



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 3J7X
EMDB ID: : EMD-6037
Title : Capsid Expansion Mechanism Of Bacteriophage T7 Revealed By Multi-State Atomic Models Derived From Cryo-EM Reconstructions
Authors : Guo, F.; Liu, Z.; Fang, P.A.; Zhang, Q.; Wright, E.T.; Wu, W.; Zhang, C.; Vago, F.; Ren, Y.; Jakata, J.; Chiu, W.; Serwer, P.; Jiang, W.
Deposited on : 2014-08-12
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

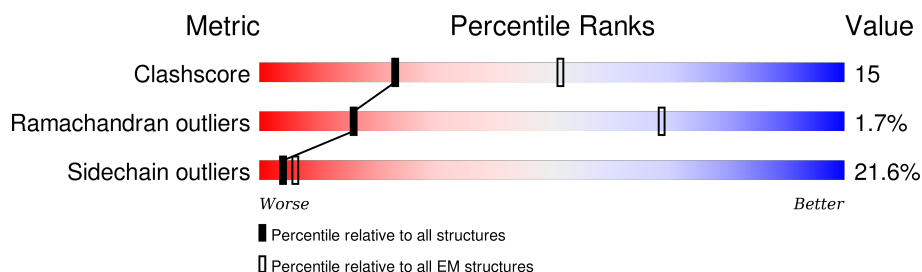
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	345	59% 32% 8% .
1	B	345	57% 34% 9% .
1	C	345	57% 33% 9% ..
1	D	345	62% 29% 8% ..
1	E	345	60% 31% 8% .
1	F	345	60% 31% 8% ..
1	G	345	61% 31% 8% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17829 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.

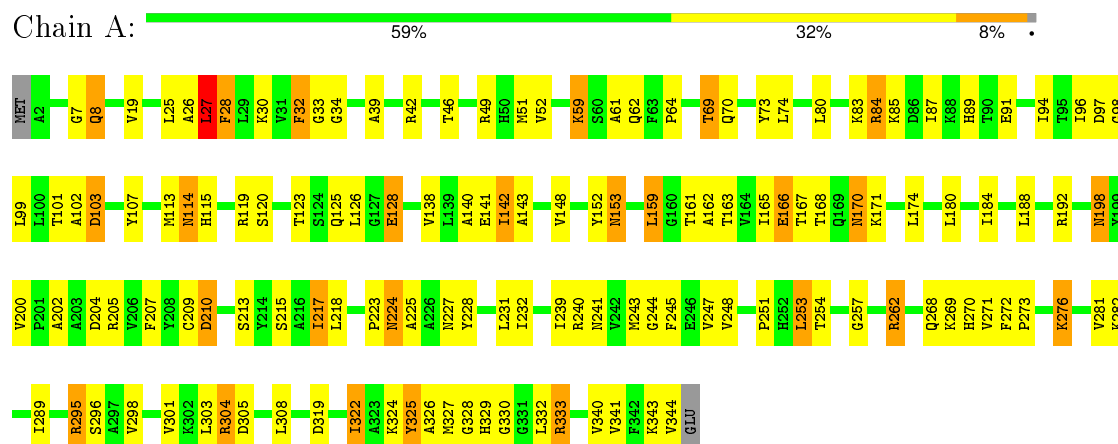
- Molecule 1 is a protein called Major capsid protein 10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	B	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	C	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	D	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	E	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	F	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	G	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		

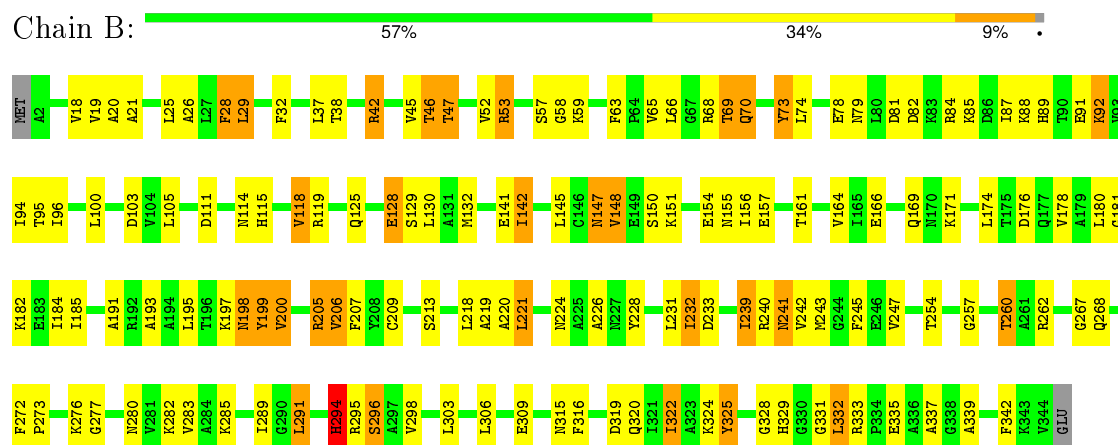
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

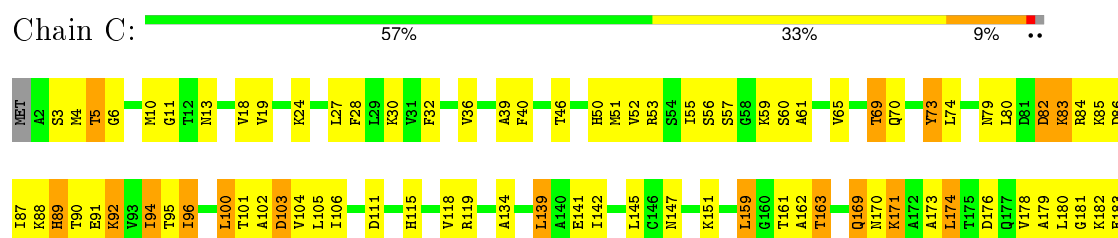
• Molecule 1: Major capsid protein 10A

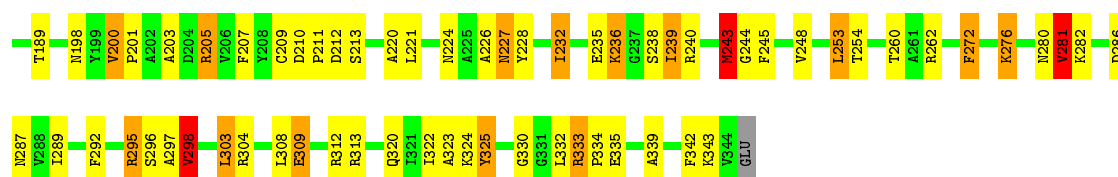


• Molecule 1: Major capsid protein 10A



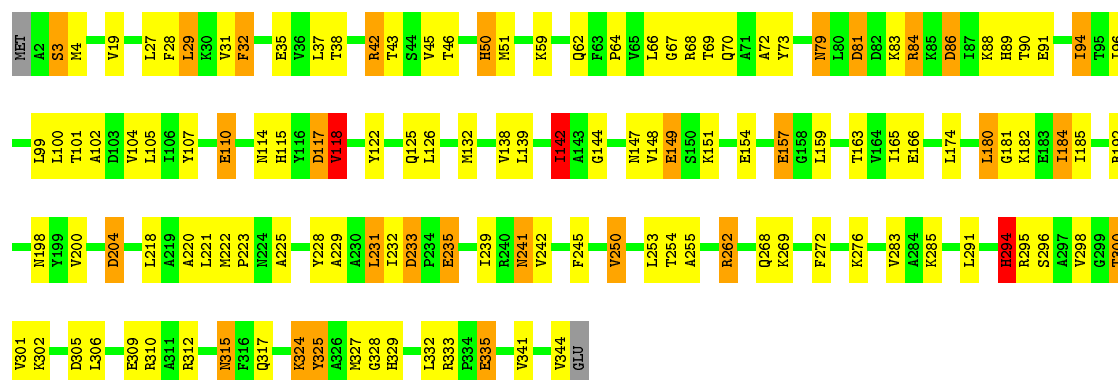
• Molecule 1: Major capsid protein 10A





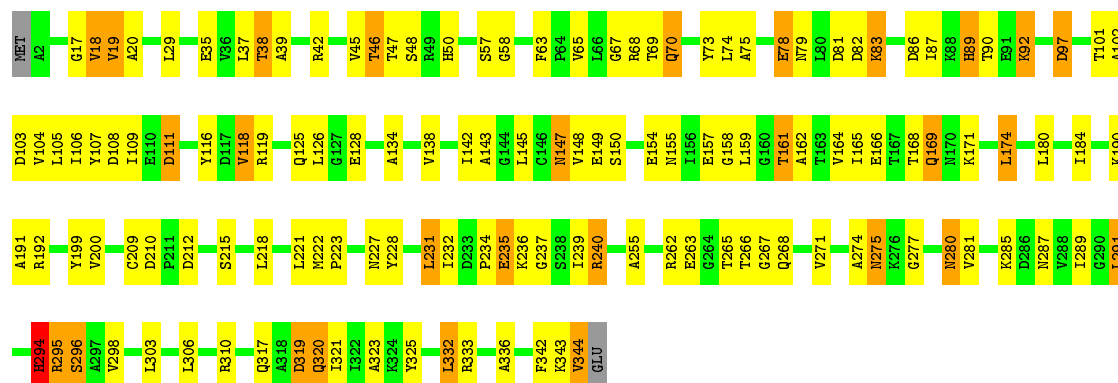
• Molecule 1: Major capsid protein 10A

Chain D: 62% 29% 8% ..



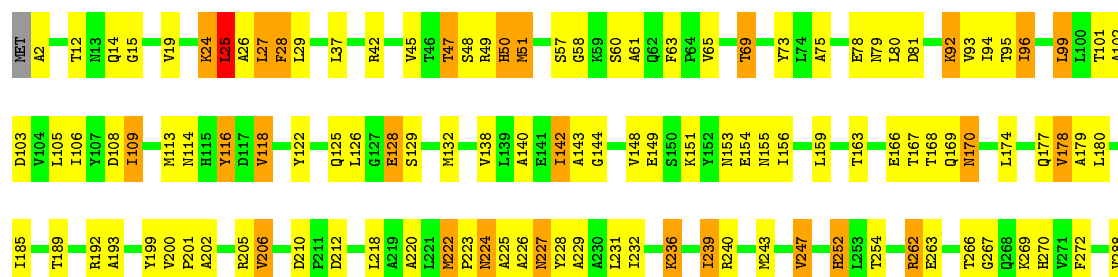
• Molecule 1: Major capsid protein 10A

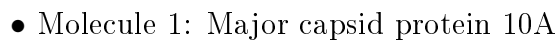
Chain E: 60% 31% 8% .



• Molecule 1: Major capsid protein 10A

Chain F: 60% 31% 8% ..





E294	A203	I109	MET
E295	D204	I109	A2
E296	R205	M143	T12
E297	F206	Y116	K16
E298	V207	R19	G17
E299	V208	Y122	V18
T300	C209	Y122	K24
L303	D210	Y122	L25
R304	P211	Q125	A26
P305	S213	L130	L27
L306	Y214	A131	F28
E309	S215	M132	V31
R340	A216	V138	E35
D819	L221	E141	T38
K324	M222	I142	R42
Y325	P223	A143	T46
G331	Y228	G144	T47
L332	A229	L145	H50
V340	A230	L146	N51
V341	L231	M147	V52
V342	I232	E154	I55
K343	D233	M155	S56
V344	E235	I156	S57
GLU	V236	E157	G58
	G237	T163	K59
	L239	V164	Q62
	F245	I165	V65
	E246	T168	L66
	E249	Q169	L80
	T254	M170	K83
	A255	K171	R84
	T260	L174	K85
	A261	I184	R89
	T265	I185	T90
	Q268	A186	E91
	V271	T189	D97
	P272	A190	G98
	P273	A191	L99
	V281	R192	L100
	V288	A193	T101
	L289	A194	A102
	G290	L195	D103
	L291	T196	
		K197	
		M198	
		Y199	
		V200	
		Z201	
		A202	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	33952	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.27	0/2582	0.57	1/3491 (0.0%)
1	B	0.27	0/2582	0.58	0/3491
1	C	0.27	0/2582	0.61	1/3491 (0.0%)
1	D	0.28	0/2582	0.60	0/3491
1	E	0.28	0/2582	0.56	0/3491
1	F	0.28	0/2582	0.59	1/3491 (0.0%)
1	G	0.27	0/2582	0.59	0/3491
All	All	0.27	0/18074	0.58	3/24437 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	9

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	LEU	CA-CB-CG	6.44	130.11	115.30
1	A	27	LEU	CA-CB-CG	5.28	127.44	115.30
1	C	100	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	GLN	Peptide
1	B	294	HIS	Peptide
1	C	238	SER	Peptide
1	C	243	MET	Peptide
1	D	294	HIS	Peptide
1	E	294	HIS	Peptide
1	F	294	HIS	Peptide
1	G	116	TYR	Peptide
1	G	294	HIS	Peptide

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	2547	0	2573	89	0
1	B	2547	0	2573	92	0
1	C	2547	0	2573	89	0
1	D	2547	0	2573	77	0
1	E	2547	0	2573	83	0
1	F	2547	0	2573	90	0
1	G	2547	0	2573	77	0
All	All	17829	0	18011	523	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 15.

All (523) 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:C:296:SER:HA	1:C:298:VAL:H	1.46	0.80
1:C:32:PHE:HA	1:D:62:GLN:H	1.45	0.79
1:C:147:ASN:HD21	1:C:282:LYS:HB2	1.49	0.77
1:C:163:THR:HB	1:C:339:ALA:H	1.49	0.77
1:A:184:ILE:HD11	1:A:289:ILE:HG21	1.66	0.76
1:E:67:GLY:H	1:E:87:ILE:HG22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HA	1:C:73:TYR:HB3	1.69	0.74
1:G:205:ARG:HB2	1:G:245:PHE:HB3	1.70	0.73
1:C:170:ASN:HB3	1:C:173:ALA:HB2	1.69	0.73
1:E:75:ALA:HB3	1:E:78:GLU:HG2	1.71	0.73
1:G:154:GLU:HG3	1:G:155:ASN:HD22	1.54	0.72
1:E:158:GLY:HA2	1:E:159:LEU:HB2	1.72	0.71
1:F:239:ILE:HD12	1:F:247:VAL:HG21	1.73	0.71
1:C:276:LYS:HG3	1:C:287:ASN:HD21	1.55	0.71
1:B:205:ARG:HA	1:B:294:HIS:HA	1.73	0.70
1:D:233:ASP:OD1	1:D:233:ASP:N	2.25	0.70
1:F:42:ARG:NH2	1:F:132:MET:SD	2.65	0.69
1:B:231:LEU:HG	1:B:232:ILE:HG23	1.74	0.69
1:E:227:ASN:H	1:F:227:ASN:HD22	1.39	0.69
1:C:198:ASN:ND2	1:C:335:GLU:O	2.25	0.69
1:G:42:ARG:NH2	1:G:132:MET:SD	2.61	0.69
1:G:42:ARG:H	1:G:42:ARG:HH11	1.40	0.68
1:A:244:GLY:H	1:F:236:LYS:H	1.41	0.68
1:A:99:LEU:HD11	1:A:324:LYS:HB2	1.75	0.68
1:G:119:ARG:H	1:G:119:ARG:HH11	1.42	0.68
1:E:102:ALA:HB1	1:E:126:LEU:HD22	1.75	0.67
1:E:215:SER:HB3	1:F:193:ALA:HB2	1.75	0.67
1:F:47:THR:OG1	1:F:48:SER:N	2.27	0.67
1:D:45:VAL:HG13	1:D:46:THR:HG23	1.77	0.67
1:A:119:ARG:NH2	1:A:319:ASP:OD1	2.27	0.67
1:E:274:ALA:HA	1:E:285:LYS:HB3	1.77	0.67
1:E:221:LEU:HD23	1:E:232:ILE:HB	1.77	0.66
1:C:103:ASP:OD1	1:D:84:ARG:NH2	2.28	0.66
1:F:96:ILE:HG22	1:F:301:VAL:HG21	1.76	0.66
1:E:275:ASN:ND2	1:E:277:GLY:O	2.28	0.66
1:G:295:ARG:C	1:G:297:ALA:HA	2.16	0.66
1:B:141:GLU:OE2	1:B:331:GLY:N	2.29	0.65
1:C:88:LYS:O	1:C:89:HIS:ND1	2.30	0.65
1:A:224:ASN:N	1:A:224:ASN:OD1	2.29	0.65
1:D:253:LEU:O	1:D:285:LYS:NZ	2.29	0.64
1:G:209:CYS:SG	1:G:213:SER:OG	2.55	0.64
1:G:51:MET:HB2	1:G:297:ALA:HB3	1.78	0.64
1:B:57:SER:OG	1:B:58:GLY:N	2.31	0.64
1:E:79:ASN:HD21	1:E:81:ASP:HB3	1.63	0.64
1:A:159:LEU:HD13	1:A:198:ASN:HA	1.78	0.63
1:E:171:LYS:HA	1:E:174:LEU:HD22	1.79	0.63
1:A:241:ASN:ND2	1:A:245:PHE:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASN:N	1:F:224:ASN:OD1	2.31	0.63
1:A:171:LYS:HA	1:A:174:LEU:HB2	1.81	0.63
1:C:254:THR:HA	1:C:272:PHE:HD2	1.64	0.63
1:C:169:GLN:HB3	1:C:343:LYS:HE2	1.80	0.63
1:D:42:ARG:NE	1:E:199:TYR:OH	2.25	0.63
1:B:37:LEU:HB2	1:C:65:VAL:HG12	1.81	0.63
1:G:209:CYS:SG	1:G:210:ASP:N	2.71	0.63
1:E:102:ALA:HB3	1:E:323:ALA:HB3	1.81	0.62
1:A:209:CYS:SG	1:A:210:ASP:N	2.72	0.62
1:D:250:VAL:HG23	1:D:253:LEU:HD23	1.82	0.62
1:C:39:ALA:HB2	1:D:67:GLY:HA2	1.80	0.62
1:C:181:GLY:HA3	1:C:220:ALA:HB2	1.81	0.62
1:C:243:MET:O	1:C:245:PHE:N	2.32	0.62
1:A:227:ASN:ND2	1:F:223:PRO:O	2.31	0.62
1:C:161:THR:OG1	1:C:162:ALA:N	2.25	0.62
1:A:223:PRO:HA	1:B:228:TYR:HE2	1.65	0.61
1:F:178:VAL:HG23	1:F:220:ALA:HA	1.82	0.61
1:A:113:MET:O	1:A:114:ASN:ND2	2.32	0.61
1:F:114:ASN:HD22	1:F:116:TYR:H	1.48	0.61
1:B:69:THR:OG1	1:B:70:GLN:N	2.33	0.61
1:A:103:ASP:HB2	1:A:322:ILE:HG22	1.82	0.60
1:D:253:LEU:C	1:D:254:THR:HG1	2.02	0.60
1:E:296:SER:OG	1:E:333:ARG:NH2	2.34	0.60
1:D:302:LYS:NZ	1:D:305:ASP:OD2	2.34	0.60
1:E:125:GLN:OE1	1:F:69:THR:OG1	2.19	0.60
1:A:96:ILE:HA	1:A:328:GLY:HA3	1.83	0.60
1:D:117:ASP:OD2	1:D:117:ASP:N	2.34	0.60
1:C:203:ALA:HA	1:C:205:ARG:HD2	1.82	0.60
1:B:294:HIS:O	1:B:295:ARG:HG2	2.02	0.60
1:C:51:MET:HG2	1:C:296:SER:HB3	1.83	0.60
1:G:38:THR:OG1	1:G:125:GLN:NE2	2.35	0.59
1:D:88:LYS:O	1:D:89:HIS:ND1	2.35	0.59
1:F:201:PRO:O	1:F:205:ARG:NH1	2.35	0.59
1:D:235:GLU:OE2	1:E:240:ARG:NH1	2.36	0.59
1:F:178:VAL:O	1:F:180:LEU:N	2.35	0.59
1:B:18:VAL:HB	1:B:21:ALA:HB2	1.84	0.59
1:G:232:ILE:HA	1:G:239:ILE:H	1.66	0.59
1:A:125:GLN:HG3	1:B:69:THR:HG22	1.83	0.59
1:A:184:ILE:HG21	1:A:217:ILE:HG12	1.83	0.59
1:E:103:ASP:OD1	1:E:262:ARG:NH2	2.36	0.59
1:D:229:ALA:HB2	1:E:228:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLN:NE2	1:B:128:GLU:OE1	2.35	0.59
1:C:295:ARG:C	1:C:297:ALA:HB3	2.24	0.58
1:D:37:LEU:HD12	1:E:65:VAL:HG12	1.85	0.58
1:G:25:LEU:HD13	1:G:25:LEU:H	1.68	0.58
1:D:117:ASP:HA	1:D:118:VAL:HG12	1.85	0.58
1:E:148:VAL:HG22	1:E:281:VAL:HG23	1.85	0.58
1:G:42:ARG:NH1	1:G:42:ARG:H	2.02	0.58
1:D:181:GLY:O	1:D:185:ILE:HG12	2.04	0.58
1:B:161:THR:OG1	1:B:337:ALA:O	2.21	0.57
1:E:143:ALA:O	1:E:147:ASN:ND2	2.38	0.57
1:B:309:GLU:HG2	1:B:322:ILE:HG12	1.87	0.57
1:C:289:ILE:HD11	1:C:342:PHE:CZ	2.39	0.57
1:D:181:GLY:HA3	1:D:220:ALA:HB2	1.86	0.57
1:A:153:ASN:OD1	1:A:153:ASN:N	2.37	0.57
1:F:202:ALA:O	1:F:205:ARG:NH1	2.38	0.57
1:A:39:ALA:HB1	1:B:68:ARG:HH21	1.67	0.56
1:B:218:LEU:HD11	1:B:232:ILE:HD13	1.88	0.56
1:B:142:ILE:HD12	1:B:291:LEU:HD13	1.88	0.56
1:D:144:GLY:O	1:D:148:VAL:HG23	2.06	0.56
1:F:92:LYS:NZ	1:F:93:VAL:O	2.38	0.56
1:F:294:HIS:O	1:F:294:HIS:ND1	2.39	0.56
1:E:319:ASP:OD2	1:E:319:ASP:N	2.38	0.56
1:B:81:ASP:OD1	1:B:82:ASP:N	2.39	0.56
1:E:266:THR:OG1	1:E:267:GLY:N	2.38	0.56
1:F:288:VAL:HA	1:F:341:VAL:HG12	1.88	0.56
1:E:42:ARG:HG2	1:F:199:TYR:CZ	2.41	0.56
1:A:168:THR:O	1:A:343:LYS:NZ	2.35	0.55
1:B:276:LYS:NZ	1:B:277:GLY:O	2.38	0.55
1:D:165:ILE:HG12	1:D:166:GLU:H	1.71	0.55
1:E:150:SER:OG	1:E:280:ASN:ND2	2.40	0.55
1:F:102:ALA:HB1	1:F:126:LEU:HD22	1.88	0.55
1:G:46:THR:HB	1:G:47:THR:HA	1.87	0.55
1:G:50:HIS:O	1:G:50:HIS:ND1	2.39	0.55
1:C:86:ASP:OD1	1:C:87:ILE:N	2.40	0.55
1:G:119:ARG:HA	1:G:122:TYR:HB2	1.89	0.55
1:A:273:PRO:HG2	1:A:281:VAL:HG21	1.89	0.55
1:G:25:LEU:HB2	1:G:26:ALA:HA	1.89	0.54
1:E:104:VAL:O	1:E:320:GLN:HB2	2.07	0.54
1:G:342:PHE:H	1:G:342:PHE:HD1	1.53	0.54
1:D:45:VAL:HG22	1:D:46:THR:H	1.73	0.54
1:E:235:GLU:O	1:E:237:GLY:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PHE:CD2	1:C:59:LYS:HB2	2.42	0.54
1:D:147:ASN:HB2	1:D:283:VAL:HG11	1.90	0.54
1:B:125:GLN:HG3	1:C:87:ILE:HD11	1.90	0.54
1:E:143:ALA:HB2	1:E:291:LEU:HD13	1.88	0.54
1:C:171:LYS:NZ	1:C:286:ASP:O	2.40	0.54
1:G:138:VAL:O	1:G:142:ILE:HG22	2.07	0.54
1:G:169:GLN:OE1	1:G:170:ASN:N	2.39	0.54
1:C:69:THR:OG1	1:C:70:GLN:N	2.41	0.54
1:G:203:ALA:O	1:G:205:ARG:N	2.41	0.53
1:B:129:SER:HB3	1:C:69:THR:HG23	1.91	0.53
1:C:235:GLU:N	1:D:242:VAL:O	2.36	0.53
1:A:223:PRO:HB3	1:B:226:ALA:HB1	1.91	0.53
1:G:273:PRO:HG2	1:G:281:VAL:HG21	1.91	0.53
1:B:180:LEU:O	1:B:184:ILE:HG12	2.08	0.53
1:C:297:ALA:H	1:C:333:ARG:HG3	1.74	0.53
1:C:111:ASP:OD1	1:C:119:ARG:NH2	2.41	0.53
1:D:333:ARG:O	1:D:335:GLU:N	2.37	0.53
1:B:65:VAL:HG22	1:B:91:GLU:HA	1.91	0.53
1:G:56:SER:OG	1:G:57:SER:N	2.42	0.52
1:D:79:ASN:OD1	1:D:79:ASN:N	2.43	0.52
1:C:226:ALA:O	1:C:227:ASN:ND2	2.42	0.52
1:A:215:SER:HB2	1:B:193:ALA:HB2	1.91	0.52
1:B:262:ARG:HD3	1:C:85:LYS:HB2	1.91	0.52
1:E:78:GLU:OE2	1:E:83:LYS:NZ	2.43	0.52
1:D:159:LEU:HB3	1:D:335:GLU:HB2	1.92	0.52
1:B:79:ASN:ND2	1:F:2:ALA:O	2.43	0.52
1:D:101:THR:OG1	1:D:102:ALA:N	2.43	0.52
1:C:262:ARG:O	1:D:70:GLN:NE2	2.43	0.52
1:F:168:THR:OG1	1:F:169:GLN:N	2.42	0.52
1:E:174:LEU:HD21	1:E:180:LEU:HD13	1.92	0.52
1:F:178:VAL:C	1:F:180:LEU:H	2.13	0.52
1:A:273:PRO:HG2	1:A:281:VAL:HG11	1.92	0.52
1:E:143:ALA:HB1	1:E:291:LEU:HD22	1.92	0.52
1:D:231:LEU:HG	1:D:232:ILE:HG23	1.92	0.52
1:G:214:TYR:CG	1:G:249:GLU:HG2	2.44	0.52
1:A:61:ALA:HB3	1:A:301:VAL:HG21	1.90	0.52
1:C:296:SER:HA	1:C:298:VAL:N	2.21	0.51
1:A:205:ARG:HD2	1:A:244:GLY:O	2.10	0.51
1:D:327:MET:SD	1:D:329:HIS:NE2	2.83	0.51
1:F:252:HIS:CD2	1:F:252:HIS:H	2.28	0.51
1:A:174:LEU:HD13	1:A:180:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:HIS:HE1	1:F:298:VAL:HG22	1.75	0.51
1:G:201:PRO:HG2	1:G:294:HIS:NE2	2.26	0.51
1:A:202:ALA:HA	1:A:205:ARG:NH2	2.25	0.51
1:A:207:PHE:HD2	1:A:247:VAL:HG22	1.74	0.51
1:F:170:ASN:OD1	1:F:170:ASN:N	2.40	0.51
1:E:180:LEU:O	1:E:184:ILE:HG12	2.10	0.51
1:D:100:LEU:HD23	1:D:325:TYR:HE2	1.75	0.51
1:F:79:ASN:OD1	1:F:80:LEU:N	2.44	0.51
1:A:240:ARG:HA	1:A:240:ARG:HH11	1.75	0.51
1:F:103:ASP:N	1:F:103:ASP:OD2	2.44	0.51
1:E:287:ASN:HB2	1:E:342:PHE:HB2	1.91	0.51
1:B:155:ASN:ND2	1:B:156:ILE:H	2.09	0.51
1:F:294:HIS:O	1:F:295:ARG:HG2	2.11	0.50
1:D:305:ASP:O	1:D:325:TYR:HB2	2.10	0.50
1:F:101:THR:OG1	1:F:102:ALA:N	2.44	0.50
1:B:156:ILE:HG23	1:B:157:GLU:H	1.75	0.50
1:A:305:ASP:O	1:A:325:TYR:HB2	2.11	0.50
1:E:108:ASP:HA	1:E:111:ASP:HB3	1.93	0.50
1:D:174:LEU:HD21	1:D:180:LEU:HD12	1.93	0.50
1:A:170:ASN:N	1:A:170:ASN:OD1	2.43	0.50
1:B:130:LEU:HD23	1:B:306:LEU:HD11	1.92	0.50
1:A:28:PHE:HB3	1:B:59:LYS:HB2	1.94	0.50
1:F:227:ASN:N	1:F:227:ASN:OD1	2.45	0.50
1:F:174:LEU:HD13	1:F:180:LEU:HB2	1.94	0.50
1:F:293:MET:HG3	1:F:295:ARG:H	1.77	0.50
1:C:36:VAL:HG23	1:D:64:PRO:HG2	1.93	0.50
1:E:343:LYS:HD3	1:E:344:VAL:HB	1.93	0.50
1:F:319:ASP:N	1:F:319:ASP:OD2	2.43	0.50
1:C:212:ASP:OD2	1:C:213:SER:N	2.44	0.50
1:F:27:LEU:HD12	1:G:91:GLU:HB3	1.94	0.50
1:G:25:LEU:HB2	1:G:26:ALA:CA	2.42	0.50
1:D:315:ASN:OD1	1:D:315:ASN:N	2.41	0.50
1:B:114:ASN:O	1:B:115:HIS:ND1	2.44	0.50
1:F:199:TYR:O	1:F:200:VAL:HB	2.11	0.50
1:E:166:GLU:HB3	1:E:343:LYS:HB2	1.93	0.49
1:B:241:ASN:N	1:B:241:ASN:OD1	2.45	0.49
1:A:74:LEU:HD11	1:F:99:LEU:HG	1.93	0.49
1:A:138:VAL:O	1:A:142:ILE:HG22	2.13	0.49
1:E:134:ALA:O	1:E:138:VAL:HG23	2.13	0.49
1:G:306:LEU:HA	1:G:325:TYR:HB2	1.95	0.49
1:G:296:SER:N	1:G:297:ALA:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ALA:HB3	1:C:94:ILE:HD11	1.94	0.49
1:G:66:LEU:HD23	1:G:89:HIS:HE1	1.77	0.49
1:B:262:ARG:O	1:C:70:GLN:NE2	2.45	0.49
1:E:97:ASP:OD1	1:E:97:ASP:N	2.46	0.49
1:B:119:ARG:NH2	1:B:319:ASP:OD2	2.45	0.49
1:A:120:SER:O	1:A:123:THR:OG1	2.23	0.49
1:E:234:PRO:O	1:E:235:GLU:HG3	2.13	0.49
1:D:3:SER:OG	1:D:4:MET:N	2.44	0.49
1:E:165:ILE:HG12	1:E:166:GLU:H	1.78	0.49
1:F:60:SER:OG	1:F:61:ALA:N	2.46	0.48
1:C:3:SER:OG	1:C:4:MET:N	2.46	0.48
1:G:51:MET:O	1:G:52:VAL:HG22	2.13	0.48
1:E:294:HIS:CE1	1:E:296:SER:HB3	2.48	0.48
1:G:24:LYS:HE3	1:G:24:LYS:H	1.77	0.48
1:B:29:LEU:HD13	1:B:29:LEU:H	1.78	0.48
1:A:327:MET:SD	1:A:329:HIS:NE2	2.75	0.48
1:A:224:ASN:HD22	1:B:182:LYS:NZ	2.11	0.48
1:G:12:THR:O	1:G:27:LEU:HB2	2.14	0.48
1:C:253:LEU:HD13	1:C:254:THR:H	1.79	0.48
1:G:203:ALA:O	1:G:205:ARG:HG3	2.13	0.48
1:F:206:VAL:HG12	1:F:293:MET:H	1.78	0.48
1:E:223:PRO:HA	1:F:228:TYR:HE1	1.78	0.48
1:C:60:SER:OG	1:C:94:ILE:O	2.25	0.48
1:G:143:ALA:O	1:G:147:ASN:HB3	2.14	0.48
1:G:186:ALA:O	1:G:189:THR:OG1	2.24	0.48
1:D:99:LEU:HD23	1:E:74:LEU:HD23	1.96	0.48
1:F:15:GLY:N	1:G:90:THR:OG1	2.46	0.48
1:A:97:ASP:OD1	1:A:98:GLY:N	2.41	0.48
1:F:205:ARG:HA	1:F:294:HIS:HA	1.96	0.48
1:F:166:GLU:HB2	1:F:341:VAL:O	2.14	0.48
1:F:149:GLU:OE1	1:F:149:GLU:N	2.44	0.48
1:B:219:ALA:HB2	1:C:189:THR:HG21	1.96	0.47
1:G:51:MET:HB3	1:G:300:THR:OG1	2.14	0.47
1:D:86:ASP:O	1:D:88:LYS:N	2.47	0.47
1:A:142:ILE:HG23	1:A:143:ALA:H	1.78	0.47
1:D:262:ARG:O	1:E:70:GLN:NE2	2.34	0.47
1:G:309:GLU:OE2	1:G:310:ARG:N	2.45	0.47
1:A:244:GLY:H	1:F:236:LYS:N	2.09	0.47
1:A:253:LEU:HD22	1:A:254:THR:H	1.80	0.47
1:C:50:HIS:H	1:C:295:ARG:NH2	2.13	0.47
1:D:232:ILE:HG22	1:D:239:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:VAL:HG22	1:E:46:THR:H	1.79	0.47
1:E:231:LEU:HD13	1:E:232:ILE:H	1.80	0.47
1:A:167:THR:HG23	1:A:168:THR:HG23	1.96	0.47
1:B:233:ASP:N	1:B:233:ASP:OD2	2.48	0.47
1:F:205:ARG:HB3	1:F:206:VAL:H	1.54	0.47
1:A:257:GLY:HA2	1:A:268:GLN:HB3	1.96	0.47
1:A:101:THR:OG1	1:A:102:ALA:N	2.48	0.47
1:C:56:SER:OG	1:C:57:SER:N	2.47	0.47
1:A:119:ARG:O	1:A:123:THR:HG23	2.14	0.47
1:C:224:ASN:HD21	1:D:182:LYS:HE2	1.80	0.47
1:E:310:ARG:HB3	1:E:321:ILE:HG13	1.96	0.47
1:B:181:GLY:O	1:B:185:ILE:HG12	2.15	0.47
1:D:89:HIS:O	1:D:90:THR:OG1	2.32	0.47
1:A:7:GLY:O	1:A:8:GLN:HB3	2.15	0.47
1:A:204:ASP:OD2	1:A:295:ARG:HB3	2.15	0.47
1:E:89:HIS:H	1:E:89:HIS:CD2	2.32	0.47
1:A:333:ARG:HB2	1:A:333:ARG:HH11	1.78	0.47
1:F:210:ASP:OD1	1:F:210:ASP:N	2.46	0.47
1:G:141:GLU:O	1:G:145:LEU:HB2	2.15	0.47
1:E:38:THR:OG1	1:E:39:ALA:N	2.48	0.47
1:C:239:ILE:HG22	1:C:240:ARG:H	1.79	0.46
1:E:97:ASP:HB3	1:F:73:TYR:CE2	2.50	0.46
1:B:147:ASN:OD1	1:B:147:ASN:N	2.47	0.46
1:G:156:ILE:HG13	1:G:157:GLU:H	1.79	0.46
1:C:235:GLU:HG3	1:D:241:ASN:HB2	1.96	0.46
1:B:150:SER:O	1:B:151:LYS:HG3	2.16	0.46
1:B:213:SER:HB2	1:B:289:ILE:HG23	1.97	0.46
1:E:106:ILE:HG22	1:E:111:ASP:HB2	1.97	0.46
1:G:165:ILE:HD12	1:G:341:VAL:HG13	1.96	0.46
1:C:308:LEU:HA	1:C:323:ALA:HA	1.96	0.46
1:B:25:LEU:HA	1:B:26:ALA:HA	1.78	0.46
1:D:294:HIS:ND1	1:D:294:HIS:O	2.49	0.46
1:E:228:TYR:HA	1:F:228:TYR:HB3	1.96	0.46
1:A:276:LYS:HA	1:A:281:VAL:HG23	1.98	0.46
1:C:159:LEU:HD22	1:C:159:LEU:H	1.81	0.46
1:E:294:HIS:HE1	1:E:296:SER:HB3	1.81	0.46
1:A:59:LYS:HD2	1:F:28:PHE:HB3	1.98	0.46
1:F:24:LYS:O	1:F:25:LEU:HD22	2.16	0.46
1:G:254:THR:HG22	1:G:272:PHE:CE2	2.51	0.46
1:C:141:GLU:HG3	1:C:145:LEU:HD12	1.98	0.46
1:G:223:PRO:HA	1:G:224:ASN:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HH21	1:B:132:MET:HG2	1.81	0.46
1:E:184:ILE:HD11	1:E:289:ILE:HG12	1.98	0.46
1:E:289:ILE:HD11	1:E:342:PHE:CD2	2.51	0.45
1:C:161:THR:HG22	1:C:334:PRO:O	2.16	0.45
1:A:223:PRO:HG2	1:B:221:LEU:HD12	1.97	0.45
1:D:229:ALA:HB2	1:E:228:TYR:CE1	2.51	0.45
1:B:291:LEU:HA	1:B:339:ALA:HA	1.99	0.45
1:G:221:LEU:O	1:G:222:MET:HB2	2.15	0.45
1:A:69:THR:OG1	1:A:70:GLN:N	2.48	0.45
1:A:224:ASN:ND2	1:B:182:LYS:HG2	2.32	0.45
1:A:209:CYS:SG	1:A:213:SER:HB2	2.56	0.45
1:E:47:THR:HA	1:E:48:SER:HA	1.56	0.45
1:A:251:PRO:HG3	1:B:199:TYR:CE1	2.51	0.45
1:D:253:LEU:O	1:D:254:THR:OG1	2.23	0.45
1:D:269:LYS:HG3	1:E:73:TYR:CE2	2.50	0.45
1:G:100:LEU:HD21	1:G:325:TYR:CE1	2.51	0.45
1:G:192:ARG:HH11	1:G:193:ALA:HA	1.81	0.45
1:F:301:VAL:O	1:F:327:MET:HB2	2.16	0.45
1:C:210:ASP:HB2	1:C:211:PRO:HD2	1.98	0.45
1:B:176:ASP:OD2	1:B:178:VAL:N	2.48	0.45
1:E:218:LEU:O	1:E:222:MET:HG3	2.16	0.45
1:B:205:ARG:HB3	1:B:206:VAL:H	1.58	0.45
1:C:207:PHE:HD1	1:C:292:PHE:HB3	1.81	0.45
1:F:12:THR:O	1:F:27:LEU:HD22	2.16	0.45
1:F:269:LYS:HB3	1:F:270:HIS:CE1	2.52	0.45
1:C:174:LEU:HD22	1:C:174:LEU:H	1.81	0.45
1:D:100:LEU:HD13	1:E:73:TYR:HD1	1.82	0.45
1:G:50:HIS:CD2	1:G:138:VAL:HG11	2.52	0.45
1:C:94:ILE:HG22	1:C:330:GLY:HA3	1.98	0.45
1:C:309:GLU:HG3	1:C:322:ILE:HG23	1.99	0.45
1:D:138:VAL:O	1:D:142:ILE:HG22	2.16	0.45
1:A:126:LEU:HA	1:B:69:THR:HG21	1.98	0.45
1:C:96:ILE:HG13	1:C:303:LEU:HD11	1.98	0.45
1:B:52:VAL:O	1:B:53:ARG:HD2	2.17	0.45
1:E:154:GLU:OE1	1:E:155:ASN:N	2.47	0.45
1:D:198:ASN:HD22	1:D:335:GLU:HG3	1.82	0.45
1:C:262:ARG:HD2	1:D:72:ALA:HB2	1.99	0.45
1:E:164:VAL:HG21	1:E:191:ALA:HB2	1.99	0.45
1:B:315:ASN:OD1	1:B:316:PHE:N	2.48	0.45
1:G:245:PHE:HB2	1:G:246:GLU:H	1.53	0.44
1:B:295:ARG:HG3	1:B:296:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:HA	1:A:225:ALA:HA	1.54	0.44
1:E:35:GLU:H	1:F:63:PHE:HE1	1.64	0.44
1:F:144:GLY:O	1:F:148:VAL:HB	2.16	0.44
1:F:225:ALA:HA	1:F:226:ALA:HA	1.62	0.44
1:D:117:ASP:HA	1:D:118:VAL:CB	2.48	0.44
1:F:200:VAL:HG13	1:F:294:HIS:CD2	2.52	0.44
1:C:209:CYS:SG	1:C:213:SER:HB2	2.57	0.44
1:F:154:GLU:OE2	1:F:155:ASN:N	2.51	0.44
1:A:184:ILE:O	1:A:188:LEU:HB2	2.18	0.44
1:F:25:LEU:N	1:F:26:ALA:HB3	2.32	0.44
1:G:254:THR:OG1	1:G:255:ALA:N	2.50	0.44
1:C:134:ALA:HB2	1:C:325:TYR:OH	2.17	0.44
1:G:230:ALA:HA	1:G:231:LEU:HA	1.63	0.44
1:B:224:ASN:HB3	1:C:182:LYS:HE2	1.98	0.44
1:A:103:ASP:OD1	1:B:84:ARG:NH1	2.39	0.44
1:F:201:PRO:HD2	1:F:294:HIS:CD2	2.52	0.44
1:B:257:GLY:HA3	1:B:268:GLN:HB3	2.00	0.44
1:C:50:HIS:HB3	1:C:52:VAL:HG23	1.98	0.44
1:A:99:LEU:HA	1:A:326:ALA:HB2	2.00	0.44
1:E:184:ILE:CD1	1:E:289:ILE:HG12	2.48	0.44
1:G:207:PHE:HB2	1:G:245:PHE:CE1	2.53	0.44
1:E:200:VAL:HG21	1:E:336:ALA:HB2	2.00	0.44
1:G:222:MET:HB3	1:G:223:PRO:CD	2.47	0.44
1:G:212:ASP:O	1:G:215:SER:OG	2.27	0.44
1:G:296:SER:OG	1:G:296:SER:O	2.33	0.44
1:G:294:HIS:O	1:G:294:HIS:CG	2.70	0.44
1:D:104:VAL:HG11	1:D:122:TYR:HD2	1.83	0.44
1:C:228:TYR:HA	1:D:228:TYR:HB3	1.99	0.44
1:G:185:ILE:O	1:G:189:THR:HG23	2.17	0.44
1:G:265:THR:O	1:G:268:GLN:HG3	2.18	0.44
1:A:42:ARG:HE	1:A:128:GLU:CD	2.20	0.44
1:A:34:GLY:HA3	1:B:63:PHE:HE1	1.83	0.44
1:F:125:GLN:O	1:F:128:GLU:HG3	2.17	0.44
1:B:164:VAL:HG21	1:B:191:ALA:HB2	2.00	0.44
1:A:166:GLU:OE2	1:A:167:THR:N	2.51	0.43
1:D:29:LEU:HD12	1:D:29:LEU:H	1.83	0.43
1:G:174:LEU:HA	1:G:174:LEU:HD23	1.86	0.43
1:A:289:ILE:HD12	1:A:340:VAL:HG22	2.00	0.43
1:B:239:ILE:HG23	1:B:240:ARG:H	1.83	0.43
1:C:221:LEU:HG	1:C:232:ILE:HD11	2.00	0.43
1:B:171:LYS:HB3	1:B:342:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:THR:OG1	1:E:162:ALA:N	2.51	0.43
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.82	0.43
1:B:89:HIS:ND1	1:B:89:HIS:O	2.50	0.43
1:B:81:ASP:O	1:B:84:ARG:HG2	2.18	0.43
1:D:50:HIS:HE1	1:D:300:THR:HG23	1.84	0.43
1:F:109:ILE:HG12	1:G:99:LEU:HG	1.99	0.43
1:B:19:VAL:HA	1:B:20:ALA:HA	1.56	0.43
1:D:204:ASP:N	1:D:204:ASP:OD1	2.51	0.43
1:C:92:LYS:HA	1:C:92:LYS:HD3	1.81	0.43
1:B:70:GLN:HB3	1:B:70:GLN:HE21	1.60	0.43
1:B:92:LYS:HD3	1:B:332:LEU:HB3	2.00	0.43
1:A:148:VAL:HG11	1:A:281:VAL:HA	2.00	0.43
1:C:101:THR:OG1	1:C:102:ALA:N	2.52	0.43
1:E:57:SER:OG	1:E:58:GLY:N	2.48	0.43
1:G:57:SER:OG	1:G:58:GLY:N	2.51	0.43
1:B:181:GLY:HA3	1:B:220:ALA:HB2	2.00	0.43
1:C:101:THR:OG1	1:C:323:ALA:O	2.19	0.43
1:F:185:ILE:O	1:F:189:THR:HG23	2.19	0.43
1:G:289:ILE:HB	1:G:340:VAL:HG23	2.01	0.43
1:F:113:MET:SD	1:G:59:LYS:HA	2.59	0.43
1:A:51:MET:HG2	1:A:296:SER:HA	2.01	0.43
1:C:178:VAL:C	1:C:180:LEU:H	2.21	0.43
1:A:165:ILE:HG12	1:A:166:GLU:H	1.83	0.43
1:E:280:ASN:O	1:E:280:ASN:ND2	2.52	0.43
1:E:69:THR:OG1	1:E:70:GLN:N	2.52	0.43
1:B:273:PRO:O	1:B:285:LYS:HB3	2.19	0.43
1:D:35:GLU:HB2	1:E:63:PHE:CD1	2.53	0.43
1:E:17:GLY:C	1:E:19:VAL:H	2.22	0.43
1:A:141:GLU:HG2	1:A:330:GLY:HA2	2.01	0.43
1:A:244:GLY:HA2	1:F:236:LYS:HB3	2.00	0.43
1:A:69:THR:HG23	1:F:129:SER:HB2	2.00	0.43
1:B:254:THR:HG21	1:B:285:LYS:HB2	2.01	0.43
1:E:19:VAL:HB	1:E:20:ALA:H	1.60	0.43
1:F:151:LYS:HE3	1:F:151:LYS:HB3	1.77	0.43
1:C:200:VAL:HA	1:C:201:PRO:HD3	1.75	0.43
1:F:122:TYR:O	1:F:126:LEU:HG	2.19	0.43
1:B:328:GLY:O	1:B:329:HIS:ND1	2.52	0.43
1:G:109:ILE:O	1:G:113:MET:HB2	2.19	0.43
1:E:255:ALA:HB1	1:E:268:GLN:HE22	1.84	0.43
1:B:294:HIS:CG	1:B:294:HIS:O	2.71	0.43
1:B:306:LEU:HD12	1:B:325:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:PRO:O	1:D:225:ALA:N	2.51	0.43
1:C:236:LYS:HG3	1:C:236:LYS:H	1.47	0.43
1:B:207:PHE:HD1	1:B:247:VAL:HG22	1.84	0.43
1:A:25:LEU:HA	1:A:26:ALA:HA	1.85	0.42
1:G:103:ASP:OD2	1:G:103:ASP:N	2.51	0.42
1:A:148:VAL:HG22	1:A:282:LYS:H	1.85	0.42
1:G:260:THR:OG1	1:G:261:ALA:N	2.51	0.42
1:F:51:MET:HB3	1:F:299:GLY:HA2	2.01	0.42
1:E:109:ILE:HD13	1:E:109:ILE:HA	1.88	0.42
1:G:154:GLU:O	1:G:155:ASN:ND2	2.52	0.42
1:C:106:ILE:HG21	1:C:119:ARG:HH21	1.82	0.42
1:D:149:GLU:HB2	1:D:151:LYS:O	2.19	0.42
1:D:255:ALA:HB1	1:D:268:GLN:OE1	2.20	0.42
1:C:51:MET:SD	1:C:53:ARG:NH2	2.93	0.42
1:B:28:PHE:CE2	1:C:59:LYS:HB2	2.54	0.42
1:F:75:ALA:HB3	1:F:78:GLU:HG3	2.00	0.42
1:B:232:ILE:HG13	1:B:233:ASP:N	2.35	0.42
1:G:222:MET:SD	1:G:229:ALA:HA	2.59	0.42
1:D:81:ASP:HA	1:D:84:ARG:NH1	2.33	0.42
1:G:142:ILE:HB	1:G:298:VAL:HG21	2.02	0.42
1:C:83:LYS:NZ	1:C:83:LYS:H	2.17	0.42
1:B:322:ILE:HD11	1:B:324:LYS:HE3	2.02	0.42
1:D:96:ILE:HA	1:D:328:GLY:HA3	2.01	0.42
1:B:103:ASP:N	1:B:103:ASP:OD1	2.53	0.42
1:A:84:ARG:HA	1:F:262:ARG:HD3	2.01	0.42
1:C:5:THR:HG22	1:C:6:GLY:H	1.85	0.42
1:G:146:CYS:HB2	1:G:331:GLY:HA3	2.02	0.42
1:E:103:ASP:N	1:E:103:ASP:OD1	2.53	0.42
1:F:266:THR:OG1	1:F:267:GLY:N	2.53	0.42
1:D:294:HIS:O	1:D:294:HIS:CG	2.72	0.41
1:C:232:ILE:H	1:C:232:ILE:HG12	1.62	0.41
1:F:239:ILE:HG22	1:F:240:ARG:H	1.85	0.41
1:C:86:ASP:C	1:C:88:LYS:H	2.23	0.41
1:F:14:GLN:HB2	1:G:89:HIS:O	2.20	0.41
1:F:24:LYS:HB3	1:F:24:LYS:HE3	1.89	0.41
1:E:92:LYS:HE2	1:E:332:LEU:HA	2.02	0.41
1:C:104:VAL:HG22	1:C:105:LEU:H	1.84	0.41
1:F:138:VAL:O	1:F:142:ILE:HG22	2.20	0.41
1:F:333:ARG:HB2	1:F:333:ARG:HH11	1.85	0.41
1:A:27:LEU:HD13	1:A:27:LEU:O	2.19	0.41
1:E:295:ARG:HD2	1:E:296:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD11	1:B:180:LEU:HD13	2.02	0.41
1:A:207:PHE:CD2	1:A:247:VAL:HG22	2.55	0.41
1:B:260:THR:OG1	1:B:267:GLY:O	2.34	0.41
1:B:198:ASN:OD1	1:B:198:ASN:N	2.51	0.41
1:B:46:THR:OG1	1:B:47:THR:N	2.53	0.41
1:D:157:GLU:CD	1:D:159:LEU:HG	2.41	0.41
1:C:207:PHE:HE2	1:C:209:CYS:HB2	1.85	0.41
1:A:140:ALA:HA	1:A:272:PHE:CZ	2.56	0.41
1:C:50:HIS:CE1	1:C:298:VAL:HB	2.55	0.41
1:E:294:HIS:O	1:E:294:HIS:CG	2.73	0.41
1:D:294:HIS:O	1:D:295:ARG:HG2	2.20	0.41
1:G:184:ILE:HB	1:G:217:ILE:HD11	2.02	0.41
1:A:32:PHE:CG	1:A:33:GLY:N	2.87	0.41
1:E:168:THR:OG1	1:E:169:GLN:N	2.53	0.41
1:E:37:LEU:O	1:F:65:VAL:HA	2.20	0.41
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.86	0.41
1:B:232:ILE:CG2	1:B:239:ILE:HA	2.51	0.41
1:B:276:LYS:HB2	1:B:276:LYS:HE2	1.92	0.41
1:B:198:ASN:HD22	1:B:335:GLU:CD	2.24	0.41
1:D:100:LEU:HD23	1:D:325:TYR:CE2	2.53	0.41
1:G:26:ALA:HB1	1:G:28:PHE:H	1.86	0.41
1:D:107:TYR:HB2	1:D:110:GLU:HB2	2.03	0.41
1:B:148:VAL:HG12	1:B:282:LYS:H	1.86	0.41
1:A:304:ARG:NE	1:A:304:ARG:HA	2.35	0.41
1:F:94:ILE:HD11	1:F:332:LEU:HD12	2.01	0.41
1:A:85:LYS:NZ	1:F:263:GLU:OE1	2.32	0.41
1:E:199:TYR:O	1:E:200:VAL:HB	2.21	0.41
1:F:222:MET:SD	1:F:223:PRO:HD2	2.61	0.41
1:G:100:LEU:HD11	1:G:130:LEU:HG	2.03	0.41
1:D:99:LEU:HD11	1:D:324:LYS:HD3	2.02	0.41
1:C:176:ASP:C	1:C:178:VAL:H	2.25	0.41
1:C:83:LYS:HZ3	1:C:83:LYS:H	1.68	0.41
1:F:143:ALA:HB3	1:F:272:PHE:HZ	1.86	0.41
1:A:269:LYS:O	1:A:270:HIS:ND1	2.53	0.41
1:F:57:SER:OG	1:F:58:GLY:N	2.52	0.41
1:C:79:ASN:OD1	1:C:82:ASP:N	2.54	0.41
1:D:125:GLN:OE1	1:E:68:ARG:HG3	2.20	0.41
1:C:11:GLY:HA3	1:C:28:PHE:CE1	2.56	0.41
1:D:59:LYS:HB3	1:D:59:LYS:HE2	1.90	0.41
1:A:62:GLN:NE2	1:A:91:GLU:OE1	2.54	0.41
1:D:222:MET:HB3	1:D:223:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:HG2	1:B:73:TYR:HE1	1.86	0.41
1:D:94:ILE:HD11	1:D:301:VAL:HG22	2.02	0.41
1:C:313:ARG:HB2	1:C:320:GLN:OE1	2.21	0.41
1:E:116:TYR:CE1	1:E:118:VAL:HG22	2.56	0.41
1:C:139:LEU:HA	1:C:139:LEU:HD13	1.90	0.41
1:D:117:ASP:HA	1:D:118:VAL:CG1	2.49	0.40
1:F:25:LEU:HB3	1:F:28:PHE:HD1	1.86	0.40
1:A:161:THR:OG1	1:A:162:ALA:N	2.54	0.40
1:G:237:GLY:HA3	1:G:238:SER:HA	1.68	0.40
1:F:228:TYR:CG	1:F:229:ALA:N	2.89	0.40
1:A:167:THR:OG1	1:A:168:THR:N	2.54	0.40
1:A:73:TYR:OH	1:F:269:LYS:NZ	2.53	0.40
1:D:231:LEU:HD13	1:D:242:VAL:HG13	2.02	0.40
1:G:214:TYR:CD1	1:G:249:GLU:HG2	2.56	0.40
1:A:64:PRO:O	1:F:37:LEU:HB3	2.21	0.40
1:C:276:LYS:O	1:C:281:VAL:HG12	2.22	0.40
1:A:224:ASN:HD22	1:B:182:LYS:HZ3	1.69	0.40
1:F:140:ALA:HA	1:F:272:PHE:CZ	2.57	0.40
1:A:262:ARG:HG3	1:B:85:LYS:HB2	2.04	0.40
1:C:96:ILE:HG13	1:C:303:LEU:HD21	2.04	0.40
1:C:178:VAL:HG22	1:C:179:ALA:H	1.86	0.40
1:D:184:ILE:HA	1:D:184:ILE:HD12	1.89	0.40
1:G:16:LYS:HD2	1:G:16:LYS:HA	1.95	0.40
1:D:31:VAL:HG22	1:D:32:PHE:H	1.87	0.40
1:A:243:MET:HE2	1:F:218:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/345 (99%)	282 (83%)	58 (17%)	1 (0%)	46	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	341/345 (99%)	279 (82%)	53 (16%)	9 (3%)	7	48
1	C	341/345 (99%)	251 (74%)	84 (25%)	6 (2%)	11	55
1	D	341/345 (99%)	275 (81%)	63 (18%)	3 (1%)	21	68
1	E	341/345 (99%)	281 (82%)	53 (16%)	7 (2%)	9	53
1	F	341/345 (99%)	276 (81%)	57 (17%)	8 (2%)	8	51
1	G	341/345 (99%)	276 (81%)	59 (17%)	6 (2%)	11	55
All	All	2387/2415 (99%)	1920 (80%)	427 (18%)	40 (2%)	16	56

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	VAL
1	D	118	VAL
1	E	18	VAL
1	F	118	VAL
1	G	52	VAL
1	B	206	VAL
1	B	232	ILE
1	E	19	VAL
1	E	236	LYS
1	E	296	SER
1	F	178	VAL
1	F	206	VAL
1	F	239	ILE
1	G	232	ILE
1	B	239	ILE
1	C	118	VAL
1	C	239	ILE
1	C	281	VAL
1	D	296	SER
1	E	239	ILE
1	G	156	ILE
1	A	19	VAL
1	B	45	VAL
1	B	199	TYR
1	C	19	VAL
1	C	244	GLY
1	C	298	VAL
1	E	118	VAL
1	F	19	VAL

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Mol	Chain	Res	Type
1	F	179	ALA
1	G	204	ASP
1	G	298	VAL
1	B	200	VAL
1	E	235	GLU
1	B	296	SER
1	F	296	SER
1	B	242	VAL
1	F	247	VAL
1	D	142	ILE
1	G	234	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/261 (99%)	205 (79%)	54 (21%)	1	11
1	B	259/261 (99%)	206 (80%)	53 (20%)	1	11
1	C	259/261 (99%)	200 (77%)	59 (23%)	1	8
1	D	259/261 (99%)	191 (74%)	68 (26%)	0	5
1	E	259/261 (99%)	207 (80%)	52 (20%)	1	12
1	F	259/261 (99%)	205 (79%)	54 (21%)	1	11
1	G	259/261 (99%)	207 (80%)	52 (20%)	1	12
All	All	1813/1827 (99%)	1421 (78%)	392 (22%)	4	9

All (392) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	PHE
1	A	30	LYS
1	A	32	PHE
1	A	46	THR
1	A	49	ARG

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Mol	Chain	Res	Type
1	A	52	VAL
1	A	59	LYS
1	A	69	THR
1	A	80	LEU
1	A	83	LYS
1	A	84	ARG
1	A	87	ILE
1	A	89	HIS
1	A	94	ILE
1	A	103	ASP
1	A	107	TYR
1	A	114	ASN
1	A	115	HIS
1	A	128	GLU
1	A	142	ILE
1	A	152	TYR
1	A	153	ASN
1	A	159	LEU
1	A	163	THR
1	A	166	GLU
1	A	170	ASN
1	A	192	ARG
1	A	198	ASN
1	A	200	VAL
1	A	210	ASP
1	A	217	ILE
1	A	218	LEU
1	A	224	ASN
1	A	228	TYR
1	A	231	LEU
1	A	232	ILE
1	A	239	ILE
1	A	248	VAL
1	A	253	LEU
1	A	262	ARG
1	A	271	VAL
1	A	276	LYS
1	A	295	ARG
1	A	298	VAL
1	A	303	LEU
1	A	304	ARG
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	322	ILE
1	A	325	TYR
1	A	332	LEU
1	A	333	ARG
1	A	341	VAL
1	A	344	VAL
1	B	28	PHE
1	B	29	LEU
1	B	32	PHE
1	B	38	THR
1	B	42	ARG
1	B	46	THR
1	B	47	THR
1	B	53	ARG
1	B	69	THR
1	B	70	GLN
1	B	73	TYR
1	B	74	LEU
1	B	78	GLU
1	B	87	ILE
1	B	88	LYS
1	B	92	LYS
1	B	94	ILE
1	B	95	THR
1	B	96	ILE
1	B	105	LEU
1	B	111	ASP
1	B	118	VAL
1	B	128	GLU
1	B	142	ILE
1	B	145	LEU
1	B	147	ASN
1	B	148	VAL
1	B	154	GLU
1	B	166	GLU
1	B	169	GLN
1	B	195	LEU
1	B	197	LYS
1	B	198	ASN
1	B	200	VAL
1	B	205	ARG
1	B	209	CYS

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Mol	Chain	Res	Type
1	B	221	LEU
1	B	241	ASN
1	B	243	MET
1	B	245	PHE
1	B	260	THR
1	B	272	PHE
1	B	280	ASN
1	B	283	VAL
1	B	291	LEU
1	B	294	HIS
1	B	298	VAL
1	B	303	LEU
1	B	320	GLN
1	B	322	ILE
1	B	325	TYR
1	B	332	LEU
1	B	333	ARG
1	C	5	THR
1	C	10	MET
1	C	13	ASN
1	C	18	VAL
1	C	24	LYS
1	C	27	LEU
1	C	30	LYS
1	C	40	PHE
1	C	46	THR
1	C	55	ILE
1	C	69	THR
1	C	73	TYR
1	C	74	LEU
1	C	80	LEU
1	C	82	ASP
1	C	83	LYS
1	C	84	ARG
1	C	89	HIS
1	C	90	THR
1	C	91	GLU
1	C	92	LYS
1	C	94	ILE
1	C	95	THR
1	C	96	ILE
1	C	100	LEU

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Mol	Chain	Res	Type
1	C	103	ASP
1	C	115	HIS
1	C	139	LEU
1	C	142	ILE
1	C	151	LYS
1	C	159	LEU
1	C	163	THR
1	C	169	GLN
1	C	171	LYS
1	C	174	LEU
1	C	183	GLU
1	C	200	VAL
1	C	205	ARG
1	C	227	ASN
1	C	232	ILE
1	C	236	LYS
1	C	243	MET
1	C	248	VAL
1	C	253	LEU
1	C	260	THR
1	C	272	PHE
1	C	276	LYS
1	C	280	ASN
1	C	281	VAL
1	C	295	ARG
1	C	298	VAL
1	C	303	LEU
1	C	304	ARG
1	C	309	GLU
1	C	312	ARG
1	C	324	LYS
1	C	325	TYR
1	C	332	LEU
1	C	333	ARG
1	D	3	SER
1	D	19	VAL
1	D	27	LEU
1	D	28	PHE
1	D	29	LEU
1	D	32	PHE
1	D	38	THR
1	D	42	ARG

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Mol	Chain	Res	Type
1	D	43	THR
1	D	50	HIS
1	D	51	MET
1	D	66	LEU
1	D	68	ARG
1	D	69	THR
1	D	73	TYR
1	D	79	ASN
1	D	81	ASP
1	D	83	LYS
1	D	84	ARG
1	D	86	ASP
1	D	91	GLU
1	D	94	ILE
1	D	105	LEU
1	D	110	GLU
1	D	114	ASN
1	D	115	HIS
1	D	117	ASP
1	D	118	VAL
1	D	126	LEU
1	D	132	MET
1	D	139	LEU
1	D	142	ILE
1	D	149	GLU
1	D	154	GLU
1	D	157	GLU
1	D	163	THR
1	D	180	LEU
1	D	184	ILE
1	D	192	ARG
1	D	200	VAL
1	D	204	ASP
1	D	218	LEU
1	D	221	LEU
1	D	231	LEU
1	D	233	ASP
1	D	235	GLU
1	D	241	ASN
1	D	245	PHE
1	D	250	VAL
1	D	262	ARG

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Mol	Chain	Res	Type
1	D	272	PHE
1	D	276	LYS
1	D	291	LEU
1	D	294	HIS
1	D	298	VAL
1	D	300	THR
1	D	306	LEU
1	D	309	GLU
1	D	310	ARG
1	D	312	ARG
1	D	315	ASN
1	D	317	GLN
1	D	324	LYS
1	D	325	TYR
1	D	332	LEU
1	D	335	GLU
1	D	341	VAL
1	D	344	VAL
1	E	18	VAL
1	E	29	LEU
1	E	38	THR
1	E	46	THR
1	E	50	HIS
1	E	70	GLN
1	E	78	GLU
1	E	82	ASP
1	E	83	LYS
1	E	86	ASP
1	E	89	HIS
1	E	90	THR
1	E	92	LYS
1	E	97	ASP
1	E	101	THR
1	E	105	LEU
1	E	107	TYR
1	E	111	ASP
1	E	119	ARG
1	E	128	GLU
1	E	142	ILE
1	E	145	LEU
1	E	147	ASN
1	E	149	GLU

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Mol	Chain	Res	Type
1	E	157	GLU
1	E	161	THR
1	E	169	GLN
1	E	174	LEU
1	E	190	LYS
1	E	192	ARG
1	E	209	CYS
1	E	210	ASP
1	E	212	ASP
1	E	231	LEU
1	E	240	ARG
1	E	263	GLU
1	E	265	THR
1	E	271	VAL
1	E	275	ASN
1	E	280	ASN
1	E	291	LEU
1	E	294	HIS
1	E	295	ARG
1	E	298	VAL
1	E	303	LEU
1	E	306	LEU
1	E	317	GLN
1	E	319	ASP
1	E	320	GLN
1	E	325	TYR
1	E	332	LEU
1	E	344	VAL
1	F	24	LYS
1	F	25	LEU
1	F	27	LEU
1	F	28	PHE
1	F	29	LEU
1	F	45	VAL
1	F	47	THR
1	F	49	ARG
1	F	50	HIS
1	F	51	MET
1	F	69	THR
1	F	81	ASP
1	F	92	LYS
1	F	95	THR

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Mol	Chain	Res	Type
1	F	96	ILE
1	F	99	LEU
1	F	105	LEU
1	F	106	ILE
1	F	108	ASP
1	F	109	ILE
1	F	116	TYR
1	F	118	VAL
1	F	128	GLU
1	F	142	ILE
1	F	153	ASN
1	F	156	ILE
1	F	159	LEU
1	F	163	THR
1	F	167	THR
1	F	170	ASN
1	F	177	GLN
1	F	192	ARG
1	F	212	ASP
1	F	222	MET
1	F	224	ASN
1	F	227	ASN
1	F	231	LEU
1	F	232	ILE
1	F	236	LYS
1	F	243	MET
1	F	252	HIS
1	F	254	THR
1	F	262	ARG
1	F	294	HIS
1	F	303	LEU
1	F	306	LEU
1	F	309	GLU
1	F	312	ARG
1	F	317	GLN
1	F	319	ASP
1	F	325	TYR
1	F	332	LEU
1	F	333	ARG
1	F	343	LYS
1	G	18	VAL
1	G	24	LYS

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Mol	Chain	Res	Type
1	G	25	LEU
1	G	31	VAL
1	G	35	GLU
1	G	38	THR
1	G	42	ARG
1	G	47	THR
1	G	50	HIS
1	G	55	ILE
1	G	62	GLN
1	G	65	VAL
1	G	66	LEU
1	G	80	LEU
1	G	83	LYS
1	G	85	LYS
1	G	89	HIS
1	G	91	GLU
1	G	97	ASP
1	G	101	THR
1	G	108	ASP
1	G	113	MET
1	G	119	ARG
1	G	142	ILE
1	G	163	THR
1	G	168	THR
1	G	169	GLN
1	G	171	LYS
1	G	190	LYS
1	G	192	ARG
1	G	195	LEU
1	G	197	LYS
1	G	199	TYR
1	G	210	ASP
1	G	228	TYR
1	G	231	LEU
1	G	235	GLU
1	G	249	GLU
1	G	271	VAL
1	G	281	VAL
1	G	288	VAL
1	G	291	LEU
1	G	295	ARG
1	G	303	LEU

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Mol	Chain	Res	Type
1	G	304	ARG
1	G	310	ARG
1	G	319	ASP
1	G	324	LYS
1	G	325	TYR
1	G	332	LEU
1	G	341	VAL
1	G	342	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	169	GLN
1	A	252	HIS
1	A	315	ASN
1	B	14	GLN
1	B	70	GLN
1	B	155	ASN
1	B	170	ASN
1	B	275	ASN
1	B	280	ASN
1	B	317	GLN
1	B	320	GLN
1	C	13	ASN
1	C	62	GLN
1	C	147	ASN
1	C	268	GLN
1	C	287	ASN
1	C	294	HIS
1	C	317	GLN
1	D	50	HIS
1	D	62	GLN
1	D	70	GLN
1	D	287	ASN
1	E	9	GLN
1	E	50	HIS
1	E	89	HIS
1	E	147	ASN
1	E	169	GLN
1	E	177	GLN
1	E	268	GLN

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Mol	Chain	Res	Type
1	E	280	ASN
1	E	287	ASN
1	F	14	GLN
1	F	114	ASN
1	F	198	ASN
1	F	252	HIS
1	G	14	GLN
1	G	62	GLN
1	G	70	GLN
1	G	89	HIS
1	G	125	GLN
1	G	155	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.