Full wwPDB EM Validation Report (i)

Mar 11, 2024 – 08:23 AM EDT

PDB ID	:	6UMM
EMDB ID	:	EMD-20820
Title	:	A complete structure of the ESX-3 translocon complex
Authors	:	Poweleit, N.; Rosenberg, O.S.
Deposited on	:	2019-10-09
Resolution	:	3.70 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 (i) 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 (i)) were used in the production of this report:

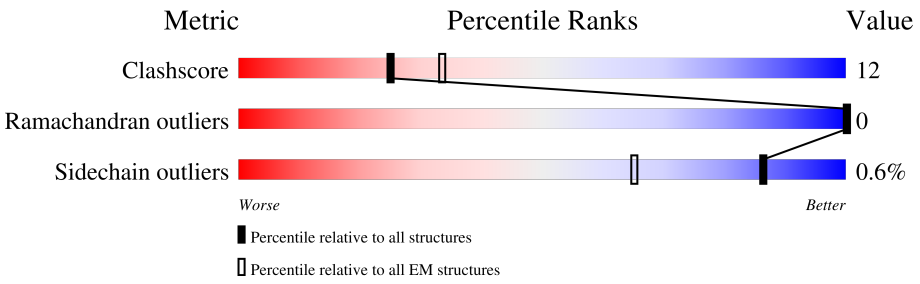
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.70 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	285	69% 31%
1	F	285	72% 27% •
2	B	475	73% 19% 7%
2	C	475	72% 23% 5%
2	G	475	69% 24% 7%
2	H	475	74% 21% 5%
3	D	81	75% 25%
3	I	81	62% 12% • 25%
4	E	403	60% 25% 15%

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Mol	Chain	Length	Quality of chain
4	J	403	57% 28% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23658 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 ESX-3 secretion system protein EccE3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	285	2169	1365	402	397	5	0	0
1	F	285	2169	1365	402	397	5	0	0

- Molecule 2 is a protein called ESX-3 secretion system protein EccD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	441	3162	2052	548	553	9	0	0
2	C	452	3238	2105	558	566	9	0	0
2	G	441	3162	2052	548	553	9	0	0
2	H	452	3238	2105	558	566	9	0	0

- Molecule 3 is a protein called ESX-3 secretion system ATPase EccB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	81	644	409	124	108	3	0	0
3	I	61	480	308	92	77	3	0	0

- Molecule 4 is a protein called ESX-3 secretion system protein EccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	343	2698	1685	504	505	4	0	0
4	J	343	2698	1685	504	505	4	0	0

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: ESX-3 secretion system protein EccE3

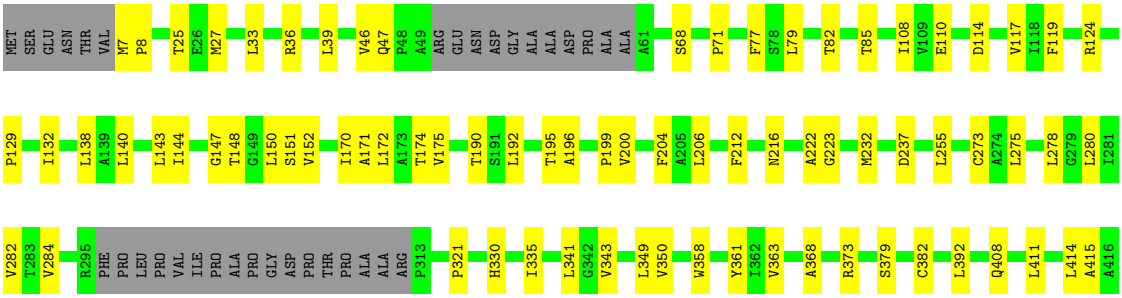
Chain A:

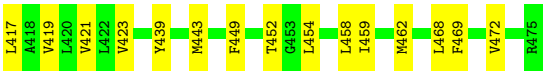
• Molecule 1: ESX-3 secretion system protein EccE3

Chain F:

• Molecule 2: ESX-3 secretion system protein EccD3

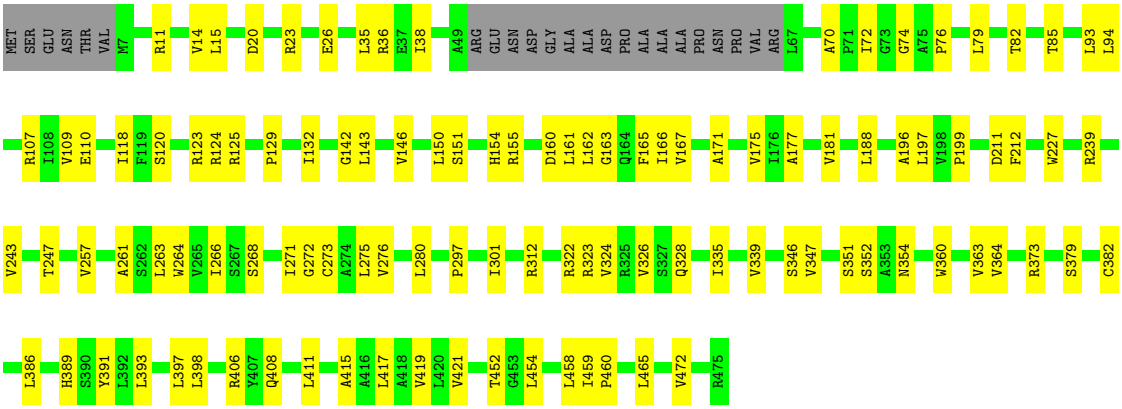
Chain B:





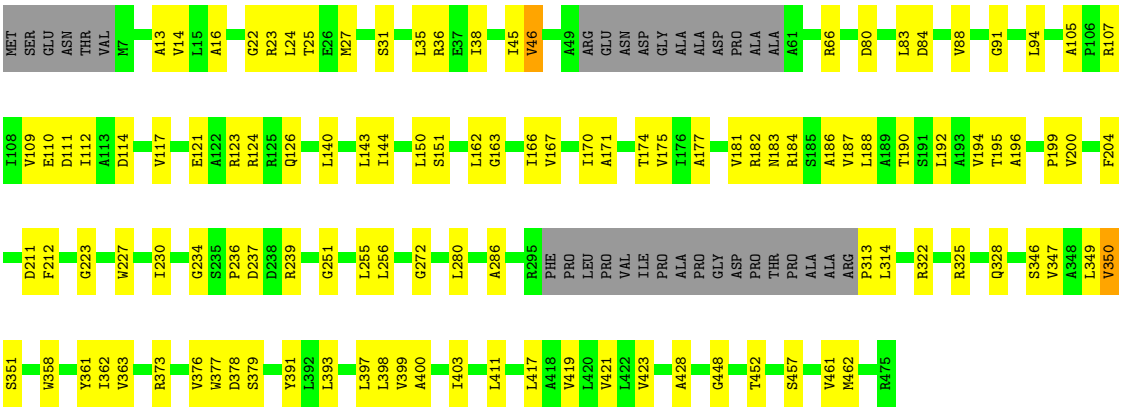
• Molecule 2: ESX-3 secretion system protein EccD3

Chain C:



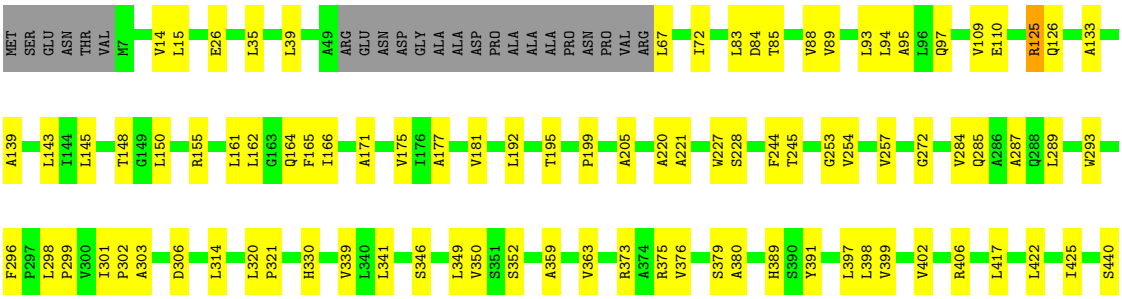
• Molecule 2: ESX-3 secretion system protein EccD3

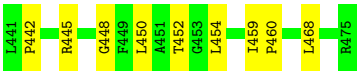
Chain G:



• Molecule 2: ESX-3 secretion system protein EccD3

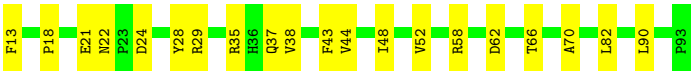
Chain H:





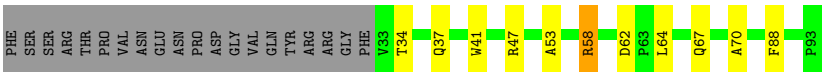
• Molecule 3: ESX-3 secretion system ATPase EccB3

Chain D:



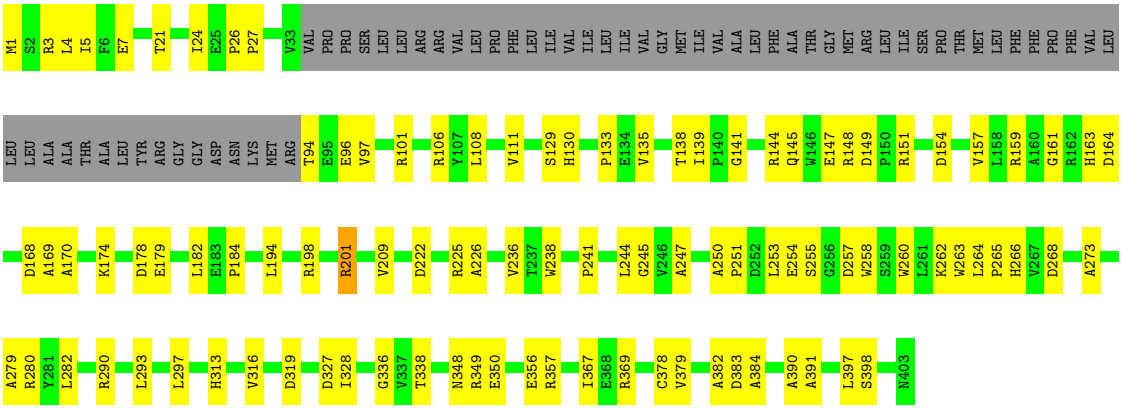
• Molecule 3: ESX-3 secretion system ATPase EccB3

Chain I:



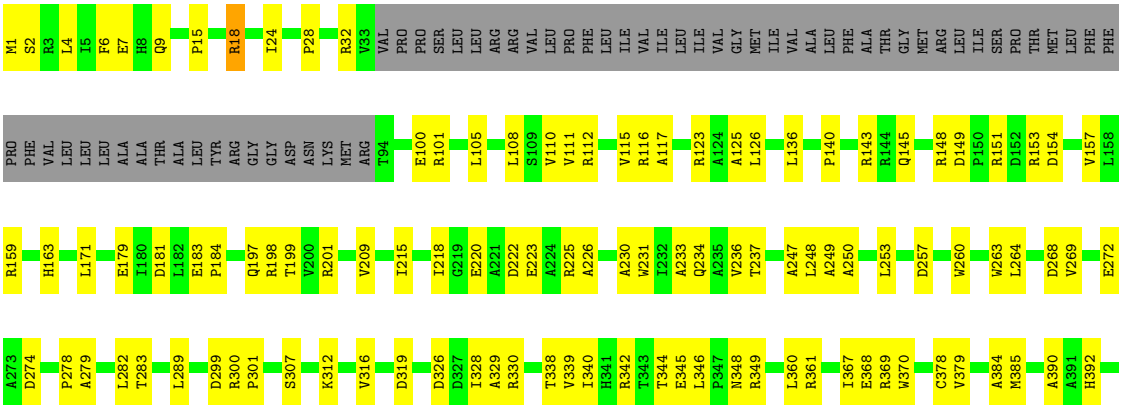
• Molecule 4: ESX-3 secretion system protein EccC3

Chain E:



• Molecule 4: ESX-3 secretion system protein EccC3

Chain J:



R399
W400
D401
S402
N403

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90479	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 ($e^-/Å^2$)	73.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.33	0/2211	0.49	0/3027
1	F	0.35	0/2211	0.51	0/3027
2	B	0.31	0/3221	0.47	0/4422
2	C	0.33	0/3303	0.45	0/4541
2	G	0.36	0/3221	0.50	1/4422 (0.0%)
2	H	0.38	0/3303	0.50	0/4541
3	D	0.37	0/658	0.47	0/889
3	I	0.36	0/489	0.49	0/660
4	E	0.33	0/2762	0.47	0/3776
4	J	0.38	0/2762	0.49	0/3776
All	All	0.35	0/24141	0.48	1/33081 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	46	VAL	C-N-CA	-5.28	108.51	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2169	0	2222	63	0
1	F	2169	0	2222	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3162	0	3346	64	0
2	C	3238	0	3423	74	0
2	G	3162	0	3346	96	0
2	H	3238	0	3423	78	0
3	D	644	0	658	25	0
3	I	480	0	507	14	0
4	E	2698	0	2671	69	0
4	J	2698	0	2671	83	0
All	All	23658	0	24489	557	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 12.

All (557) 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:G:350:VAL:CG1	2:G:397:LEU:HD21	1.84	1.06
2:G:350:VAL:HG11	2:G:397:LEU:HD21	1.43	0.98
2:G:272:GLY:C	2:G:349:LEU:HD23	1.96	0.85
2:G:350:VAL:CG1	2:G:397:LEU:CD2	2.55	0.84
2:G:272:GLY:CA	2:G:349:LEU:HD23	2.08	0.84
2:C:280:LEU:HD22	2:C:458:LEU:HD23	1.61	0.83
2:G:272:GLY:HA3	2:G:349:LEU:HD23	1.59	0.82
1:A:82:VAL:HG11	1:A:89:GLN:HE22	1.45	0.80
2:G:346:SER:O	2:G:350:VAL:HB	1.83	0.79
1:F:62:ARG:HD2	1:F:264:ARG:HD2	1.63	0.78
2:G:358:TRP:HD1	2:G:461:VAL:HG23	1.49	0.78
2:G:347:VAL:HA	2:G:350:VAL:HG12	1.66	0.78
2:G:398:LEU:HD11	2:H:150:LEU:HD13	1.68	0.76
2:G:31:SER:HB2	2:G:83:LEU:HB2	1.69	0.75
4:E:348:ASN:H	4:E:350:GLU:HG3	1.52	0.74
2:G:350:VAL:HG13	2:G:397:LEU:CD2	2.17	0.74
2:B:46:VAL:HG13	2:B:47:GLN:HG3	1.70	0.72
2:G:350:VAL:CG2	2:G:363:VAL:HG21	2.19	0.72
2:G:421:VAL:HG21	2:H:143:LEU:HD22	1.72	0.72
4:J:225:ARG:NH2	4:J:257:ASP:OD2	2.23	0.72
4:J:116:ARG:NH2	4:J:197:GLN:OE1	2.24	0.71
2:B:39:LEU:HD11	2:B:68:SER:HA	1.73	0.70
1:F:174:THR:HG22	1:F:271:ASN:HD21	1.57	0.69
4:E:1:MET:N	4:E:398:SER:OG	2.26	0.69
2:G:349:LEU:HD12	2:G:349:LEU:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:9:GLN:HE21	4:J:143:ARG:HG3	1.57	0.69
2:B:25:THR:HG22	2:B:46:VAL:HG23	1.76	0.68
2:H:72:ILE:HD11	2:H:93:LEU:HD22	1.76	0.68
1:A:188:ALA:HA	1:A:193:VAL:HG22	1.75	0.68
1:F:47:MET:SD	1:F:55:ARG:NH1	2.68	0.67
2:B:280:LEU:HD12	2:B:373:ARG:HH12	1.59	0.67
2:H:459:ILE:HG23	2:H:460:PRO:HD3	1.77	0.67
1:A:197:TYR:HE2	1:A:256:LEU:HD13	1.60	0.67
2:H:346:SER:HB3	2:H:363:VAL:HG13	1.78	0.66
1:A:211:GLU:HB3	1:A:253:LEU:HD13	1.78	0.65
4:E:247:ALA:HB3	4:E:316:VAL:HG12	1.78	0.65
3:D:58:ARG:HB3	4:E:106:ARG:HD3	1.77	0.65
2:H:205:ALA:HB2	2:H:220:ALA:HB2	1.78	0.65
4:J:236:VAL:HG11	4:J:264:LEU:HD21	1.79	0.65
1:A:138:ARG:NE	2:C:110:GLU:OE2	2.24	0.65
2:C:346:SER:HB3	2:C:363:VAL:HG13	1.78	0.65
2:G:350:VAL:HG13	2:G:397:LEU:HD22	1.78	0.64
4:J:225:ARG:NH1	4:J:319:ASP:OD2	2.30	0.64
2:G:361:TYR:HH	2:G:457:SER:HG	1.45	0.64
2:B:449:PHE:HA	2:B:452:THR:HG22	1.80	0.63
4:E:130:HIS:HE1	4:E:157:VAL:HG23	1.64	0.63
1:A:82:VAL:HG22	1:A:166:VAL:HG12	1.81	0.63
1:F:134:ALA:O	1:F:138:ARG:NH1	2.29	0.62
2:B:152:VAL:HG23	2:B:206:LEU:HD11	1.81	0.62
4:J:1:MET:HG2	4:J:278:PRO:HD2	1.82	0.62
4:J:222:ASP:OD1	4:J:223:GLU:N	2.30	0.62
2:B:143:LEU:HB2	2:C:421:VAL:HG21	1.81	0.61
4:J:348:ASN:OD1	4:J:349:ARG:NH1	2.33	0.61
1:F:78:VAL:HG13	1:F:148:THR:HG22	1.83	0.61
2:B:190:THR:HG21	2:B:237:ASP:HB3	1.83	0.61
1:F:196:ALA:H	1:F:263:HIS:HD2	1.49	0.61
2:H:125:ARG:HH11	2:H:125:ARG:H	1.46	0.61
2:C:26:GLU:HB3	4:E:263:TRP:CZ2	2.36	0.61
1:F:96:TYR:CE1	1:F:99:ARG:HD2	2.35	0.61
4:E:148:ARG:NE	4:E:154:ASP:OD2	2.33	0.61
4:E:226:ALA:HB1	4:E:384:ALA:HB1	1.83	0.61
2:G:23:ARG:HH21	2:H:109:VAL:HG21	1.65	0.60
1:A:189:ASP:OD2	1:A:242:ARG:NH1	2.34	0.60
1:A:219:GLU:OE2	1:A:221:TRP:NE1	2.35	0.60
4:E:356:GLU:HG2	4:E:357:ARG:HG3	1.83	0.60
1:A:77:THR:HB	1:A:125:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:ILE:HD11	2:C:93:LEU:HD22	1.83	0.59
4:J:226:ALA:HB1	4:J:384:ALA:HB1	1.83	0.59
4:E:369:ARG:HG3	4:E:378:CYS:HB2	1.83	0.59
2:G:421:VAL:HG12	2:H:139:ALA:HB1	1.85	0.59
2:C:268:SER:HA	2:C:271:ILE:HD12	1.84	0.59
2:B:150:LEU:HD22	2:C:398:LEU:HD11	1.85	0.59
3:D:22:ASN:ND2	3:D:24:ASP:OD1	2.30	0.59
2:G:350:VAL:HG13	2:G:350:VAL:O	2.02	0.59
4:E:273:ALA:HA	4:E:279:ALA:H	1.68	0.59
3:I:53:ALA:HB3	3:I:64:LEU:HD11	1.85	0.59
2:C:181:VAL:HG21	2:C:188:LEU:HD22	1.85	0.58
4:J:136:LEU:HD21	4:J:234:GLN:HE22	1.66	0.58
4:J:326:ASP:O	4:J:330:ARG:NH2	2.37	0.58
3:D:35:ARG:NH1	2:H:445:ARG:HH22	2.02	0.58
4:E:26:PRO:HD3	4:E:174:LYS:HB3	1.84	0.58
4:E:253:LEU:HG	4:E:254:GLU:HG3	1.86	0.58
2:B:335:ILE:HD12	2:B:382:CYS:HB3	1.86	0.57
4:J:301:PRO:HG3	4:J:307:SER:HB3	1.85	0.57
2:B:408:GLN:HA	2:B:411:LEU:HD12	1.87	0.57
2:C:74:GLY:HA2	2:C:107:ARG:HH12	1.69	0.57
2:H:303:ALA:HB3	2:H:306:ASP:HB2	1.86	0.57
1:A:128:ALA:HB2	1:A:144:LEU:HD22	1.87	0.57
1:A:199:VAL:HB	1:A:237:VAL:HG23	1.85	0.57
2:C:452:THR:HG23	3:D:70:ALA:HB2	1.87	0.57
2:G:31:SER:OG	2:G:84:ASP:OD1	2.23	0.57
4:J:361:ARG:NH1	4:J:368:GLU:OE1	2.38	0.57
4:J:319:ASP:OD1	4:J:342:ARG:HD3	2.05	0.56
2:C:82:THR:O	2:C:85:THR:OG1	2.23	0.56
4:E:209:VAL:HG23	4:E:338:THR:HG21	1.87	0.56
1:A:36:ALA:O	1:A:40:LEU:HB2	2.05	0.56
4:E:225:ARG:NE	4:E:319:ASP:OD2	2.37	0.56
4:J:199:THR:OG1	4:J:201:ARG:NH1	2.38	0.56
2:G:25:THR:HG22	2:H:109:VAL:HA	1.87	0.56
2:B:119:PHE:HB2	2:C:324:VAL:HG21	1.88	0.56
2:H:352:SER:O	2:H:406:ARG:NH2	2.39	0.56
4:E:159:ARG:HH21	4:E:161:GLY:HA2	1.71	0.56
1:F:67:ASP:OD2	1:F:67:ASP:N	2.39	0.56
2:C:129:PRO:HA	2:C:132:ILE:HG22	1.88	0.56
2:G:272:GLY:C	2:G:349:LEU:CD2	2.73	0.56
2:H:272:GLY:HA3	2:H:349:LEU:HG	1.88	0.56
1:A:134:ALA:HA	2:C:118:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:352:SER:OG	2:C:354:ASN:OD1	2.20	0.55
1:F:197:TYR:HD1	1:F:258:PRO:HA	1.71	0.55
1:F:4:ARG:NH2	1:F:40:LEU:O	2.39	0.55
4:E:129:SER:O	4:E:148:ARG:NH2	2.40	0.55
4:J:171:LEU:HB2	4:J:198:ARG:NH1	2.21	0.55
2:C:36:ARG:N	2:C:79:LEU:O	2.40	0.55
1:A:172:VAL:H	1:A:273:LEU:HD11	1.72	0.55
2:C:163:GLY:O	2:C:167:VAL:HG22	2.07	0.55
2:G:346:SER:O	2:G:350:VAL:CB	2.53	0.55
1:A:47:MET:HE3	1:A:51:THR:HG22	1.89	0.55
1:F:186:GLY:H	1:F:263:HIS:CE1	2.25	0.55
1:F:52:ARG:HH22	1:F:260:ARG:HH11	1.55	0.55
1:A:173:ASP:N	1:A:173:ASP:OD1	2.41	0.54
4:J:248:LEU:HD11	4:J:250:ALA:HB2	1.88	0.54
3:D:28:TYR:CD2	3:I:58:ARG:HD2	2.42	0.54
4:J:349:ARG:H	4:J:370:TRP:HZ2	1.55	0.54
4:J:6:PHE:HB2	4:J:400:TRP:HB3	1.89	0.54
3:D:18:PRO:HD2	4:J:110:VAL:HG11	1.89	0.54
3:D:90:LEU:HD12	3:I:88:PHE:HZ	1.72	0.54
2:H:125:ARG:HD3	2:H:125:ARG:N	2.22	0.54
2:B:417:LEU:O	2:B:421:VAL:HG23	2.07	0.54
2:G:31:SER:OG	2:G:31:SER:O	2.24	0.54
1:F:128:ALA:HB2	1:F:144:LEU:HD13	1.89	0.54
1:A:75:ARG:HG3	1:A:275:THR:HB	1.89	0.54
2:H:379:SER:OG	2:H:380:ALA:N	2.39	0.54
4:J:369:ARG:HG3	4:J:378:CYS:HB2	1.89	0.54
2:G:16:ALA:O	2:G:22:GLY:HA3	2.06	0.54
2:G:373:ARG:O	2:G:376:VAL:HG12	2.08	0.54
4:J:345:GLU:OE2	4:J:345:GLU:N	2.41	0.54
2:C:142:GLY:O	2:C:146:VAL:HG12	2.08	0.54
2:C:154:HIS:CE1	2:C:160:ASP:HB3	2.43	0.53
2:C:155:ARG:HB2	2:C:163:GLY:HA3	1.91	0.53
3:D:13:PHE:N	4:J:100:GLU:OE2	2.41	0.53
2:G:105:ALA:HB3	4:J:123:ARG:HH22	1.72	0.53
2:H:155:ARG:HD3	2:H:164:GLN:HG3	1.90	0.53
4:J:215:ILE:HD12	4:J:340:ILE:HG12	1.89	0.53
1:A:103:THR:H	1:A:131:ASN:HD22	1.57	0.53
2:G:363:VAL:HG13	2:G:393:LEU:HD11	1.91	0.53
4:J:4:LEU:HB3	4:J:399:ARG:O	2.08	0.53
2:C:154:HIS:HE1	2:C:160:ASP:HB3	1.74	0.53
2:G:350:VAL:HG21	2:G:363:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:280:LEU:HD12	2:G:373:ARG:HH12	1.72	0.53
2:B:421:VAL:HG21	2:C:143:LEU:HB2	1.91	0.53
2:G:110:GLU:CD	2:G:110:GLU:H	2.12	0.53
2:G:195:THR:O	2:G:199:PRO:HD2	2.09	0.53
2:H:35:LEU:HD23	2:H:39:LEU:HD21	1.91	0.53
2:B:419:VAL:O	2:B:423:VAL:HG23	2.08	0.52
2:C:272:GLY:O	2:C:276:VAL:HG23	2.09	0.52
2:C:408:GLN:HA	2:C:411:LEU:HD12	1.91	0.52
2:G:121:GLU:HG2	2:G:124:ARG:HH21	1.74	0.52
1:A:175:PRO:HB3	1:A:221:TRP:CE2	2.44	0.52
3:I:34:THR:H	3:I:37:GLN:HG3	1.74	0.52
4:J:268:ASP:OD1	4:J:268:ASP:N	2.42	0.52
2:G:204:PHE:CD2	2:G:223:GLY:HA3	2.45	0.52
2:C:297:PRO:HD3	2:C:323:ARG:HH11	1.74	0.52
1:F:47:MET:HE3	1:F:52:ARG:HE	1.75	0.52
2:H:171:ALA:O	2:H:175:VAL:HG23	2.09	0.52
2:G:143:LEU:HD13	2:H:417:LEU:HD22	1.91	0.52
2:B:82:THR:HB	2:B:85:THR:HG23	1.92	0.52
2:C:391:TYR:CE1	2:C:417:LEU:HD11	2.44	0.51
1:F:196:ALA:H	1:F:263:HIS:CD2	2.27	0.51
4:E:168:ASP:OD2	4:E:169:ALA:N	2.43	0.51
1:F:82:VAL:HG12	1:F:85:ALA:H	1.75	0.51
1:F:253:LEU:HB2	1:F:256:LEU:HD21	1.92	0.51
1:A:28:TRP:O	1:A:32:VAL:HG12	2.10	0.51
2:H:440:SER:OG	2:H:442:PRO:HD2	2.10	0.51
2:G:391:TYR:CE2	2:G:417:LEU:HD11	2.46	0.51
1:F:160:ARG:NH2	1:F:166:VAL:O	2.41	0.51
2:C:415:ALA:O	2:C:419:VAL:HG23	2.11	0.51
1:F:193:VAL:HG21	1:F:246:ARG:HD2	1.92	0.51
1:A:79:VAL:HG12	1:A:123:SER:HB2	1.93	0.51
1:A:219:GLU:HG2	1:A:242:ARG:HB3	1.93	0.51
2:H:67:LEU:N	2:H:97:GLN:O	2.44	0.51
2:B:415:ALA:O	2:B:419:VAL:HG23	2.10	0.51
1:F:122:ILE:HD12	1:F:155:LEU:HD21	1.92	0.50
4:E:135:VAL:O	4:E:138:THR:HG22	2.10	0.50
4:E:268:ASP:HA	4:E:280:ARG:HA	1.93	0.50
2:H:35:LEU:HB3	2:H:39:LEU:HD23	1.92	0.50
2:H:391:TYR:HE1	2:H:417:LEU:HD21	1.75	0.50
1:F:29:VAL:HA	1:F:32:VAL:HG12	1.91	0.50
3:I:58:ARG:H	3:I:58:ARG:HD3	1.76	0.50
1:A:105:ASP:HB2	1:A:127:ASP:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:PHE:HA	2:B:216:ASN:ND2	2.27	0.50
1:F:114:ALA:HB2	1:F:219:GLU:OE2	2.11	0.50
2:G:378:ASP:N	2:G:378:ASP:OD1	2.44	0.50
2:H:302:PRO:O	3:I:37:GLN:NE2	2.38	0.50
4:E:258:TRP:NE1	4:E:319:ASP:OD2	2.41	0.50
1:F:90:LEU:O	1:F:94:VAL:HG12	2.12	0.50
2:G:23:ARG:HE	2:H:109:VAL:HG11	1.76	0.50
1:A:75:ARG:NH1	1:A:127:ASP:OD2	2.30	0.50
2:B:25:THR:HB	2:C:109:VAL:HG12	1.94	0.50
4:E:222:ASP:N	4:E:222:ASP:OD1	2.45	0.50
1:A:21:TRP:CD1	1:A:26:GLN:HB3	2.47	0.49
2:G:150:LEU:HD22	2:H:398:LEU:HD11	1.92	0.49
2:H:303:ALA:HA	3:I:37:GLN:NE2	2.27	0.49
1:A:83:ASP:HB2	1:A:165:THR:HG23	1.94	0.49
4:J:300:ARG:NH1	4:J:312:LYS:O	2.45	0.49
2:B:129:PRO:HA	2:B:132:ILE:HD12	1.94	0.49
1:F:93:VAL:O	1:F:107:VAL:HG11	2.12	0.49
1:F:235:LEU:O	1:F:282:ALA:HB3	2.12	0.49
1:A:184:TRP:NE1	1:A:260:ARG:HB2	2.27	0.49
3:D:13:PHE:HE2	4:J:32:ARG:HH22	1.61	0.49
1:F:96:TYR:HE1	1:F:99:ARG:HD2	1.76	0.49
2:G:192:LEU:HA	2:G:195:THR:HG22	1.94	0.49
2:G:328:GLN:NE2	2:G:379:SER:OG	2.46	0.49
4:J:249:ALA:HB2	4:J:289:LEU:HD22	1.95	0.49
4:E:21:THR:HG22	4:E:170:ALA:HB3	1.95	0.49
2:H:84:ASP:OD2	2:H:85:THR:N	2.46	0.49
1:A:197:TYR:HB2	1:A:257:THR:O	2.11	0.49
4:E:313:HIS:CD2	4:E:336:GLY:HA2	2.48	0.49
2:C:20:ASP:OD1	2:C:20:ASP:N	2.46	0.49
2:C:243:VAL:O	2:C:247:THR:HG23	2.13	0.49
4:E:262:LYS:NZ	4:E:280:ARG:HH11	2.11	0.49
2:G:83:LEU:HD22	2:G:88:VAL:HG21	1.95	0.49
2:G:170:ILE:O	2:G:174:THR:HG22	2.12	0.49
4:J:218:ILE:HB	4:J:361:ARG:HB2	1.94	0.49
1:A:106:LYS:HG2	1:A:125:THR:OG1	2.13	0.48
2:B:71:PRO:HD3	2:B:77:PHE:CE1	2.48	0.48
2:C:360:TRP:O	2:C:364:VAL:HG12	2.12	0.48
2:G:175:VAL:HG13	2:G:227:TRP:CZ3	2.48	0.48
2:H:376:VAL:HG21	3:I:67:GLN:NE2	2.28	0.48
1:F:25:THR:O	1:F:29:VAL:HG13	2.12	0.48
1:A:112:ARG:HG3	1:A:221:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:347:VAL:O	2:C:351:SER:HB3	2.13	0.48
4:E:149:ASP:O	4:E:151:ARG:N	2.46	0.48
4:E:262:LYS:HZ2	4:E:280:ARG:HH11	1.58	0.48
2:G:190:THR:HG21	2:G:237:ASP:HB2	1.95	0.48
1:A:94:VAL:O	1:A:97:LEU:HD23	2.13	0.48
2:B:379:SER:HB2	2:B:382:CYS:SG	2.53	0.48
2:B:414:LEU:HD22	2:C:150:LEU:HD23	1.95	0.48
4:E:225:ARG:NH1	4:E:319:ASP:OD1	2.35	0.48
4:E:241:PRO:HG3	4:E:266:HIS:CD2	2.49	0.48
4:E:244:LEU:HD12	4:E:245:GLY:H	1.78	0.48
1:F:94:VAL:O	1:F:97:LEU:HD23	2.13	0.48
2:H:83:LEU:HD22	2:H:88:VAL:HG11	1.95	0.48
2:H:359:ALA:O	2:H:363:VAL:HG23	2.13	0.48
2:G:204:PHE:HD2	2:G:223:GLY:HA3	1.79	0.48
2:H:450:LEU:O	2:H:454:LEU:HB2	2.13	0.48
1:A:235:LEU:O	1:A:282:ALA:HB3	2.13	0.48
1:F:77:THR:HB	1:F:125:THR:HB	1.95	0.48
3:I:62:ASP:OD2	3:I:62:ASP:N	2.46	0.48
1:A:25:THR:O	1:A:29:VAL:HG23	2.13	0.47
2:C:120:SER:HA	2:C:123:ARG:NH1	2.30	0.47
2:C:123:ARG:NH2	2:C:124:ARG:HH12	2.11	0.47
2:C:301:ILE:HG22	3:D:37:GLN:HG2	1.95	0.47
4:E:7:GLU:N	4:E:7:GLU:OE1	2.47	0.47
2:G:457:SER:O	2:G:461:VAL:HG12	2.14	0.47
1:F:235:LEU:HD12	1:F:236:THR:H	1.79	0.47
2:G:351:SER:OG	2:G:400:ALA:HB1	2.13	0.47
2:G:448:GLY:O	2:G:452:THR:HG23	2.15	0.47
2:C:35:LEU:HD23	2:C:38:ILE:HD11	1.96	0.47
1:F:182:GLU:HA	1:F:187:VAL:HG12	1.96	0.47
2:H:375:ARG:NH2	2:H:448:GLY:HA2	2.29	0.47
1:A:106:LYS:NZ	1:A:108:ARG:HE	2.13	0.47
2:H:221:ALA:HB2	2:H:254:VAL:HG13	1.95	0.47
2:H:373:ARG:HG2	3:I:67:GLN:NE2	2.30	0.47
4:J:269:VAL:HG13	4:J:272:GLU:HB2	1.95	0.47
2:G:35:LEU:HD23	2:G:38:ILE:HD11	1.95	0.47
2:H:299:PRO:HG2	3:I:41:TRP:CD1	2.49	0.47
4:J:149:ASP:O	4:J:151:ARG:N	2.38	0.47
3:D:62:ASP:O	3:D:66:THR:HG23	2.15	0.47
1:A:33:SER:O	1:A:37:VAL:HG23	2.15	0.47
1:A:197:TYR:CE2	1:A:256:LEU:HD13	2.44	0.47
2:G:14:VAL:HA	2:G:94:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:140:LEU:O	2:G:144:ILE:HG12	2.14	0.47
4:J:24:ILE:HD11	4:J:171:LEU:HD22	1.97	0.47
2:C:14:VAL:HA	2:C:94:LEU:O	2.15	0.47
4:E:4:LEU:HD12	4:E:5:ILE:H	1.79	0.47
1:F:80:LEU:HB2	1:F:122:ILE:HG13	1.97	0.47
2:G:190:THR:O	2:G:194:VAL:HG13	2.15	0.47
2:B:140:LEU:O	2:B:144:ILE:HG13	2.16	0.47
1:F:74:HIS:HD2	1:F:129:VAL:HG23	1.79	0.47
2:B:27:MET:HB3	2:B:27:MET:HE3	1.82	0.46
4:E:164:ASP:OD1	4:E:201:ARG:HA	2.16	0.46
2:G:399:VAL:O	2:G:403:ILE:HG12	2.15	0.46
1:A:205:LEU:O	1:A:208:VAL:HB	2.15	0.46
2:G:188:LEU:HD23	2:G:188:LEU:HA	1.75	0.46
2:H:289:LEU:O	2:H:293:TRP:HB2	2.15	0.46
1:A:6:ALA:HB1	2:B:459:ILE:HG13	1.98	0.46
1:A:223:ALA:HB3	1:A:270:LEU:HD11	1.98	0.46
2:C:11:ARG:NH2	2:C:26:GLU:OE2	2.48	0.46
2:C:162:LEU:O	2:C:166:ILE:HG22	2.15	0.46
2:C:393:LEU:O	2:C:397:LEU:HG	2.16	0.46
2:H:301:ILE:HG23	4:J:184:PRO:HB2	1.97	0.46
2:C:263:LEU:HB3	2:C:264:TRP:CE3	2.51	0.46
2:C:273:CYS:SG	2:C:465:LEU:HD22	2.56	0.46
2:C:328:GLN:HE22	3:D:52:VAL:HG13	1.81	0.46
2:G:163:GLY:O	2:G:167:VAL:HG12	2.16	0.46
4:E:265:PRO:HG2	4:E:266:HIS:HD2	1.81	0.46
1:F:93:VAL:HG11	1:F:109:ILE:HD11	1.98	0.46
1:F:218:GLU:N	1:F:242:ARG:O	2.49	0.46
4:E:27:PRO:HD2	4:E:182:LEU:HD13	1.97	0.46
4:J:140:PRO:HA	4:J:145:GLN:HG3	1.98	0.46
1:A:23:THR:O	1:A:27:ARG:HG2	2.16	0.45
4:E:130:HIS:HB3	4:E:159:ARG:HB3	1.98	0.45
2:G:27:MET:SD	2:G:45:ILE:HG21	2.56	0.45
2:G:151:SER:OG	2:G:167:VAL:HB	2.15	0.45
2:H:287:ALA:HB2	3:I:53:ALA:HB2	1.98	0.45
2:B:39:LEU:HD12	2:B:79:LEU:HD11	1.99	0.45
2:B:204:PHE:CD1	2:B:223:GLY:HA3	2.52	0.45
2:G:177:ALA:O	2:G:181:VAL:HG22	2.16	0.45
2:C:352:SER:O	2:C:406:ARG:NH2	2.49	0.45
4:E:397:LEU:HD23	4:E:397:LEU:HA	1.75	0.45
2:H:89:VAL:HG21	4:J:399:ARG:HE	1.79	0.45
4:J:7:GLU:N	4:J:7:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:163:HIS:HB2	4:E:379:VAL:HA	1.98	0.45
2:H:399:VAL:HA	2:H:402:VAL:HG12	1.98	0.45
4:J:108:LEU:HA	4:J:111:VAL:HG12	1.98	0.45
4:J:148:ARG:HD3	4:J:154:ASP:O	2.15	0.45
4:E:194:LEU:HB3	4:E:198:ARG:HH11	1.80	0.45
2:H:192:LEU:HA	2:H:195:THR:HG22	1.97	0.45
1:A:103:THR:H	1:A:131:ASN:ND2	2.14	0.45
3:D:38:VAL:HG21	2:H:445:ARG:HG3	1.98	0.45
2:H:350:VAL:HG23	2:H:397:LEU:HD21	1.98	0.45
2:B:458:LEU:O	2:B:462:MET:HB2	2.17	0.45
4:E:108:LEU:HA	4:E:108:LEU:HD12	1.80	0.45
1:F:52:ARG:HH22	1:F:260:ARG:NH1	2.13	0.45
2:B:275:LEU:HD11	2:B:341:LEU:HD22	1.98	0.45
2:B:343:VAL:HG21	2:B:392:LEU:HD22	1.98	0.45
2:G:107:ARG:NH2	4:J:116:ARG:HD2	2.31	0.45
2:H:253:GLY:O	2:H:257:VAL:HG23	2.17	0.45
2:B:25:THR:HG23	2:B:27:MET:HE1	1.99	0.45
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.86	0.45
2:G:362:ILE:HD13	2:G:462:MET:HG2	1.99	0.45
2:G:109:VAL:HG13	4:J:112:ARG:HD3	1.99	0.45
3:I:47:ARG:NH1	4:J:105:LEU:HD13	2.32	0.45
1:A:106:LYS:NZ	1:A:108:ARG:HH21	2.14	0.44
1:F:185:ARG:NH2	1:F:246:ARG:HH11	2.16	0.44
4:J:231:TRP:HH2	4:J:360:LEU:HD11	1.81	0.44
2:C:301:ILE:HG23	4:E:184:PRO:HB2	2.00	0.44
1:F:21:TRP:CE2	1:F:30:LEU:HD22	2.53	0.44
1:F:126:VAL:HG23	1:F:144:LEU:HD11	1.99	0.44
2:H:177:ALA:O	2:H:181:VAL:HG12	2.17	0.44
2:H:468:LEU:HD23	2:H:468:LEU:HA	1.84	0.44
4:J:183:GLU:OE1	4:J:184:PRO:HD2	2.17	0.44
2:B:358:TRP:HA	2:B:361:TYR:HB3	1.98	0.44
2:C:335:ILE:HD13	2:C:335:ILE:HA	1.86	0.44
4:J:260:TRP:CE3	4:J:390:ALA:HB1	2.51	0.44
1:A:58:ALA:O	1:A:62:ARG:HG2	2.17	0.44
2:B:273:CYS:HB2	2:B:462:MET:HG3	1.99	0.44
2:C:261:ALA:HA	2:C:266:ILE:HG12	1.99	0.44
2:H:26:GLU:HB3	4:J:263:TRP:CZ2	2.53	0.44
4:J:348:ASN:HD21	4:J:349:ARG:NH2	2.15	0.44
1:A:96:TYR:CD1	1:A:99:ARG:HD2	2.53	0.44
1:F:176:LEU:HB3	1:F:267:LEU:HB3	1.99	0.44
1:A:30:LEU:O	1:A:34:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:ASP:HB3	1:F:230:PRO:HD3	1.99	0.44
1:F:150:VAL:HG11	2:H:110:GLU:HG3	1.99	0.44
2:G:111:ASP:OD1	2:G:112:ILE:N	2.48	0.44
1:A:113:ASP:HB3	1:A:220:THR:HG23	1.99	0.44
1:A:196:ALA:H	1:A:263:HIS:HD2	1.65	0.44
2:B:148:THR:O	2:B:152:VAL:HG12	2.18	0.44
2:H:284:VAL:HG13	2:H:285:GLN:HG3	2.00	0.44
4:J:15:PRO:HG2	4:J:125:ALA:HA	2.00	0.44
4:J:220:GLU:CD	4:J:220:GLU:H	2.20	0.44
1:A:82:VAL:HG21	1:A:122:ILE:HG13	2.00	0.44
2:B:27:MET:SD	2:B:27:MET:N	2.91	0.44
2:B:439:TYR:HB3	2:B:443:MET:HB2	1.99	0.44
2:C:459:ILE:N	2:C:460:PRO:HD2	2.33	0.44
2:G:411:LEU:HD23	2:H:150:LEU:HD21	2.00	0.44
2:H:397:LEU:HA	2:H:397:LEU:HD23	1.66	0.44
4:J:316:VAL:HG23	4:J:339:VAL:HA	1.99	0.44
2:G:181:VAL:HG23	2:G:181:VAL:O	2.18	0.43
2:H:289:LEU:O	2:H:293:TRP:CB	2.66	0.43
4:J:115:VAL:HG21	4:J:171:LEU:HD11	1.99	0.43
4:E:253:LEU:HD12	4:E:262:LYS:HZ1	1.83	0.43
4:E:273:ALA:HA	4:E:279:ALA:N	2.33	0.43
4:J:257:ASP:OD1	4:J:257:ASP:N	2.51	0.43
2:B:33:LEU:HD11	2:C:15:LEU:HD22	2.00	0.43
3:D:44:VAL:O	3:D:48:ILE:HG13	2.19	0.43
2:G:13:ALA:HB1	2:G:24:LEU:HD11	2.00	0.43
2:B:110:GLU:OE1	2:B:110:GLU:N	2.52	0.43
2:B:192:LEU:HA	2:B:195:THR:HG22	2.00	0.43
3:D:13:PHE:HE2	4:J:32:ARG:NH2	2.15	0.43
1:F:83:ASP:HB2	1:F:84:PRO:HD3	2.01	0.43
4:J:179:GLU:HB2	4:J:181:ASP:OD2	2.18	0.43
2:C:211:ASP:OD1	2:C:212:PHE:N	2.51	0.43
2:G:286:ALA:HB3	2:G:377:TRP:CZ2	2.54	0.43
2:H:245:THR:OG1	2:H:330:HIS:HD2	2.02	0.43
4:J:344:THR:O	4:J:346:LEU:HD12	2.18	0.43
1:A:224:LEU:HG	1:A:237:VAL:HG12	2.01	0.43
2:G:313:PRO:HB2	2:G:314:LEU:HD12	1.99	0.43
2:G:350:VAL:HG23	2:G:363:VAL:HG21	2.00	0.43
2:C:161:LEU:HG	2:C:165:PHE:CE1	2.53	0.43
4:J:159:ARG:HG2	4:J:234:GLN:HG2	2.00	0.43
3:D:29:ARG:NH2	2:G:126:GLN:HB3	2.34	0.43
4:E:367:ILE:HG13	4:E:382:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:358:TRP:CD1	2:G:461:VAL:HG23	2.39	0.43
2:H:14:VAL:HA	2:H:94:LEU:O	2.19	0.43
2:B:368:ALA:HB3	2:B:454:LEU:HD21	2.01	0.43
2:G:114:ASP:HA	2:G:117:VAL:HG12	2.01	0.43
2:H:314:LEU:HD23	2:H:314:LEU:O	2.18	0.43
4:J:274:ASP:N	4:J:279:ALA:HB2	2.33	0.43
2:B:36:ARG:HG3	2:B:79:LEU:HD12	2.01	0.43
3:D:13:PHE:HB2	4:J:28:PRO:HB3	2.01	0.43
4:J:299:ASP:OD1	4:J:299:ASP:N	2.52	0.43
2:C:373:ARG:HB3	2:C:386:LEU:HD13	2.01	0.42
4:E:141:GLY:N	4:E:145:GLN:OE1	2.24	0.42
2:G:182:ARG:HH12	2:G:234:GLY:HA3	1.84	0.42
4:J:253:LEU:HD13	4:J:282:LEU:HB3	2.01	0.42
1:A:44:TRP:HB3	1:A:52:ARG:HH21	1.83	0.42
1:A:106:LYS:HZ3	1:A:108:ARG:HE	1.65	0.42
3:D:18:PRO:HD2	4:J:110:VAL:CG1	2.48	0.42
2:G:196:ALA:O	2:G:200:VAL:HG22	2.19	0.42
4:J:112:ARG:CG	4:J:116:ARG:HH12	2.32	0.42
2:B:196:ALA:C	2:B:199:PRO:HD2	2.40	0.42
2:B:196:ALA:O	2:B:200:VAL:HG22	2.19	0.42
2:C:379:SER:HB3	2:C:382:CYS:SG	2.59	0.42
1:F:104:CYS:HA	1:F:126:VAL:HG12	2.01	0.42
2:G:151:SER:HB2	2:G:166:ILE:HB	2.02	0.42
4:J:328:ILE:HG13	4:J:329:ALA:H	1.83	0.42
2:B:469:PHE:HA	2:B:472:VAL:HG22	2.01	0.42
2:C:151:SER:OG	2:C:167:VAL:HG13	2.20	0.42
3:D:35:ARG:HH11	2:H:445:ARG:HH22	1.67	0.42
1:F:104:CYS:SG	1:F:124:LEU:HD12	2.59	0.42
2:G:280:LEU:HD12	2:G:373:ARG:NH1	2.34	0.42
2:G:398:LEU:HD11	2:H:150:LEU:CD1	2.45	0.42
2:H:26:GLU:HB3	4:J:263:TRP:HZ2	1.85	0.42
2:H:89:VAL:HG21	4:J:399:ARG:NE	2.35	0.42
2:H:161:LEU:HB3	2:H:165:PHE:CE2	2.54	0.42
1:A:225:GLU:OE2	1:A:278:LEU:HG	2.20	0.42
2:B:468:LEU:O	2:B:472:VAL:HG13	2.19	0.42
4:E:3:ARG:HD2	4:E:3:ARG:HA	1.71	0.42
4:E:268:ASP:OD2	4:E:268:ASP:N	2.50	0.42
2:G:211:ASP:OD2	2:G:212:PHE:N	2.52	0.42
2:H:162:LEU:O	2:H:166:ILE:HG22	2.19	0.42
4:J:148:ARG:NH1	4:J:157:VAL:O	2.52	0.42
1:A:108:ARG:HG2	1:A:123:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:ALA:O	2:C:181:VAL:HG12	2.20	0.42
2:C:239:ARG:HA	2:C:239:ARG:HD3	1.65	0.42
4:E:94:THR:N	4:E:96:GLU:HG2	2.35	0.42
1:F:99:ARG:HG3	2:G:91:GLY:HA3	2.01	0.42
4:J:108:LEU:HA	4:J:108:LEU:HD12	1.76	0.42
1:A:221:TRP:O	1:A:239:ALA:HA	2.19	0.42
2:B:170:ILE:O	2:B:174:THR:HG22	2.20	0.42
2:B:349:LEU:HD12	2:B:350:VAL:HG23	2.02	0.42
2:B:468:LEU:HD23	2:B:468:LEU:HA	1.84	0.42
2:G:162:LEU:O	2:G:166:ILE:HG12	2.19	0.42
2:H:422:LEU:HA	2:H:425:ILE:HG22	2.02	0.42
2:B:138:LEU:HD23	2:B:138:LEU:HA	1.86	0.42
2:B:350:VAL:HG21	2:B:363:VAL:HG21	2.02	0.42
2:B:417:LEU:HG	2:C:143:LEU:HD13	2.02	0.42
2:C:322:ARG:O	2:C:326:VAL:HG23	2.20	0.42
4:E:139:ILE:HD13	4:E:139:ILE:HA	1.89	0.42
4:J:171:LEU:HB2	4:J:198:ARG:HH12	1.85	0.42
4:J:247:ALA:HB3	4:J:316:VAL:HG12	2.02	0.42
2:B:147:GLY:O	2:B:151:SER:OG	2.26	0.42
4:E:260:TRP:CZ3	4:E:390:ALA:HB1	2.55	0.42
2:H:341:LEU:HD23	2:H:341:LEU:HA	1.91	0.42
4:J:136:LEU:O	4:J:140:PRO:HD3	2.20	0.42
2:C:257:VAL:HG11	2:C:275:LEU:CD2	2.50	0.42
3:D:43:PHE:CD2	4:E:101:ARG:HD3	2.55	0.42
3:D:82:LEU:HA	3:D:82:LEU:HD23	1.88	0.42
4:E:97:VAL:O	4:E:101:ARG:HG2	2.19	0.42
4:E:236:VAL:HG23	4:E:266:HIS:CG	2.55	0.42
4:E:260:TRP:HB2	4:E:391:ALA:HA	2.02	0.42
1:F:125:THR:OG1	1:F:126:VAL:N	2.53	0.42
4:J:233:ALA:O	4:J:237:THR:HG22	2.20	0.42
1:A:52:ARG:HH22	1:A:260:ARG:CZ	2.33	0.41
2:C:171:ALA:O	2:C:175:VAL:HG13	2.20	0.41
4:E:194:LEU:HD22	4:E:198:ARG:NH1	2.35	0.41
2:G:251:GLY:O	2:G:255:LEU:HB2	2.20	0.41
4:J:253:LEU:HD11	4:J:283:THR:O	2.21	0.41
1:A:44:TRP:CB	1:A:52:ARG:HE	2.32	0.41
2:B:114:ASP:HA	2:B:117:VAL:HG12	2.01	0.41
2:C:196:ALA:C	2:C:199:PRO:HD2	2.41	0.41
1:F:57:LEU:HD23	1:F:57:LEU:HA	1.88	0.41
2:G:171:ALA:O	2:G:175:VAL:HG23	2.20	0.41
2:B:7:MET:HA	2:B:8:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ALA:O	2:B:175:VAL:HG22	2.20	0.41
2:G:14:VAL:HG23	2:G:46:VAL:HG11	2.02	0.41
1:A:29:VAL:O	1:A:33:SER:OG	2.26	0.41
2:B:280:LEU:O	2:B:284:VAL:HG12	2.21	0.41
2:C:70:ALA:HB2	2:C:76:PRO:HA	2.03	0.41
2:C:301:ILE:O	3:D:37:GLN:NE2	2.53	0.41
3:D:21:GLU:OE2	4:J:18:ARG:NH2	2.54	0.41
2:G:187:VAL:HG22	2:G:239:ARG:HH12	1.86	0.41
1:F:106:LYS:HG3	1:F:125:THR:HG22	2.02	0.41
2:H:298:LEU:HG	2:H:299:PRO:HD2	2.01	0.41
1:A:92:VAL:HG23	1:A:93:VAL:HG23	2.02	0.41
1:A:103:THR:O	1:A:103:THR:OG1	2.37	0.41
2:C:339:VAL:HG13	2:C:389:HIS:CD2	2.55	0.41
4:E:255:SER:OG	4:E:257:ASP:OD1	2.38	0.41
4:E:290:ARG:HD2	4:E:327:ASP:O	2.20	0.41
1:F:109:ILE:HG12	1:F:122:ILE:HG22	2.02	0.41
2:G:36:ARG:HH12	2:G:80:ASP:HB3	1.86	0.41
2:G:419:VAL:O	2:G:423:VAL:HG23	2.20	0.41
2:H:452:THR:HG23	3:I:70:ALA:HB2	2.02	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.90	0.41
2:B:222:ALA:HA	2:B:255:LEU:HD12	2.01	0.41
2:C:454:LEU:HD23	2:C:454:LEU:HA	1.83	0.41
4:E:24:ILE:HG12	4:E:111:VAL:HG11	2.02	0.41
4:E:144:ARG:HH11	4:E:238:TRP:HH2	1.69	0.41
1:F:82:VAL:HG11	1:F:89:GLN:HE22	1.86	0.41
2:G:256:LEU:HD23	2:G:256:LEU:HA	1.73	0.41
2:G:428:ALA:HB1	2:H:133:ALA:HA	2.02	0.41
2:H:126:GLN:CD	2:H:126:GLN:H	2.24	0.41
2:H:339:VAL:HG22	2:H:389:HIS:HB2	2.03	0.41
4:J:230:ALA:HA	4:J:385:MET:SD	2.61	0.41
4:E:147:GLU:OE2	4:E:238:TRP:HZ3	2.03	0.41
1:F:193:VAL:HB	1:F:247:PRO:HD3	2.03	0.41
4:J:163:HIS:HB2	4:J:379:VAL:HA	2.03	0.41
2:C:72:ILE:HD11	2:C:93:LEU:HB3	2.03	0.41
2:C:151:SER:HG	2:C:167:VAL:HG13	1.86	0.41
2:C:197:LEU:HD23	2:C:227:TRP:HD1	1.85	0.41
2:C:472:VAL:HG21	3:D:82:LEU:HD22	2.02	0.41
4:E:236:VAL:HG21	4:E:264:LEU:HD22	2.03	0.41
4:E:250:ALA:HB1	4:E:251:PRO:HD2	2.03	0.41
4:E:293:LEU:HG	4:E:297:LEU:HD23	2.03	0.41
4:E:316:VAL:HG21	4:E:328:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:66:ARG:NH2	4:J:392:HIS:HE1	2.19	0.41
2:G:183:ASN:OD1	2:G:184:ARG:N	2.54	0.41
2:G:186:ALA:HB1	2:G:236:PRO:HB2	2.03	0.41
2:G:227:TRP:HE3	2:G:230:ILE:HD11	1.86	0.41
2:G:361:TYR:HD2	2:G:461:VAL:HG21	1.85	0.41
2:H:35:LEU:O	2:H:39:LEU:HD23	2.21	0.41
2:H:171:ALA:HA	2:H:199:PRO:HB2	2.02	0.41
2:H:289:LEU:HD23	2:H:289:LEU:HA	1.74	0.41
2:H:320:LEU:N	2:H:321:PRO:HD2	2.35	0.41
4:J:209:VAL:HG13	4:J:338:THR:OG1	2.21	0.41
4:J:367:ILE:HB	4:J:379:VAL:HG22	2.02	0.41
2:B:172:LEU:HA	2:B:175:VAL:HG22	2.03	0.41
2:B:232:MET:SD	2:B:330:HIS:HE1	2.45	0.41
3:D:22:ASN:HB2	4:J:117:ALA:HB2	2.02	0.41
1:F:108:ARG:NH2	1:F:269:ALA:O	2.54	0.41
2:H:145:LEU:O	2:H:148:THR:OG1	2.37	0.41
1:A:196:ALA:H	1:A:263:HIS:CD2	2.39	0.40
2:B:192:LEU:HA	2:B:192:LEU:HD23	1.83	0.40
4:J:101:ARG:NH2	4:J:183:GLU:OE1	2.52	0.40
1:A:132:LEU:HD21	2:B:321:PRO:HA	2.02	0.40
4:E:133:PRO:HG3	4:E:383:ASP:HB2	2.04	0.40
4:E:178:ASP:OD1	4:E:179:GLU:N	2.49	0.40
1:F:74:HIS:CD2	1:F:129:VAL:HG23	2.54	0.40
1:F:102:ILE:HG21	1:F:151:VAL:HG21	2.03	0.40
2:G:322:ARG:HA	2:G:325:ARG:NH2	2.35	0.40
2:H:228:SER:OG	2:H:244:PHE:O	2.35	0.40
1:A:192:GLY:HA2	1:A:244:SER:O	2.22	0.40
2:B:108:ILE:HD11	4:E:201:ARG:HH21	1.85	0.40
2:H:15:LEU:HG	2:H:95:ALA:HA	2.03	0.40
4:J:126:LEU:HD23	4:J:126:LEU:HA	1.78	0.40
4:E:262:LYS:HD3	4:E:282:LEU:HD12	2.02	0.40
2:G:227:TRP:CE3	2:G:230:ILE:HD11	2.57	0.40
2:H:175:VAL:HG13	2:H:227:TRP:CZ3	2.56	0.40
2:B:278:LEU:O	2:B:282:VAL:HG23	2.22	0.40
2:C:79:LEU:HD12	2:C:79:LEU:H	1.86	0.40
2:C:93:LEU:HD23	2:C:94:LEU:N	2.37	0.40
4:E:348:ASN:O	4:E:349:ARG:HB2	2.22	0.40
1:F:159:LEU:HD23	1:F:159:LEU:HA	1.80	0.40
1:F:197:TYR:CD1	1:F:258:PRO:HA	2.55	0.40
4:J:2:SER:HB3	4:J:401:ASP:CG	2.42	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	283/285 (99%)	272 (96%)	11 (4%)	0	100	100
1	F	283/285 (99%)	275 (97%)	8 (3%)	0	100	100
2	B	435/475 (92%)	421 (97%)	14 (3%)	0	100	100
2	C	448/475 (94%)	430 (96%)	18 (4%)	0	100	100
2	G	435/475 (92%)	413 (95%)	22 (5%)	0	100	100
2	H	448/475 (94%)	426 (95%)	22 (5%)	0	100	100
3	D	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
3	I	59/81 (73%)	56 (95%)	3 (5%)	0	100	100
4	E	339/403 (84%)	312 (92%)	27 (8%)	0	100	100
4	J	339/403 (84%)	314 (93%)	25 (7%)	0	100	100
All	All	3148/3438 (92%)	2996 (95%)	152 (5%)	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	224/224 (100%)	223 (100%)	1 (0%)	91	95
1	F	224/224 (100%)	222 (99%)	2 (1%)	78	88
2	B	317/342 (93%)	316 (100%)	1 (0%)	92	96
2	C	325/342 (95%)	322 (99%)	3 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	317/342 (93%)	315 (99%)	2 (1%)	86	93
2	H	325/342 (95%)	323 (99%)	2 (1%)	86	93
3	D	70/70 (100%)	70 (100%)	0	100	100
3	I	52/70 (74%)	51 (98%)	1 (2%)	57	76
4	E	281/332 (85%)	280 (100%)	1 (0%)	91	95
4	J	281/332 (85%)	279 (99%)	2 (1%)	84	91
All	All	2416/2620 (92%)	2401 (99%)	15 (1%)	86	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
2	B	124	ARG
2	C	23	ARG
2	C	125	ARG
2	C	312	ARG
4	E	201	ARG
1	F	74	HIS
1	F	106	LYS
2	G	123	ARG
2	G	350	VAL
2	H	125	ARG
2	H	296	PHE
3	I	58	ARG
4	J	18	ARG
4	J	153	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	89	GLN
1	A	263	HIS
2	B	154	HIS
2	B	328	GLN
2	B	408	GLN
2	C	154	HIS
2	C	216	ASN
2	C	328	GLN

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Mol	Chain	Res	Type
2	C	330	HIS
3	D	37	GLN
4	E	29	GLN
4	E	130	HIS
4	E	187	HIS
4	E	266	HIS
4	E	271	ASN
4	E	313	HIS
1	F	74	HIS
1	F	89	GLN
1	F	263	HIS
1	F	271	ASN
2	G	47	GLN
2	G	154	HIS
2	G	328	GLN
2	G	330	HIS
2	G	389	HIS
2	H	330	HIS
3	I	67	GLN
4	J	130	HIS
4	J	234	GLN
4	J	266	HIS
4	J	313	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.