Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 01:45 AM EST

PDB ID	:	6XO4
EMDB ID	:	EMD-22276
Title	:	CryoEM structure of Eastern Equine Encephalitis (EEEV) VLP
Authors	:	Binshtein, E.; Crowe, J.E.
Deposited on	:	2020-07-06
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

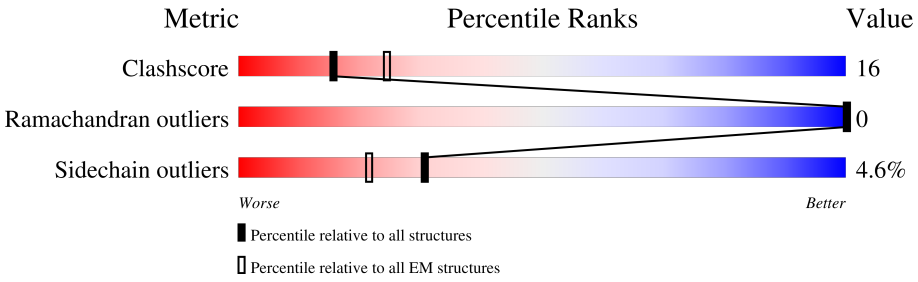
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	441	69% 27%
1	D	441	70% 27%
1	G	441	69% 28%
1	J	441	70% 27%
2	B	420	59% 38%
2	E	420	57% 40%
2	H	420	58% 38%
2	K	420	58% 39%
3	C	261	43% 13% 42%

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Mol	Chain	Length	Quality of chain
3	F	261	45% 11% 42%
3	I	261	43% 13% 42%
3	L	261	44% 13% 42%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30900 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 Togavirin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3307	2111	549	627	20		
1	D	433	Total	C	N	O	S	0	0
			3307	2111	549	627	20		
1	G	433	Total	C	N	O	S	0	0
			3307	2111	549	627	20		
1	J	433	Total	C	N	O	S	0	0
			3307	2111	549	627	20		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	TYR	TRP	conflict	UNP Q88678
D	89	TYR	TRP	conflict	UNP Q88678
G	89	TYR	TRP	conflict	UNP Q88678
J	89	TYR	TRP	conflict	UNP Q88678

- Molecule 2 is a protein called Togavirin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	E	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	H	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	K	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		

- Molecule 3 is a protein called Togavirin.

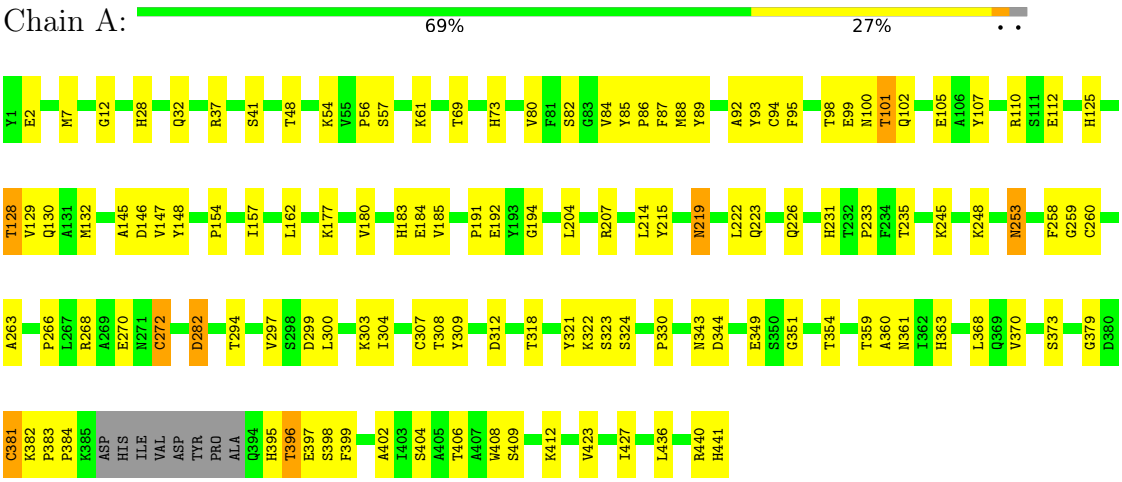
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		
3	F	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		
3	I	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		
3	L	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

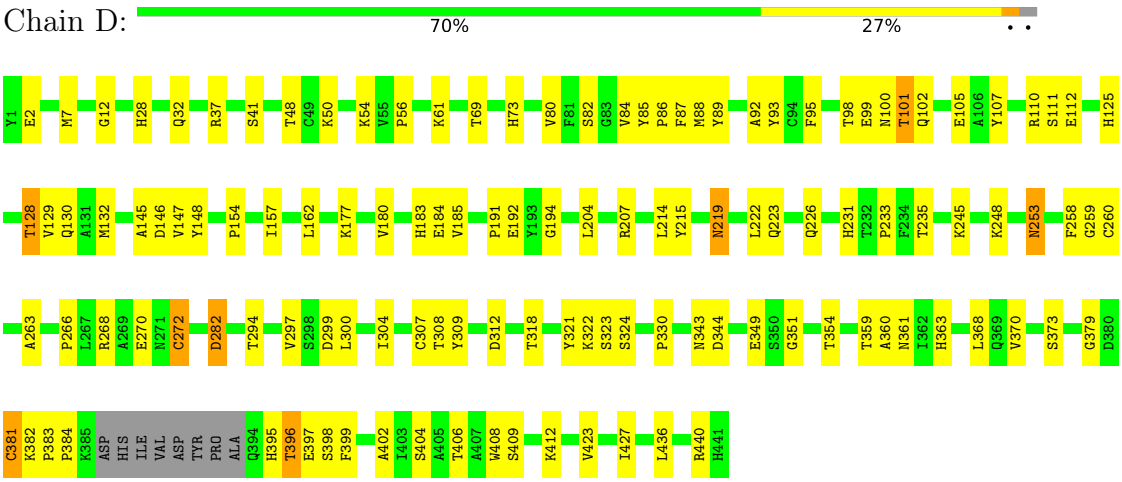
• Molecule 1: Togavirin

Chain A:



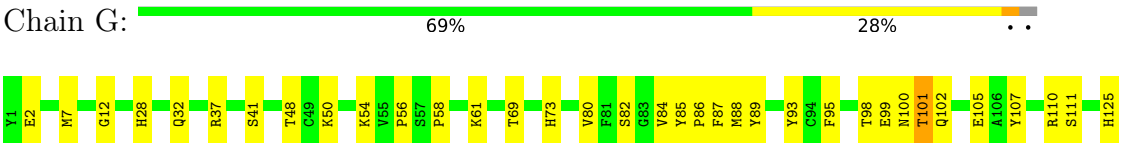
• Molecule 1: Togavirin

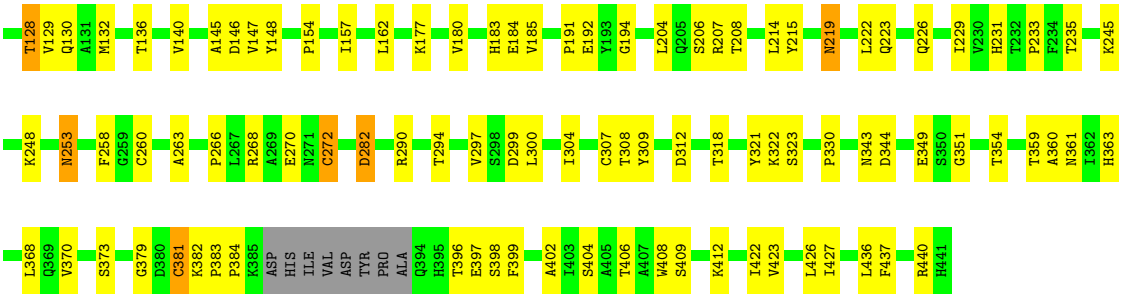
Chain D:



• Molecule 1: Togavirin

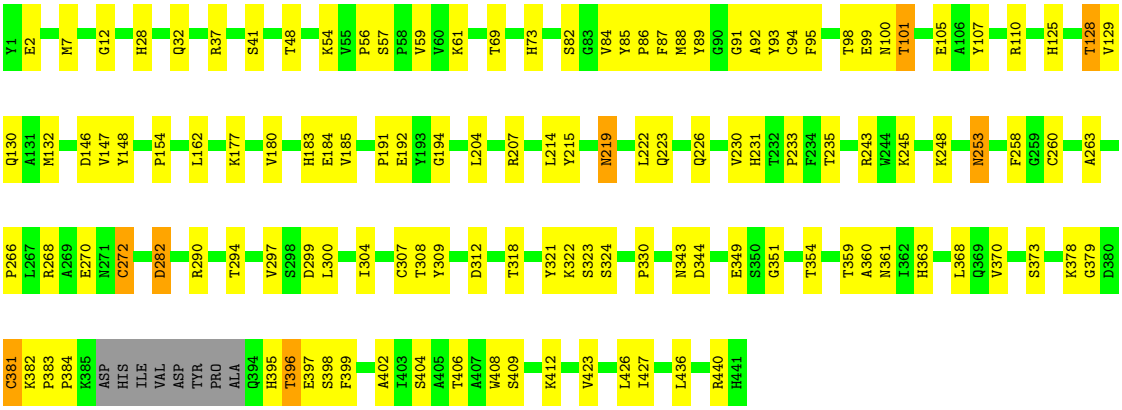
Chain G:





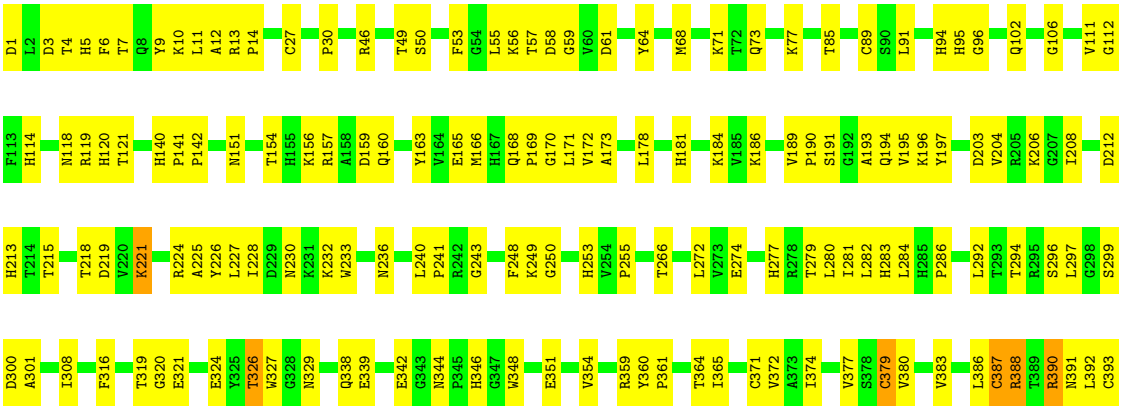
• Molecule 1: Togavirin

Chain J:



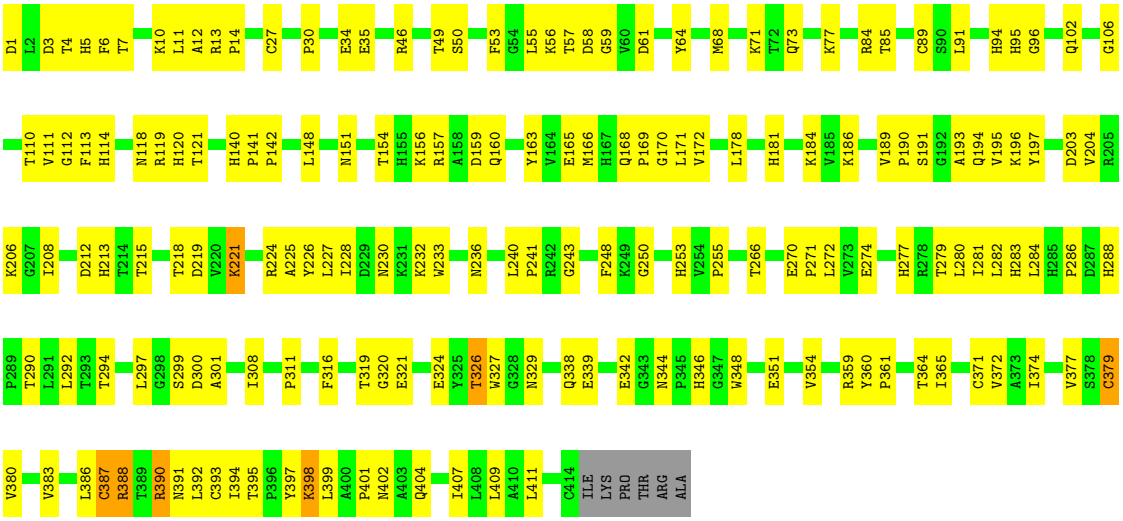
• Molecule 2: Togavirin

Chain B:



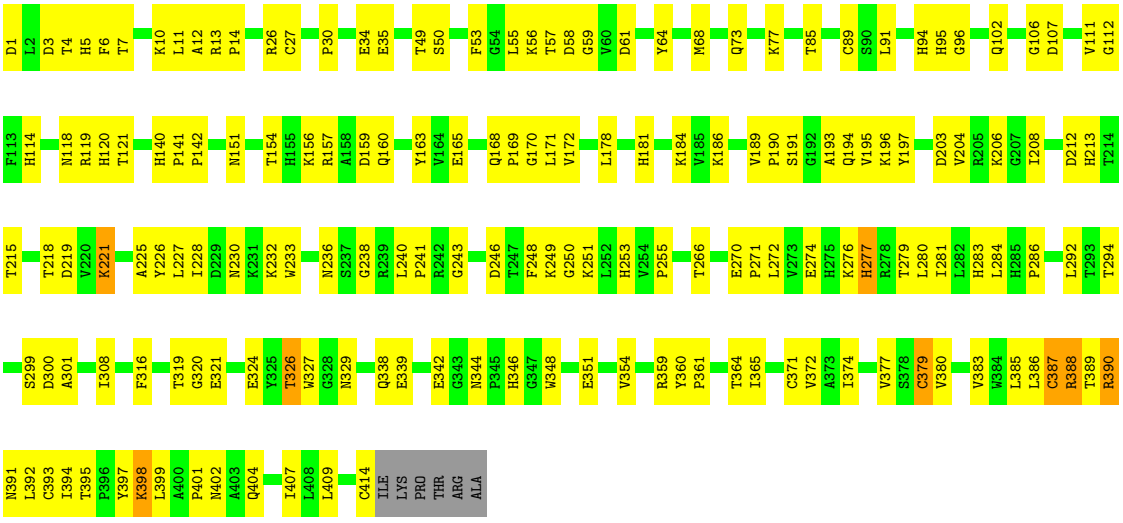
• Molecule 2: Togavirin

Chain E:



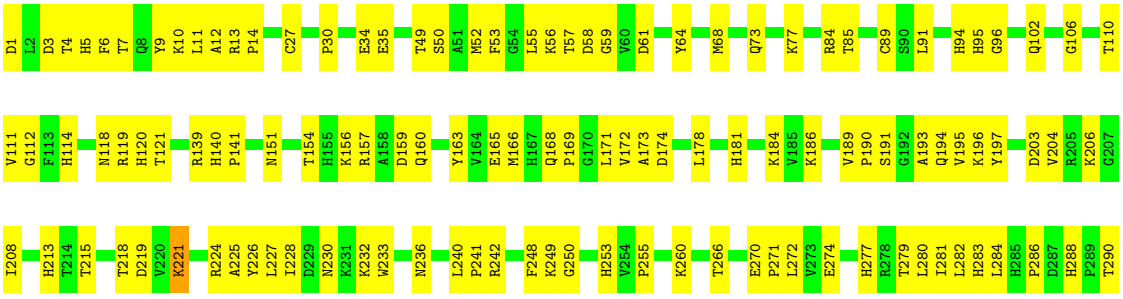
• Molecule 2: Togavirin

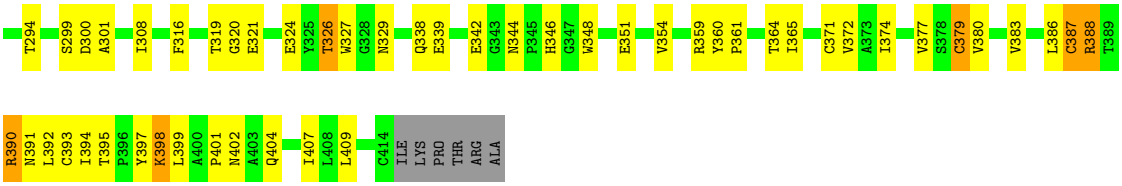
Chain H:



• Molecule 2: Togavirin

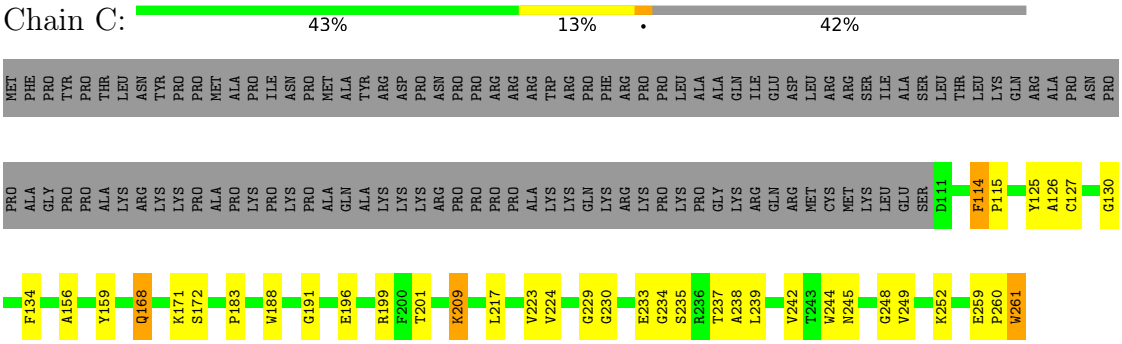
Chain K:





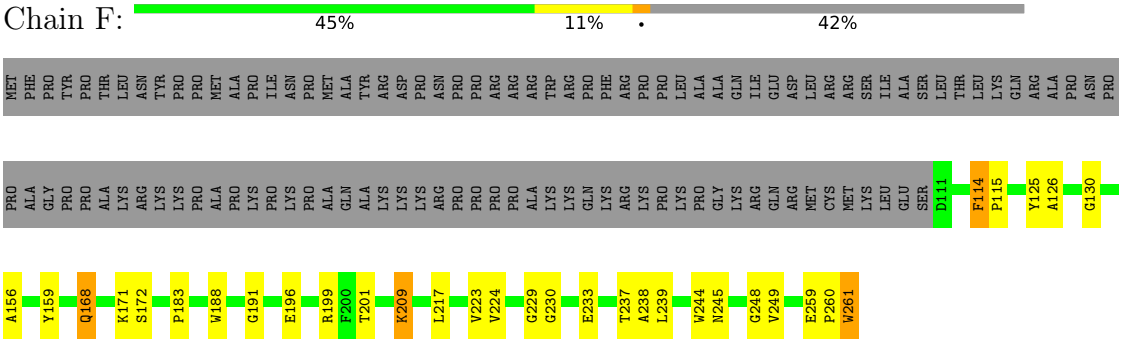
• Molecule 3: Togavirin

Chain C:



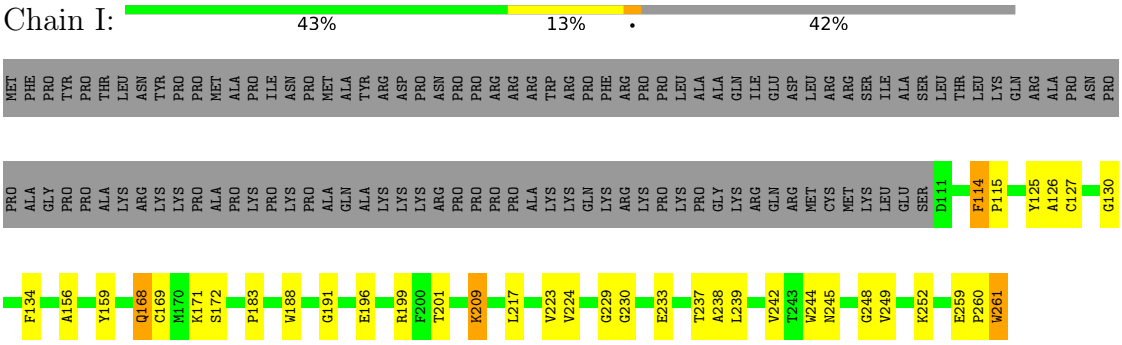
• Molecule 3: Togavirin

Chain F:



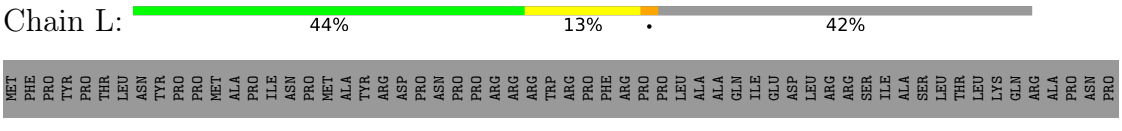
• Molecule 3: Togavirin

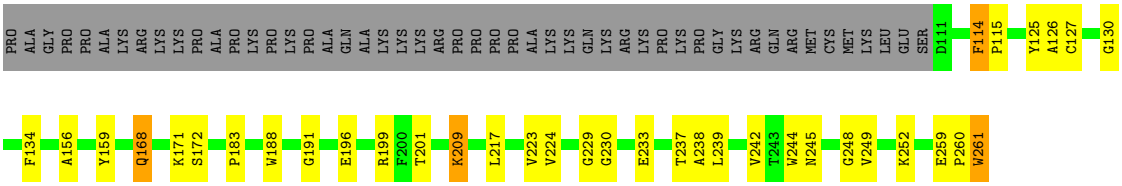
Chain I:



• Molecule 3: Togavirin

Chain L:




PRO ALA GLY PRO PRO ALA LYS ARG LYS LYS PRO ALA PRO LYS PRO LYS PRO ALA GLN ALA LYS LYS LYS ARG PRO PRO PRO PRO ALA LYS LYS GLN LYS ARG LYS PRO LYS PRO GLY LYS ARG GLN ARG MET CYS MET LYS LEU GLU SER D111 F114 P115 Y125 A126 C127 G130
F134 A156 Y159 Q168 K171 S172 P183 W188 G191 E196 R199 F200 T201 K209 L217 V223 V224 G229 G230 E233 T237 A238 L239 V242 T243 W244 N245 G248 V249 K252 E259 P260 W261

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.37	0/3396	0.49	0/4630
1	D	0.37	0/3396	0.49	0/4630
1	G	0.37	0/3396	0.49	0/4630
1	J	0.37	0/3396	0.49	0/4630
2	B	0.35	0/3347	0.48	0/4565
2	E	0.35	0/3347	0.48	0/4565
2	H	0.35	0/3347	0.48	0/4565
2	K	0.35	0/3347	0.48	0/4565
3	C	0.29	0/1192	0.46	0/1615
3	F	0.29	0/1192	0.46	0/1615
3	I	0.29	0/1192	0.46	0/1615
3	L	0.29	0/1192	0.46	0/1615
All	All	0.35	0/31740	0.48	0/43240

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	3307	0	3226	89	0
1	D	3307	0	3226	85	0
1	G	3307	0	3226	94	0
1	J	3307	0	3226	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3253	0	3218	130	0
2	E	3253	0	3218	131	0
2	H	3253	0	3218	135	0
2	K	3253	0	3218	136	0
3	C	1165	0	1146	24	0
3	F	1165	0	1146	17	0
3	I	1165	0	1146	24	0
3	L	1165	0	1146	19	0
All	All	30900	0	30360	926	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 16.

All (926) 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:D:92:ALA:HB1	2:E:224:ARG:HD2	1.50	0.93
3:C:235:SER:H	3:I:169:CYS:HA	1.38	0.87
1:D:82:SER:HA	1:D:100:ASN:HA	1.58	0.84
1:J:82:SER:HA	1:J:100:ASN:HA	1.58	0.84
1:G:82:SER:HA	1:G:100:ASN:HA	1.58	0.83
1:A:82:SER:HA	1:A:100:ASN:HA	1.59	0.83
1:J:426:LEU:HD21	2:K:386:LEU:HD23	1.64	0.79
1:J:253:ASN:OD1	1:J:253:ASN:N	2.18	0.76
1:G:426:LEU:HD21	2:H:386:LEU:HD23	1.66	0.76
3:L:217:LEU:HA	3:L:223:VAL:HA	1.68	0.75
2:K:14:PRO:HB2	2:K:68:MET:HG2	1.69	0.75
2:B:383:VAL:HA	2:B:386:LEU:HD12	1.69	0.75
3:C:217:LEU:HA	3:C:223:VAL:HA	1.68	0.75
2:H:383:VAL:HA	2:H:386:LEU:HD12	1.69	0.75
2:E:14:PRO:HB2	2:E:68:MET:HG2	1.69	0.74
2:K:383:VAL:HA	2:K:386:LEU:HD12	1.69	0.74
2:H:14:PRO:HB2	2:H:68:MET:HG2	1.69	0.74
2:B:14:PRO:HB2	2:B:68:MET:HG2	1.69	0.74
2:E:383:VAL:HA	2:E:386:LEU:HD12	1.69	0.74
3:C:168:GLN:HA	3:C:171:LYS:HB2	1.70	0.74
3:L:168:GLN:HA	3:L:171:LYS:HB2	1.70	0.74
3:I:217:LEU:HA	3:I:223:VAL:HA	1.68	0.73
3:I:168:GLN:HA	3:I:171:LYS:HB2	1.70	0.73
1:D:110:ARG:HG2	1:D:204:LEU:HD21	1.71	0.73
3:F:217:LEU:HA	3:F:223:VAL:HA	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:HIS:HB3	2:B:55:LEU:HD11	1.71	0.73
2:K:5:HIS:HB3	2:K:55:LEU:HD11	1.71	0.72
1:D:258:PHE:HE1	2:E:299:SER:HA	1.54	0.72
1:J:110:ARG:HG2	1:J:204:LEU:HD21	1.71	0.72
2:H:5:HIS:HB3	2:H:55:LEU:HD11	1.72	0.72
2:K:1:ASP:OD2	2:K:4:THR:OG1	2.07	0.72
3:F:168:GLN:HA	3:F:171:LYS:HB2	1.70	0.71
3:C:114:PHE:O	3:C:126:ALA:N	2.24	0.71
2:E:1:ASP:OD2	2:E:4:THR:OG1	2.07	0.71
1:G:110:ARG:HG2	1:G:204:LEU:HD21	1.71	0.71
2:E:61:ASP:OD2	2:E:77:LYS:NZ	2.24	0.71
1:G:253:ASN:OD1	1:G:253:ASN:N	2.18	0.71
2:B:1:ASP:OD2	2:B:4:THR:OG1	2.07	0.71
2:E:5:HIS:HB3	2:E:55:LEU:HD11	1.71	0.71
3:I:114:PHE:O	3:I:126:ALA:N	2.24	0.71
3:L:114:PHE:O	3:L:126:ALA:N	2.24	0.70
3:F:114:PHE:O	3:F:126:ALA:N	2.24	0.70
1:A:110:ARG:HG2	1:A:204:LEU:HD21	1.71	0.70
2:B:61:ASP:OD2	2:B:77:LYS:NZ	2.24	0.70
2:E:360:TYR:HB2	2:E:364:THR:HG23	1.74	0.70
2:H:1:ASP:OD2	2:H:4:THR:OG1	2.07	0.70
1:J:323:SER:HB3	1:J:349:GLU:HA	1.74	0.70
2:K:360:TYR:HB2	2:K:364:THR:HG23	1.74	0.70
1:G:258:PHE:HE1	2:H:299:SER:HA	1.57	0.70
2:H:61:ASP:OD2	2:H:77:LYS:NZ	2.24	0.69
1:D:323:SER:HB3	1:D:349:GLU:HA	1.74	0.69
1:G:323:SER:HB3	1:G:349:GLU:HA	1.74	0.69
2:K:61:ASP:OD2	2:K:77:LYS:NZ	2.24	0.69
1:D:112:GLU:OE2	2:E:46:ARG:NH2	2.26	0.69
2:H:360:TYR:HB2	2:H:364:THR:HG23	1.74	0.69
1:A:323:SER:HB3	1:A:349:GLU:HA	1.74	0.68
2:B:360:TYR:HB2	2:B:364:THR:HG23	1.74	0.68
2:B:14:PRO:HD2	2:B:73:GLN:HE22	1.59	0.68
1:J:91:GLY:HA2	2:K:174:ASP:HA	1.75	0.68
3:C:235:SER:H	3:I:169:CYS:CA	2.06	0.68
2:H:14:PRO:HD2	2:H:73:GLN:HE22	1.59	0.68
2:E:14:PRO:HD2	2:E:73:GLN:HE22	1.59	0.68
2:E:360:TYR:O	2:E:364:THR:OG1	2.09	0.68
2:K:402:ASN:O	2:K:404:GLN:NE2	2.22	0.67
1:A:307:CYS:HB3	1:A:382:LYS:HE2	1.77	0.67
2:B:360:TYR:O	2:B:364:THR:OG1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:ASN:OD1	1:D:253:ASN:N	2.18	0.67
1:D:307:CYS:HB3	1:D:382:LYS:HE2	1.77	0.67
2:K:274:GLU:HB3	2:K:281:ILE:HB	1.77	0.67
1:J:307:CYS:HB3	1:J:382:LYS:HE2	1.77	0.66
1:G:222:LEU:O	1:G:223:GLN:NE2	2.28	0.66
1:G:307:CYS:HB3	1:G:382:LYS:HE2	1.77	0.66
2:K:14:PRO:HD2	2:K:73:GLN:HE22	1.59	0.66
2:E:274:GLU:HB3	2:E:281:ILE:HB	1.77	0.66
1:A:258:PHE:HE1	2:B:299:SER:HA	1.60	0.66
2:B:274:GLU:HB3	2:B:281:ILE:HB	1.77	0.66
2:H:274:GLU:HB3	2:H:281:ILE:HB	1.77	0.66
1:A:222:LEU:O	1:A:223:GLN:NE2	2.28	0.65
2:E:56:LYS:NZ	2:E:57:THR:OG1	2.30	0.65
1:J:222:LEU:O	1:J:223:GLN:NE2	2.28	0.65
2:H:181:HIS:HD2	2:H:186:LYS:HD3	1.62	0.65
3:L:130:GLY:HA2	3:L:172:SER:HA	1.79	0.65
1:A:253:ASN:OD1	1:A:253:ASN:N	2.18	0.65
3:F:130:GLY:HA2	3:F:172:SER:HA	1.79	0.65
2:K:181:HIS:HD2	2:K:186:LYS:HD3	1.62	0.65
3:I:130:GLY:HA2	3:I:172:SER:HA	1.79	0.65
2:B:181:HIS:HD2	2:B:186:LYS:HD3	1.62	0.65
2:H:56:LYS:NZ	2:H:57:THR:OG1	2.30	0.65
2:B:404:GLN:HG3	3:C:248:GLY:O	1.97	0.65
2:E:181:HIS:HD2	2:E:186:LYS:HD3	1.62	0.64
2:B:56:LYS:NZ	2:B:57:THR:OG1	2.30	0.64
2:K:56:LYS:NZ	2:K:57:THR:OG1	2.30	0.64
1:D:222:LEU:O	1:D:223:GLN:NE2	2.28	0.64
1:J:37:ARG:NH2	1:J:130:GLN:OE1	2.31	0.64
2:B:402:ASN:O	2:B:404:GLN:NE2	2.22	0.64
2:E:165:GLU:OE2	2:E:236:ASN:ND2	2.25	0.64
1:A:245:LYS:O	1:A:248:LYS:NZ	2.31	0.63
1:D:184:GLU:N	1:D:184:GLU:OE1	2.32	0.63
2:E:402:ASN:O	2:E:404:GLN:NE2	2.22	0.63
1:G:184:GLU:N	1:G:184:GLU:OE1	2.32	0.63
1:G:258:PHE:CE1	2:H:299:SER:HA	2.33	0.63
1:J:245:LYS:O	1:J:248:LYS:NZ	2.32	0.63
1:A:37:ARG:NH2	1:A:130:GLN:OE1	2.31	0.63
1:G:245:LYS:O	1:G:248:LYS:NZ	2.31	0.63
2:H:118:ASN:OD1	2:H:119:ARG:N	2.32	0.63
1:A:184:GLU:N	1:A:184:GLU:OE1	2.32	0.63
1:D:37:ARG:NH2	1:D:130:GLN:OE1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:184:GLU:OE1	1:J:184:GLU:N	2.32	0.63
3:C:130:GLY:HA2	3:C:172:SER:HA	1.79	0.63
2:K:159:ASP:OD1	2:K:160:GLN:N	2.32	0.63
2:B:118:ASN:OD1	2:B:119:ARG:N	2.32	0.63
2:B:159:ASP:OD1	2:B:160:GLN:N	2.32	0.63
2:E:159:ASP:OD1	2:E:160:GLN:N	2.32	0.63
1:G:37:ARG:NH2	1:G:130:GLN:OE1	2.31	0.62
2:K:360:TYR:O	2:K:364:THR:OG1	2.09	0.62
1:G:404:SER:HA	1:G:408:TRP:HE3	1.64	0.62
2:E:321:GLU:OE1	2:E:321:GLU:N	2.31	0.62
2:K:321:GLU:OE1	2:K:321:GLU:N	2.31	0.62
1:D:245:LYS:O	1:D:248:LYS:NZ	2.32	0.62
2:E:118:ASN:OD1	2:E:119:ARG:N	2.32	0.62
2:H:402:ASN:O	2:H:404:GLN:NE2	2.22	0.62
2:K:118:ASN:OD1	2:K:119:ARG:N	2.32	0.62
1:G:426:LEU:HD11	2:H:386:LEU:HG	1.82	0.62
1:A:112:GLU:OE2	2:B:46:ARG:NH2	2.33	0.62
1:A:92:ALA:HB1	2:B:224:ARG:HD2	1.81	0.62
2:B:168:GLN:NE2	2:B:230:ASN:OD1	2.33	0.62
1:A:404:SER:HA	1:A:408:TRP:HE3	1.64	0.62
1:D:404:SER:HA	1:D:408:TRP:HE3	1.64	0.62
2:E:68:MET:SD	2:E:73:GLN:NE2	2.73	0.62
2:H:159:ASP:OD1	2:H:160:GLN:N	2.32	0.62
1:D:259:GLY:HA3	2:E:297:LEU:HD22	1.82	0.61
2:E:168:GLN:NE2	2:E:230:ASN:OD1	2.33	0.61
2:H:168:GLN:NE2	2:H:230:ASN:OD1	2.33	0.61
1:A:73:HIS:CG	1:A:107:TYR:HE1	2.18	0.61
3:F:230:GLY:HA3	3:F:239:LEU:HA	1.81	0.61
2:K:68:MET:SD	2:K:73:GLN:NE2	2.73	0.61
1:D:73:HIS:CG	1:D:107:TYR:HE1	2.19	0.61
2:B:165:GLU:OE2	2:B:236:ASN:ND2	2.25	0.61
3:I:230:GLY:HA3	3:I:239:LEU:HA	1.81	0.61
2:K:168:GLN:NE2	2:K:230:ASN:OD1	2.33	0.61
2:E:189:VAL:HG12	2:E:191:SER:H	1.65	0.61
2:B:68:MET:SD	2:B:73:GLN:NE2	2.73	0.61
2:H:68:MET:SD	2:H:73:GLN:NE2	2.73	0.61
2:K:189:VAL:HG12	2:K:191:SER:H	1.65	0.61
3:C:230:GLY:HA3	3:C:239:LEU:HA	1.81	0.61
1:G:73:HIS:CG	1:G:107:TYR:HE1	2.18	0.61
1:J:404:SER:HA	1:J:408:TRP:HE3	1.64	0.61
1:A:360:ALA:HB2	1:A:397:GLU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:230:GLY:HA3	3:L:239:LEU:HA	1.81	0.61
2:B:189:VAL:HG12	2:B:191:SER:H	1.65	0.60
2:K:392:LEU:O	2:K:395:THR:OG1	2.18	0.60
1:G:260:CYS:HB3	1:G:272:CYS:HA	1.83	0.60
1:J:73:HIS:CG	1:J:107:TYR:HE1	2.18	0.60
1:D:260:CYS:HB3	1:D:272:CYS:HA	1.83	0.60
3:C:235:SER:N	3:I:169:CYS:HA	2.12	0.60
2:H:165:GLU:OE2	2:H:236:ASN:ND2	2.25	0.60
2:H:321:GLU:OE1	2:H:321:GLU:N	2.31	0.60
2:E:344:ASN:ND2	2:E:346:HIS:O	2.35	0.59
2:E:392:LEU:O	2:E:395:THR:OG1	2.18	0.59
2:H:189:VAL:HG12	2:H:191:SER:H	1.65	0.59
1:G:88:MET:H	1:G:93:TYR:HD1	1.50	0.59
1:J:360:ALA:HB2	1:J:397:GLU:HB3	1.83	0.59
1:A:260:CYS:HB3	1:A:272:CYS:HA	1.83	0.59
2:B:344:ASN:ND2	2:B:346:HIS:O	2.35	0.59
1:D:88:MET:H	1:D:93:TYR:HD1	1.50	0.59
1:D:360:ALA:HB2	1:D:397:GLU:HB3	1.83	0.59
2:H:344:ASN:ND2	2:H:346:HIS:O	2.35	0.59
2:K:344:ASN:ND2	2:K:346:HIS:O	2.35	0.59
1:J:88:MET:H	1:J:93:TYR:HD1	1.50	0.59
1:D:370:VAL:O	1:D:373:SER:OG	2.16	0.59
2:E:387:CYS:O	2:E:391:ASN:ND2	2.36	0.59
1:G:128:THR:OG1	1:G:129:VAL:N	2.36	0.59
1:G:360:ALA:HB2	1:G:397:GLU:HB3	1.83	0.58
2:B:387:CYS:O	2:B:391:ASN:ND2	2.36	0.58
1:J:260:CYS:HB3	1:J:272:CYS:HA	1.83	0.58
1:J:258:PHE:HE1	2:K:299:SER:HA	1.67	0.58
1:J:266:PRO:HG2	1:J:268:ARG:HG3	1.86	0.58
1:A:266:PRO:HG2	1:A:268:ARG:HG3	1.85	0.58
2:B:392:LEU:O	2:B:395:THR:OG1	2.18	0.58
2:H:387:CYS:O	2:H:391:ASN:ND2	2.36	0.58
1:G:266:PRO:HG2	1:G:268:ARG:HG3	1.85	0.58
2:B:196:LYS:HE3	2:B:228:ILE:HD11	1.86	0.58
2:H:196:LYS:HE3	2:H:228:ILE:HD11	1.86	0.58
2:H:360:TYR:O	2:H:364:THR:OG1	2.09	0.58
1:A:128:THR:OG1	1:A:129:VAL:N	2.36	0.58
1:D:128:THR:OG1	1:D:129:VAL:N	2.36	0.58
2:K:387:CYS:O	2:K:391:ASN:ND2	2.36	0.58
1:A:88:MET:H	1:A:93:TYR:HD1	1.51	0.58
1:J:426:LEU:HD11	2:K:386:LEU:HG	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:370:VAL:O	1:J:373:SER:OG	2.16	0.57
1:J:92:ALA:HB1	2:K:224:ARG:HD2	1.86	0.57
1:J:128:THR:OG1	1:J:129:VAL:N	2.36	0.57
2:K:165:GLU:OE2	2:K:236:ASN:ND2	2.25	0.57
2:H:388:ARG:HA	2:H:391:ASN:HD22	1.70	0.57
1:D:304:ILE:HG21	1:D:379:GLY:HA2	1.87	0.57
1:J:321:TYR:CZ	1:J:323:SER:HA	2.40	0.57
1:D:321:TYR:CZ	1:D:323:SER:HA	2.40	0.57
1:G:321:TYR:CZ	1:G:323:SER:HA	2.40	0.57
1:D:266:PRO:HG2	1:D:268:ARG:HG3	1.86	0.57
2:K:196:LYS:HE3	2:K:228:ILE:HD11	1.86	0.57
2:B:168:GLN:NE2	2:B:169:PRO:O	2.37	0.56
2:B:279:THR:OG1	2:B:280:LEU:N	2.38	0.56
1:A:304:ILE:HG21	1:A:379:GLY:HA2	1.87	0.56
2:B:91:LEU:HD23	2:B:91:LEU:H	1.70	0.56
2:E:196:LYS:HE3	2:E:228:ILE:HD11	1.86	0.56
1:G:370:VAL:O	1:G:373:SER:OG	2.16	0.56
2:H:279:THR:OG1	2:H:280:LEU:N	2.38	0.56
2:K:388:ARG:HA	2:K:391:ASN:HD22	1.70	0.56
1:A:321:TYR:CZ	1:A:323:SER:HA	2.40	0.56
1:D:307:CYS:SG	1:D:308:THR:N	2.79	0.56
2:E:279:THR:OG1	2:E:280:LEU:N	2.39	0.56
2:E:388:ARG:HA	2:E:391:ASN:HD22	1.70	0.56
2:K:168:GLN:NE2	2:K:169:PRO:O	2.37	0.56
2:H:240:LEU:HD12	2:H:241:PRO:HD2	1.87	0.56
1:G:304:ILE:HG21	1:G:379:GLY:HA2	1.87	0.56
2:H:30:PRO:O	2:H:50:SER:OG	2.20	0.56
2:H:197:TYR:HE1	2:H:204:VAL:HB	1.71	0.56
2:K:186:LYS:HA	2:K:213:HIS:HB3	1.88	0.56
2:H:186:LYS:HA	2:H:213:HIS:HB3	1.88	0.56
3:F:233:GLU:HB2	3:F:237:THR:HA	1.88	0.56
1:J:307:CYS:SG	1:J:308:THR:N	2.79	0.56
2:K:91:LEU:H	2:K:91:LEU:HD23	1.70	0.56
2:K:197:TYR:HE1	2:K:204:VAL:HB	1.71	0.56
2:E:56:LYS:HG2	2:E:57:THR:H	1.71	0.56
1:G:229:ILE:HD12	2:H:26:ARG:HH22	1.71	0.56
2:H:91:LEU:HD23	2:H:91:LEU:H	1.70	0.56
1:J:361:ASN:ND2	1:J:402:ALA:O	2.39	0.56
2:K:196:LYS:HB3	2:K:226:TYR:HB2	1.88	0.56
1:A:361:ASN:ND2	1:A:402:ALA:O	2.39	0.55
1:G:12:GLY:O	1:G:32:GLN:NE2	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:196:LYS:HB3	2:H:226:TYR:HB2	1.88	0.55
1:J:12:GLY:O	1:J:32:GLN:NE2	2.29	0.55
2:K:30:PRO:O	2:K:50:SER:OG	2.20	0.55
1:A:307:CYS:SG	1:A:308:THR:N	2.79	0.55
2:B:56:LYS:HG2	2:B:57:THR:H	1.71	0.55
2:B:240:LEU:HD12	2:B:241:PRO:HD2	1.87	0.55
2:E:197:TYR:HE1	2:E:204:VAL:HB	1.71	0.55
1:G:2:GLU:HA	1:G:282:ASP:HA	1.89	0.55
1:G:307:CYS:SG	1:G:308:THR:N	2.79	0.55
2:B:388:ARG:HA	2:B:391:ASN:HD22	1.70	0.55
2:B:190:PRO:HD2	2:B:193:ALA:HB3	1.89	0.55
2:B:197:TYR:HE1	2:B:204:VAL:HB	1.71	0.55
2:B:348:TRP:N	2:B:351:GLU:OE2	2.40	0.55
1:D:180:VAL:HG22	1:D:185:VAL:HG12	1.89	0.55
1:D:361:ASN:ND2	1:D:402:ALA:O	2.39	0.55
2:E:91:LEU:HD23	2:E:91:LEU:H	1.70	0.55
3:L:233:GLU:HB2	3:L:237:THR:HA	1.88	0.55
2:B:321:GLU:OE1	2:B:321:GLU:N	2.31	0.55
1:G:361:ASN:ND2	1:G:402:ALA:O	2.39	0.55
2:K:326:THR:OG1	2:K:327:TRP:N	2.40	0.55
2:B:186:LYS:HA	2:B:213:HIS:HB3	1.88	0.55
2:B:300:ASP:OD1	2:B:301:ALA:N	2.40	0.55
1:D:226:GLN:N	1:D:226:GLN:OE1	2.40	0.55
2:E:190:PRO:HD2	2:E:193:ALA:HB3	1.89	0.55
1:J:180:VAL:HG22	1:J:185:VAL:HG12	1.89	0.55
2:E:240:LEU:HD12	2:E:241:PRO:HD2	1.87	0.55
1:G:226:GLN:N	1:G:226:GLN:OE1	2.40	0.55
1:A:2:GLU:HA	1:A:282:ASP:HA	1.89	0.55
1:A:180:VAL:HG22	1:A:185:VAL:HG12	1.89	0.55
1:J:2:GLU:HA	1:J:282:ASP:HA	1.89	0.55
2:K:56:LYS:HG2	2:K:57:THR:H	1.71	0.55
2:K:240:LEU:HD12	2:K:241:PRO:HD2	1.87	0.55
2:E:186:LYS:HA	2:E:213:HIS:HB3	1.88	0.54
3:F:115:PRO:HA	3:F:125:TYR:HA	1.89	0.54
2:H:56:LYS:HG2	2:H:57:THR:H	1.71	0.54
2:H:326:THR:OG1	2:H:327:TRP:N	2.40	0.54
1:J:304:ILE:HG21	1:J:379:GLY:HA2	1.87	0.54
2:K:300:ASP:OD1	2:K:301:ALA:N	2.40	0.54
3:L:115:PRO:HA	3:L:125:TYR:HA	1.89	0.54
2:H:190:PRO:HD2	2:H:193:ALA:HB3	1.89	0.54
3:I:233:GLU:HB2	3:I:237:THR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:THR:OG1	2:B:327:TRP:N	2.40	0.54
1:D:2:GLU:HA	1:D:282:ASP:HA	1.89	0.54
2:E:196:LYS:HB3	2:E:226:TYR:HB2	1.88	0.54
1:G:180:VAL:HG22	1:G:185:VAL:HG12	1.89	0.54
2:H:300:ASP:OD1	2:H:301:ALA:N	2.40	0.54
3:I:115:PRO:HA	3:I:125:TYR:HA	1.89	0.54
2:E:348:TRP:N	2:E:351:GLU:OE2	2.40	0.54
1:A:436:LEU:O	1:A:440:ARG:HG2	2.08	0.54
2:B:196:LYS:HB3	2:B:226:TYR:HB2	1.88	0.54
2:E:300:ASP:OD1	2:E:301:ALA:N	2.40	0.54
2:H:342:GLU:OE1	2:H:342:GLU:N	2.31	0.54
2:K:348:TRP:N	2:K:351:GLU:OE2	2.40	0.54
1:A:226:GLN:N	1:A:226:GLN:OE1	2.40	0.54
1:D:312:ASP:OD1	1:D:312:ASP:N	2.37	0.54
1:G:343:ASN:OD1	1:G:343:ASN:N	2.41	0.54
2:H:85:THR:HG22	2:H:106:GLY:HA3	1.90	0.54
2:H:118:ASN:OD1	2:H:120:HIS:N	2.33	0.54
2:K:390:ARG:O	2:K:394:ILE:HG12	2.08	0.54
2:B:30:PRO:O	2:B:50:SER:OG	2.20	0.54
3:C:115:PRO:HA	3:C:125:TYR:HA	1.90	0.54
3:C:233:GLU:HB2	3:C:237:THR:HA	1.88	0.54
2:K:279:THR:OG1	2:K:280:LEU:N	2.38	0.54
1:A:61:LYS:HG3	1:A:101:THR:HG21	1.90	0.54
2:E:30:PRO:O	2:E:50:SER:OG	2.20	0.54
2:E:326:THR:OG1	2:E:327:TRP:N	2.40	0.54
1:G:263:ALA:HB3	1:G:268:ARG:HB2	1.90	0.54
2:K:118:ASN:OD1	2:K:120:HIS:N	2.33	0.54
2:B:390:ARG:O	2:B:394:ILE:HG12	2.08	0.53
1:D:61:LYS:HG3	1:D:101:THR:HG21	1.90	0.53
1:G:436:LEU:O	1:G:440:ARG:HG2	2.08	0.53
1:J:436:LEU:O	1:J:440:ARG:HG2	2.08	0.53
2:K:190:PRO:HD2	2:K:193:ALA:HB3	1.89	0.53
1:G:61:LYS:HG3	1:G:101:THR:HG21	1.90	0.53
1:A:263:ALA:HB3	1:A:268:ARG:HB2	1.90	0.53
1:D:436:LEU:O	1:D:440:ARG:HG2	2.08	0.53
2:H:348:TRP:N	2:H:351:GLU:OE2	2.40	0.53
1:A:312:ASP:OD1	1:A:312:ASP:N	2.37	0.53
1:D:263:ALA:HB3	1:D:268:ARG:HB2	1.90	0.53
1:D:343:ASN:OD1	1:D:343:ASN:N	2.41	0.53
2:H:390:ARG:O	2:H:394:ILE:HG12	2.08	0.53
2:E:85:THR:HG22	2:E:106:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:311:PRO:HG2	1:J:243:ARG:HD2	1.89	0.53
2:E:390:ARG:O	2:E:394:ILE:HG12	2.08	0.53
1:A:343:ASN:OD1	1:A:343:ASN:N	2.41	0.53
2:B:286:PRO:HG3	2:B:308:ILE:HG22	1.91	0.53
2:B:168:GLN:HA	2:B:233:TRP:CD1	2.44	0.53
2:E:168:GLN:NE2	2:E:169:PRO:O	2.37	0.53
3:F:156:ALA:HB3	3:F:159:TYR:HB2	1.91	0.53
2:E:172:VAL:HG13	2:E:227:LEU:HB3	1.91	0.53
2:E:181:HIS:HB2	2:E:186:LYS:HB2	1.91	0.53
2:H:286:PRO:HG3	2:H:308:ILE:HG22	1.91	0.53
2:H:392:LEU:O	2:H:395:THR:OG1	2.18	0.53
1:J:226:GLN:OE1	1:J:226:GLN:N	2.40	0.53
2:K:172:VAL:HG13	2:K:227:LEU:HB3	1.91	0.53
3:C:156:ALA:HB3	3:C:159:TYR:HB2	1.91	0.53
2:E:168:GLN:HA	2:E:233:TRP:CD1	2.44	0.53
2:K:181:HIS:HB2	2:K:186:LYS:HB2	1.91	0.53
2:B:11:LEU:HB3	2:B:233:TRP:HE3	1.75	0.53
1:D:12:GLY:O	1:D:32:GLN:NE2	2.30	0.53
1:D:318:THR:HG22	1:D:354:THR:HB	1.91	0.53
2:E:11:LEU:HB3	2:E:233:TRP:HE3	1.74	0.53
2:E:286:PRO:HG3	2:E:308:ILE:HG22	1.91	0.53
2:H:351:GLU:O	2:H:354:VAL:HG12	2.09	0.53
3:L:183:PRO:HB3	3:L:196:GLU:HB2	1.92	0.53
1:A:207:ARG:NE	1:A:215:TYR:OH	2.43	0.52
2:B:85:THR:HG22	2:B:106:GLY:HA3	1.90	0.52
2:B:181:HIS:HB2	2:B:186:LYS:HB2	1.91	0.52
1:D:86:PRO:HD2	1:D:95:PHE:HB3	1.92	0.52
1:J:318:THR:HG22	1:J:354:THR:HB	1.91	0.52
2:K:11:LEU:HB3	2:K:233:TRP:HE3	1.74	0.52
2:B:351:GLU:O	2:B:354:VAL:HG12	2.09	0.52
2:E:94:HIS:O	2:E:157:ARG:NH1	2.37	0.52
2:E:351:GLU:O	2:E:354:VAL:HG12	2.09	0.52
1:J:61:LYS:HG3	1:J:101:THR:HG21	1.90	0.52
2:H:11:LEU:HB3	2:H:233:TRP:HE3	1.74	0.52
3:I:156:ALA:HB3	3:I:159:TYR:HB2	1.91	0.52
3:C:183:PRO:HB3	3:C:196:GLU:HB2	1.92	0.52
1:G:318:THR:HG22	1:G:354:THR:HB	1.91	0.52
2:H:56:LYS:HZ2	2:H:58:ASP:H	1.57	0.52
2:H:89:CYS:HB3	2:H:102:GLN:O	2.10	0.52
1:A:318:THR:HG22	1:A:354:THR:HB	1.91	0.52
1:A:321:TYR:HD2	1:A:351:GLY:HA3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:5:HIS:HE1	2:K:157:ARG:HB3	1.75	0.52
2:B:118:ASN:OD1	2:B:120:HIS:N	2.33	0.52
2:B:172:VAL:HG13	2:B:227:LEU:HB3	1.91	0.52
1:G:207:ARG:NE	1:G:215:TYR:OH	2.43	0.52
2:H:168:GLN:NE2	2:H:169:PRO:O	2.37	0.52
2:H:168:GLN:HA	2:H:233:TRP:CD1	2.44	0.52
1:J:207:ARG:NE	1:J:215:TYR:OH	2.42	0.52
2:K:351:GLU:O	2:K:354:VAL:HG12	2.09	0.52
2:E:5:HIS:HE1	2:E:157:ARG:HB3	1.75	0.52
2:E:89:CYS:HB3	2:E:102:GLN:O	2.10	0.52
2:H:171:LEU:HD12	2:H:226:TYR:HB3	1.91	0.52
2:K:171:LEU:HD12	2:K:226:TYR:HB3	1.91	0.52
2:K:342:GLU:OE1	2:K:342:GLU:N	2.31	0.52
2:B:5:HIS:HE1	2:B:157:ARG:HB3	1.75	0.52
2:B:171:LEU:HD12	2:B:226:TYR:HB3	1.91	0.52
2:E:204:VAL:HG11	2:E:208:ILE:HG23	1.92	0.52
3:F:183:PRO:HB3	3:F:196:GLU:HB2	1.92	0.52
1:D:207:ARG:NE	1:D:215:TYR:OH	2.42	0.52
2:H:5:HIS:HE1	2:H:157:ARG:HB3	1.75	0.52
2:H:181:HIS:HB2	2:H:186:LYS:HB2	1.91	0.52
1:A:86:PRO:HD2	1:A:95:PHE:HB3	1.92	0.51
1:D:183:HIS:O	1:D:183:HIS:ND1	2.43	0.51
3:I:183:PRO:HB3	3:I:196:GLU:HB2	1.92	0.51
2:H:172:VAL:HG13	2:H:227:LEU:HB3	1.91	0.51
2:K:168:GLN:HA	2:K:233:TRP:CD1	2.44	0.51
2:K:286:PRO:HG3	2:K:308:ILE:HG22	1.91	0.51
1:A:183:HIS:O	1:A:183:HIS:ND1	2.43	0.51
3:F:244:TRP:HB3	3:F:248:GLY:HA2	1.93	0.51
1:J:183:HIS:ND1	1:J:183:HIS:O	2.43	0.51
2:B:204:VAL:HG11	2:B:208:ILE:HG23	1.92	0.51
2:E:118:ASN:OD1	2:E:120:HIS:N	2.33	0.51
1:G:312:ASP:OD1	1:G:312:ASP:N	2.37	0.51
1:G:321:TYR:HD2	1:G:351:GLY:HA3	1.75	0.51
2:K:94:HIS:O	2:K:157:ARG:NH1	2.37	0.51
3:C:244:TRP:HB3	3:C:248:GLY:HA2	1.93	0.51
1:G:183:HIS:O	1:G:183:HIS:ND1	2.43	0.51
1:J:263:ALA:HB3	1:J:268:ARG:HB2	1.91	0.51
1:J:321:TYR:HD2	1:J:351:GLY:HA3	1.75	0.51
2:K:85:THR:HG22	2:K:106:GLY:HA3	1.90	0.51
2:K:404:GLN:HG3	3:L:248:GLY:O	2.11	0.51
3:L:156:ALA:HB3	3:L:159:TYR:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ALA:O	2:B:232:LYS:NZ	2.43	0.51
2:E:171:LEU:HD12	2:E:226:TYR:HB3	1.91	0.51
2:H:204:VAL:HG11	2:H:208:ILE:HG23	1.92	0.51
2:K:89:CYS:HB3	2:K:102:GLN:O	2.10	0.51
1:A:89:TYR:OH	2:B:71:LYS:HG2	2.10	0.51
2:B:89:CYS:HB3	2:B:102:GLN:O	2.10	0.51
1:J:86:PRO:HD2	1:J:95:PHE:HB3	1.92	0.51
1:G:86:PRO:HD2	1:G:95:PHE:HB3	1.92	0.51
1:G:426:LEU:HB3	2:H:385:LEU:HG	1.92	0.51
2:H:197:TYR:CE1	2:H:204:VAL:HB	2.46	0.51
1:A:381:CYS:C	1:A:382:LYS:HD2	2.32	0.51
1:J:343:ASN:OD1	1:J:343:ASN:N	2.41	0.51
1:J:381:CYS:C	1:J:382:LYS:HD2	2.31	0.51
1:A:12:GLY:O	1:A:32:GLN:NE2	2.29	0.51
2:B:342:GLU:OE1	2:B:342:GLU:N	2.31	0.51
2:E:197:TYR:CE1	2:E:204:VAL:HB	2.46	0.51
2:B:181:HIS:CD2	2:B:186:LYS:HD3	2.46	0.50
2:B:219:ASP:HB2	2:B:221:LYS:HE2	1.93	0.50
1:D:321:TYR:HD2	1:D:351:GLY:HA3	1.75	0.50
2:K:197:TYR:CE1	2:K:204:VAL:HB	2.46	0.50
2:K:219:ASP:HB2	2:K:221:LYS:HE2	1.93	0.50
2:E:342:GLU:OE1	2:E:342:GLU:N	2.31	0.50
1:J:92:ALA:HB1	2:K:224:ARG:HB3	1.92	0.50
3:L:244:TRP:HB3	3:L:248:GLY:HA2	1.93	0.50
2:B:197:TYR:CE1	2:B:204:VAL:HB	2.46	0.50
1:J:359:THR:OG1	1:J:360:ALA:N	2.45	0.50
3:I:244:TRP:HB3	3:I:248:GLY:HA2	1.93	0.50
1:D:359:THR:OG1	1:D:360:ALA:N	2.45	0.50
1:D:381:CYS:C	1:D:382:LYS:HD2	2.32	0.50
3:C:234:GLY:HA3	3:I:169:CYS:HA	1.93	0.50
1:D:219:ASN:O	1:D:219:ASN:ND2	2.43	0.50
2:H:184:LYS:HA	2:H:218:THR:HA	1.94	0.50
2:H:276:LYS:NZ	2:H:277:HIS:O	2.37	0.50
1:A:370:VAL:O	1:A:373:SER:OG	2.16	0.49
2:B:151:ASN:OD1	2:B:151:ASN:N	2.45	0.49
2:B:184:LYS:HA	2:B:218:THR:HA	1.94	0.49
1:G:381:CYS:C	1:G:382:LYS:HD2	2.32	0.49
2:H:14:PRO:HD2	2:H:73:GLN:NE2	2.27	0.49
2:K:204:VAL:HG11	2:K:208:ILE:HG23	1.92	0.49
2:H:219:ASP:HB2	2:H:221:LYS:HE2	1.93	0.49
2:K:151:ASN:OD1	2:K:151:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:THR:OG1	1:G:360:ALA:N	2.45	0.49
1:J:192:GLU:OE1	1:J:192:GLU:N	2.45	0.49
3:F:199:ARG:HB2	3:F:238:ALA:HB1	1.95	0.49
1:A:359:THR:OG1	1:A:360:ALA:N	2.45	0.49
2:B:377:VAL:HA	2:B:380:VAL:HG22	1.95	0.49
2:B:407:ILE:HG22	2:B:409:LEU:HD23	1.95	0.49
2:E:377:VAL:HA	2:E:380:VAL:HG22	1.95	0.49
1:G:192:GLU:N	1:G:192:GLU:OE1	2.45	0.49
2:K:6:PHE:O	2:K:10:LYS:N	2.46	0.49
2:K:11:LEU:HB2	2:K:166:MET:HE1	1.94	0.49
2:B:56:LYS:HZ2	2:B:58:ASP:H	1.60	0.49
2:E:219:ASP:HB2	2:E:221:LYS:HE2	1.93	0.49
1:G:50:LYS:O	1:G:111:SER:OG	2.20	0.49
2:H:94:HIS:O	2:H:157:ARG:NH1	2.37	0.49
2:H:407:ILE:HG22	2:H:409:LEU:HD23	1.95	0.49
2:B:6:PHE:O	2:B:10:LYS:N	2.46	0.49
2:E:184:LYS:HA	2:E:218:THR:HA	1.94	0.49
2:E:233:TRP:CD1	2:E:248:PHE:HD1	2.31	0.49
1:A:192:GLU:N	1:A:192:GLU:OE1	2.45	0.49
1:D:192:GLU:N	1:D:192:GLU:OE1	2.45	0.49
2:H:6:PHE:O	2:H:10:LYS:N	2.46	0.49
2:B:233:TRP:CD1	2:B:248:PHE:HD1	2.31	0.49
2:H:377:VAL:HA	2:H:380:VAL:HG22	1.95	0.49
2:E:49:THR:OG1	2:E:50:SER:N	2.46	0.48
2:H:233:TRP:CD1	2:H:248:PHE:HD1	2.31	0.48
2:K:14:PRO:HD2	2:K:73:GLN:NE2	2.27	0.48
2:B:49:THR:OG1	2:B:50:SER:N	2.46	0.48
2:K:233:TRP:CD1	2:K:248:PHE:HD1	2.31	0.48
2:B:284:LEU:HD13	2:B:327:TRP:CZ3	2.49	0.48
2:E:6:PHE:O	2:E:10:LYS:N	2.46	0.48
2:E:151:ASN:N	2:E:151:ASN:OD1	2.45	0.48
2:K:184:LYS:HA	2:K:218:THR:HA	1.94	0.48
2:E:407:ILE:HG22	2:E:409:LEU:HD23	1.95	0.48
2:H:284:LEU:HD13	2:H:327:TRP:CZ3	2.49	0.48
2:K:284:LEU:HD13	2:K:327:TRP:CZ3	2.49	0.48
3:I:199:ARG:HB2	3:I:238:ALA:HB1	1.94	0.48
3:L:199:ARG:HB2	3:L:238:ALA:HB1	1.94	0.48
3:C:199:ARG:HB2	3:C:238:ALA:HB1	1.94	0.48
1:D:398:SER:OG	1:D:399:PHE:N	2.47	0.48
2:E:12:ALA:O	2:E:232:LYS:NZ	2.43	0.48
2:E:284:LEU:HD13	2:E:327:TRP:CZ3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:56:LYS:HZ2	2:K:58:ASP:H	1.61	0.48
3:F:245:ASN:HB3	3:F:249:VAL:HB	1.96	0.48
1:D:299:ASP:HB3	1:D:322:LYS:HB3	1.95	0.48
3:L:245:ASN:HB3	3:L:249:VAL:HB	1.96	0.48
1:A:299:ASP:HB3	1:A:322:LYS:HB3	1.95	0.48
2:B:14:PRO:HD2	2:B:73:GLN:NE2	2.27	0.48
2:B:380:VAL:HA	2:B:383:VAL:HG22	1.96	0.48
3:C:188:TRP:HB3	3:C:191:GLY:O	2.14	0.48
2:E:380:VAL:HA	2:E:383:VAL:HG22	1.96	0.48
3:I:209:LYS:HA	3:I:261:TRP:HA	1.96	0.48
2:B:154:THR:HG21	2:B:156:LYS:NZ	2.29	0.48
2:E:141:PRO:HA	2:E:142:PRO:HD3	1.80	0.48
1:G:299:ASP:HB3	1:G:322:LYS:HB3	1.95	0.48
1:J:398:SER:OG	1:J:399:PHE:N	2.47	0.48
2:B:3:ASP:OD1	2:B:3:ASP:N	2.47	0.47
3:C:245:ASN:HB3	3:C:249:VAL:HB	1.96	0.47
2:E:154:THR:HG21	2:E:156:LYS:NZ	2.29	0.47
2:H:154:THR:HG21	2:H:156:LYS:NZ	2.29	0.47
3:I:245:ASN:HB3	3:I:249:VAL:HB	1.96	0.47
2:E:360:TYR:CB	2:E:364:THR:HG23	2.44	0.47
1:G:229:ILE:HD12	2:H:26:ARG:NH2	2.29	0.47
2:H:151:ASN:N	2:H:151:ASN:OD1	2.45	0.47
3:I:188:TRP:HB3	3:I:191:GLY:O	2.14	0.47
2:K:49:THR:OG1	2:K:50:SER:N	2.46	0.47
1:A:132:MET:HA	1:A:146:ASP:HA	1.96	0.47
2:E:181:HIS:CD2	2:E:186:LYS:HD3	2.46	0.47
1:G:398:SER:OG	1:G:399:PHE:N	2.47	0.47
1:D:132:MET:HA	1:D:146:ASP:HA	1.96	0.47
2:H:181:HIS:CD2	2:H:186:LYS:HD3	2.46	0.47
2:K:154:THR:HG21	2:K:156:LYS:NZ	2.29	0.47
1:A:309:TYR:OH	1:A:384:PRO:HB3	2.15	0.47
1:D:309:TYR:OH	1:D:384:PRO:HB3	2.15	0.47
3:F:188:TRP:HB3	3:F:191:GLY:O	2.14	0.47
3:F:209:LYS:HA	3:F:261:TRP:HA	1.96	0.47
1:G:56:PRO:HD2	1:G:105:GLU:HG2	1.96	0.47
1:G:132:MET:HA	1:G:146:ASP:HA	1.96	0.47
1:D:50:LYS:O	1:D:111:SER:OG	2.20	0.47
2:E:11:LEU:HB2	2:E:166:MET:HE1	1.97	0.47
1:A:330:PRO:HA	1:A:344:ASP:HA	1.97	0.47
1:A:398:SER:OG	1:A:399:PHE:N	2.47	0.47
2:B:272:LEU:HD13	2:B:272:LEU:HA	1.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:107:ASP:HB3	2:K:139:ARG:HG2	1.97	0.47
1:J:299:ASP:HB3	1:J:322:LYS:HB3	1.95	0.47
1:J:309:TYR:OH	1:J:384:PRO:HB3	2.15	0.47
2:K:377:VAL:HA	2:K:380:VAL:HG22	1.95	0.47
2:K:380:VAL:HA	2:K:383:VAL:HG22	1.96	0.47
1:D:177:LYS:HD3	1:D:191:PRO:HD2	1.97	0.47
1:J:177:LYS:HD3	1:J:191:PRO:HD2	1.97	0.47
2:K:360:TYR:CB	2:K:364:THR:HG23	2.44	0.47
2:K:407:ILE:HG22	2:K:409:LEU:HD23	1.95	0.47
1:A:219:ASN:O	1:A:219:ASN:ND2	2.43	0.47
2:H:380:VAL:HA	2:H:383:VAL:HG22	1.96	0.47
3:L:188:TRP:HB3	3:L:191:GLY:O	2.14	0.47
2:B:141:PRO:HA	2:B:142:PRO:HD3	1.80	0.46
3:C:209:LYS:HA	3:C:261:TRP:HA	1.96	0.46
1:D:56:PRO:HD2	1:D:105:GLU:HG2	1.96	0.46
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.74	0.46
1:G:297:VAL:HG13	1:G:321:TYR:CE1	2.51	0.46
1:J:92:ALA:CB	2:K:224:ARG:HB3	2.46	0.46
1:A:177:LYS:HD3	1:A:191:PRO:HD2	1.97	0.46
1:J:219:ASN:O	1:J:219:ASN:ND2	2.43	0.46
2:K:319:THR:OG1	2:K:320:GLY:N	2.49	0.46
2:K:359:ARG:HG3	2:K:360:TYR:CE1	2.51	0.46
3:L:209:LYS:HA	3:L:261:TRP:HA	1.96	0.46
2:E:359:ARG:HG3	2:E:360:TYR:CE1	2.51	0.46
1:J:258:PHE:CE1	2:K:299:SER:HA	2.49	0.46
1:J:312:ASP:OD1	1:J:312:ASP:N	2.37	0.46
2:K:3:ASP:N	2:K:3:ASP:OD1	2.47	0.46
2:K:13:ARG:HB2	2:K:73:GLN:NE2	2.31	0.46
1:A:297:VAL:HG13	1:A:321:TYR:CE1	2.51	0.46
1:D:297:VAL:HG12	1:D:300:LEU:HD11	1.97	0.46
2:H:13:ARG:HB2	2:H:73:GLN:NE2	2.31	0.46
1:J:132:MET:HA	1:J:146:ASP:HA	1.96	0.46
1:J:330:PRO:HA	1:J:344:ASP:HA	1.97	0.46
2:K:181:HIS:CD2	2:K:186:LYS:HD3	2.46	0.46
1:A:56:PRO:HD2	1:A:105:GLU:HG2	1.96	0.46
2:B:165:GLU:HA	2:B:250:GLY:O	2.16	0.46
1:D:297:VAL:HG13	1:D:321:TYR:CE1	2.51	0.46
2:E:165:GLU:HA	2:E:250:GLY:O	2.16	0.46
1:J:297:VAL:HG12	1:J:300:LEU:HD11	1.97	0.46
2:B:178:LEU:HD21	2:B:225:ALA:HB2	1.98	0.46
1:D:330:PRO:HA	1:D:344:ASP:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:CYS:O	2:E:383:VAL:HG13	2.16	0.46
1:J:297:VAL:HG13	1:J:321:TYR:CE1	2.51	0.46
2:K:12:ALA:O	2:K:232:LYS:NZ	2.43	0.46
2:B:13:ARG:HB2	2:B:73:GLN:NE2	2.31	0.46
1:D:194:GLY:HA2	1:D:215:TYR:CD2	2.51	0.46
2:E:13:ARG:HB2	2:E:73:GLN:NE2	2.31	0.46
2:E:319:THR:OG1	2:E:320:GLY:N	2.48	0.46
1:G:309:TYR:OH	1:G:384:PRO:HB3	2.15	0.46
1:G:321:TYR:OH	1:G:323:SER:HA	2.16	0.46
2:H:379:CYS:O	2:H:383:VAL:HG13	2.16	0.46
1:A:297:VAL:HG12	1:A:300:LEU:HD11	1.97	0.46
2:B:94:HIS:O	2:B:157:ARG:NH1	2.37	0.46
1:D:321:TYR:N	1:D:351:GLY:O	2.49	0.46
2:H:53:PHE:N	2:H:96:GLY:O	2.48	0.46
2:H:165:GLU:HA	2:H:250:GLY:O	2.16	0.46
2:H:359:ARG:HG3	2:H:360:TYR:CE1	2.51	0.46
2:K:379:CYS:O	2:K:383:VAL:HG13	2.16	0.46
3:L:229:GLY:HA2	3:L:260:PRO:HA	1.98	0.46
2:B:319:THR:OG1	2:B:320:GLY:N	2.48	0.46
1:D:321:TYR:OH	1:D:323:SER:HA	2.16	0.46
2:E:14:PRO:HD2	2:E:73:GLN:NE2	2.27	0.46
2:E:398:LYS:HG2	2:E:399:LEU:N	2.31	0.46
1:J:56:PRO:HD2	1:J:105:GLU:HG2	1.96	0.46
2:K:53:PHE:N	2:K:96:GLY:O	2.48	0.46
2:K:165:GLU:HA	2:K:250:GLY:O	2.16	0.46
2:K:398:LYS:HG2	2:K:399:LEU:N	2.31	0.46
1:A:321:TYR:OH	1:A:323:SER:HA	2.16	0.46
2:E:178:LEU:HD21	2:E:225:ALA:HB2	1.98	0.46
1:G:426:LEU:HD22	2:H:389:THR:OG1	2.15	0.46
1:J:194:GLY:HA2	1:J:215:TYR:CD2	2.51	0.46
1:J:426:LEU:HD21	2:K:386:LEU:CD2	2.43	0.46
2:B:112:GLY:HA3	2:B:121:THR:HG22	1.98	0.45
2:B:388:ARG:HA	2:B:388:ARG:HD3	1.80	0.45
1:G:177:LYS:HD3	1:G:191:PRO:HD2	1.97	0.45
1:G:297:VAL:HG12	1:G:300:LEU:HD11	1.97	0.45
1:J:57:SER:HB3	2:K:242:ARG:HB2	1.97	0.45
2:K:112:GLY:HA3	2:K:121:THR:HG22	1.98	0.45
2:K:194:GLN:HB2	2:K:228:ILE:HB	1.98	0.45
1:A:321:TYR:N	1:A:351:GLY:O	2.49	0.45
2:B:359:ARG:HG3	2:B:360:TYR:CE1	2.51	0.45
2:B:379:CYS:O	2:B:383:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:ASP:OD1	2:E:3:ASP:N	2.47	0.45
3:F:229:GLY:HA2	3:F:260:PRO:HA	1.97	0.45
1:G:330:PRO:HA	1:G:344:ASP:HA	1.97	0.45
1:J:92:ALA:H	2:K:173:ALA:HB1	1.80	0.45
1:J:321:TYR:OH	1:J:323:SER:HA	2.16	0.45
2:H:3:ASP:N	2:H:3:ASP:OD1	2.47	0.45
3:C:229:GLY:HA2	3:C:260:PRO:HA	1.97	0.45
1:J:86:PRO:O	1:J:93:TYR:HB3	2.16	0.45
1:G:321:TYR:N	1:G:351:GLY:O	2.49	0.45
2:H:374:ILE:HA	2:H:377:VAL:HG12	1.99	0.45
1:J:84:VAL:H	1:J:99:GLU:HB2	1.82	0.45
2:B:53:PHE:N	2:B:96:GLY:O	2.48	0.45
1:D:84:VAL:H	1:D:99:GLU:HB2	1.82	0.45
1:D:307:CYS:SG	1:D:382:LYS:HG3	2.57	0.45
1:G:194:GLY:HA2	1:G:215:TYR:CD2	2.51	0.45
1:G:437:PHE:HE1	2:H:398:LYS:HE3	1.81	0.45
2:H:359:ARG:HG3	2:H:360:TYR:CD1	2.52	0.45
1:A:436:LEU:O	1:A:440:ARG:NH1	2.50	0.45
2:B:374:ILE:HA	2:B:377:VAL:HG12	1.99	0.45
1:G:307:CYS:SG	1:G:382:LYS:HG3	2.57	0.45
2:H:112:GLY:HA3	2:H:121:THR:HG22	1.98	0.45
2:H:319:THR:OG1	2:H:320:GLY:N	2.48	0.45
3:I:229:GLY:HA2	3:I:260:PRO:HA	1.97	0.45
2:K:374:ILE:HA	2:K:377:VAL:HG12	1.99	0.45
1:A:194:GLY:HA2	1:A:215:TYR:CD2	2.51	0.45
1:A:307:CYS:SG	1:A:382:LYS:HG3	2.57	0.45
2:E:53:PHE:N	2:E:96:GLY:O	2.48	0.45
2:E:112:GLY:HA3	2:E:121:THR:HG22	1.98	0.45
1:G:219:ASN:O	1:G:219:ASN:ND2	2.43	0.45
2:H:398:LYS:HG2	2:H:399:LEU:N	2.31	0.45
2:H:212:ASP:OD1	2:H:213:HIS:N	2.46	0.45
1:J:307:CYS:O	1:J:383:PRO:HD2	2.17	0.45
1:J:321:TYR:N	1:J:351:GLY:O	2.49	0.45
2:K:178:LEU:HD21	2:K:225:ALA:HB2	1.98	0.45
2:B:7:THR:HA	2:B:10:LYS:HD3	1.99	0.44
2:H:49:THR:OG1	2:H:50:SER:N	2.46	0.44
2:H:394:ILE:HA	2:H:397:TYR:CE2	2.52	0.44
1:J:307:CYS:SG	1:J:382:LYS:HG3	2.57	0.44
1:A:86:PRO:O	1:A:93:TYR:HB3	2.16	0.44
2:B:163:TYR:HB3	2:B:253:HIS:HA	2.00	0.44
2:B:194:GLN:HB2	2:B:228:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:ARG:HG3	2:B:360:TYR:CD1	2.52	0.44
2:E:56:LYS:HZ2	2:E:58:ASP:H	1.63	0.44
2:E:398:LYS:O	2:E:401:PRO:HD2	2.18	0.44
1:G:307:CYS:O	1:G:383:PRO:HD2	2.17	0.44
1:G:436:LEU:O	1:G:440:ARG:NH1	2.50	0.44
2:H:11:LEU:HB3	2:H:233:TRP:CE3	2.53	0.44
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.74	0.44
1:D:86:PRO:O	1:D:93:TYR:HB3	2.16	0.44
2:E:374:ILE:HA	2:E:377:VAL:HG12	1.99	0.44
2:E:394:ILE:HA	2:E:397:TYR:CE2	2.52	0.44
2:H:194:GLN:HB2	2:H:228:ILE:HB	1.98	0.44
1:J:344:ASP:OD1	1:J:344:ASP:N	2.51	0.44
2:K:7:THR:HA	2:K:10:LYS:HD3	1.99	0.44
2:K:359:ARG:HG3	2:K:360:TYR:CD1	2.52	0.44
2:B:398:LYS:HG2	2:B:399:LEU:N	2.31	0.44
1:D:307:CYS:O	1:D:383:PRO:HD2	2.17	0.44
1:D:436:LEU:O	1:D:440:ARG:NH1	2.50	0.44
1:G:344:ASP:N	1:G:344:ASP:OD1	2.51	0.44
2:H:7:THR:O	2:H:10:LYS:NZ	2.36	0.44
1:A:84:VAL:H	1:A:99:GLU:HB2	1.82	0.44
2:B:11:LEU:HB3	2:B:233:TRP:CE3	2.53	0.44
2:E:359:ARG:HG3	2:E:360:TYR:CD1	2.52	0.44
1:G:84:VAL:H	1:G:99:GLU:HB2	1.82	0.44
2:K:394:ILE:HA	2:K:397:TYR:CE2	2.52	0.44
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.69	0.44
1:G:437:PHE:CE1	2:H:398:LYS:HE3	2.52	0.44
2:H:7:THR:HA	2:H:10:LYS:HD3	1.99	0.44
2:K:11:LEU:HB3	2:K:233:TRP:CE3	2.53	0.44
3:C:235:SER:HB3	3:I:169:CYS:O	2.18	0.44
1:G:86:PRO:O	1:G:93:TYR:HB3	2.16	0.44
2:H:163:TYR:HB3	2:H:253:HIS:HA	2.00	0.44
2:H:178:LEU:HD21	2:H:225:ALA:HB2	1.98	0.44
1:A:154:PRO:HA	1:A:162:LEU:O	2.18	0.43
2:E:194:GLN:HB2	2:E:228:ILE:HB	1.98	0.43
1:G:154:PRO:HA	1:G:162:LEU:O	2.18	0.43
1:J:154:PRO:HA	1:J:162:LEU:O	2.18	0.43
1:A:259:GLY:HA3	2:B:297:LEU:HD22	2.00	0.43
2:B:361:PRO:O	2:B:365:ILE:HD13	2.18	0.43
2:B:394:ILE:HA	2:B:397:TYR:CE2	2.52	0.43
2:E:7:THR:HA	2:E:10:LYS:HD3	1.99	0.43
1:G:162:LEU:HD23	1:G:162:LEU:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:361:PRO:O	2:K:365:ILE:HD13	2.18	0.43
2:B:140:HIS:CG	2:B:141:PRO:HD2	2.53	0.43
2:H:140:HIS:CG	2:H:141:PRO:HD2	2.53	0.43
2:H:361:PRO:O	2:H:365:ILE:HD13	2.19	0.43
1:J:260:CYS:HB2	1:J:270:GLU:O	2.19	0.43
1:A:344:ASP:OD1	1:A:344:ASP:N	2.51	0.43
2:B:390:ARG:NH1	2:B:390:ARG:HB3	2.34	0.43
2:E:288:HIS:O	2:E:290:THR:OG1	2.31	0.43
2:B:272:LEU:HB2	2:B:283:HIS:HB2	2.00	0.43
2:B:398:LYS:O	2:B:401:PRO:HD2	2.18	0.43
2:E:11:LEU:HB3	2:E:233:TRP:CE3	2.53	0.43
1:G:260:CYS:HB2	1:G:270:GLU:O	2.18	0.43
1:J:378:LYS:HE2	1:J:378:LYS:HB2	1.87	0.43
1:J:436:LEU:O	1:J:440:ARG:NH1	2.50	0.43
2:K:95:HIS:ND1	2:K:255:PRO:HB3	2.34	0.43
2:K:390:ARG:HB3	2:K:390:ARG:NH1	2.34	0.43
1:A:260:CYS:HB2	1:A:270:GLU:O	2.18	0.43
1:A:360:ALA:HB1	1:A:399:PHE:CE2	2.54	0.43
2:H:95:HIS:ND1	2:H:255:PRO:HB3	2.34	0.43
2:K:391:ASN:O	2:K:395:THR:HG23	2.19	0.43
2:K:398:LYS:O	2:K:401:PRO:HD2	2.18	0.43
1:A:307:CYS:O	1:A:383:PRO:HD2	2.18	0.43
2:B:360:TYR:CB	2:B:364:THR:HG23	2.44	0.43
2:B:391:ASN:O	2:B:395:THR:HG23	2.19	0.43
1:D:344:ASP:OD1	1:D:344:ASP:N	2.51	0.43
2:K:163:TYR:HB3	2:K:253:HIS:HA	2.00	0.43
2:K:387:CYS:SG	2:K:388:ARG:N	2.92	0.43
2:K:388:ARG:HA	2:K:388:ARG:HD3	1.80	0.43
2:H:195:VAL:HG22	2:H:208:ILE:O	2.19	0.43
1:J:110:ARG:HG3	1:J:214:LEU:HD21	2.01	0.43
2:K:140:HIS:CG	2:K:141:PRO:HD2	2.53	0.43
1:A:94:CYS:SG	2:B:173:ALA:HB2	2.59	0.43
2:B:9:TYR:OH	2:B:53:PHE:O	2.31	0.43
2:B:95:HIS:ND1	2:B:255:PRO:HB3	2.34	0.43
1:D:260:CYS:HB2	1:D:270:GLU:O	2.18	0.43
1:D:409:SER:HA	1:D:412:LYS:HG2	2.01	0.43
2:E:391:ASN:O	2:E:395:THR:HG23	2.19	0.43
2:H:360:TYR:CB	2:H:364:THR:HG23	2.44	0.43
2:H:391:ASN:O	2:H:395:THR:HG23	2.19	0.43
2:H:398:LYS:O	2:H:401:PRO:HD2	2.18	0.43
2:K:388:ARG:O	2:K:392:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HG3	1:A:214:LEU:HD21	2.01	0.43
2:E:195:VAL:HG22	2:E:208:ILE:O	2.19	0.43
1:J:59:VAL:HG21	2:K:242:ARG:HH21	1.84	0.43
1:D:154:PRO:HA	1:D:162:LEU:O	2.18	0.42
2:E:197:TYR:CE2	2:E:203:ASP:HB3	2.54	0.42
2:E:388:ARG:HA	2:E:388:ARG:HD3	1.80	0.42
2:E:388:ARG:O	2:E:392:LEU:HG	2.19	0.42
2:H:388:ARG:O	2:H:392:LEU:HG	2.19	0.42
1:J:94:CYS:HA	2:K:226:TYR:CE1	2.54	0.42
1:J:162:LEU:HA	1:J:162:LEU:HD23	1.74	0.42
1:D:259:GLY:CA	2:E:297:LEU:HD22	2.48	0.42
2:E:95:HIS:ND1	2:E:255:PRO:HB3	2.34	0.42
2:E:140:HIS:CG	2:E:141:PRO:HD2	2.53	0.42
2:E:212:ASP:OD1	2:E:213:HIS:N	2.46	0.42
2:E:272:LEU:HB2	2:E:283:HIS:HB2	2.00	0.42
1:G:409:SER:HA	1:G:412:LYS:HG2	2.01	0.42
2:H:390:ARG:HB3	2:H:390:ARG:NH1	2.34	0.42
1:J:290:ARG:HA	1:J:290:ARG:HD3	1.81	0.42
2:K:56:LYS:HB2	2:K:64:TYR:CD2	2.55	0.42
2:K:197:TYR:CE2	2:K:203:ASP:HB3	2.54	0.42
2:K:260:LYS:HE2	2:K:260:LYS:HB2	1.92	0.42
1:D:110:ARG:HG3	1:D:214:LEU:HD21	2.01	0.42
2:E:163:TYR:HB3	2:E:253:HIS:HA	2.00	0.42
1:G:110:ARG:HG3	1:G:214:LEU:HD21	2.01	0.42
2:H:58:ASP:OD1	2:H:59:GLY:N	2.52	0.42
2:H:387:CYS:SG	2:H:388:ARG:N	2.92	0.42
2:H:390:ARG:HB3	2:H:390:ARG:HH11	1.84	0.42
1:J:360:ALA:HB1	1:J:399:PHE:CE2	2.54	0.42
2:K:114:HIS:CE1	2:K:119:ARG:HE	2.38	0.42
2:K:154:THR:HG21	2:K:156:LYS:HZ1	1.82	0.42
2:B:195:VAL:HG22	2:B:208:ILE:O	2.19	0.42
2:B:388:ARG:O	2:B:392:LEU:HG	2.19	0.42
2:E:58:ASP:OD1	2:E:59:GLY:N	2.52	0.42
2:E:114:HIS:CE1	2:E:119:ARG:HE	2.38	0.42
2:E:361:PRO:O	2:E:365:ILE:HD13	2.19	0.42
1:G:206:SER:OG	1:G:208:THR:O	2.30	0.42
2:H:12:ALA:O	2:H:232:LYS:NZ	2.43	0.42
2:H:272:LEU:HD13	2:H:272:LEU:HA	1.83	0.42
2:K:272:LEU:HB2	2:K:283:HIS:HB2	2.00	0.42
2:B:294:THR:HG21	2:B:316:PHE:CZ	2.55	0.42
2:E:148:LEU:HD23	2:E:148:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:HIS:CD2	1:G:233:PRO:HD3	2.55	0.42
1:G:426:LEU:HB3	2:H:389:THR:HG21	2.00	0.42
2:K:195:VAL:HG22	2:K:208:ILE:O	2.19	0.42
2:K:390:ARG:HB3	2:K:390:ARG:HH11	1.84	0.42
1:A:307:CYS:N	1:A:382:LYS:HE2	2.35	0.42
2:B:58:ASP:OD1	2:B:59:GLY:N	2.52	0.42
2:B:114:HIS:CE1	2:B:119:ARG:HE	2.38	0.42
2:E:390:ARG:NH1	2:E:390:ARG:HB3	2.34	0.42
1:G:307:CYS:N	1:G:382:LYS:HE2	2.35	0.42
2:H:114:HIS:CE1	2:H:119:ARG:HE	2.38	0.42
2:H:141:PRO:HA	2:H:142:PRO:HD3	1.80	0.42
1:J:147:VAL:HG22	1:J:148:TYR:O	2.20	0.42
1:A:258:PHE:CE1	2:B:299:SER:HA	2.47	0.42
2:B:197:TYR:CE2	2:B:203:ASP:HB3	2.54	0.42
2:B:411:LEU:HD13	2:B:411:LEU:HA	1.94	0.42
1:D:360:ALA:HB1	1:D:399:PHE:CE2	2.54	0.42
2:E:387:CYS:SG	2:E:388:ARG:N	2.92	0.42
2:H:294:THR:HG21	2:H:316:PHE:CZ	2.55	0.42
1:J:231:HIS:CD2	1:J:233:PRO:HD3	2.55	0.42
1:D:231:HIS:CD2	1:D:233:PRO:HD3	2.54	0.42
1:G:360:ALA:HB1	1:G:399:PHE:CE2	2.54	0.42
2:H:56:LYS:HB2	2:H:64:TYR:CD2	2.55	0.42
2:H:272:LEU:HB2	2:H:283:HIS:HB2	2.00	0.42
1:A:147:VAL:HG22	1:A:148:TYR:O	2.20	0.42
2:B:390:ARG:HB3	2:B:390:ARG:HH11	1.84	0.42
2:E:56:LYS:HB2	2:E:64:TYR:CD2	2.55	0.42
2:E:294:THR:HG21	2:E:316:PHE:CZ	2.55	0.42
1:G:58:PRO:HD3	2:H:238:GLY:HA2	2.02	0.42
2:E:390:ARG:HB3	2:E:390:ARG:HH11	1.84	0.42
1:G:147:VAL:HG22	1:G:148:TYR:O	2.20	0.42
1:J:54:LYS:HG2	1:J:107:TYR:HD2	1.85	0.42
2:B:7:THR:O	2:B:10:LYS:NZ	2.36	0.41
2:B:292:LEU:HD13	2:B:327:TRP:HE3	1.85	0.41
2:B:387:CYS:SG	2:B:388:ARG:N	2.92	0.41
2:E:266:THR:O	2:E:329:ASN:ND2	2.53	0.41
1:G:54:LYS:HG2	1:G:107:TYR:HD2	1.85	0.41
2:K:288:HIS:O	2:K:290:THR:OG1	2.31	0.41
1:A:231:HIS:CD2	1:A:233:PRO:HD3	2.55	0.41
1:D:85:TYR:CE2	1:D:98:THR:HA	2.55	0.41
2:E:34:GLU:C	2:E:35:GLU:HG3	2.41	0.41
2:H:292:LEU:HD13	2:H:327:TRP:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:7:THR:O	2:K:10:LYS:NZ	2.36	0.41
2:K:34:GLU:C	2:K:35:GLU:HG3	2.41	0.41
1:A:363:HIS:NE2	1:A:406:THR:HG23	2.35	0.41
1:A:409:SER:HA	1:A:412:LYS:HG2	2.01	0.41
1:D:409:SER:O	1:D:412:LYS:HG2	2.20	0.41
2:H:249:LYS:HA	2:H:249:LYS:HD3	1.91	0.41
1:A:303:LYS:HD2	1:A:303:LYS:HA	1.88	0.41
1:A:409:SER:OG	1:A:412:LYS:NZ	2.54	0.41
1:A:441:HIS:HB2	2:H:414:CYS:SG	2.60	0.41
1:D:147:VAL:HG22	1:D:148:TYR:O	2.20	0.41
1:D:307:CYS:N	1:D:382:LYS:HE2	2.35	0.41
1:D:423:VAL:O	1:D:427:ILE:HG12	2.20	0.41
2:E:156:LYS:HE2	2:E:159:ASP:HB2	2.03	0.41
3:F:114:PHE:N	3:F:126:ALA:O	2.24	0.41
1:G:80:VAL:HA	1:G:102:GLN:O	2.21	0.41
1:G:85:TYR:CE2	1:G:98:THR:HA	2.55	0.41
1:G:290:ARG:HA	1:G:290:ARG:HD3	1.81	0.41
1:G:363:HIS:NE2	1:G:406:THR:HG23	2.35	0.41
2:H:197:TYR:CE2	2:H:203:ASP:HB3	2.54	0.41
1:J:423:VAL:O	1:J:427:ILE:HG12	2.20	0.41
2:K:249:LYS:HA	2:K:249:LYS:HD3	1.91	0.41
2:K:266:THR:O	2:K:329:ASN:ND2	2.53	0.41
2:K:371:CYS:SG	2:K:372:VAL:N	2.94	0.41
1:D:145:ALA:HB3	1:D:157:ILE:HG12	2.03	0.41
2:E:170:GLY:HA3	2:E:243:GLY:H	1.86	0.41
2:E:282:LEU:HD23	2:E:282:LEU:HA	1.69	0.41
1:J:85:TYR:CE2	1:J:98:THR:HA	2.55	0.41
1:J:409:SER:OG	1:J:412:LYS:NZ	2.54	0.41
1:A:85:TYR:CE2	1:A:98:THR:HA	2.55	0.41
1:A:409:SER:O	1:A:412:LYS:HG2	2.20	0.41
2:B:212:ASP:OD1	2:B:213:HIS:N	2.46	0.41
1:D:323:SER:OG	1:D:324:SER:N	2.54	0.41
1:D:363:HIS:NE2	1:D:406:THR:HG23	2.35	0.41
1:D:395:HIS:CE1	1:D:396:THR:HG22	2.56	0.41
1:D:409:SER:OG	1:D:412:LYS:NZ	2.54	0.41
2:E:402:ASN:HB3	2:E:404:GLN:HG2	2.03	0.41
1:G:145:ALA:HB3	1:G:157:ILE:HG12	2.03	0.41
1:G:423:VAL:O	1:G:427:ILE:HG12	2.20	0.41
1:J:409:SER:O	1:J:412:LYS:HG2	2.20	0.41
2:K:294:THR:HG21	2:K:316:PHE:CZ	2.55	0.41
3:L:242:VAL:HA	3:L:252:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:THR:O	2:B:329:ASN:ND2	2.53	0.41
2:B:371:CYS:SG	2:B:372:VAL:N	2.94	0.41
2:E:7:THR:O	2:E:10:LYS:HG2	2.21	0.41
2:H:7:THR:O	2:H:10:LYS:HG2	2.21	0.41
2:H:266:THR:O	2:H:329:ASN:ND2	2.53	0.41
1:J:307:CYS:N	1:J:382:LYS:HE2	2.35	0.41
1:J:363:HIS:NE2	1:J:406:THR:HG23	2.35	0.41
2:K:9:TYR:OH	2:K:53:PHE:O	2.31	0.41
1:A:80:VAL:HA	1:A:102:GLN:O	2.21	0.41
1:G:89:TYR:O	1:G:89:TYR:CG	2.73	0.41
2:K:402:ASN:HB3	2:K:404:GLN:HG2	2.03	0.41
2:B:7:THR:O	2:B:10:LYS:HG2	2.21	0.41
2:B:11:LEU:HB2	2:B:166:MET:HE1	2.03	0.41
2:B:56:LYS:HB2	2:B:64:TYR:CD2	2.55	0.41
1:D:80:VAL:HA	1:D:102:GLN:O	2.21	0.41
1:D:89:TYR:O	1:D:89:TYR:CG	2.73	0.41
2:E:292:LEU:HD13	2:E:327:TRP:HE3	1.85	0.41
2:E:371:CYS:SG	2:E:372:VAL:N	2.94	0.41
1:G:409:SER:O	1:G:412:LYS:HG2	2.20	0.41
1:G:422:ILE:HD11	2:H:386:LEU:HD21	2.03	0.41
2:H:34:GLU:C	2:H:35:GLU:HG3	2.41	0.41
2:H:246:ASP:OD1	2:H:246:ASP:N	2.54	0.41
2:H:371:CYS:SG	2:H:372:VAL:N	2.94	0.41
3:I:242:VAL:HA	3:I:252:LYS:HA	2.02	0.41
1:J:41:SER:OG	1:J:125:HIS:HB2	2.21	0.41
1:J:323:SER:OG	1:J:324:SER:N	2.54	0.41
1:J:395:HIS:CE1	1:J:396:THR:HG22	2.56	0.41
2:K:7:THR:O	2:K:10:LYS:HG2	2.21	0.41
2:K:58:ASP:OD1	2:K:59:GLY:N	2.52	0.41
2:K:282:LEU:HD23	2:K:282:LEU:HA	1.69	0.41
1:A:145:ALA:HB3	1:A:157:ILE:HG12	2.03	0.41
3:C:242:VAL:HA	3:C:252:LYS:HA	2.02	0.41
1:D:41:SER:OG	1:D:125:HIS:HB2	2.21	0.41
1:D:54:LYS:HG2	1:D:107:TYR:HD2	1.85	0.41
1:G:41:SER:OG	1:G:125:HIS:HB2	2.21	0.41
2:H:170:GLY:HA3	2:H:243:GLY:H	1.86	0.41
1:J:409:SER:HA	1:J:412:LYS:HG2	2.01	0.41
1:A:54:LYS:HG2	1:A:107:TYR:HD2	1.85	0.40
1:A:89:TYR:O	1:A:89:TYR:CG	2.73	0.40
2:B:11:LEU:O	2:B:233:TRP:N	2.46	0.40
2:B:186:LYS:HA	2:B:186:LYS:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:VAL:HA	2:H:190:PRO:HD3	1.94	0.40
2:K:52:MET:HB3	2:K:52:MET:HE3	1.95	0.40
1:A:41:SER:OG	1:A:125:HIS:HB2	2.21	0.40
1:A:382:LYS:HA	1:A:382:LYS:HE3	2.04	0.40
1:A:395:HIS:CE1	1:A:396:THR:HG22	2.56	0.40
2:B:170:GLY:HA3	2:B:243:GLY:H	1.86	0.40
1:D:89:TYR:OH	2:E:71:LYS:HG2	2.22	0.40
2:E:84:ARG:NH2	2:E:110:THR:HG21	2.36	0.40
2:E:169:PRO:HD3	2:E:233:TRP:HA	2.03	0.40
1:G:136:THR:HG23	1:G:140:VAL:O	2.22	0.40
2:H:270:GLU:OE1	2:H:271:PRO:HD2	2.21	0.40
3:I:114:PHE:N	3:I:126:ALA:O	2.24	0.40
2:K:84:ARG:NH2	2:K:110:THR:HG21	2.36	0.40
2:K:270:GLU:OE1	2:K:271:PRO:HD2	2.21	0.40
3:L:127:CYS:O	3:L:134:PHE:HB2	2.22	0.40
1:A:323:SER:OG	1:A:324:SER:N	2.54	0.40
1:A:423:VAL:O	1:A:427:ILE:HG12	2.20	0.40
2:B:402:ASN:HB3	2:B:404:GLN:HG2	2.03	0.40
3:C:127:CYS:O	3:C:134:PHE:HB2	2.22	0.40
3:C:245:ASN:N	3:C:249:VAL:O	2.55	0.40
2:E:270:GLU:OE1	2:E:271:PRO:HD2	2.21	0.40
2:E:411:LEU:HD13	2:E:411:LEU:HA	1.94	0.40
1:G:409:SER:OG	1:G:412:LYS:NZ	2.54	0.40
2:H:163:TYR:HE2	2:H:251:LYS:HZ2	1.70	0.40
2:K:156:LYS:HE2	2:K:159:ASP:HB2	2.03	0.40
2:B:249:LYS:HA	2:B:249:LYS:HD3	1.91	0.40
2:E:11:LEU:O	2:E:233:TRP:N	2.46	0.40
3:F:245:ASN:N	3:F:249:VAL:O	2.55	0.40
2:H:140:HIS:ND1	2:H:141:PRO:O	2.55	0.40
2:H:169:PRO:HD3	2:H:233:TRP:HA	2.03	0.40
3:I:127:CYS:O	3:I:134:PHE:HB2	2.22	0.40
3:I:245:ASN:N	3:I:249:VAL:O	2.55	0.40
1:J:89:TYR:O	1:J:89:TYR:CG	2.73	0.40
1:J:230:VAL:HG21	2:K:241:PRO:HD3	2.03	0.40
3:L:245:ASN:N	3:L:249:VAL:O	2.55	0.40
1:A:57:SER:HB3	2:B:240:LEU:O	2.22	0.40
2:B:296:SER:O	2:B:297:LEU:HD23	2.22	0.40
2:E:113:PHE:O	2:E:120:HIS:HB2	2.22	0.40
2:E:272:LEU:HD13	2:E:272:LEU:HA	1.83	0.40
1:G:382:LYS:HE3	1:G:382:LYS:HA	2.03	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	429/441 (97%)	387 (90%)	42 (10%)	0	100	100
1	D	429/441 (97%)	386 (90%)	43 (10%)	0	100	100
1	G	429/441 (97%)	386 (90%)	43 (10%)	0	100	100
1	J	429/441 (97%)	387 (90%)	42 (10%)	0	100	100
2	B	412/420 (98%)	362 (88%)	50 (12%)	0	100	100
2	E	412/420 (98%)	361 (88%)	51 (12%)	0	100	100
2	H	412/420 (98%)	360 (87%)	52 (13%)	0	100	100
2	K	412/420 (98%)	362 (88%)	50 (12%)	0	100	100
3	C	149/261 (57%)	134 (90%)	15 (10%)	0	100	100
3	F	149/261 (57%)	134 (90%)	15 (10%)	0	100	100
3	I	149/261 (57%)	134 (90%)	15 (10%)	0	100	100
3	L	149/261 (57%)	134 (90%)	15 (10%)	0	100	100
All	All	3960/4488 (88%)	3527 (89%)	433 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	363/371 (98%)	347 (96%)	16 (4%)	28	54
1	D	363/371 (98%)	347 (96%)	16 (4%)	28	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	363/371 (98%)	347 (96%)	16 (4%)	28	54
1	J	363/371 (98%)	347 (96%)	16 (4%)	28	54
2	B	362/367 (99%)	346 (96%)	16 (4%)	28	54
2	E	362/367 (99%)	346 (96%)	16 (4%)	28	54
2	H	362/367 (99%)	346 (96%)	16 (4%)	28	54
2	K	362/367 (99%)	346 (96%)	16 (4%)	28	54
3	C	125/221 (57%)	118 (94%)	7 (6%)	21	48
3	F	125/221 (57%)	118 (94%)	7 (6%)	21	48
3	I	125/221 (57%)	118 (94%)	7 (6%)	21	48
3	L	125/221 (57%)	118 (94%)	7 (6%)	21	48
All	All	3400/3836 (89%)	3244 (95%)	156 (5%)	31	54

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	28	HIS
1	A	48	THR
1	A	69	THR
1	A	87	PHE
1	A	101	THR
1	A	128	THR
1	A	219	ASN
1	A	235	THR
1	A	253	ASN
1	A	272	CYS
1	A	282	ASP
1	A	294	THR
1	A	368	LEU
1	A	381	CYS
1	A	396	THR
2	B	27	CYS
2	B	111	VAL
2	B	206	LYS
2	B	215	THR
2	B	221	LYS
2	B	277	HIS
2	B	324	GLU

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Mol	Chain	Res	Type
2	B	326	THR
2	B	338	GLN
2	B	339	GLU
2	B	379	CYS
2	B	387	CYS
2	B	388	ARG
2	B	390	ARG
2	B	393	CYS
2	B	398	LYS
3	C	114	PHE
3	C	168	GLN
3	C	201	THR
3	C	209	LYS
3	C	224	VAL
3	C	259	GLU
3	C	261	TRP
1	D	7	MET
1	D	28	HIS
1	D	48	THR
1	D	69	THR
1	D	87	PHE
1	D	101	THR
1	D	128	THR
1	D	219	ASN
1	D	235	THR
1	D	253	ASN
1	D	272	CYS
1	D	282	ASP
1	D	294	THR
1	D	368	LEU
1	D	381	CYS
1	D	396	THR
2	E	27	CYS
2	E	111	VAL
2	E	206	LYS
2	E	215	THR
2	E	221	LYS
2	E	277	HIS
2	E	324	GLU
2	E	326	THR
2	E	338	GLN
2	E	339	GLU

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Mol	Chain	Res	Type
2	E	379	CYS
2	E	387	CYS
2	E	388	ARG
2	E	390	ARG
2	E	393	CYS
2	E	398	LYS
3	F	114	PHE
3	F	168	GLN
3	F	201	THR
3	F	209	LYS
3	F	224	VAL
3	F	259	GLU
3	F	261	TRP
1	G	7	MET
1	G	28	HIS
1	G	48	THR
1	G	69	THR
1	G	87	PHE
1	G	101	THR
1	G	128	THR
1	G	219	ASN
1	G	235	THR
1	G	253	ASN
1	G	272	CYS
1	G	282	ASP
1	G	294	THR
1	G	368	LEU
1	G	381	CYS
1	G	396	THR
2	H	27	CYS
2	H	111	VAL
2	H	206	LYS
2	H	215	THR
2	H	221	LYS
2	H	277	HIS
2	H	324	GLU
2	H	326	THR
2	H	338	GLN
2	H	339	GLU
2	H	379	CYS
2	H	387	CYS
2	H	388	ARG

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Mol	Chain	Res	Type
2	H	390	ARG
2	H	393	CYS
2	H	398	LYS
3	I	114	PHE
3	I	168	GLN
3	I	201	THR
3	I	209	LYS
3	I	224	VAL
3	I	259	GLU
3	I	261	TRP
1	J	7	MET
1	J	28	HIS
1	J	48	THR
1	J	69	THR
1	J	87	PHE
1	J	101	THR
1	J	128	THR
1	J	219	ASN
1	J	235	THR
1	J	253	ASN
1	J	272	CYS
1	J	282	ASP
1	J	294	THR
1	J	368	LEU
1	J	381	CYS
1	J	396	THR
2	K	27	CYS
2	K	111	VAL
2	K	206	LYS
2	K	215	THR
2	K	221	LYS
2	K	277	HIS
2	K	324	GLU
2	K	326	THR
2	K	338	GLN
2	K	339	GLU
2	K	379	CYS
2	K	387	CYS
2	K	388	ARG
2	K	390	ARG
2	K	393	CYS
2	K	398	LYS

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Mol	Chain	Res	Type
3	L	114	PHE
3	L	168	GLN
3	L	201	THR
3	L	209	LYS
3	L	224	VAL
3	L	259	GLU
3	L	261	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	361	ASN
1	A	363	HIS
2	B	73	GLN
2	B	120	HIS
2	B	181	HIS
1	D	271	ASN
1	D	361	ASN
1	D	363	HIS
2	E	73	GLN
2	E	120	HIS
2	E	181	HIS
1	G	271	ASN
1	G	361	ASN
1	G	363	HIS
2	H	73	GLN
2	H	120	HIS
2	H	181	HIS
1	J	271	ASN
1	J	361	ASN
1	J	363	HIS
2	K	73	GLN
2	K	120	HIS
2	K	181	HIS

5.3.3 RNA

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 monosaccharides 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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22276. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.