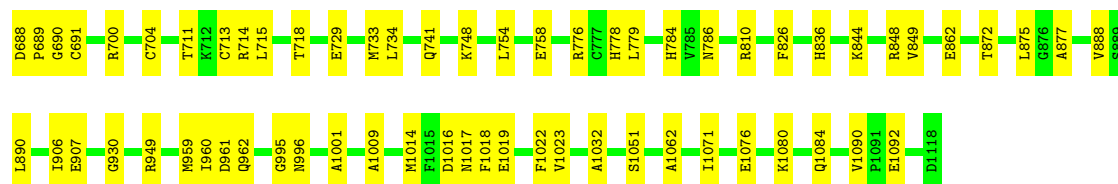
• Molecule 2: Glycoprotein

Chain H: 79% 20%



• Molecule 2: Glycoprotein

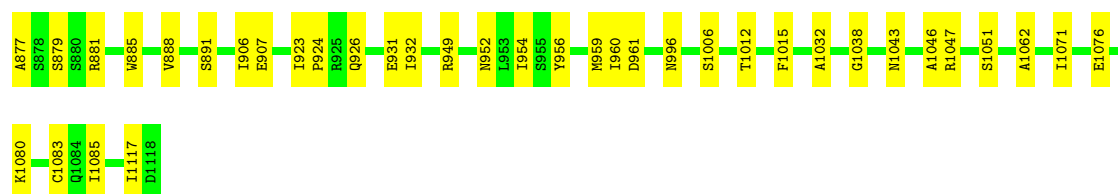
Chain J: 85% 15%



• Molecule 2: Glycoprotein

Chain L: 83% 17%





• Molecule 2: Glycoprotein

Chain N: 82% 17%



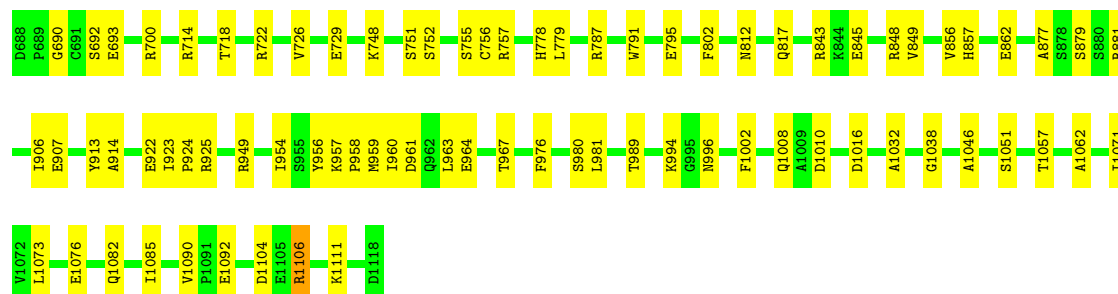
• Molecule 2: Glycoprotein

Chain P: 83% 17%



• Molecule 2: Glycoprotein

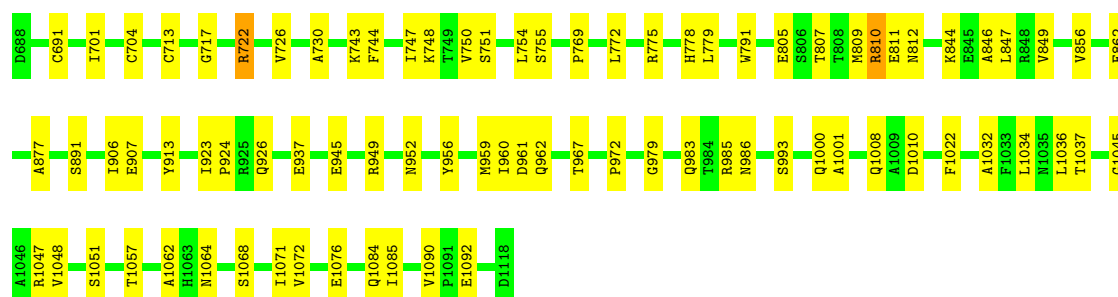
Chain R: 82% 18%



• Molecule 2: Glycoprotein

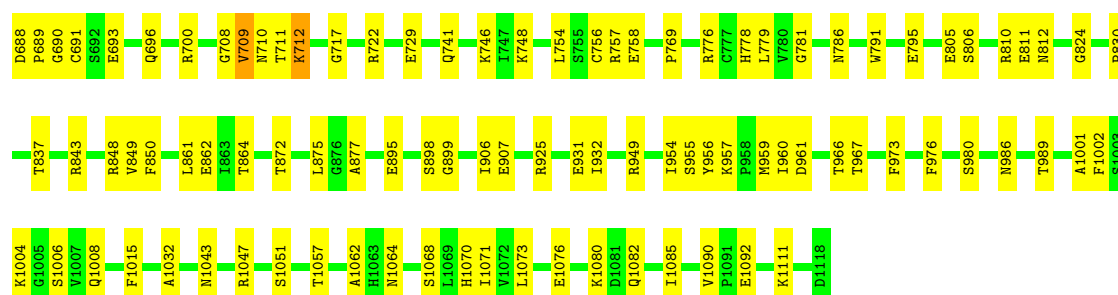
Chain T: 81% 19%





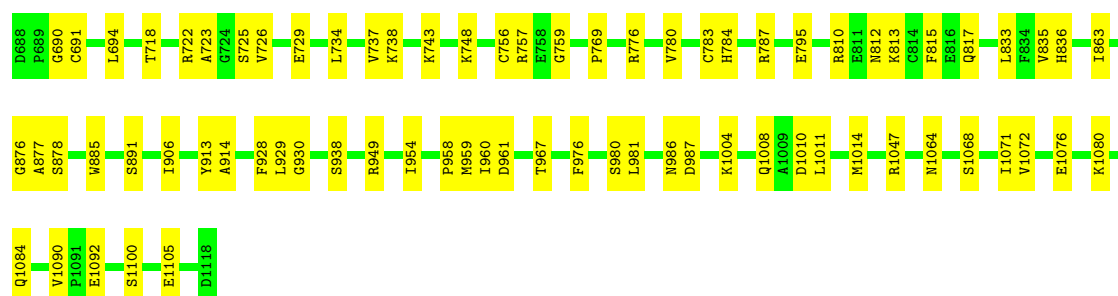
• Molecule 2: Glycoprotein

Chain V: 78% 22%



• Molecule 2: Glycoprotein

Chain Y: 83% 17%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.24	0/2373	0.40	0/3193
1	C	0.24	0/2373	0.40	0/3193
1	E	0.24	0/2373	0.40	0/3193
1	G	0.24	0/2373	0.41	0/3193
1	I	0.24	0/2373	0.40	0/3193
1	K	0.24	0/2373	0.41	0/3193
1	M	0.24	0/2373	0.40	0/3193
1	O	0.24	0/2373	0.40	0/3193
1	Q	0.24	0/2373	0.40	0/3193
1	S	0.24	0/2373	0.41	0/3193
1	U	0.24	0/2373	0.41	0/3193
1	X	0.24	0/2373	0.41	0/3193
2	B	0.24	0/3332	0.42	0/4503
2	D	0.24	0/3332	0.42	0/4503
2	F	0.24	0/3332	0.42	0/4503
2	H	0.24	0/3332	0.43	0/4503
2	J	0.24	0/3332	0.43	0/4503
2	L	0.24	0/3332	0.42	0/4503
2	N	0.24	0/3332	0.42	0/4503
2	P	0.24	0/3332	0.42	0/4503
2	R	0.24	0/3332	0.42	0/4503
2	T	0.24	0/3332	0.43	0/4503
2	V	0.24	0/3332	0.42	0/4503
2	Y	0.24	0/3332	0.42	0/4503
All	All	0.24	0/68460	0.42	0/92352

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 ⓘ

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	2324	0	2259	25	0
1	C	2324	0	2259	19	0
1	E	2324	0	2259	22	0
1	G	2324	0	2259	26	0
1	I	2324	0	2259	28	0
1	K	2324	0	2259	23	0
1	M	2324	0	2259	23	0
1	O	2324	0	2259	25	0
1	Q	2324	0	2259	23	0
1	S	2324	0	2259	28	0
1	U	2324	0	2259	31	0
1	X	2324	0	2259	32	0
2	B	3272	0	3143	41	0
2	D	3272	0	3143	44	0
2	F	3272	0	3143	43	0
2	H	3272	0	3143	47	0
2	J	3272	0	3143	33	0
2	L	3272	0	3143	38	0
2	N	3272	0	3143	39	0
2	P	3272	0	3143	37	0
2	R	3272	0	3143	40	0
2	T	3272	0	3143	44	0
2	V	3272	0	3143	50	0
2	Y	3272	0	3143	38	0
All	All	67152	0	64824	766	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 6.

All (766) 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:L:1062:ALA:HB3	2:L:1071:ILE:HB	1.71	0.73
2:J:1062:ALA:HB3	2:J:1071:ILE:HB	1.71	0.71
2:F:691:CYS:HA	2:F:729:GLU:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1062:ALA:HB3	2:N:1071:ILE:HB	1.74	0.69
1:I:262:ASN:HD22	1:I:326:VAL:HG22	1.58	0.69
1:X:261:ASN:HD21	1:X:265:LYS:HB2	1.57	0.69
2:H:785:VAL:O	2:H:789:LEU:HB2	1.93	0.68
2:P:1062:ALA:HB3	2:P:1071:ILE:HB	1.76	0.67
1:S:359:LEU:H	2:T:772:LEU:HG	1.60	0.67
2:D:843:ARG:HG3	2:D:845:GLU:H	1.60	0.67
2:J:690:GLY:HA3	2:J:1084:GLN:HA	1.77	0.67
2:T:1062:ALA:HB3	2:T:1071:ILE:HB	1.77	0.67
1:E:261:ASN:HD21	1:E:265:LYS:HB2	1.59	0.66
2:T:748:LYS:HB3	2:T:862:GLU:HB3	1.78	0.66
2:B:691:CYS:HA	2:B:729:GLU:HB2	1.78	0.66
2:R:748:LYS:HB3	2:R:862:GLU:HB3	1.78	0.65
2:T:791:TRP:HE1	2:T:812:ASN:HB3	1.60	0.65
2:N:691:CYS:HA	2:N:729:GLU:HB2	1.79	0.64
2:T:805:GLU:OE2	2:T:810:ARG:NH2	2.30	0.64
2:B:722:ARG:HH22	2:B:1008:GLN:HG3	1.63	0.64
2:D:1064:ASN:HD21	2:D:1068:SER:H	1.44	0.64
1:K:261:ASN:HD21	1:K:265:LYS:HB2	1.62	0.63
2:F:890:LEU:HD11	2:F:1009:ALA:HB1	1.81	0.63
2:F:1104:ASP:OD2	2:F:1106:ARG:NH1	2.31	0.63
1:E:412:LYS:HD2	1:E:426:THR:HG21	1.81	0.62
1:C:367:LEU:HD12	1:C:422:ALA:HB2	1.82	0.62
1:X:438:ASN:HB2	2:Y:780:VAL:HG22	1.81	0.62
2:B:785:VAL:O	2:B:789:LEU:HB2	1.99	0.62
2:V:1062:ALA:HB3	2:V:1071:ILE:HB	1.80	0.62
1:A:336:LEU:HD13	1:A:465:LYS:HD3	1.82	0.62
2:H:1104:ASP:OD2	2:H:1106:ARG:NH1	2.32	0.62
1:S:231:LEU:HD23	1:S:237:ASN:HD21	1.64	0.61
2:N:1104:ASP:OD2	2:N:1106:ARG:NH1	2.33	0.61
2:D:1104:ASP:OD2	2:D:1106:ARG:NH1	2.33	0.61
1:G:321:VAL:HG22	1:G:466:ARG:HG2	1.82	0.61
2:R:1062:ALA:HB3	2:R:1071:ILE:HB	1.81	0.61
2:V:848:ARG:NH2	2:V:907:GLU:OE1	2.33	0.61
2:L:701:ILE:HD12	2:L:717:GLY:HA3	1.83	0.60
2:T:730:ALA:HB3	2:T:747:ILE:HB	1.83	0.60
1:G:377:HIS:HB3	1:I:285:ARG:HH21	1.65	0.60
1:C:426:THR:HB	1:C:429:TYR:HB2	1.84	0.60
1:A:174:GLN:HG3	1:A:294:LYS:HB3	1.83	0.60
2:H:730:ALA:HB3	2:H:747:ILE:HB	1.84	0.60
1:Q:316:THR:HG23	1:Q:355:TYR:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:316:THR:HG23	1:S:355:TYR:HB2	1.83	0.60
1:Q:261:ASN:HD21	1:Q:265:LYS:HB2	1.67	0.60
1:S:374:CYS:HA	1:S:434:CYS:HA	1.84	0.60
1:E:197:LYS:HA	1:E:204:GLN:HE22	1.67	0.59
2:H:848:ARG:NH2	2:H:907:GLU:OE1	2.33	0.59
1:E:427:ALA:HB1	1:G:283:PHE:HB3	1.84	0.59
2:D:1076:GLU:HB3	2:D:1080:LYS:HG3	1.85	0.59
2:D:748:LYS:HB3	2:D:862:GLU:HB3	1.83	0.59
1:A:446:GLN:HE21	1:A:449:GLY:HA2	1.68	0.59
2:B:849:VAL:HG22	2:B:906:ILE:HG12	1.85	0.59
1:Q:197:LYS:HA	1:Q:204:GLN:HE22	1.68	0.59
2:B:906:ILE:HB	2:B:914:ALA:HB3	1.85	0.59
2:H:805:GLU:OE2	2:H:810:ARG:NH2	2.35	0.59
1:U:362:LYS:HD3	1:U:444:GLN:HB2	1.85	0.59
1:Q:342:VAL:HG22	1:Q:461:ARG:HG2	1.85	0.58
2:J:718:THR:HG22	2:J:1014:MET:HG2	1.85	0.58
2:J:849:VAL:HG22	2:J:906:ILE:HG12	1.84	0.58
2:H:849:VAL:HG22	2:H:906:ILE:HG12	1.86	0.58
2:J:754:LEU:HB2	2:J:1001:ALA:HB3	1.86	0.58
1:S:197:LYS:HA	1:S:204:GLN:HE22	1.68	0.58
2:D:989:THR:HB	2:D:1002:PHE:HB2	1.86	0.58
1:X:159:ARG:HE	1:X:184:TYR:HA	1.68	0.58
2:H:691:CYS:H	2:H:1084:GLN:HA	1.68	0.58
1:K:426:THR:HB	1:K:429:TYR:HB2	1.86	0.58
2:F:992:ALA:O	2:F:1000:GLN:NE2	2.37	0.57
1:I:255:GLN:NE2	1:I:271:CYS:O	2.34	0.57
1:A:358:LYS:NZ	1:A:360:ASP:OD2	2.37	0.57
2:D:729:GLU:HG2	2:D:748:LYS:HA	1.86	0.57
2:F:805:GLU:OE1	2:F:810:ARG:NH2	2.36	0.57
2:R:756:CYS:SG	2:R:757:ARG:N	2.78	0.57
2:J:1032:ALA:HB3	2:J:1051:SER:HB2	1.86	0.57
2:B:1006:SER:OG	2:B:1008:GLN:NE2	2.38	0.57
2:D:752:SER:HG	2:D:857:HIS:HE2	1.47	0.57
1:M:374:CYS:HA	1:M:434:CYS:HA	1.86	0.57
1:K:201:PRO:HG2	2:L:802:PHE:HB3	1.86	0.57
2:T:1032:ALA:HB3	2:T:1051:SER:HB3	1.85	0.57
1:C:255:GLN:HB2	1:C:271:CYS:HB2	1.85	0.57
2:D:849:VAL:HG22	2:D:906:ILE:HG12	1.86	0.57
2:P:848:ARG:NH2	2:P:907:GLU:OE1	2.38	0.57
2:P:791:TRP:HE1	2:P:812:ASN:HB3	1.70	0.57
1:X:232:GLN:HE22	1:X:275:TYR:HD2	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:302:LEU:HD12	1:I:456:CYS:HB3	1.86	0.57
1:K:197:LYS:HA	1:K:204:GLN:HE22	1.69	0.57
1:K:212:LEU:HD23	1:K:258:HIS:HD2	1.69	0.57
1:U:305:GLN:HE22	1:U:443:VAL:HB	1.70	0.57
2:L:1038:GLY:HA3	2:L:1046:ALA:HA	1.86	0.57
2:D:1062:ALA:HB3	2:D:1071:ILE:HB	1.87	0.56
2:H:890:LEU:HD11	2:H:1009:ALA:HB1	1.86	0.56
1:M:196:GLU:O	1:M:204:GLN:NE2	2.38	0.56
2:V:957:LYS:NZ	2:V:966:THR:OG1	2.38	0.56
2:B:696:GLN:NE2	2:B:733:MET:SD	2.77	0.56
2:D:741:GLN:HE21	2:D:1024:GLY:HA2	1.70	0.56
2:R:913:TYR:HB2	2:R:981:LEU:HD12	1.87	0.56
2:N:849:VAL:HG22	2:N:906:ILE:HG12	1.87	0.56
1:O:324:VAL:HG23	1:O:464:VAL:HG22	1.88	0.56
2:Y:784:HIS:HD2	2:Y:787:ARG:HH21	1.54	0.56
1:K:271:CYS:HB3	1:K:275:TYR:HB2	1.87	0.56
1:E:300:GLN:NE2	1:E:460:GLU:OE1	2.39	0.56
1:U:261:ASN:HD21	1:U:265:LYS:HB2	1.69	0.56
1:C:252:ASN:O	1:C:254:TYR:N	2.38	0.56
1:G:467:GLU:OE1	2:J:1017:ASN:ND2	2.38	0.56
2:R:906:ILE:HB	2:R:914:ALA:HB3	1.88	0.56
1:X:263:ASP:OD1	1:X:352:LYS:NZ	2.38	0.56
1:G:442:ILE:HG23	1:G:453:LYS:HD2	1.88	0.56
1:O:405:ILE:HA	1:O:424:GLU:HB2	1.88	0.56
2:F:885:TRP:HH2	2:F:1013:LEU:HD22	1.71	0.56
1:C:412:LYS:HD2	1:C:426:THR:HG21	1.88	0.56
2:F:806:SER:O	2:F:810:ARG:NH1	2.39	0.56
2:N:923:ILE:HD12	2:N:924:PRO:HD2	1.88	0.56
2:B:775:ARG:NH1	2:B:777:CYS:SG	2.78	0.55
1:C:278:THR:HG22	1:C:285:ARG:HD2	1.87	0.55
2:D:926:GLN:NE2	2:D:951:PRO:O	2.39	0.55
1:I:374:CYS:HA	1:I:434:CYS:HA	1.87	0.55
1:O:255:GLN:NE2	1:O:271:CYS:O	2.36	0.55
1:S:158:LEU:HD12	1:S:159:ARG:HG3	1.87	0.55
1:S:302:LEU:HD12	1:S:456:CYS:HB3	1.87	0.55
1:X:246:MET:HG2	1:X:462:VAL:HG12	1.88	0.55
1:A:261:ASN:HD21	1:A:265:LYS:HB2	1.70	0.55
2:P:879:SER:OG	2:P:881:ARG:NH1	2.40	0.55
2:R:849:VAL:HG22	2:R:906:ILE:HG12	1.88	0.55
2:L:842:VAL:HG23	2:L:843:ARG:HD2	1.88	0.55
2:V:849:VAL:HG22	2:V:906:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ARG:NH2	1:C:209:HIS:O	2.40	0.55
1:A:230:ASP:O	1:A:237:ASN:ND2	2.40	0.55
2:R:693:GLU:HG2	2:R:722:ARG:HB2	1.89	0.55
2:R:989:THR:HB	2:R:1002:PHE:HB2	1.89	0.55
1:U:250:CYS:N	1:U:281:CYS:SG	2.79	0.55
2:F:1062:ALA:HB3	2:F:1071:ILE:HB	1.88	0.55
2:P:690:GLY:H	2:P:1085:ILE:HG12	1.71	0.55
1:A:374:CYS:HA	1:A:434:CYS:HA	1.89	0.55
1:M:358:LYS:NZ	1:M:360:ASP:OD2	2.40	0.55
2:L:828:VAL:HG11	1:M:337:SER:HA	1.89	0.55
2:Y:734:LEU:HB3	2:Y:743:LYS:HB2	1.87	0.55
2:F:1032:ALA:HB3	2:F:1051:SER:HB2	1.88	0.55
2:N:756:CYS:SG	2:N:757:ARG:N	2.80	0.55
1:C:300:GLN:NE2	1:C:460:GLU:OE1	2.40	0.54
2:R:729:GLU:HG2	2:R:748:LYS:HA	1.88	0.54
1:U:327:GLN:NE2	1:U:353:LYS:O	2.38	0.54
1:S:183:THR:HG23	1:S:185:ALA:H	1.73	0.54
2:N:879:SER:OG	2:N:881:ARG:NH1	2.40	0.54
2:V:989:THR:HB	2:V:1002:PHE:HB2	1.89	0.54
1:G:161:ARG:NH2	1:G:209:HIS:O	2.40	0.54
2:D:992:ALA:O	2:D:1000:GLN:NE2	2.41	0.54
2:F:849:VAL:HG22	2:F:906:ILE:HG12	1.88	0.54
2:H:843:ARG:NH1	2:J:1014:MET:SD	2.81	0.54
1:K:277:LEU:HD13	1:K:281:CYS:HB2	1.88	0.54
1:Q:201:PRO:HG2	2:R:802:PHE:HB3	1.90	0.54
2:V:843:ARG:NH1	2:Y:1014:MET:SD	2.80	0.54
1:A:362:LYS:NZ	2:B:961:ASP:OD2	2.40	0.54
2:D:756:CYS:SG	2:D:757:ARG:N	2.81	0.54
2:L:748:LYS:HB3	2:L:862:GLU:HB3	1.89	0.54
1:O:376:GLU:HA	1:O:432:ALA:HA	1.89	0.54
2:P:875:LEU:HD21	2:P:888:VAL:HG23	1.89	0.54
2:F:729:GLU:HG2	2:F:748:LYS:HA	1.89	0.54
2:H:1034:LEU:HD23	2:H:1049:CYS:HB3	1.89	0.54
2:H:879:SER:OG	2:H:881:ARG:NH1	2.39	0.54
2:N:926:GLN:NE2	2:N:951:PRO:O	2.41	0.54
2:R:817:GLN:HE22	2:R:958:PRO:HB3	1.72	0.54
2:T:993:SER:HB2	2:T:1000:GLN:HB3	1.89	0.54
2:T:701:ILE:HD12	2:T:717:GLY:HA3	1.90	0.54
2:J:741:GLN:NE2	2:J:1023:VAL:O	2.40	0.53
2:P:756:CYS:SG	2:P:757:ARG:N	2.81	0.53
2:B:1062:ALA:HB3	2:B:1071:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:975:VAL:HA	2:D:978:ARG:HG2	1.90	0.53
2:F:906:ILE:HB	2:F:914:ALA:HB3	1.90	0.53
2:Y:756:CYS:SG	2:Y:757:ARG:N	2.81	0.53
1:I:248:THR:HB	1:I:299:LEU:HD22	1.89	0.53
2:L:756:CYS:SG	2:L:757:ARG:N	2.82	0.53
1:A:367:LEU:HD22	1:A:422:ALA:HB2	1.91	0.53
2:L:693:GLU:HG3	2:L:722:ARG:HB3	1.90	0.53
1:S:263:ASP:OD1	1:S:352:LYS:NZ	2.39	0.53
1:M:373:VAL:HG13	1:M:437:ALA:HB2	1.90	0.53
2:N:1038:GLY:HA3	2:N:1046:ALA:HA	1.89	0.53
2:L:688:ASP:HB2	2:L:1083:CYS:HB2	1.91	0.53
1:A:255:GLN:NE2	1:A:271:CYS:O	2.41	0.53
1:C:327:GLN:NE2	1:C:353:LYS:O	2.41	0.53
2:D:691:CYS:HA	2:D:729:GLU:HB2	1.91	0.53
2:V:1032:ALA:HB3	2:V:1051:SER:HB3	1.90	0.53
1:I:206:TYR:HE1	2:J:776:ARG:HH22	1.57	0.53
2:L:1047:ARG:HG2	2:L:1085:ILE:HG12	1.91	0.53
2:P:722:ARG:NH2	2:P:1008:GLN:OE1	2.41	0.53
2:D:704:CYS:HA	2:D:713:CYS:HA	1.89	0.53
2:F:690:GLY:HA3	2:F:1084:GLN:HA	1.91	0.53
2:T:983:GLN:OE1	2:T:985:ARG:NH2	2.42	0.53
1:U:263:ASP:OD1	1:U:352:LYS:NZ	2.40	0.53
1:C:349:LYS:NZ	1:C:350:ASN:OD1	2.41	0.52
1:G:261:ASN:HD21	1:G:265:LYS:HB2	1.74	0.52
2:L:1032:ALA:HB3	2:L:1051:SER:HB3	1.91	0.52
2:B:756:CYS:SG	2:B:757:ARG:N	2.82	0.52
2:D:923:ILE:HD12	2:D:924:PRO:HD2	1.91	0.52
1:M:263:ASP:OD1	1:M:352:LYS:NZ	2.39	0.52
1:X:259:TYR:HB3	1:X:299:LEU:HD12	1.91	0.52
1:U:403:PRO:HB2	1:U:424:GLU:HB3	1.89	0.52
2:Y:769:PRO:HG3	2:Y:967:THR:HG23	1.91	0.52
2:Y:813:LYS:HB2	2:Y:835:VAL:HB	1.91	0.52
1:C:323:GLU:HG2	1:C:328:ALA:HA	1.91	0.52
2:L:923:ILE:HD12	2:L:924:PRO:HD2	1.91	0.52
1:M:255:GLN:NE2	1:M:271:CYS:O	2.35	0.52
2:P:704:CYS:HA	2:P:713:CYS:HA	1.90	0.52
2:P:849:VAL:HG22	2:P:906:ILE:HG12	1.91	0.52
1:U:230:ASP:O	1:U:237:ASN:ND2	2.42	0.52
2:D:722:ARG:NH1	2:D:1010:ASP:OD1	2.40	0.52
2:L:849:VAL:HG22	2:L:906:ILE:HG12	1.92	0.52
2:N:795:GLU:O	2:N:812:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:926:GLN:NE2	2:T:952:ASN:O	2.43	0.52
2:Y:694:LEU:HD21	2:Y:1072:VAL:HG12	1.92	0.52
1:A:275:TYR:HB3	1:A:284:CYS:HB3	1.91	0.52
2:B:701:ILE:HD12	2:B:717:GLY:HA3	1.91	0.52
2:H:704:CYS:HA	2:H:713:CYS:HA	1.91	0.52
1:S:277:LEU:O	1:S:285:ARG:NH2	2.42	0.52
2:V:691:CYS:HA	2:V:729:GLU:HB2	1.91	0.52
2:Y:722:ARG:NH2	2:Y:1008:GLN:OE1	2.42	0.52
2:H:1076:GLU:OE1	2:H:1080:LYS:NZ	2.41	0.52
1:S:376:GLU:HB2	1:S:397:PHE:HB2	1.92	0.52
2:F:1071:ILE:HA	2:F:1084:GLN:HE22	1.75	0.52
2:F:700:ARG:HD3	2:F:701:ILE:HG23	1.90	0.52
1:S:248:THR:HB	1:S:299:LEU:HD22	1.92	0.52
1:I:261:ASN:HD21	1:I:265:LYS:HB2	1.75	0.52
2:J:890:LEU:HD11	2:J:1009:ALA:HB1	1.92	0.52
1:K:446:GLN:HE21	1:K:449:GLY:HA2	1.75	0.52
2:L:691:CYS:HA	2:L:729:GLU:HB2	1.91	0.51
1:X:374:CYS:HA	1:X:434:CYS:HA	1.92	0.51
2:Y:691:CYS:HA	2:Y:729:GLU:HB2	1.92	0.51
2:T:1090:VAL:HG22	2:T:1092:GLU:H	1.75	0.51
1:A:176:ASP:HB2	1:A:180:LYS:HE2	1.92	0.51
2:J:1076:GLU:OE1	2:J:1080:LYS:NZ	2.43	0.51
1:U:166:HIS:H	1:U:214:GLU:HG2	1.74	0.51
1:E:319:LYS:NZ	2:H:1016:ASP:OD2	2.42	0.51
2:J:848:ARG:NH2	2:J:907:GLU:OE1	2.34	0.51
1:A:197:LYS:HA	1:A:204:GLN:HE22	1.76	0.51
1:A:376:GLU:HB2	1:A:397:PHE:HB2	1.92	0.51
2:D:906:ILE:HB	2:D:914:ALA:HB3	1.93	0.51
1:Q:336:LEU:HD13	1:Q:465:LYS:HB3	1.92	0.51
2:T:979:GLY:HA2	2:T:983:GLN:HE22	1.76	0.51
2:Y:987:ASP:O	2:Y:1004:LYS:NZ	2.43	0.51
1:I:347:VAL:HG22	1:I:353:LYS:HA	1.92	0.51
2:J:711:THR:HB	2:J:1022:PHE:HB2	1.92	0.51
2:J:729:GLU:HG2	2:J:748:LYS:HA	1.93	0.51
2:R:755:SER:N	2:R:856:VAL:O	2.42	0.51
1:S:167:ASN:HD22	1:S:182:VAL:HG21	1.76	0.51
1:E:330:LYS:HD2	2:H:714:ARG:HH22	1.76	0.51
1:G:278:THR:HG22	1:G:285:ARG:HD3	1.93	0.51
2:H:957:LYS:HB2	2:H:964:GLU:HB3	1.92	0.51
2:N:848:ARG:NH2	2:N:907:GLU:OE1	2.36	0.51
2:N:806:SER:O	2:N:810:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:344:PRO:HG2	1:Q:356:LEU:HB2	1.92	0.51
2:R:848:ARG:NH2	2:R:907:GLU:OE1	2.37	0.51
1:X:278:THR:HG22	1:X:285:ARG:HD3	1.93	0.51
2:B:785:VAL:O	2:B:789:LEU:CB	2.59	0.51
2:F:722:ARG:NH1	2:F:1010:ASP:OD1	2.43	0.51
2:J:758:GLU:OE2	2:J:848:ARG:NH2	2.43	0.51
2:B:690:GLY:H	2:B:1084:GLN:HA	1.76	0.50
2:B:729:GLU:HG2	2:B:748:LYS:HA	1.94	0.50
1:C:261:ASN:HD21	1:C:265:LYS:HB2	1.76	0.50
2:L:1076:GLU:OE1	2:L:1080:LYS:NZ	2.43	0.50
1:Q:316:THR:OG1	1:Q:327:GLN:OE1	2.29	0.50
2:V:806:SER:O	2:V:810:ARG:NH1	2.44	0.50
2:L:690:GLY:HA3	2:L:1085:ILE:H	1.76	0.50
2:P:746:LYS:HB2	2:P:864:THR:HB	1.94	0.50
2:J:691:CYS:HA	2:J:729:GLU:HB2	1.93	0.50
2:R:692:SER:OG	2:R:693:GLU:OE1	2.29	0.50
2:R:923:ILE:HD12	2:R:924:PRO:HD2	1.94	0.50
1:E:307:SER:HB3	1:E:455:LEU:HD23	1.94	0.50
2:R:787:ARG:NH2	2:R:795:GLU:OE2	2.45	0.50
1:S:316:THR:HG22	1:S:318:MET:H	1.77	0.50
1:Q:358:LYS:NZ	1:Q:446:GLN:OE1	2.45	0.50
1:G:336:LEU:HD11	1:G:465:LYS:HB3	1.93	0.50
1:I:379:GLY:HA2	1:K:286:GLN:H	1.76	0.50
1:I:376:GLU:HB3	1:I:397:PHE:HB2	1.94	0.50
1:O:261:ASN:HD21	1:O:265:LYS:HB2	1.76	0.50
2:V:830:PRO:HG2	2:Y:938:SER:HB3	1.94	0.50
2:F:957:LYS:HB2	2:F:964:GLU:HB2	1.94	0.50
2:L:891:SER:HB2	2:L:1012:THR:HG23	1.92	0.50
1:U:324:VAL:HG23	1:U:464:VAL:HG22	1.93	0.50
2:D:811:GLU:OE2	2:D:956:TYR:OH	2.29	0.49
2:N:1071:ILE:HA	2:N:1084:GLN:HE22	1.77	0.49
2:T:754:LEU:HB2	2:T:1001:ALA:HB3	1.94	0.49
2:V:769:PRO:HG3	2:V:967:THR:HG23	1.94	0.49
1:A:159:ARG:NH2	1:A:183:THR:O	2.41	0.49
2:D:754:LEU:HB2	2:D:1001:ALA:HB3	1.93	0.49
2:P:805:GLU:OE2	2:P:810:ARG:NH2	2.45	0.49
2:B:848:ARG:NH2	2:B:907:GLU:OE1	2.33	0.49
1:K:376:GLU:HG3	1:K:397:PHE:HB2	1.93	0.49
2:L:747:ILE:HD12	2:L:863:ILE:HG12	1.94	0.49
2:V:837:THR:HG21	2:V:954:ILE:HG21	1.95	0.49
1:C:263:ASP:OD1	1:C:352:LYS:NZ	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:VAL:HG13	1:C:437:ALA:HB2	1.95	0.49
2:J:1090:VAL:HG22	2:J:1092:GLU:H	1.77	0.49
1:S:376:GLU:OE1	1:S:395:LYS:NZ	2.37	0.49
2:H:775:ARG:NH1	2:H:825:CYS:SG	2.85	0.49
1:K:159:ARG:HH21	1:K:186:GLY:H	1.59	0.49
2:T:811:GLU:OE2	2:T:956:TYR:OH	2.27	0.49
2:Y:795:GLU:O	2:Y:812:ASN:ND2	2.39	0.49
2:H:926:GLN:NE2	2:H:952:ASN:O	2.46	0.49
2:R:879:SER:OG	2:R:881:ARG:NH1	2.41	0.49
2:D:858:LYS:NZ	2:D:860:THR:OG1	2.45	0.49
2:R:1032:ALA:HB3	2:R:1051:SER:HB3	1.95	0.49
1:S:159:ARG:NH2	1:S:183:THR:O	2.40	0.49
1:G:302:LEU:HD12	1:G:456:CYS:HB3	1.95	0.49
1:O:161:ARG:NH1	1:O:207:ALA:O	2.45	0.49
2:R:722:ARG:NH1	2:R:1010:ASP:OD1	2.46	0.49
2:B:817:GLN:HE22	2:B:958:PRO:HB2	1.77	0.48
1:I:309:ASP:HB2	1:I:453:LYS:HE3	1.95	0.48
1:S:468:LEU:HD12	2:T:844:LYS:HG2	1.95	0.48
2:V:693:GLU:HG2	2:V:722:ARG:HB3	1.95	0.48
1:A:336:LEU:HD22	1:A:465:LYS:HB3	1.94	0.48
1:C:197:LYS:HA	1:C:204:GLN:HE22	1.78	0.48
2:D:1059:SER:HA	2:D:1074:PRO:HA	1.95	0.48
2:P:1090:VAL:HG22	2:P:1092:GLU:H	1.78	0.48
2:B:733:MET:HG3	2:B:744:PHE:HE1	1.77	0.48
1:E:194:LEU:HA	1:E:200:PHE:HD2	1.78	0.48
1:I:156:PRO:HD3	1:I:438:ASN:H	1.78	0.48
1:I:242:GLU:HG2	1:I:326:VAL:HG21	1.94	0.48
1:X:361:LEU:HG	1:X:445:ILE:HG13	1.93	0.48
2:H:957:LYS:HG2	2:J:996:ASN:HD21	1.77	0.48
2:T:1045:GLY:HA3	2:T:1085:ILE:HD11	1.95	0.48
2:Y:863:ILE:HG21	2:Y:885:TRP:HE1	1.78	0.48
2:D:976:PHE:O	2:D:980:SER:OG	2.28	0.48
1:E:344:PRO:HB3	1:E:459:TYR:HE1	1.79	0.48
2:H:722:ARG:NH2	2:H:1008:GLN:OE1	2.46	0.48
2:P:913:TYR:HB2	2:P:981:LEU:HD12	1.94	0.48
2:R:1090:VAL:HG22	2:R:1092:GLU:H	1.79	0.48
1:I:412:LYS:HD2	1:I:426:THR:HG21	1.95	0.48
1:O:273:PRO:HA	1:O:274:LYS:HA	1.47	0.48
2:P:1023:VAL:HG22	2:P:1025:ALA:H	1.78	0.48
1:S:273:PRO:HA	1:S:274:LYS:HA	1.53	0.48
2:F:950:ALA:HB3	2:F:953:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:776:ARG:NH2	2:L:799:GLU:OE2	2.46	0.48
1:O:426:THR:HB	1:O:429:TYR:HB2	1.96	0.48
2:R:959:MET:O	2:R:961:ASP:N	2.47	0.48
2:J:784:HIS:HD1	2:J:786:ASN:H	1.61	0.48
1:X:208:HIS:HB3	1:X:440:SER:HB2	1.96	0.48
2:F:791:TRP:HE1	2:F:812:ASN:HB3	1.79	0.47
2:F:891:SER:HB2	2:F:1010:ASP:HB2	1.96	0.47
2:J:715:LEU:HD11	2:J:734:LEU:HD22	1.96	0.47
1:K:367:LEU:HD22	1:K:422:ALA:HB2	1.96	0.47
2:L:926:GLN:NE2	2:L:952:ASN:O	2.47	0.47
2:P:817:GLN:HE22	2:P:958:PRO:HB2	1.79	0.47
2:F:776:ARG:HD2	2:F:780:VAL:HG11	1.96	0.47
2:L:730:ALA:HB3	2:L:747:ILE:HB	1.97	0.47
2:R:1057:THR:HA	2:R:1076:GLU:HA	1.96	0.47
2:Y:723:ALA:HB2	2:Y:1011:LEU:HG	1.95	0.47
2:Y:913:TYR:HB2	2:Y:981:LEU:HD12	1.96	0.47
1:G:321:VAL:HA	1:G:466:ARG:HA	1.95	0.47
2:H:791:TRP:HE1	2:H:812:ASN:HB3	1.79	0.47
2:L:755:SER:N	2:L:856:VAL:O	2.47	0.47
1:O:342:VAL:HG22	1:O:461:ARG:HG2	1.95	0.47
2:P:795:GLU:O	2:P:812:ASN:ND2	2.48	0.47
2:T:744:PHE:HZ	2:T:1072:VAL:HG13	1.80	0.47
1:E:263:ASP:OD1	1:E:352:LYS:NZ	2.42	0.47
1:I:365:GLU:HG3	2:J:826:PHE:HD1	1.79	0.47
2:P:723:ALA:HB2	2:P:1011:LEU:HG	1.97	0.47
2:V:898:SER:OG	2:V:899:GLY:N	2.48	0.47
2:Y:1064:ASN:HD21	2:Y:1068:SER:H	1.62	0.47
2:Y:737:VAL:HG23	2:Y:738:LYS:HG2	1.96	0.47
2:B:795:GLU:O	2:B:812:ASN:ND2	2.45	0.47
2:F:904:SER:HB2	2:F:916:VAL:HB	1.96	0.47
2:H:1090:VAL:HG22	2:H:1092:GLU:H	1.79	0.47
1:M:305:GLN:NE2	1:M:454:PRO:O	2.37	0.47
1:Q:212:LEU:HD23	1:Q:258:HIS:HD2	1.78	0.47
1:U:273:PRO:HA	1:U:274:LYS:HA	1.56	0.47
2:B:959:MET:O	2:B:961:ASP:N	2.47	0.47
1:O:243:LYS:NZ	1:O:281:CYS:O	2.36	0.47
2:P:1064:ASN:ND2	2:P:1068:SER:OG	2.47	0.47
1:S:246:MET:HG2	1:S:462:VAL:HG12	1.96	0.47
2:T:849:VAL:HG22	2:T:906:ILE:HG12	1.96	0.47
2:V:712:LYS:HD2	2:V:712:LYS:H	1.80	0.47
2:Y:1090:VAL:HG22	2:Y:1092:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:991:ALA:HB3	2:B:1000:GLN:HE21	1.80	0.47
1:E:246:MET:HG2	1:E:462:VAL:HG12	1.96	0.47
2:F:704:CYS:HA	2:F:713:CYS:HA	1.96	0.47
1:G:321:VAL:HG11	1:G:324:VAL:HB	1.95	0.47
2:H:844:LYS:NZ	2:J:1016:ASP:OD1	2.48	0.47
2:T:923:ILE:HD12	2:T:924:PRO:HD2	1.96	0.47
1:U:222:ALA:HB3	1:U:265:LYS:HG2	1.97	0.47
2:V:754:LEU:HB2	2:V:1001:ALA:HB3	1.97	0.47
2:V:729:GLU:OE2	2:V:748:LYS:NZ	2.37	0.47
2:B:1038:GLY:HA3	2:B:1046:ALA:HA	1.97	0.47
2:B:954:ILE:HA	2:B:967:THR:HG22	1.97	0.47
2:F:717:GLY:H	2:F:1015:PHE:HB2	1.79	0.47
2:F:959:MET:O	2:F:961:ASP:N	2.48	0.47
1:O:349:LYS:NZ	1:O:350:ASN:OD1	2.41	0.47
1:X:259:TYR:HB2	1:X:300:GLN:HE22	1.79	0.47
1:I:275:TYR:HB3	1:I:284:CYS:HB3	1.96	0.47
1:M:246:MET:SD	1:M:300:GLN:NE2	2.88	0.47
1:M:324:VAL:HG23	1:M:464:VAL:HG22	1.96	0.47
2:V:1006:SER:OG	2:V:1043:ASN:ND2	2.45	0.47
2:V:690:GLY:H	2:V:1085:ILE:HG12	1.80	0.47
1:E:426:THR:HB	1:E:429:TYR:HB2	1.97	0.47
2:N:1057:THR:HA	2:N:1076:GLU:HA	1.96	0.47
2:R:692:SER:OG	2:R:729:GLU:O	2.29	0.47
1:S:321:VAL:HG22	1:S:466:ARG:HG2	1.97	0.47
2:V:711:THR:HB	2:V:741:GLN:HE22	1.80	0.47
2:V:955:SER:OG	2:V:957:LYS:NZ	2.48	0.47
2:D:700:ARG:HG3	2:D:701:ILE:HG23	1.96	0.46
2:H:748:LYS:HB3	2:H:862:GLU:HB3	1.97	0.46
2:L:837:THR:HG21	2:L:954:ILE:HG21	1.97	0.46
1:M:261:ASN:HD21	1:M:265:LYS:HB2	1.79	0.46
1:M:273:PRO:HA	1:M:274:LYS:HA	1.52	0.46
1:Q:321:VAL:HG22	1:Q:466:ARG:HG2	1.97	0.46
2:T:959:MET:O	2:T:961:ASP:N	2.48	0.46
1:X:255:GLN:NE2	1:X:271:CYS:O	2.35	0.46
2:D:714:ARG:HD2	2:D:1017:ASN:ND2	2.30	0.46
2:F:725:SER:OG	2:F:726:VAL:N	2.48	0.46
2:H:806:SER:O	2:H:810:ARG:NH1	2.48	0.46
2:V:746:LYS:HB2	2:V:864:THR:HB	1.96	0.46
2:Y:954:ILE:HA	2:Y:967:THR:HG22	1.96	0.46
2:B:879:SER:OG	2:B:881:ARG:NH1	2.47	0.46
1:C:344:PRO:HG2	1:C:356:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:959:MET:O	2:D:961:ASP:N	2.48	0.46
2:H:959:MET:O	2:H:961:ASP:N	2.48	0.46
1:G:259:TYR:HB3	1:G:299:LEU:HD12	1.98	0.46
2:R:954:ILE:HA	2:R:967:THR:HG22	1.97	0.46
2:V:976:PHE:O	2:V:980:SER:OG	2.31	0.46
1:X:197:LYS:HA	1:X:204:GLN:HE22	1.79	0.46
1:X:210:ARG:NH2	1:X:370:ASP:OD2	2.49	0.46
2:Y:959:MET:O	2:Y:961:ASP:N	2.48	0.46
2:B:976:PHE:O	2:B:980:SER:OG	2.33	0.46
2:H:711:THR:O	2:H:741:GLN:NE2	2.48	0.46
1:O:313:LYS:H	1:O:313:LYS:HD2	1.80	0.46
2:R:690:GLY:HA3	2:R:1085:ILE:H	1.81	0.46
2:V:959:MET:O	2:V:961:ASP:N	2.49	0.46
2:F:1037:THR:O	2:F:1047:ARG:N	2.46	0.46
1:K:323:GLU:HG2	1:K:328:ALA:HA	1.98	0.46
2:R:791:TRP:HE1	2:R:812:ASN:HB3	1.81	0.46
1:X:362:LYS:HE3	1:X:444:GLN:HB2	1.97	0.46
2:D:725:SER:HA	2:D:1007:VAL:HB	1.98	0.46
2:N:712:LYS:H	2:N:712:LYS:HD2	1.80	0.46
1:O:250:CYS:HB2	1:O:281:CYS:HB3	1.78	0.46
2:T:1071:ILE:HA	2:T:1084:GLN:HE22	1.81	0.46
2:Y:891:SER:HB3	2:Y:1010:ASP:HB2	1.97	0.46
1:I:276:GLU:OE2	1:I:285:ARG:NE	2.46	0.46
1:K:259:TYR:HB3	1:K:299:LEU:HD12	1.98	0.46
1:K:348:PHE:HZ	1:K:447:VAL:HG21	1.81	0.46
2:V:756:CYS:SG	2:V:757:ARG:N	2.89	0.46
2:V:758:GLU:OE2	2:V:848:ARG:NH1	2.48	0.46
2:Y:815:PHE:HB2	2:Y:833:LEU:HD23	1.98	0.46
2:T:1057:THR:HA	2:T:1076:GLU:HA	1.97	0.46
2:Y:725:SER:OG	2:Y:726:VAL:N	2.48	0.46
2:D:710:ASN:ND2	2:D:1022:PHE:O	2.39	0.45
2:R:752:SER:HG	2:R:857:HIS:HE2	1.63	0.45
2:V:1064:ASN:ND2	2:V:1068:SER:OG	2.44	0.45
1:A:302:LEU:HD12	1:A:456:CYS:HB3	1.98	0.45
2:B:714:ARG:HD3	2:B:1017:ASN:HD21	1.80	0.45
1:E:273:PRO:HA	1:E:274:LYS:HA	1.55	0.45
2:F:1026:ALA:HB3	2:F:1102:ASP:HA	1.97	0.45
1:K:255:GLN:HG3	1:K:271:CYS:HB2	1.98	0.45
1:M:250:CYS:N	1:M:281:CYS:SG	2.89	0.45
1:M:426:THR:HB	1:M:429:TYR:HB2	1.97	0.45
1:Q:222:ALA:HB3	1:Q:265:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:323:GLU:HB3	1:X:465:LYS:HD2	1.98	0.45
2:H:795:GLU:O	2:H:812:ASN:ND2	2.48	0.45
1:I:451:TRP:NE1	2:J:962:GLN:OE1	2.44	0.45
2:T:807:THR:O	2:T:945:GLU:N	2.49	0.45
1:U:312:SER:HA	1:U:351:SER:HB3	1.98	0.45
1:O:307:SER:HB3	1:O:455:LEU:HD23	1.98	0.45
2:P:843:ARG:HH12	2:R:718:THR:HG21	1.81	0.45
1:S:363:THR:O	2:T:775:ARG:NH2	2.49	0.45
1:X:232:GLN:HE21	1:X:284:CYS:HB2	1.82	0.45
1:A:202:LEU:HD21	1:A:303:PHE:HD1	1.81	0.45
2:L:1006:SER:OG	2:L:1043:ASN:ND2	2.43	0.45
2:L:959:MET:O	2:L:961:ASP:N	2.50	0.45
1:Q:324:VAL:HG23	1:Q:464:VAL:HG22	1.97	0.45
2:B:1032:ALA:HB3	2:B:1051:SER:HB3	1.98	0.45
1:I:252:ASN:O	1:I:254:TYR:N	2.44	0.45
2:N:991:ALA:HB3	2:N:1002:PHE:HE2	1.82	0.45
2:P:690:GLY:HA3	2:P:1084:GLN:HA	1.98	0.45
1:Q:250:CYS:N	1:Q:281:CYS:SG	2.90	0.45
2:R:976:PHE:O	2:R:980:SER:OG	2.33	0.45
1:U:175:GLU:HB3	1:U:294:LYS:HE3	1.96	0.45
1:U:206:TYR:HE1	2:V:776:ARG:HH12	1.63	0.45
2:Y:718:THR:OG1	2:Y:1014:MET:SD	2.69	0.45
1:A:250:CYS:N	1:A:281:CYS:SG	2.90	0.45
2:F:875:LEU:HD11	2:F:888:VAL:HG13	1.98	0.45
1:I:398:ASP:OD2	1:I:400:SER:OG	2.26	0.45
1:K:460:GLU:HG2	1:K:462:VAL:HG13	1.98	0.45
2:L:811:GLU:OE2	2:L:956:TYR:OH	2.32	0.45
2:N:754:LEU:HB2	2:N:1001:ALA:HB3	1.98	0.45
2:D:769:PRO:HG3	2:D:967:THR:HG23	1.98	0.45
2:P:755:SER:N	2:P:856:VAL:O	2.50	0.45
2:T:810:ARG:HD3	2:T:810:ARG:H	1.81	0.45
2:V:1076:GLU:OE2	2:V:1080:LYS:NZ	2.41	0.45
1:X:242:GLU:HA	1:X:326:VAL:HG11	1.99	0.45
1:I:167:ASN:HD22	1:I:182:VAL:HG21	1.82	0.45
1:Q:321:VAL:HG11	1:Q:324:VAL:HB	1.99	0.45
1:U:347:VAL:HG22	1:U:353:LYS:HA	1.99	0.45
1:X:273:PRO:HA	1:X:274:LYS:HA	1.50	0.45
1:G:271:CYS:HB3	1:G:275:TYR:HB2	1.99	0.45
2:J:704:CYS:HA	2:J:713:CYS:HA	1.98	0.45
2:P:843:ARG:NH2	2:P:971:ASP:OD2	2.50	0.45
1:S:368:LEU:HD12	1:S:441:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:708:GLY:C	2:V:710:ASN:H	2.19	0.45
2:V:795:GLU:O	2:V:812:ASN:ND2	2.49	0.45
2:J:959:MET:O	2:J:961:ASP:N	2.50	0.44
1:O:316:THR:HG22	1:O:318:MET:H	1.82	0.44
1:O:412:LYS:HD2	1:O:426:THR:HG21	1.97	0.44
2:Y:1100:SER:HB3	2:Y:1105:GLU:HA	1.98	0.44
2:D:1038:GLY:HA3	2:D:1046:ALA:HA	1.98	0.44
1:E:408:HIS:HD2	1:E:426:THR:HG22	1.82	0.44
1:G:250:CYS:HB2	1:G:281:CYS:HB3	1.68	0.44
1:G:277:LEU:HD13	1:G:281:CYS:HB2	1.99	0.44
2:L:875:LEU:HD11	2:L:888:VAL:HG13	1.98	0.44
2:P:850:PHE:HE1	2:P:907:GLU:HB2	1.81	0.44
1:A:273:PRO:HA	1:A:274:LYS:HA	1.54	0.44
2:H:692:SER:HB3	2:H:728:ALA:HB1	1.99	0.44
2:H:913:TYR:HB2	2:H:981:LEU:HD12	1.99	0.44
2:N:725:SER:HA	2:N:1007:VAL:HB	1.97	0.44
2:Y:729:GLU:HG2	2:Y:748:LYS:HA	1.99	0.44
2:P:694:LEU:HD22	2:P:1070:HIS:HB3	1.98	0.44
1:U:275:TYR:HE1	1:U:286:GLN:HE21	1.64	0.44
1:G:412:LYS:HB2	1:G:430:ALA:HA	1.99	0.44
2:H:708:GLY:C	2:H:710:ASN:H	2.20	0.44
2:N:729:GLU:HG2	2:N:748:LYS:HA	1.98	0.44
1:U:183:THR:OG1	1:U:184:TYR:N	2.50	0.44
1:U:278:THR:HG22	1:U:285:ARG:HD2	1.99	0.44
2:V:931:GLU:HG3	2:V:932:ILE:HG13	1.99	0.44
2:B:805:GLU:OE1	2:B:810:ARG:NH2	2.45	0.44
1:O:159:ARG:NH2	1:O:186:GLY:O	2.50	0.44
2:V:717:GLY:H	2:V:1015:PHE:HB2	1.82	0.44
1:C:278:THR:OG1	1:C:280:ASP:OD1	2.31	0.44
2:H:1037:THR:O	2:H:1047:ARG:N	2.50	0.44
1:I:273:PRO:HA	1:I:274:LYS:HA	1.50	0.44
2:J:862:GLU:HA	2:J:872:THR:HA	1.99	0.44
2:N:811:GLU:OE2	2:N:956:TYR:OH	2.35	0.44
2:N:959:MET:O	2:N:961:ASP:N	2.51	0.44
2:F:754:LEU:HB2	2:F:1001:ALA:HB3	1.99	0.44
2:N:931:GLU:HG3	2:N:932:ILE:HG13	1.99	0.44
2:P:916:VAL:HG12	2:P:918:GLU:HG2	1.99	0.44
1:Q:316:THR:HG22	1:Q:318:MET:H	1.82	0.44
2:B:891:SER:HB2	2:B:1012:THR:HG23	2.00	0.44
2:F:873:ILE:HB	2:F:881:ARG:HG3	1.99	0.44
2:P:959:MET:O	2:P:961:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1073:LEU:HD22	2:V:1082:GLN:HB3	2.00	0.44
1:X:175:GLU:OE1	1:X:189:SER:OG	2.29	0.44
1:E:379:GLY:HA3	1:G:286:GLN:HB2	2.00	0.43
1:E:438:ASN:HD21	2:F:780:VAL:HA	1.82	0.43
1:G:344:PRO:HB3	1:G:459:TYR:HD1	1.83	0.43
1:M:426:THR:O	1:M:428:GLN:N	2.51	0.43
2:T:846:ALA:HB3	2:T:937:GLU:HG3	1.99	0.43
1:E:180:LYS:HA	1:E:181:PRO:HA	1.87	0.43
2:J:875:LEU:HD11	2:J:888:VAL:HG22	1.99	0.43
1:O:377:HIS:CE1	1:O:433:TYR:HB2	2.53	0.43
2:R:722:ARG:NH2	2:R:1008:GLN:OE1	2.51	0.43
2:R:843:ARG:HG3	2:R:845:GLU:H	1.82	0.43
1:C:273:PRO:HA	1:C:274:LYS:HA	1.45	0.43
2:H:701:ILE:HB	2:H:717:GLY:HA3	1.99	0.43
2:R:1038:GLY:HA3	2:R:1046:ALA:HA	2.00	0.43
2:B:1064:ASN:ND2	2:B:1068:SER:OG	2.52	0.43
2:F:747:ILE:HG23	2:F:863:ILE:HG12	2.01	0.43
2:F:778:HIS:ND1	2:F:779:LEU:HG	2.33	0.43
2:H:1045:GLY:HA3	2:H:1085:ILE:HD11	2.00	0.43
2:J:810:ARG:HD2	2:J:836:HIS:CE1	2.53	0.43
1:S:410:SER:OG	1:S:411:LYS:N	2.49	0.43
2:V:778:HIS:ND1	2:V:779:LEU:HG	2.34	0.43
2:B:775:ARG:NH1	2:B:825:CYS:SG	2.91	0.43
2:D:931:GLU:HG3	2:D:932:ILE:HG13	2.00	0.43
2:F:876:GLY:O	2:F:878:SER:N	2.52	0.43
1:K:278:THR:OG1	1:K:280:ASP:OD1	2.35	0.43
2:L:863:ILE:HG21	2:L:885:TRP:HE1	1.83	0.43
2:R:956:TYR:HD1	2:R:963:LEU:HD21	1.82	0.43
1:X:247:LYS:O	1:X:461:ARG:NH1	2.44	0.43
2:H:715:LEU:HD21	2:H:734:LEU:HD21	2.00	0.43
2:L:879:SER:OG	2:L:881:ARG:NH1	2.48	0.43
2:L:931:GLU:HG3	2:L:932:ILE:HG13	1.99	0.43
1:Q:362:LYS:NZ	1:Q:364:GLU:OE2	2.52	0.43
1:U:361:LEU:HG	1:U:445:ILE:HG13	2.01	0.43
1:X:339:ALA:O	1:X:464:VAL:N	2.50	0.43
2:L:717:GLY:H	2:L:1015:PHE:HB2	1.83	0.43
1:M:246:MET:HG3	1:M:462:VAL:HG12	2.01	0.43
1:O:180:LYS:HA	1:O:181:PRO:HA	1.87	0.43
1:S:158:LEU:HD13	1:S:195:LEU:HD22	2.01	0.43
1:S:316:THR:OG1	1:S:327:GLN:OE1	2.37	0.43
2:B:861:LEU:HD12	2:B:875:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:994:LYS:HD2	2:D:994:LYS:H	1.84	0.43
2:F:747:ILE:HG13	2:F:863:ILE:HG23	1.99	0.43
1:K:366:ASN:HD22	1:K:367:LEU:H	1.66	0.43
1:O:278:THR:HG22	1:O:285:ARG:HG2	2.01	0.43
2:H:732:LEU:HB3	2:H:745:LEU:HB3	2.01	0.43
1:X:410:SER:OG	1:X:411:LYS:N	2.50	0.43
2:F:848:ARG:NH2	2:F:907:GLU:OE1	2.36	0.43
1:Q:273:PRO:HA	1:Q:274:LYS:HA	1.51	0.43
2:T:778:HIS:ND1	2:T:779:LEU:HG	2.34	0.43
2:T:755:SER:N	2:T:856:VAL:O	2.52	0.43
2:Y:1076:GLU:OE2	2:Y:1080:LYS:NZ	2.46	0.43
2:D:1003:SER:OG	2:D:1004:LYS:N	2.48	0.42
2:H:921:SER:HB2	2:H:928:PHE:HE2	1.84	0.42
1:M:201:PRO:HG2	2:N:802:PHE:HB3	2.00	0.42
2:T:1036:LEU:HD12	2:T:1048:VAL:HG23	2.01	0.42
1:Q:278:THR:OG1	1:Q:280:ASP:OD1	2.26	0.42
1:Q:346:ALA:HB2	1:Q:356:LEU:HD11	2.01	0.42
1:U:251:PRO:HB2	1:U:252:ASN:H	1.61	0.42
2:V:1057:THR:HA	2:V:1076:GLU:HA	2.00	0.42
1:A:208:HIS:CE1	1:A:438:ASN:H	2.37	0.42
1:A:278:THR:HG22	1:A:285:ARG:HD3	2.00	0.42
2:D:778:HIS:ND1	2:D:779:LEU:HG	2.34	0.42
2:H:874:ASP:OD1	2:H:874:ASP:N	2.53	0.42
2:N:815:PHE:HB2	2:N:833:LEU:HD23	2.02	0.42
2:P:688:ASP:HB2	2:P:689:PRO:HD3	2.01	0.42
2:V:688:ASP:HB2	2:V:689:PRO:HD3	2.01	0.42
1:I:262:ASN:O	1:I:327:GLN:NE2	2.52	0.42
2:P:811:GLU:OE2	2:P:956:TYR:OH	2.31	0.42
2:Y:691:CYS:HB3	2:Y:694:LEU:HD11	2.02	0.42
2:J:778:HIS:ND1	2:J:779:LEU:HG	2.34	0.42
1:K:276:GLU:OE2	1:K:285:ARG:NH1	2.52	0.42
2:N:1081:ASP:OD1	2:N:1081:ASP:N	2.52	0.42
2:N:1089:THR:HG23	2:N:1090:VAL:HG13	2.02	0.42
1:U:172:MET:HA	1:U:174:GLN:HE22	1.84	0.42
2:B:811:GLU:OE2	2:B:956:TYR:OH	2.36	0.42
2:B:757:ARG:HD3	2:B:853:ILE:HB	2.02	0.42
2:F:906:ILE:HD11	2:F:929:LEU:HD21	2.01	0.42
2:L:707:GLU:HB2	2:L:712:LYS:HD3	2.02	0.42
2:N:776:ARG:HD2	2:N:780:VAL:HG11	2.02	0.42
2:P:715:LEU:HD11	2:P:734:LEU:HD12	2.02	0.42
2:T:891:SER:HB3	2:T:1010:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:348:PHE:HZ	1:U:447:VAL:HG21	1.84	0.42
1:U:367:LEU:HD22	1:U:422:ALA:HB2	2.00	0.42
1:X:345:PHE:HA	1:X:355:TYR:HA	2.02	0.42
2:B:827:ASN:ND2	2:B:829:ASN:OD1	2.53	0.42
1:G:273:PRO:HA	1:G:274:LYS:HA	1.45	0.42
1:G:444:GLN:HA	1:G:453:LYS:HA	2.01	0.42
1:S:358:LYS:NZ	1:S:360:ASP:OD2	2.53	0.42
1:X:262:ASN:HD21	1:X:327:GLN:HB3	1.84	0.42
2:Y:776:ARG:HD2	2:Y:780:VAL:HG11	2.00	0.42
1:E:225:ASP:HA	1:E:226:PRO:HA	1.91	0.42
2:F:874:ASP:OD1	2:F:874:ASP:N	2.53	0.42
2:H:718:THR:OG1	2:H:1014:MET:SD	2.66	0.42
2:H:688:ASP:HB2	2:H:689:PRO:HD3	2.02	0.42
1:Q:271:CYS:HB3	1:Q:275:TYR:HB2	2.01	0.42
2:T:907:GLU:HG3	2:T:913:TYR:HE1	1.85	0.42
2:H:1062:ALA:HB3	2:H:1071:ILE:HB	2.01	0.42
2:J:714:ARG:HD3	2:J:1019:GLU:HA	2.01	0.42
2:N:1006:SER:HB3	2:N:1008:GLN:HE22	1.85	0.42
2:P:1064:ASN:HD21	2:P:1068:SER:H	1.68	0.42
2:P:691:CYS:HA	2:P:729:GLU:HB2	2.01	0.42
2:T:959:MET:HB2	2:T:962:GLN:HB2	2.02	0.42
2:V:862:GLU:HA	2:V:872:THR:HA	2.02	0.42
1:A:347:VAL:HG22	1:A:353:LYS:HA	2.01	0.42
2:D:714:ARG:NH1	2:D:1019:GLU:HB2	2.35	0.42
2:P:1076:GLU:HB2	2:P:1080:LYS:HG3	2.02	0.42
2:V:696:GLN:HE22	2:V:1070:HIS:CE1	2.38	0.42
1:U:154:GLU:HG3	2:V:781:GLY:H	1.85	0.42
1:X:230:ASP:OD2	1:X:233:SER:OG	2.36	0.42
2:D:1034:LEU:HD21	2:D:1051:SER:HB2	2.02	0.41
1:M:271:CYS:HB3	1:M:275:TYR:HB2	2.02	0.41
2:P:712:LYS:HG2	2:P:1021:ASP:HB3	2.02	0.41
1:S:169:ILE:HA	1:S:169:ILE:HD12	1.94	0.41
2:T:1064:ASN:HD21	2:T:1068:SER:H	1.67	0.41
2:T:722:ARG:NH2	2:T:1008:GLN:OE1	2.53	0.41
2:V:850:PHE:HE1	2:V:907:GLU:HB2	1.85	0.41
2:B:754:LEU:HB2	2:B:1001:ALA:HB3	2.01	0.41
2:H:843:ARG:NH2	2:H:971:ASP:OD2	2.53	0.41
1:K:412:LYS:HD2	1:K:426:THR:HG21	2.01	0.41
1:U:275:TYR:HB3	1:U:284:CYS:HB3	2.02	0.41
1:X:403:PRO:HG3	1:X:409:GLY:HA3	2.01	0.41
1:X:302:LEU:HD13	1:X:456:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:844:LYS:NZ	2:F:1016:ASP:OD1	2.49	0.41
1:G:429:TYR:OH	1:I:233:SER:O	2.33	0.41
1:M:230:ASP:HB3	1:M:233:SER:HB2	2.01	0.41
1:O:277:LEU:HD13	1:O:281:CYS:HB2	2.03	0.41
2:P:857:HIS:CD2	2:P:895:GLU:HB2	2.54	0.41
2:V:791:TRP:HE1	2:V:812:ASN:HB3	1.85	0.41
2:V:973:PHE:HA	2:V:976:PHE:HB3	2.02	0.41
1:X:180:LYS:HA	1:X:181:PRO:HA	1.87	0.41
2:H:778:HIS:ND1	2:H:779:LEU:HG	2.35	0.41
1:Q:278:THR:HG22	1:Q:285:ARG:HD3	2.01	0.41
1:O:319:LYS:HE2	2:R:1016:ASP:HB3	2.03	0.41
2:T:726:VAL:HG22	2:T:751:SER:HA	2.03	0.41
1:G:158:LEU:HD22	1:G:195:LEU:HD22	2.02	0.41
1:I:183:THR:HG23	1:I:185:ALA:H	1.85	0.41
1:K:412:LYS:HB2	1:K:430:ALA:HA	2.03	0.41
1:M:183:THR:HG23	1:M:185:ALA:H	1.85	0.41
2:T:1034:LEU:HD21	2:T:1051:SER:HB2	2.01	0.41
2:V:1006:SER:HG	2:V:1043:ASN:HD22	1.67	0.41
2:Y:876:GLY:O	2:Y:878:SER:N	2.54	0.41
2:D:815:PHE:HB2	2:D:833:LEU:HD23	2.03	0.41
1:M:258:HIS:HA	1:M:268:SER:HA	2.02	0.41
2:R:778:HIS:ND1	2:R:779:LEU:HG	2.35	0.41
2:T:1037:THR:O	2:T:1047:ARG:N	2.50	0.41
1:U:180:LYS:HA	1:U:181:PRO:HA	1.88	0.41
2:Y:928:PHE:O	2:Y:930:GLY:N	2.54	0.41
2:D:722:ARG:NH2	2:D:1008:GLN:OE1	2.54	0.41
2:H:752:SER:OG	2:H:857:HIS:NE2	2.54	0.41
1:I:251:PRO:HB2	1:I:252:ASN:H	1.58	0.41
2:J:688:ASP:HB2	2:J:689:PRO:HD3	2.01	0.41
2:L:721:ILE:HD13	2:L:730:ALA:HB1	2.02	0.41
2:L:729:GLU:HG2	2:L:748:LYS:HA	2.02	0.41
1:O:460:GLU:HG2	1:O:462:VAL:HG13	2.03	0.41
1:C:346:ALA:HB2	1:C:356:LEU:HD11	2.02	0.41
2:L:850:PHE:HE1	2:L:907:GLU:HB2	1.84	0.41
2:N:688:ASP:HA	2:N:689:PRO:HD3	1.95	0.41
2:R:907:GLU:HG3	2:R:913:TYR:CE1	2.55	0.41
2:T:847:LEU:HD12	2:T:972:PRO:HB2	2.03	0.41
1:U:335:GLN:HB2	1:U:468:LEU:HB3	2.03	0.41
2:V:805:GLU:OE2	2:V:810:ARG:NH2	2.53	0.41
2:D:817:GLN:HE22	2:D:958:PRO:HB2	1.86	0.41
1:E:174:GLN:HB3	1:E:294:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:698:SER:HB3	2:F:701:ILE:HG12	2.03	0.41
1:G:319:LYS:HD3	2:J:1018:PHE:HD1	1.86	0.41
1:M:169:ILE:HA	1:M:169:ILE:HD12	1.94	0.41
1:S:378:LYS:HG3	1:S:393:GLU:HG2	2.03	0.41
2:T:743:LYS:HD3	2:T:1022:PHE:HD1	1.86	0.41
1:U:161:ARG:NH2	1:U:209:HIS:O	2.54	0.41
1:U:302:LEU:HD12	1:U:456:CYS:HB3	2.02	0.41
2:V:954:ILE:HA	2:V:967:THR:HG22	2.02	0.41
2:Y:690:GLY:H	2:Y:1084:GLN:HA	1.86	0.41
1:A:410:SER:OG	1:A:411:LYS:N	2.51	0.41
2:B:1115:ILE:HD12	2:B:1115:ILE:HA	1.96	0.41
2:B:706:THR:HA	2:B:711:THR:HA	2.03	0.41
1:E:324:VAL:HG23	1:E:464:VAL:HG22	2.03	0.41
1:G:206:TYR:OH	1:G:363:THR:OG1	2.35	0.41
2:H:706:THR:HA	2:H:711:THR:HA	2.02	0.41
1:K:273:PRO:HA	1:K:274:LYS:HA	1.44	0.41
2:N:1028:SER:OG	2:N:1102:ASP:OD2	2.35	0.41
2:N:778:HIS:ND1	2:N:779:LEU:HG	2.36	0.41
2:N:959:MET:HB2	2:N:962:GLN:HB2	2.03	0.41
2:P:743:LYS:HE3	2:P:1022:PHE:HB2	2.02	0.41
2:R:726:VAL:HG22	2:R:751:SER:HA	2.03	0.41
1:U:216:VAL:HG22	1:U:221:ILE:HB	2.03	0.41
2:V:861:LEU:HD12	2:V:875:LEU:HD12	2.03	0.41
1:G:206:TYR:HH	1:G:363:THR:HG1	1.64	0.41
2:N:691:CYS:HB3	2:N:694:LEU:HD11	2.03	0.41
2:N:876:GLY:O	2:N:878:SER:N	2.54	0.41
2:D:880:SER:N	2:N:966:THR:OG1	2.52	0.41
2:Y:1071:ILE:HG23	2:Y:1084:GLN:HE22	1.86	0.41
1:A:464:VAL:HG12	1:A:466:ARG:HG3	2.04	0.40
2:B:694:LEU:HD11	2:B:733:MET:HB2	2.02	0.40
1:E:273:PRO:HB3	1:E:274:LYS:HD3	2.03	0.40
2:F:976:PHE:O	2:F:980:SER:OG	2.33	0.40
2:H:744:PHE:HZ	2:H:1072:VAL:HB	1.85	0.40
1:I:360:ASP:HB2	1:I:446:GLN:HB3	2.03	0.40
2:N:708:GLY:O	2:N:710:ASN:N	2.54	0.40
2:N:809:MET:HB2	2:N:839:LEU:HB2	2.03	0.40
1:Q:362:LYS:HB3	1:Q:444:GLN:HB2	2.03	0.40
2:T:810:ARG:NH1	2:T:945:GLU:OE1	2.47	0.40
2:D:898:SER:OG	2:D:899:GLY:N	2.52	0.40
2:R:957:LYS:HD3	2:R:964:GLU:HB2	2.03	0.40
2:V:811:GLU:OE2	2:V:956:TYR:OH	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:169:ILE:HA	1:X:169:ILE:HD12	1.94	0.40
2:Y:810:ARG:HD2	2:Y:836:HIS:HE1	1.86	0.40
2:B:769:PRO:HG3	2:B:967:THR:HG23	2.03	0.40
2:H:786:ASN:O	2:H:790:SER:OG	2.38	0.40
2:L:737:VAL:HG13	2:L:738:LYS:HG2	2.03	0.40
1:O:374:CYS:HA	1:O:434:CYS:HA	2.03	0.40
2:V:1090:VAL:HG22	2:V:1092:GLU:H	1.86	0.40
2:Y:906:ILE:HB	2:Y:914:ALA:HB3	2.04	0.40
2:Y:976:PHE:O	2:Y:980:SER:OG	2.32	0.40
2:B:850:PHE:HE1	2:B:907:GLU:HB2	1.86	0.40
2:F:756:CYS:SG	2:F:757:ARG:N	2.94	0.40
2:N:932:ILE:HD12	2:N:969:LEU:HD13	2.04	0.40
1:O:440:SER:OG	1:O:441:GLY:N	2.51	0.40
2:P:922:GLU:O	2:P:933:ARG:NH1	2.54	0.40
2:R:1073:LEU:HD22	2:R:1082:GLN:HB3	2.03	0.40
2:R:1104:ASP:O	2:R:1106:ARG:NH1	2.54	0.40
2:T:704:CYS:HA	2:T:713:CYS:HA	2.04	0.40
1:X:158:LEU:HD22	1:X:207:ALA:HB3	2.04	0.40
2:L:1117:ILE:HD12	2:L:1117:ILE:HA	1.97	0.40
1:M:225:ASP:HA	1:M:226:PRO:HA	1.93	0.40
2:N:850:PHE:HE1	2:N:907:GLU:HB2	1.86	0.40
2:T:691:CYS:H	2:T:1084:GLN:HA	1.86	0.40
2:T:769:PRO:HG3	2:T:967:THR:HG23	2.02	0.40
2:V:722:ARG:HH21	2:V:1008:GLN:HA	1.85	0.40
2:Y:817:GLN:HE22	2:Y:958:PRO:HB2	1.87	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%)	252 (85%)	42 (14%)	1 (0%)	43	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	295/316 (93%)	262 (89%)	30 (10%)	3 (1%)	17	60
1	E	295/316 (93%)	253 (86%)	40 (14%)	2 (1%)	24	67
1	G	295/316 (93%)	259 (88%)	33 (11%)	3 (1%)	17	60
1	I	295/316 (93%)	258 (88%)	33 (11%)	4 (1%)	12	52
1	K	295/316 (93%)	251 (85%)	41 (14%)	3 (1%)	17	60
1	M	295/316 (93%)	245 (83%)	43 (15%)	7 (2%)	6	40
1	O	295/316 (93%)	262 (89%)	29 (10%)	4 (1%)	12	52
1	Q	295/316 (93%)	249 (84%)	44 (15%)	2 (1%)	24	67
1	S	295/316 (93%)	261 (88%)	32 (11%)	2 (1%)	24	67
1	U	295/316 (93%)	250 (85%)	40 (14%)	5 (2%)	10	49
1	X	295/316 (93%)	256 (87%)	39 (13%)	0	100	100
2	B	429/431 (100%)	377 (88%)	48 (11%)	4 (1%)	19	61
2	D	429/431 (100%)	385 (90%)	40 (9%)	4 (1%)	19	61
2	F	429/431 (100%)	375 (87%)	50 (12%)	4 (1%)	19	61
2	H	429/431 (100%)	378 (88%)	47 (11%)	4 (1%)	19	61
2	J	429/431 (100%)	382 (89%)	43 (10%)	4 (1%)	19	61
2	L	429/431 (100%)	383 (89%)	43 (10%)	3 (1%)	24	67
2	N	429/431 (100%)	383 (89%)	39 (9%)	7 (2%)	11	50
2	P	429/431 (100%)	385 (90%)	40 (9%)	4 (1%)	19	61
2	R	429/431 (100%)	378 (88%)	48 (11%)	3 (1%)	24	67
2	T	429/431 (100%)	380 (89%)	44 (10%)	5 (1%)	14	56
2	V	429/431 (100%)	368 (86%)	55 (13%)	6 (1%)	12	52
2	Y	429/431 (100%)	375 (87%)	48 (11%)	6 (1%)	12	52
All	All	8688/8964 (97%)	7607 (88%)	991 (11%)	90 (1%)	22	60

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	709	VAL
2	V	709	VAL
2	F	877	ALA
2	H	877	ALA
1	I	251	PRO
1	I	439	GLY

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Mol	Chain	Res	Type
2	N	877	ALA
2	N	960	ILE
2	N	1017	ASN
2	P	759	GLY
1	U	251	PRO
1	U	311	GLY
2	Y	877	ALA
2	Y	929	LEU
1	C	322	CYS
2	D	960	ILE
1	E	427	ALA
2	F	809	MET
1	G	427	ALA
1	I	410	SER
2	J	877	ALA
2	J	960	ILE
1	K	427	ALA
2	L	877	ALA
1	M	311	GLY
1	M	410	SER
1	M	427	ALA
1	M	439	GLY
1	O	322	CYS
1	O	329	LEU
2	P	960	ILE
2	P	986	ASN
1	Q	282	ASN
2	R	922	GLU
2	T	809	MET
2	T	877	ALA
2	T	960	ILE
1	U	265	LYS
2	Y	986	ASN
1	A	329	LEU
2	B	960	ILE
1	C	237	ASN
2	D	986	ASN
2	F	960	ILE
2	H	759	GLY
2	H	960	ILE
1	I	329	LEU
1	K	265	LYS

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Mol	Chain	Res	Type
2	L	960	ILE
1	M	329	LEU
2	N	709	VAL
2	N	986	ASN
1	O	164	LYS
2	R	960	ILE
2	T	986	ASN
1	U	237	ASN
2	V	877	ALA
2	V	960	ILE
2	Y	960	ILE
2	B	759	GLY
2	D	759	GLY
1	G	232	GLN
2	L	759	GLY
1	M	440	SER
2	N	759	GLY
1	O	439	GLY
2	P	877	ALA
1	S	233	SER
1	S	322	CYS
2	V	986	ASN
1	C	253	ASP
2	R	877	ALA
2	V	895	GLU
2	Y	759	GLY
2	Y	783	CYS
2	D	750	VAL
1	E	311	GLY
1	G	439	GLY
1	K	236	GLY
1	Q	311	GLY
2	T	750	VAL
2	B	750	VAL
2	J	930	GLY
1	M	334	GLY
2	N	750	VAL
2	V	824	GLY
2	B	896	GLY
2	J	995	GLY
1	U	326	VAL
2	F	759	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	259/271 (96%)	258 (100%)	1 (0%)	92	95
1	C	259/271 (96%)	257 (99%)	2 (1%)	83	92
1	E	259/271 (96%)	256 (99%)	3 (1%)	74	87
1	G	259/271 (96%)	258 (100%)	1 (0%)	92	95
1	I	259/271 (96%)	257 (99%)	2 (1%)	83	92
1	K	259/271 (96%)	258 (100%)	1 (0%)	92	95
1	M	259/271 (96%)	257 (99%)	2 (1%)	83	92
1	O	259/271 (96%)	255 (98%)	4 (2%)	67	85
1	Q	259/271 (96%)	257 (99%)	2 (1%)	83	92
1	S	259/271 (96%)	258 (100%)	1 (0%)	92	95
1	U	259/271 (96%)	257 (99%)	2 (1%)	83	92
1	X	259/271 (96%)	257 (99%)	2 (1%)	83	92
2	B	371/371 (100%)	367 (99%)	4 (1%)	76	88
2	D	371/371 (100%)	367 (99%)	4 (1%)	76	88
2	F	371/371 (100%)	368 (99%)	3 (1%)	83	92
2	H	371/371 (100%)	368 (99%)	3 (1%)	83	92
2	J	371/371 (100%)	367 (99%)	4 (1%)	76	88
2	L	371/371 (100%)	367 (99%)	4 (1%)	76	88
2	N	371/371 (100%)	369 (100%)	2 (0%)	90	95
2	P	371/371 (100%)	368 (99%)	3 (1%)	83	92
2	R	371/371 (100%)	363 (98%)	8 (2%)	55	77
2	T	371/371 (100%)	368 (99%)	3 (1%)	83	92
2	V	371/371 (100%)	362 (98%)	9 (2%)	52	75
2	Y	371/371 (100%)	369 (100%)	2 (0%)	90	95
All	All	7560/7704 (98%)	7488 (99%)	72 (1%)	80	89

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	ASN
2	B	810	ARG
2	B	925	ARG
2	B	1017	ASN
2	B	1065	LYS
1	C	285	ARG
1	C	378	LYS
2	D	710	ASN
2	D	733	MET
2	D	994	LYS
2	D	1017	ASN
1	E	172	MET
1	E	378	LYS
1	E	438	ASN
2	F	700	ARG
2	F	844	LYS
2	F	949	ARG
1	G	378	LYS
2	H	709	VAL
2	H	925	ARG
2	H	949	ARG
1	I	285	ARG
1	I	315	LYS
2	J	700	ARG
2	J	733	MET
2	J	844	LYS
2	J	949	ARG
1	K	366	ASN
2	L	810	ARG
2	L	844	LYS
2	L	949	ARG
2	L	996	ASN
1	M	315	LYS
1	M	438	ASN
2	N	712	LYS
2	N	949	ARG
1	O	285	ARG
1	O	313	LYS
1	O	330	LYS
1	O	438	ASN
2	P	700	ARG
2	P	810	ARG
2	P	949	ARG

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Mol	Chain	Res	Type
1	Q	331	LYS
1	Q	438	ASN
2	R	700	ARG
2	R	714	ARG
2	R	925	ARG
2	R	949	ARG
2	R	994	LYS
2	R	996	ASN
2	R	1106	ARG
2	R	1111	LYS
1	S	378	LYS
2	T	722	ARG
2	T	810	ARG
2	T	949	ARG
1	U	285	ARG
1	U	358	LYS
2	V	700	ARG
2	V	709	VAL
2	V	712	LYS
2	V	786	ASN
2	V	925	ARG
2	V	949	ARG
2	V	1004	LYS
2	V	1047	ARG
2	V	1111	LYS
1	X	270	LYS
1	X	362	LYS
2	Y	949	ARG
2	Y	1047	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	208	HIS
1	A	438	ASN
1	A	446	GLN
2	B	817	GLN
2	B	1008	GLN
2	B	1017	ASN
2	B	1084	GLN
1	C	204	GLN

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Mol	Chain	Res	Type
2	D	741	GLN
2	D	817	GLN
2	D	829	ASN
2	D	944	HIS
2	D	1017	ASN
2	D	1084	GLN
1	E	204	GLN
1	E	408	HIS
1	E	438	ASN
2	F	817	GLN
2	F	840	GLN
2	F	1084	GLN
1	G	166	HIS
2	H	817	GLN
2	H	901	ASN
2	H	1084	GLN
1	I	166	HIS
1	I	167	ASN
1	I	204	GLN
1	I	232	GLN
1	I	327	GLN
1	I	446	GLN
2	J	1000	GLN
2	J	1084	GLN
1	K	174	GLN
1	K	204	GLN
1	K	366	ASN
1	K	377	HIS
1	K	438	ASN
1	K	446	GLN
2	L	996	ASN
2	L	1000	GLN
2	L	1063	HIS
2	L	1084	GLN
1	M	157	HIS
2	N	1008	GLN
2	N	1084	GLN
1	O	431	ASN
2	P	1064	ASN
2	P	1084	GLN
1	Q	166	HIS
1	Q	204	GLN

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Mol	Chain	Res	Type
1	Q	438	ASN
2	R	817	GLN
2	R	1000	GLN
2	R	1084	GLN
1	S	160	ASN
1	S	166	HIS
1	S	204	GLN
1	S	237	ASN
2	T	817	GLN
2	T	901	ASN
2	T	1084	GLN
1	U	174	GLN
1	U	204	GLN
1	U	208	HIS
1	U	286	GLN
1	U	305	GLN
2	V	786	ASN
2	V	857	HIS
2	V	1070	HIS
2	V	1084	GLN
1	X	204	GLN
1	X	232	GLN
1	X	377	HIS
1	X	436	HIS
2	Y	784	HIS
2	Y	836	HIS
2	Y	1084	GLN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.