



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 15, 2018 – 07:51 AM EST

PDB ID : 5YFP  
EMDB ID: : EMD-6827  
Title : Cryo-EM Structure of the Exocyst Complex  
Authors : Mei, K.; Li, Y.; Wang, S.; Shao, G.; Wang, J.; Ding, Y.; Luo, G.; Yue, P.; Liu, J.J.; Wang, X.; Dong, M.Q.; Guo, W.; Wang, H.W.  
Deposited on : 2017-09-21  
Resolution : 4.40 Å(reported)  
Based on PDB ID : 2FJI, 2B1E, 2A2F, 5H11, 1ZC4, 2D2S, ?

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

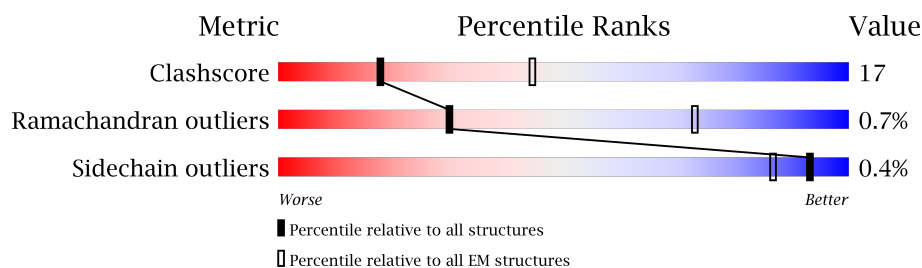
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	1336	
2	B	971	
3	C	805	
4	D	1065	
5	E	871	
6	F	910	
7	G	623	
8	H	753	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33096 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 Exocyst complex component SEC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	672	Total	C	N	O	0	0
			3345	2001	672	672		

- Molecule 2 is a protein called Exocyst complex component SEC5.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	928	Total	C	N	O	0	0
			4610	2755	927	928		

- Molecule 3 is a protein called Exocyst complex component SEC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	794	Total	C	N	O	S	0	0
			4994	3097	892	989	16		

- Molecule 4 is a protein called Exocyst complex component SEC8.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	954	Total	C	N	O	0	0
			4739	2831	954	954		

- Molecule 5 is a protein called Exocyst complex component SEC10.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	776	Total	C	N	O	0	0
			3860	2308	776	776		

- Molecule 6 is a protein called Exocyst complex component SEC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	725	Total	C	N	O	0	0
			3612	2162	725	725		

- Molecule 7 is a protein called Exocyst complex component EXO70.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	615	Total	C	N	O	S	0	0
			4696	2968	809	902	17		

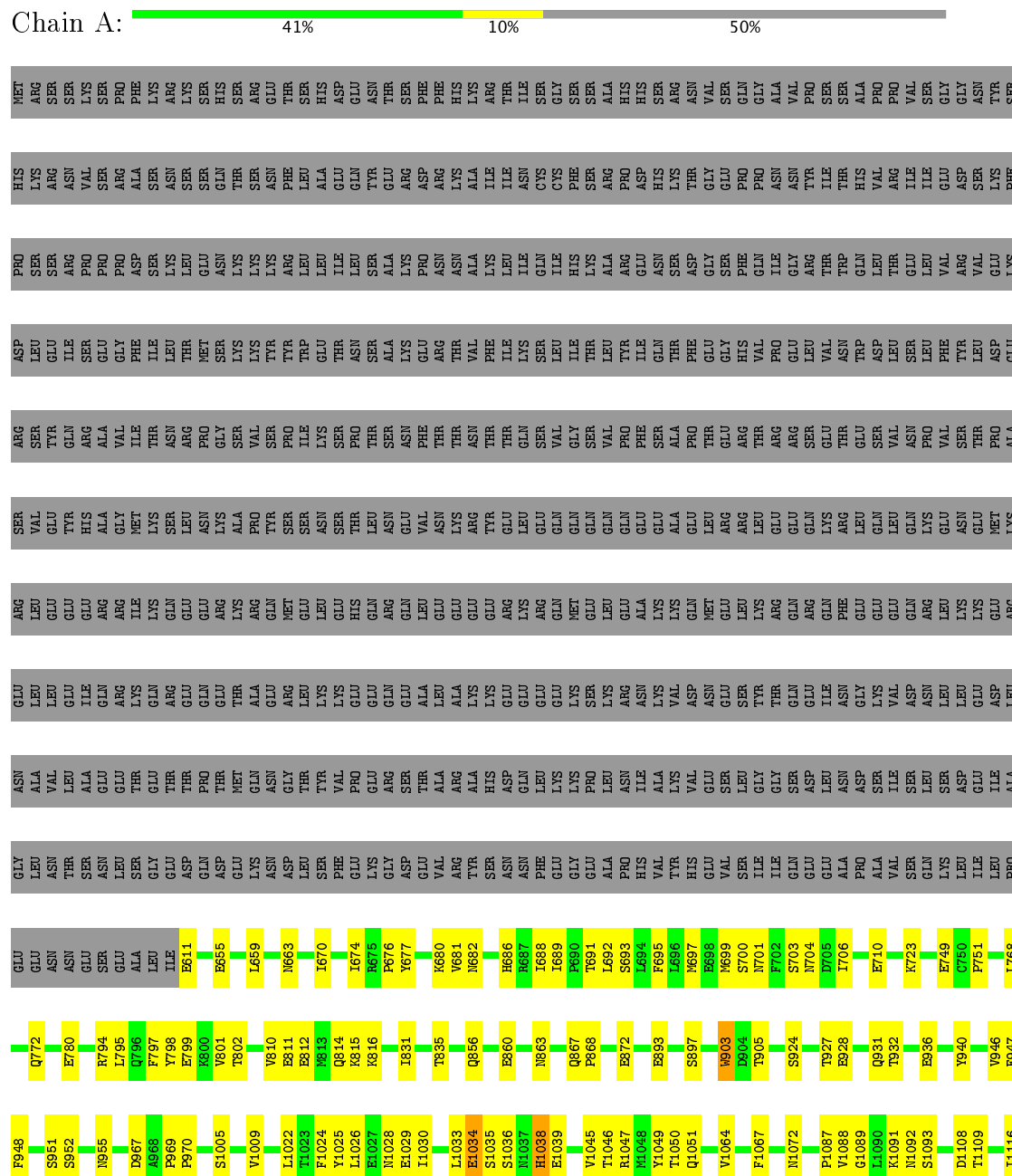
- Molecule 8 is a protein called Exocyst complex component EXO84.

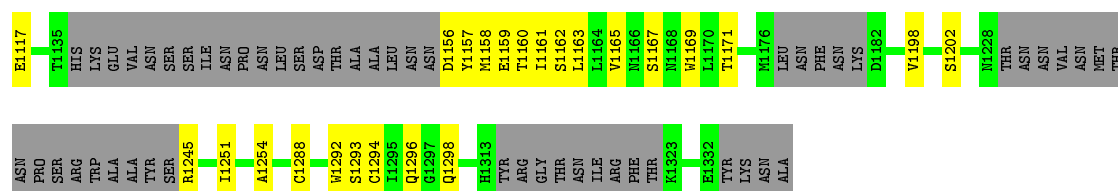
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	518	Total	C	N	O	S	0	0
			3240	2002	591	643	4		

### 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 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.

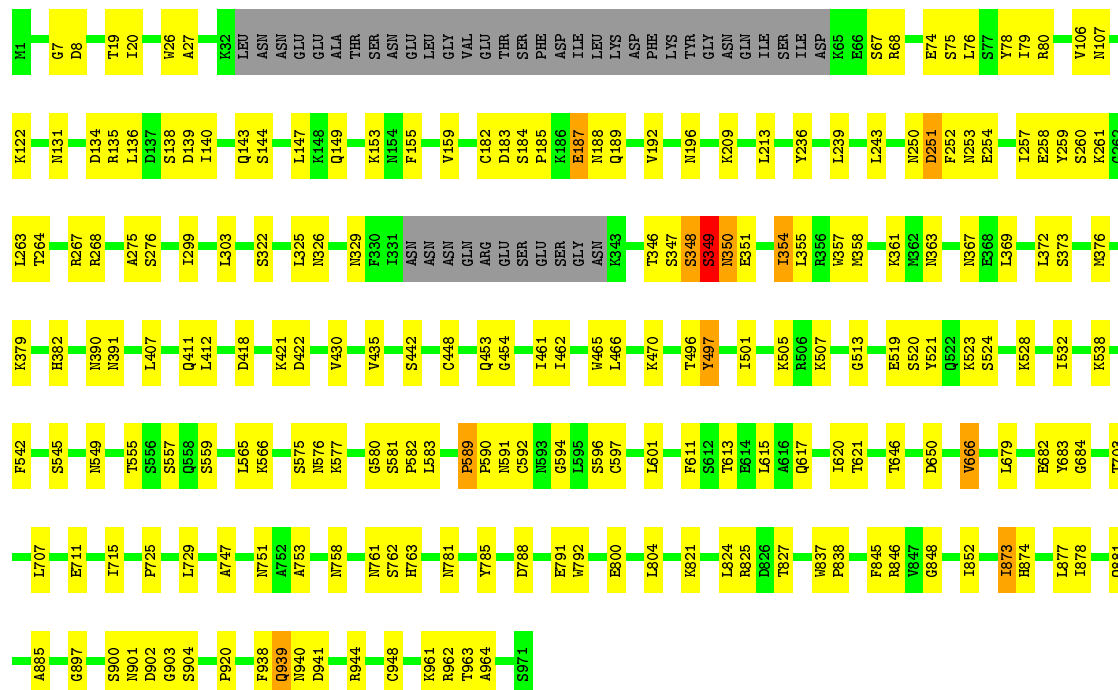
- Molecule 1: Exocyst complex component SEC3





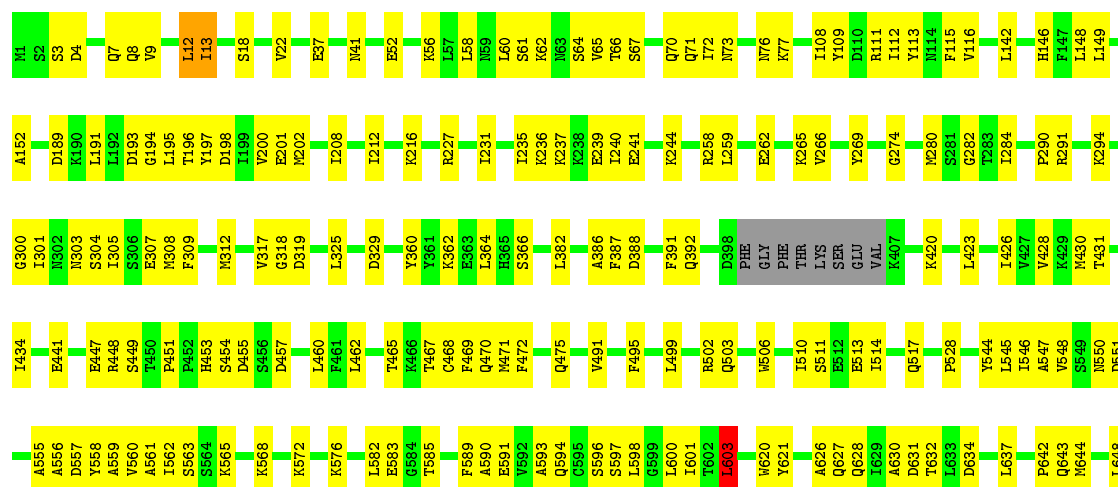
• Molecule 2: Exocyst complex component SEC5

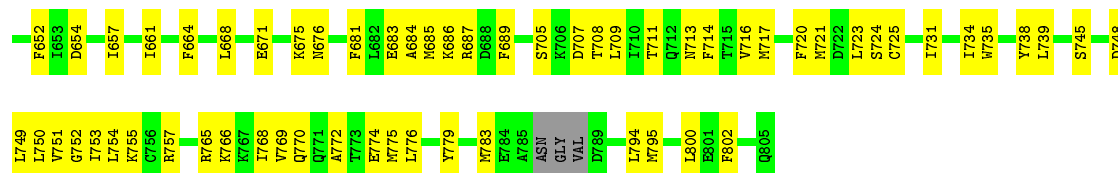
Chain B: 74% 20% . .



• Molecule 3: Exocyst complex component SEC6

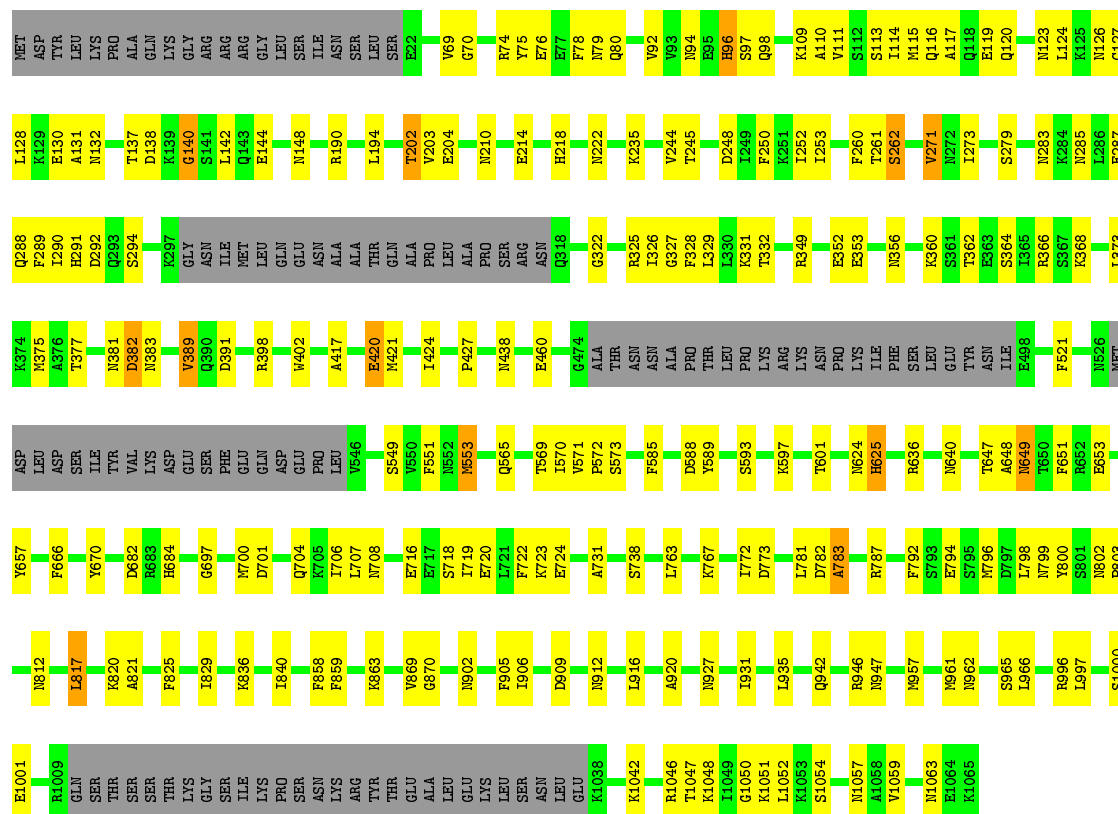
Chain C: 68% 30% . .





### • Molecule 4: Exocyst complex component SEC8

Chain D:



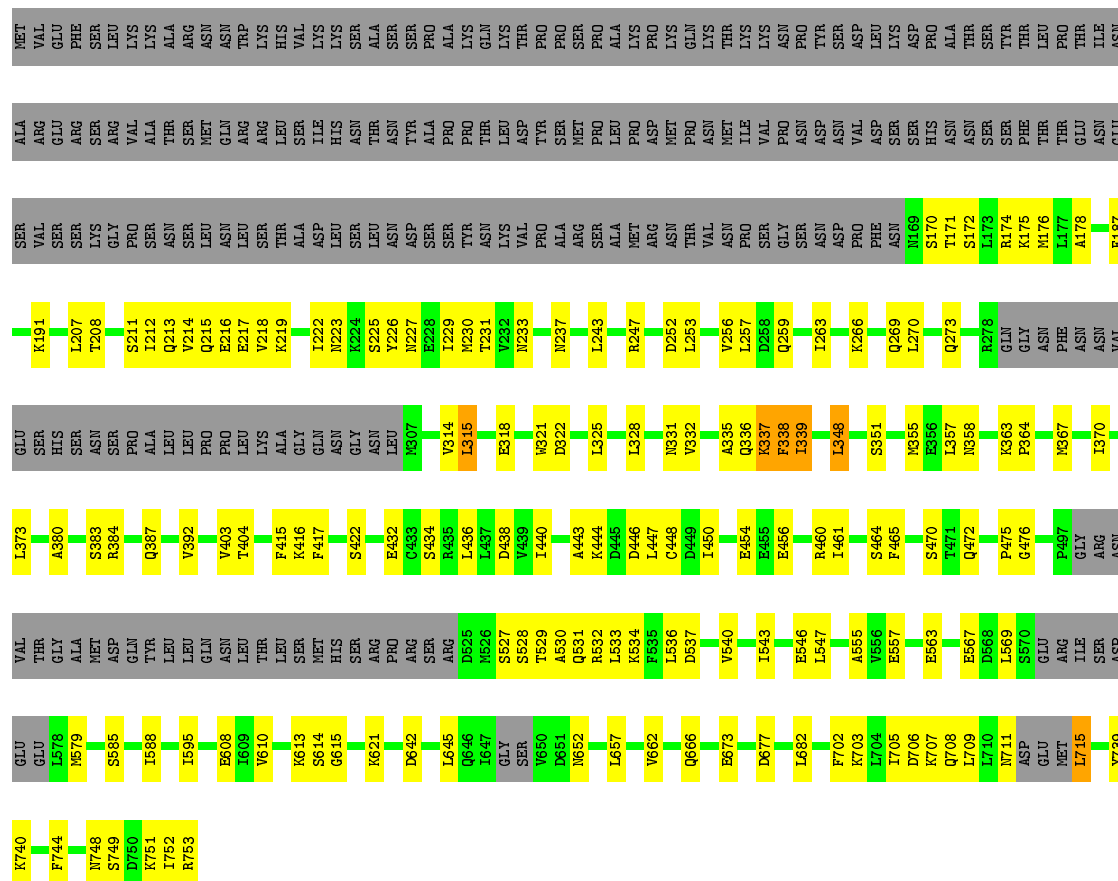
### • Molecule 5: Exocyst complex component SEC10

Chain E:









## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	343342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The defocus value of each image was determined by CTFFIND3.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.28	0/3340	0.63	4/4659 (0.1%)
2	B	0.33	0/4607	0.71	13/6427 (0.2%)
3	C	0.31	0/5043	0.61	1/6885 (0.0%)
4	D	0.33	0/4734	0.75	7/6601 (0.1%)
5	E	0.27	0/3857	0.56	2/5383 (0.0%)
6	F	0.29	0/3607	0.61	5/5034 (0.1%)
7	G	0.37	0/4768	0.63	3/6443 (0.0%)
8	H	0.41	0/3253	0.65	2/4443 (0.0%)
All	All	0.33	0/33209	0.65	37/45875 (0.1%)

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	11
2	B	0	41
3	C	0	8
4	D	0	43
5	E	0	6
6	F	0	13
7	G	0	9
8	H	0	12
All	All	0	143

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	758	ASN	C-N-CA	7.96	155.41	122.00
1	A	1116	ILE	C-N-CA	7.77	141.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	444	ILE	C-N-CA	7.20	139.70	121.70
7	G	153	LEU	CA-CB-CG	-6.69	99.91	115.30
4	D	649	ASN	C-N-CA	6.38	137.65	121.70
6	F	275	SER	C-N-CA	6.32	137.51	121.70
7	G	111	LEU	CA-CB-CG	6.26	129.69	115.30
2	B	715	ILE	N-CA-C	6.06	127.37	111.00
8	H	472	GLN	C-N-CA	5.96	136.61	121.70
5	E	243	TYR	C-N-CA	5.90	136.45	121.70
2	B	496	THR	C-N-CA	5.88	136.39	121.70
5	E	316	THR	C-N-CA	5.84	136.30	121.70
4	D	262	SER	N-CA-C	-5.82	95.29	111.00
7	G	300	ASN	C-N-CA	5.79	136.18	121.70
1	A	1038	HIS	C-N-CA	5.77	136.13	121.70
4	D	260	PHE	C-N-CA	5.68	135.91	121.70
4	D	382	ASP	C-N-CA	5.62	135.75	121.70
4	D	782	ASP	C-N-CA	5.62	135.75	121.70
2	B	940	ASN	N-CA-C	5.49	125.83	111.00
2	B	346	THR	N-CA-C	5.44	125.69	111.00
3	C	603	LEU	CA-CB-CG	-5.41	102.86	115.30
1	A	1109	THR	C-N-CA	5.36	135.11	121.70
6	F	281	ASN	N-CA-C	5.32	125.37	111.00
2	B	513	GLY	C-N-CA	5.31	134.98	121.70
2	B	497	TYR	C-N-CA	5.30	134.96	121.70
2	B	555	THR	C-N-CA	5.26	134.86	121.70
2	B	187	GLU	C-N-CA	5.25	134.82	121.70
4	D	783	ALA	N-CA-C	5.24	125.13	111.00
6	F	276	LYS	N-CA-C	5.16	124.93	111.00
1	A	903	TRP	C-N-CA	5.13	134.52	121.70
8	H	715	LEU	CA-CB-CG	5.11	127.06	115.30
2	B	523	LYS	C-N-CA	5.10	134.46	121.70
2	B	252	PHE	C-N-CA	5.09	134.42	121.70
4	D	271	VAL	C-N-CA	5.05	134.34	121.70
2	B	679	LEU	C-N-CA	5.05	134.32	121.70
2	B	122	LYS	C-N-CA	5.03	134.27	121.70
6	F	469	GLU	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (143) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1039	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	1064	VAL	Peptide
1	A	1117	GLU	Peptide
1	A	749	GLU	Peptide
1	A	780	GLU	Peptide
1	A	946	VAL	Peptide
1	A	947	PHE	Peptide
1	A	948	PHE	Peptide
1	A	955	ASN	Peptide
1	A	967	ASP	Peptide
2	B	184	SER	Peptide
2	B	187	GLU	Peptide
2	B	236	TYR	Peptide
2	B	251	ASP	Peptide
2	B	268	ARG	Peptide
2	B	347	SER	Peptide
2	B	348	SER	Peptide
2	B	349	SER	Peptide
2	B	350	ASN	Peptide
2	B	354	ILE	Peptide
2	B	407	LEU	Peptide
2	B	411	GLN	Peptide
2	B	418	ASP	Peptide
2	B	430	VAL	Peptide
2	B	435	VAL	Peptide
2	B	442	SER	Peptide
2	B	448	CYS	Peptide
2	B	453	GLN	Peptide
2	B	454	GLY	Peptide
2	B	507	LYS	Peptide
2	B	519	GLU	Peptide
2	B	524	SER	Peptide
2	B	557	SER	Peptide
2	B	559	SER	Peptide
2	B	577	LYS	Peptide
2	B	580	GLY	Peptide
2	B	581	SER	Peptide
2	B	589	PRO	Peptide
2	B	591	ASN	Peptide
2	B	592	CYS	Peptide
2	B	666	VAL	Peptide
2	B	703	THR	Peptide
2	B	711	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	753	ALA	Peptide
2	B	761	ASN	Peptide
2	B	763	HIS	Peptide
2	B	788	ASP	Peptide
2	B	791	GLU	Peptide
2	B	792	TRP	Peptide
2	B	873	ILE	Peptide
2	B	939	GLN	Peptide
3	C	12	LEU	Peptide
3	C	13	ILE	Peptide
3	C	284	ILE	Peptide
3	C	294	LYS	Peptide
3	C	319	ASP	Peptide
3	C	453	HIS	Peptide
3	C	454	SER	Peptide
3	C	603	LEU	Peptide
4	D	1057	ASN	Peptide
4	D	137	THR	Peptide
4	D	138	ASP	Peptide
4	D	140	GLY	Peptide
4	D	142	LEU	Peptide
4	D	202	THR	Peptide
4	D	235	LYS	Peptide
4	D	244	VAL	Peptide
4	D	248	ASP	Peptide
4	D	250	PHE	Peptide
4	D	261	THR	Peptide
4	D	262	SER	Peptide
4	D	271	VAL	Peptide
4	D	273	ILE	Peptide
4	D	373	LEU	Peptide
4	D	375	MET	Peptide
4	D	377	THR	Peptide
4	D	383	ASN	Peptide
4	D	389	VAL	Peptide
4	D	420	GLU	Peptide
4	D	438	ASN	Peptide
4	D	460	GLU	Peptide
4	D	549	SER	Peptide
4	D	551	PHE	Peptide
4	D	553	MET	Peptide
4	D	570	ILE	Peptide

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Mol	Chain	Res	Type	Group
4	D	571	VAL	Peptide
4	D	585	PHE	Peptide
4	D	624	ASN	Peptide
4	D	625	HIS	Peptide
4	D	651	PHE	Peptide
4	D	682	ASP	Peptide
4	D	707	LEU	Peptide
4	D	731	ALA	Peptide
4	D	781	LEU	Peptide
4	D	787	ARG	Peptide
4	D	792	PHE	Peptide
4	D	799	ASN	Peptide
4	D	802	ASN	Peptide
4	D	812	ASN	Peptide
4	D	817	LEU	Peptide
4	D	863	LYS	Peptide
4	D	96	HIS	Peptide
5	E	179	ILE	Peptide
5	E	24	LEU	Peptide
5	E	315	GLU	Peptide
5	E	36	ASP	Peptide
5	E	564	SER	Peptide
5	E	753	LEU	Peptide
6	F	280	THR	Peptide
6	F	295	GLU	Peptide
6	F	345	TYR	Peptide
6	F	410	ASN	Peptide
6	F	415	PHE	Peptide
6	F	444	ILE	Peptide
6	F	445	ASP	Peptide
6	F	53	VAL	Peptide
6	F	599	ASN	Peptide
6	F	600	ASP	Peptide
6	F	601	ILE	Peptide
6	F	643	ASN	Peptide
6	F	75	ASN	Peptide
7	G	153	LEU	Peptide
7	G	175	GLU	Peptide
7	G	190	HIS	Peptide
7	G	230	ALA	Peptide
7	G	259	ASP	Peptide
7	G	261	TYR	Peptide

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Mol	Chain	Res	Type	Group
7	G	262	SER	Peptide
7	G	300	ASN	Peptide
7	G	317	LYS	Peptide
8	H	314	VAL	Peptide
8	H	315	LEU	Peptide
8	H	336	GLN	Peptide
8	H	337	LYS	Peptide
8	H	338	PHE	Peptide
8	H	339	ILE	Peptide
8	H	348	LEU	Peptide
8	H	387	GLN	Peptide
8	H	454	GLU	Peptide
8	H	470	SER	Peptide
8	H	652	ASN	Peptide
8	H	708	GLN	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	3345	0	1403	67	0
2	B	4610	0	1926	83	0
3	C	4994	0	3576	172	0
4	D	4739	0	2011	90	0
5	E	3860	0	1635	120	0
6	F	3612	0	1508	83	0
7	G	4696	0	4483	186	0
8	H	3240	0	2433	84	0
All	All	33096	0	18975	874	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 17.

All (874) 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)
3:C:506:TRP:O	3:C:510:ILE:HB	1.54	1.06
3:C:558:TYR:O	3:C:562:ILE:HB	1.60	1.00
3:C:714:PHE:CD2	3:C:714:PHE:CZ	2.38	0.99
3:C:544:TYR:CG	3:C:544:TYR:CE2	2.40	0.97
3:C:557:ASP:O	3:C:561:ALA:HB3	1.66	0.96
8:H:530:ALA:O	8:H:534:LYS:HB2	1.69	0.92
7:G:546:LYS:O	7:G:550:ARG:HB3	1.68	0.92
3:C:555:ALA:O	3:C:559:ALA:HB3	1.70	0.91
7:G:589:TYR:O	7:G:593:TYR:HB3	1.71	0.91
7:G:33:LEU:O	7:G:37:ALA:HB3	1.74	0.87
3:C:561:ALA:O	3:C:565:LYS:HB2	1.74	0.87
4:D:127:CYS:O	4:D:131:ALA:HB3	1.74	0.86
7:G:543:GLU:O	7:G:547:GLU:HB2	1.75	0.86
7:G:106:LYS:O	7:G:110:MET:HB2	1.73	0.86
7:G:210:ILE:O	7:G:214:MET:HB2	1.77	0.85
7:G:105:HIS:O	7:G:109:ASP:HB2	1.78	0.83
7:G:351:ARG:O	7:G:355:LYS:HB2	1.78	0.82
7:G:307:GLU:O	7:G:310:GLU:HB3	1.79	0.82
3:C:774:GLU:CA	3:C:774:GLU:CG	2.56	0.82
3:C:766:LYS:O	3:C:770:GLN:HB2	1.80	0.82
8:H:380:ALA:HA	8:H:392:VAL:O	1.81	0.80
3:C:457:ASP:CA	3:C:457:ASP:CG	2.51	0.79
8:H:351:SER:HA	8:H:370:ILE:O	1.81	0.79
7:G:84:TYR:O	7:G:88:LEU:HB2	1.83	0.77
7:G:588:MET:O	7:G:592:PHE:HB3	1.84	0.77
3:C:556:ALA:O	3:C:560:VAL:HB	1.84	0.76
3:C:765:ARG:O	3:C:769:VAL:HB	1.86	0.74
7:G:331:GLN:O	7:G:335:GLN:HB2	1.88	0.73
7:G:287:PHE:O	7:G:291:LEU:HB2	1.89	0.72
7:G:253:GLU:O	7:G:257:VAL:HB	1.89	0.71
7:G:211:LEU:O	7:G:215:ALA:HB2	1.89	0.71
7:G:347:ASP:O	7:G:351:ARG:HB2	1.92	0.70
3:C:630:ALA:O	3:C:634:ASP:HB2	1.92	0.70
3:C:471:MET:SD	3:C:471:MET:CB	2.81	0.69
3:C:546:ILE:HG21	3:C:644:MET:HA	1.73	0.69
7:G:340:VAL:O	7:G:344:LEU:HB2	1.93	0.69
3:C:559:ALA:O	3:C:563:SER:HB2	1.93	0.68
3:C:572:LYS:O	3:C:576:LYS:HB2	1.93	0.68
7:G:520:ARG:O	7:G:524:ALA:HB2	1.92	0.68
7:G:591:ARG:O	7:G:595:ARG:HB2	1.92	0.68
3:C:648:LEU:O	3:C:652:PHE:HB2	1.94	0.67
3:C:671:GLU:HG2	3:C:755:LYS:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:491:VAL:O	3:C:495:PHE:HB2	1.96	0.65
7:G:158:PRO:HG3	7:G:212:LYS:HD3	1.78	0.65
7:G:98:LYS:O	7:G:102:GLN:HB3	1.97	0.64
3:C:686:LYS:O	3:C:689:PHE:HB3	1.98	0.64
7:G:390:LEU:O	7:G:423:HIS:ND1	2.30	0.64
3:C:661:ILE:HD12	3:C:713:ASN:HB3	1.80	0.64
7:G:470:GLN:HA	7:G:515:MET:HG2	1.80	0.63
3:C:561:ALA:O	3:C:565:LYS:CB	2.46	0.63
8:H:533:LEU:HA	8:H:536:LEU:HB2	1.81	0.63
7:G:184:TRP:O	7:G:188:TYR:CB	2.47	0.63
3:C:716:VAL:O	3:C:720:PHE:HB3	1.99	0.63
6:F:711:GLU:HA	6:F:715:ALA:HB3	1.81	0.63
3:C:517:GLN:HB3	3:C:603:LEU:HD13	1.80	0.62
7:G:98:LYS:O	7:G:102:GLN:CB	2.47	0.62
2:B:357:TRP:O	2:B:361:LYS:N	2.25	0.62
7:G:324:LEU:HG	7:G:327:TYR:HB2	1.81	0.62
8:H:403:VAL:HA	8:H:416:LYS:HA	1.80	0.62
3:C:317:VAL:H	3:C:318:GLY:HA2	1.64	0.62
7:G:290:ASN:HA	7:G:293:ILE:HG22	1.82	0.62
3:C:491:VAL:O	3:C:495:PHE:CB	2.48	0.61
3:C:716:VAL:O	3:C:720:PHE:CB	2.48	0.61
7:G:488:GLU:HG2	7:G:489:LYS:HG3	1.82	0.61
4:D:140:GLY:O	4:D:144:GLU:N	2.29	0.61
7:G:283:TYR:O	7:G:287:PHE:HB2	2.00	0.61
1:A:611:GLU:N	2:B:261:LYS:O	2.33	0.61
7:G:142:GLU:HA	7:G:145:LEU:HD12	1.83	0.61
7:G:306:PHE:O	7:G:309:VAL:HB	2.01	0.61
3:C:423:LEU:HD23	3:C:491:VAL:HG23	1.83	0.60
6:F:90:ASP:O	6:F:94:GLY:HA3	2.00	0.60
3:C:72:ILE:O	3:C:76:ASN:CB	2.49	0.60
7:G:305:SER:O	7:G:308:LEU:HB2	2.00	0.60
7:G:359:ILE:O	7:G:445:LYS:NZ	2.32	0.60
7:G:330:LEU:O	7:G:334:THR:CB	2.49	0.60
4:D:716:GLU:O	4:D:720:GLU:CB	2.50	0.60
7:G:546:LYS:O	7:G:550:ARG:CB	2.47	0.60
8:H:528:SER:O	8:H:532:ARG:HB2	2.01	0.60
3:C:66:THR:O	3:C:70:GLN:CB	2.50	0.60
7:G:352:ILE:HG22	7:G:441:ASN:HD22	1.67	0.60
6:F:315:SER:O	6:F:319:PHE:CB	2.49	0.60
3:C:585:THR:O	3:C:589:PHE:N	2.35	0.60
7:G:252:ASN:O	7:G:256:LEU:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:283:TYR:O	7:G:287:PHE:CB	2.50	0.59
1:A:1288:CYS:O	1:A:1292:TRP:N	2.35	0.59
3:C:430:MET:O	3:C:434:ILE:HB	2.01	0.59
5:E:108:ILE:O	5:E:112:ASN:CB	2.51	0.59
7:G:287:PHE:O	7:G:291:LEU:CB	2.50	0.59
8:H:321:TRP:O	8:H:325:LEU:CB	2.50	0.59
7:G:441:ASN:OD1	7:G:444:ARG:NH1	2.35	0.59
7:G:447:GLN:HE22	7:G:458:VAL:HA	1.67	0.59
4:D:116:GLN:O	4:D:120:GLN:N	2.34	0.59
2:B:725:PRO:O	2:B:729:LEU:N	2.35	0.59
8:H:543:ILE:HG23	8:H:555:ALA:HB1	1.84	0.59
3:C:734:ILE:O	3:C:738:TYR:HB3	2.02	0.59
5:E:200:LYS:O	5:E:204:ILE:CB	2.51	0.59
4:D:287:GLU:O	4:D:291:HIS:CB	2.51	0.58
3:C:468:CYS:SG	3:C:502:ARG:NH1	2.76	0.58
4:D:109:LYS:O	4:D:113:SER:N	2.35	0.58
3:C:676:ASN:ND2	3:C:725:CYS:O	2.36	0.58
7:G:34:LYS:O	7:G:38:ALA:HB2	2.03	0.58
7:G:184:TRP:O	7:G:188:TYR:HB2	2.03	0.58
4:D:349:ARG:O	4:D:353:GLU:CB	2.52	0.58
7:G:388:GLY:O	7:G:392:ALA:HB2	2.03	0.58
3:C:73:ASN:O	3:C:77:LYS:CB	2.52	0.58
4:D:144:GLU:O	4:D:148:ASN:N	2.34	0.58
3:C:565:LYS:O	3:C:568:LYS:NZ	2.33	0.58
8:H:207:LEU:O	8:H:211:SER:CB	2.51	0.58
3:C:745:SER:HB2	3:C:795:MET:HB3	1.86	0.58
4:D:947:ASN:O	8:H:707:LYS:NZ	2.34	0.58
5:E:99:SER:O	5:E:103:ALA:HB2	2.04	0.58
6:F:624:ASN:O	6:F:628:PHE:CB	2.52	0.57
3:C:559:ALA:O	3:C:563:SER:CB	2.52	0.57
3:C:735:TRP:O	3:C:739:LEU:CB	2.52	0.57
4:D:916:LEU:O	4:D:920:ALA:HB2	2.05	0.57
4:D:957:MET:O	4:D:961:MET:CB	2.51	0.57
6:F:700:ASP:N	6:F:760:ASN:O	2.37	0.57
7:G:516:VAL:HG13	7:G:581:ILE:HG12	1.87	0.57
2:B:781:ASN:O	2:B:785:TYR:CB	2.52	0.57
5:E:653:LEU:O	5:E:657:SER:CB	2.53	0.57
4:D:521:PHE:HA	5:E:756:LYS:HA	1.87	0.57
7:G:146:ARG:NH2	7:G:194:GLU:OE1	2.37	0.57
8:H:331:ASN:O	8:H:335:ALA:N	2.34	0.57
3:C:468:CYS:O	3:C:472:PHE:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:653:GLU:O	4:D:657:TYR:N	2.38	0.57
6:F:394:ASP:O	6:F:398:LYS:CB	2.53	0.57
7:G:419:ASN:HB3	7:G:421:GLU:HG2	1.86	0.57
7:G:85:GLU:OE1	7:G:133:HIS:NE2	2.37	0.57
3:C:590:ALA:O	3:C:593:ALA:HB3	2.04	0.57
4:D:565:GLN:O	4:D:569:THR:N	2.37	0.57
4:D:700:MET:O	4:D:704:GLN:N	2.38	0.56
7:G:610:THR:HG1	7:G:613:GLU:H	1.52	0.56
8:H:355:MET:HA	8:H:367:MET:HA	1.85	0.56
8:H:443:ALA:O	8:H:447:LEU:CB	2.53	0.56
3:C:4:ASP:O	3:C:8:GLN:N	2.36	0.56
5:E:75:ARG:O	5:E:79:SER:N	2.37	0.56
5:E:73:TYR:O	5:E:77:PHE:CB	2.53	0.56
7:G:189:PHE:HA	7:G:192:ASN:HB2	1.87	0.56
7:G:27:PHE:O	7:G:31:LYS:CB	2.53	0.56
7:G:346:ARG:HG2	7:G:401:TRP:HA	1.87	0.56
5:E:112:ASN:O	5:E:116:LEU:CB	2.54	0.56
2:B:873:ILE:O	2:B:877:LEU:CB	2.54	0.56
3:C:60:LEU:O	3:C:64:SER:CB	2.53	0.56
4:D:706:ILE:N	4:D:708:ASN:O	2.39	0.56
6:F:864:ILE:O	6:F:868:VAL:CB	2.54	0.56
7:G:330:LEU:O	7:G:334:THR:HB	2.05	0.56
7:G:9:GLU:O	7:G:13:LEU:CB	2.53	0.56
2:B:646:THR:O	2:B:650:ASP:CB	2.54	0.56
3:C:208:ILE:H	3:C:212:ILE:H	1.54	0.56
3:C:627:GLN:NE2	3:C:631:ASP:OD2	2.38	0.56
7:G:447:GLN:NE2	7:G:457:ASP:O	2.39	0.56
8:H:219:LYS:O	8:H:223:ASN:CB	2.54	0.56
1:A:682:ASN:O	1:A:686:HIS:CB	2.54	0.56
2:B:538:LYS:O	2:B:542:PHE:CB	2.54	0.56
2:B:800:GLU:O	2:B:804:LEU:N	2.33	0.56
5:E:433:SER:O	5:E:438:ILE:N	2.37	0.56
6:F:607:ARG:O	6:F:611:GLU:N	2.38	0.56
7:G:352:ILE:O	7:G:356:ALA:CB	2.54	0.56
8:H:215:GLN:O	8:H:219:LYS:CB	2.54	0.55
8:H:546:GLU:HB3	8:H:555:ALA:HB2	1.87	0.55
3:C:752:GLY:HA3	3:C:800:LEU:HD23	1.87	0.55
4:D:126:ASN:O	4:D:130:GLU:CB	2.53	0.55
5:E:599:ILE:O	5:E:603:LEU:CB	2.54	0.55
7:G:589:TYR:OH	7:G:609:TYR:O	2.23	0.55
1:A:1072:ASN:O	1:A:1245:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:LYS:O	3:C:66:THR:CB	2.54	0.55
3:C:685:MET:HB3	3:C:721:MET:HG2	1.89	0.55
4:D:666:PHE:O	4:D:670:TYR:CB	2.54	0.55
6:F:217:LEU:O	6:F:221:TYR:CB	2.55	0.55
7:G:319:LEU:HB3	7:G:322:LYS:HZ1	1.71	0.55
5:E:685:GLN:O	5:E:689:MET:CB	2.54	0.55
3:C:705:SER:HA	3:C:708:THR:HB	1.88	0.55
6:F:725:VAL:O	6:F:729:LEU:N	2.39	0.55
5:E:749:SER:O	5:E:753:LEU:N	2.38	0.55
7:G:347:ASP:O	7:G:351:ARG:CB	2.55	0.55
1:A:1251:ILE:HA	1:A:1254:ALA:HB2	1.89	0.55
5:E:267:VAL:O	5:E:270:SER:C	2.45	0.55
5:E:83:GLU:O	5:E:87:LEU:N	2.37	0.55
7:G:352:ILE:O	7:G:356:ALA:HB3	2.07	0.55
8:H:444:LYS:HA	8:H:448:CYS:H	1.70	0.55
8:H:533:LEU:O	8:H:537:ASP:N	2.39	0.55
3:C:388:ASP:O	3:C:392:GLN:CB	2.55	0.55
4:D:1047:THR:O	4:D:1051:LYS:CB	2.55	0.55
5:E:33:LEU:O	5:E:37:HIS:N	2.40	0.55
5:E:163:GLU:O	5:E:167:ARG:CB	2.55	0.55
7:G:114:ILE:O	7:G:121:ARG:N	2.39	0.55
8:H:434:SER:O	8:H:438:ASP:CB	2.55	0.55
4:D:697:GLY:O	4:D:701:ASP:CB	2.55	0.55
7:G:16:SER:O	7:G:20:GLN:N	2.38	0.55
7:G:507:LEU:HD23	7:G:510:ARG:HH12	1.72	0.55
1:A:1067:PHE:O	1:A:1245:ARG:N	2.40	0.54
3:C:240:ILE:O	3:C:244:LYS:N	2.39	0.54
3:C:280:MET:HA	3:C:282:GLY:HA3	1.88	0.54
5:E:576:MET:O	5:E:580:VAL:CB	2.55	0.54
6:F:275:SER:HA	6:F:277:MET:H	1.71	0.54
7:G:377:SER:HA	7:G:380:ARG:HG2	1.88	0.54
1:A:1030:ILE:O	1:A:1035:SER:N	2.35	0.54
3:C:8:GLN:O	3:C:12:LEU:CB	2.54	0.54
5:E:736:ILE:O	5:E:740:ASN:CB	2.55	0.54
8:H:528:SER:HA	8:H:531:GLN:HB3	1.89	0.54
8:H:608:GLU:OE1	8:H:610:VAL:N	2.40	0.54
1:A:1156:ASP:O	1:A:1160:THR:N	2.40	0.54
4:D:763:LEU:O	4:D:767:LYS:CB	2.56	0.54
5:E:105:GLN:O	5:E:109:HIS:CB	2.55	0.54
6:F:244:ASN:O	6:F:248:GLY:N	2.41	0.54
8:H:269:GLN:O	8:H:273:GLN:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:285:ASN:O	4:D:289:PHE:CB	2.55	0.54
6:F:461:LEU:O	6:F:465:VAL:N	2.40	0.54
2:B:131:ASN:O	2:B:135:ARG:N	2.40	0.54
2:B:259:TYR:O	2:B:263:LEU:CB	2.56	0.54
3:C:304:SER:O	3:C:308:MET:CB	2.55	0.54
4:D:124:LEU:O	4:D:128:LEU:CB	2.55	0.54
4:D:364:SER:O	4:D:368:LYS:CB	2.55	0.54
5:E:78:GLU:O	5:E:82:LYS:N	2.39	0.54
1:A:1046:THR:O	1:A:1050:THR:CB	2.55	0.54
2:B:149:GLN:HA	2:B:153:LYS:H	1.71	0.54
2:B:939:GLN:HA	2:B:941:ASP:H	1.72	0.54
3:C:300:GLY:O	3:C:304:SER:CB	2.55	0.54
5:E:797:TYR:HA	5:E:800:ALA:HB3	1.90	0.54
7:G:34:LYS:O	7:G:38:ALA:CB	2.56	0.54
7:G:174:TYR:HD1	7:G:178:GLN:HE22	1.55	0.54
7:G:19:LEU:O	7:G:23:SER:N	2.41	0.54
5:E:740:ASN:O	5:E:744:LEU:CB	2.56	0.54
7:G:589:TYR:O	7:G:593:TYR:CB	2.50	0.54
3:C:462:LEU:N	3:C:551:ASP:OD2	2.41	0.54
3:C:598:LEU:HA	3:C:601:ILE:HD12	1.89	0.54
3:C:668:LEU:HD13	3:C:749:LEU:HD11	1.90	0.54
3:C:751:VAL:O	3:C:755:LYS:N	2.41	0.54
6:F:737:LEU:O	6:F:741:PHE:CB	2.55	0.54
3:C:142:LEU:O	3:C:146:HIS:CB	2.56	0.54
5:E:708:PHE:O	5:E:712:LEU:CB	2.56	0.54
6:F:711:GLU:O	6:F:716:SER:N	2.40	0.54
6:F:754:THR:H	6:F:758:ILE:H	1.54	0.54
8:H:744:PHE:O	8:H:748:ASN:HB2	2.08	0.54
2:B:134:ASP:O	2:B:138:SER:CB	2.57	0.53
6:F:389:LEU:O	6:F:393:GLN:N	2.41	0.53
3:C:572:LYS:O	3:C:576:LYS:CB	2.57	0.53
4:D:905:PHE:O	4:D:909:ASP:CB	2.57	0.53
5:E:412:ILE:O	5:E:416:THR:N	2.41	0.53
5:E:701:ILE:O	5:E:705:SER:CB	2.56	0.53
5:E:769:LEU:O	5:E:773:LEU:N	2.40	0.53
7:G:195:GLY:O	7:G:199:GLN:CB	2.55	0.53
8:H:706:ASP:HA	8:H:709:LEU:HD13	1.90	0.53
2:B:139:ASP:O	2:B:143:GLN:CB	2.57	0.53
4:D:389:VAL:HA	4:D:391:ASP:H	1.73	0.53
5:E:318:MET:O	5:E:322:ILE:N	2.41	0.53
5:E:705:SER:O	5:E:709:SER:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:SER:O	5:E:83:GLU:N	2.42	0.53
6:F:738:THR:O	6:F:742:MET:CB	2.56	0.53
3:C:18:SER:O	3:C:22:VAL:N	2.36	0.53
3:C:648:LEU:O	3:C:652:PHE:CB	2.57	0.53
6:F:133:LYS:O	6:F:137:ARG:CB	2.56	0.53
1:A:1025:TYR:O	1:A:1029:GLU:N	2.40	0.53
2:B:747:ALA:O	2:B:751:ASN:CB	2.56	0.53
4:D:325:ARG:O	4:D:329:LEU:CB	2.57	0.53
8:H:461:ILE:O	8:H:465:PHE:CB	2.57	0.53
1:A:706:ILE:O	1:A:710:GLU:CB	2.56	0.53
5:E:199:MET:O	5:E:203:LEU:CB	2.57	0.53
3:C:194:GLY:O	3:C:198:ASP:CB	2.57	0.53
3:C:236:LYS:O	3:C:240:ILE:CB	2.57	0.53
3:C:628:GLN:O	3:C:632:THR:HB	2.08	0.53
4:D:123:ASN:O	4:D:127:CYS:CB	2.56	0.53
4:D:417:ALA:O	4:D:421:MET:CB	2.57	0.53
5:E:104:THR:O	5:E:108:ILE:CB	2.57	0.53
5:E:187:LYS:N	5:E:190:LYS:O	2.41	0.53
5:E:396:SER:O	5:E:400:TYR:CB	2.57	0.53
7:G:184:TRP:O	7:G:188:TYR:HB3	2.09	0.53
4:D:352:GLU:O	4:D:356:ASN:CB	2.57	0.53
5:E:608:LEU:O	5:E:613:SER:N	2.38	0.53
6:F:257:GLU:O	6:F:261:ILE:CB	2.57	0.53
5:E:316:THR:HA	5:E:318:MET:H	1.74	0.53
8:H:456:GLU:O	8:H:460:ARG:CB	2.57	0.53
2:B:944:ARG:O	2:B:948:CYS:CB	2.57	0.53
4:D:362:THR:O	4:D:366:ARG:CB	2.57	0.53
5:E:86:ASN:O	5:E:90:GLU:N	2.42	0.53
6:F:840:ASN:O	6:F:844:ILE:CB	2.57	0.53
7:G:466:ASN:HD21	7:G:472:ILE:HD12	1.74	0.53
5:E:773:LEU:O	5:E:778:SER:N	2.36	0.52
7:G:195:GLY:O	7:G:199:GLN:HB2	2.09	0.52
7:G:161:PRO:HG3	7:G:213:CYS:HB3	1.91	0.52
1:A:1159:GLU:O	1:A:1163:LEU:CB	2.57	0.52
1:A:688:ILE:O	1:A:692:LEU:N	2.39	0.52
2:B:239:LEU:O	2:B:243:LEU:CB	2.58	0.52
5:E:684:SER:O	5:E:688:LYS:CB	2.57	0.52
6:F:194:VAL:O	6:F:198:LEU:CB	2.57	0.52
2:B:136:LEU:O	2:B:140:ILE:CB	2.57	0.52
3:C:555:ALA:O	3:C:559:ALA:CB	2.52	0.52
4:D:279:SER:O	4:D:283:ASN:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:720:GLU:O	4:D:724:GLU:CB	2.58	0.52
4:D:912:ASN:O	4:D:916:LEU:CB	2.57	0.52
5:E:660:ILE:O	5:E:664:PHE:CB	2.57	0.52
6:F:308:GLN:O	6:F:312:PHE:N	2.40	0.52
8:H:171:THR:O	8:H:175:LYS:CB	2.57	0.52
1:A:693:SER:O	1:A:697:MET:CB	2.58	0.52
2:B:363:ASN:O	2:B:367:ASN:CB	2.57	0.52
3:C:61:SER:O	3:C:65:VAL:CB	2.58	0.52
7:G:427:LEU:HG	7:G:496:LEU:HD23	1.91	0.52
5:E:379:TYR:O	5:E:383:LEU:CB	2.58	0.52
5:E:620:GLU:O	5:E:624:TRP:N	2.42	0.52
7:G:104:VAL:O	7:G:108:ASP:HB2	2.09	0.52
8:H:749:SER:HA	8:H:752:ILE:HD12	1.91	0.52
6:F:141:SER:O	6:F:145:LEU:CB	2.57	0.52
8:H:613:LYS:NZ	8:H:677:ASP:OD2	2.38	0.52
5:E:586:ARG:O	5:E:590:LEU:CB	2.58	0.52
7:G:492:LEU:HA	7:G:495:MET:HB2	1.92	0.52
2:B:597:CYS:O	2:B:601:LEU:CB	2.58	0.52
3:C:735:TRP:O	3:C:739:LEU:HB3	2.09	0.52
4:D:996:ARG:O	4:D:1000:SER:CB	2.58	0.52
5:E:369:ARG:O	5:E:373:SER:CB	2.58	0.52
6:F:863:LYS:O	6:F:867:PHE:CB	2.58	0.52
7:G:203:VAL:O	7:G:207:SER:CB	2.58	0.52
8:H:187:PHE:O	8:H:191:LYS:N	2.38	0.52
8:H:357:LEU:HA	8:H:364:PRO:HA	1.91	0.52
8:H:432:GLU:O	8:H:436:LEU:CB	2.58	0.52
4:D:821:ALA:O	4:D:825:PHE:CB	2.58	0.51
6:F:603:ASN:O	6:F:607:ARG:N	2.44	0.51
2:B:143:GLN:O	2:B:147:LEU:CB	2.59	0.51
2:B:192:VAL:O	2:B:196:ASN:N	2.40	0.51
3:C:191:LEU:O	3:C:195:LEU:CB	2.58	0.51
5:E:650:THR:O	5:E:654:ASP:CB	2.59	0.51
6:F:841:GLU:O	6:F:845:ARG:CB	2.58	0.51
6:F:881:VAL:O	6:F:885:SER:CB	2.58	0.51
7:G:8:ASP:O	7:G:12:VAL:CB	2.58	0.51
7:G:272:LEU:HD23	7:G:322:LYS:HG2	1.92	0.51
7:G:316:LYS:O	7:G:320:ARG:NH1	2.43	0.51
7:G:374:ASP:O	7:G:378:ARG:HB2	2.10	0.51
3:C:387:PHE:O	3:C:391:PHE:CB	2.58	0.51
3:C:426:ILE:HG23	3:C:475:GLN:HE21	1.76	0.51
3:C:448:ARG:HH22	3:C:513:GLU:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:768:ILE:O	3:C:772:ALA:CB	2.58	0.51
5:E:619:LEU:O	5:E:623:TYR:N	2.44	0.51
5:E:655:LEU:O	5:E:659:SER:CB	2.59	0.51
6:F:226:PHE:O	6:F:230:VAL:CB	2.58	0.51
8:H:226:TYR:O	8:H:230:MET:CB	2.58	0.51
8:H:318:GLU:O	8:H:322:ASP:CB	2.58	0.51
3:C:499:LEU:HD23	3:C:502:ARG:HD3	1.92	0.51
3:C:627:GLN:O	3:C:631:ASP:HB2	2.11	0.51
7:G:543:GLU:O	7:G:547:GLU:CB	2.53	0.51
8:H:170:SER:O	8:H:174:ARG:CB	2.59	0.51
8:H:557:GLU:OE2	8:H:621:LYS:NZ	2.40	0.51
2:B:354:ILE:HA	2:B:357:TRP:H	1.76	0.51
3:C:112:ILE:O	3:C:116:VAL:CB	2.58	0.51
3:C:465:THR:HG23	3:C:502:ARG:HH22	1.74	0.51
5:E:739:VAL:O	5:E:743:ASN:CB	2.59	0.51
8:H:348:LEU:HA	8:H:373:LEU:HA	1.92	0.51
4:D:113:SER:O	4:D:117:ALA:N	2.40	0.51
5:E:82:LYS:O	5:E:86:ASN:N	2.42	0.51
6:F:111:THR:O	6:F:115:GLU:CB	2.58	0.51
7:G:520:ARG:O	7:G:524:ALA:CB	2.59	0.51
7:G:588:MET:O	7:G:592:PHE:CB	2.56	0.51
8:H:233:ASN:O	8:H:237:ASN:CB	2.59	0.51
1:A:1288:CYS:O	1:A:1293:SER:N	2.42	0.51
2:B:613:THR:O	2:B:617:GLN:CB	2.59	0.51
3:C:559:ALA:HB1	3:C:582:LEU:HD22	1.93	0.51
4:D:128:LEU:O	4:D:132:ASN:CB	2.59	0.51
8:H:404:THR:N	8:H:415:PHE:O	2.43	0.51
4:D:927:ASN:O	4:D:931:ILE:N	2.42	0.51
2:B:611:PHE:O	2:B:615:LEU:CB	2.59	0.51
4:D:997:LEU:O	4:D:1001:GLU:CB	2.59	0.51
5:E:346:HIS:O	5:E:351:PHE:N	2.44	0.51
5:E:642:PHE:O	5:E:646:ILE:CB	2.58	0.51
6:F:865:GLN:O	6:F:869:SER:CB	2.58	0.51
7:G:114:ILE:HA	7:G:121:ARG:HG2	1.93	0.51
7:G:30:ASN:O	7:G:34:LYS:CB	2.59	0.51
7:G:310:GLU:O	7:G:313:ASN:HB2	2.11	0.51
1:A:1024:PHE:O	1:A:1028:ASN:N	2.43	0.50
3:C:67:SER:O	3:C:71:GLN:CB	2.58	0.50
5:E:686:ILE:O	5:E:690:GLU:CB	2.59	0.50
6:F:269:GLN:O	6:F:273:THR:CB	2.59	0.50
8:H:225:SER:O	8:H:229:ILE:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:SER:O	2:B:264:THR:CB	2.59	0.50
4:D:322:GLY:O	4:D:326:ILE:CB	2.59	0.50
4:D:92:VAL:O	4:D:96:HIS:N	2.36	0.50
5:E:578:LYS:O	5:E:582:GLU:CB	2.59	0.50
1:A:1158:MET:O	1:A:1162:SER:CB	2.60	0.50
4:D:110:ALA:O	4:D:114:ILE:N	2.42	0.50
6:F:333:ASN:O	6:F:337:GLU:CB	2.59	0.50
7:G:161:PRO:HD2	7:G:217:LEU:HG	1.94	0.50
8:H:208:THR:O	8:H:212:ILE:CB	2.59	0.50
2:B:140:ILE:O	2:B:144:SER:CB	2.59	0.50
3:C:262:GLU:H	3:C:265:LYS:H	1.58	0.50
3:C:305:ILE:O	3:C:309:PHE:CB	2.60	0.50
4:D:328:PHE:O	4:D:332:THR:CB	2.60	0.50
6:F:735:ASP:O	6:F:739:ARG:N	2.43	0.50
7:G:339:GLN:O	7:G:343:SER:CB	2.59	0.50
8:H:214:VAL:O	8:H:218:VAL:CB	2.59	0.50
8:H:460:ARG:O	8:H:464:SER:CB	2.60	0.50
1:A:794:ARG:O	1:A:798:TYR:CB	2.59	0.50
2:B:349:SER:O	2:B:351:GLU:N	2.36	0.50
3:C:637:LEU:HD21	3:C:652:PHE:HE2	1.75	0.50
5:E:397:LEU:O	5:E:401:PHE:CB	2.60	0.50
5:E:768:GLU:O	5:E:772:LEU:N	2.41	0.50
7:G:162:GLN:HB2	7:G:217:LEU:HD21	1.93	0.50
8:H:703:LYS:O	8:H:707:LYS:HB2	2.10	0.50
1:A:1087:PRO:O	1:A:1091:LYS:CB	2.59	0.50
5:E:156:GLN:O	5:E:160:GLN:CB	2.60	0.50
6:F:634:GLU:O	6:F:638:PHE:N	2.42	0.50
7:G:13:LEU:O	7:G:17:GLN:N	2.41	0.50
8:H:529:THR:HG22	8:H:569:LEU:HD13	1.93	0.50
1:A:893:GLU:O	1:A:897:SER:CB	2.59	0.50
5:E:384:HIS:O	5:E:388:THR:CB	2.60	0.50
5:E:574:ASP:O	5:E:578:LYS:CB	2.60	0.50
7:G:199:GLN:NE2	7:G:267:SER:OG	2.45	0.50
7:G:258:ASP:HA	7:G:261:TYR:HE2	1.77	0.50
7:G:339:GLN:O	7:G:343:SER:HB2	2.12	0.50
1:A:697:MET:O	1:A:701:ASN:CB	2.59	0.50
1:A:812:GLU:O	1:A:816:LYS:CB	2.60	0.50
3:C:108:ILE:O	3:C:112:ILE:CB	2.59	0.50
3:C:661:ILE:HA	3:C:664:PHE:HB3	1.93	0.50
1:A:1047:ARG:O	1:A:1051:GLN:CB	2.60	0.50
2:B:897:GLY:O	2:B:938:PHE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:360:TYR:O	3:C:364:LEU:CB	2.59	0.50
5:E:697:LEU:O	5:E:701:ILE:CB	2.60	0.50
5:E:696:ILE:O	5:E:700:THR:CB	2.60	0.50
3:C:235:ILE:O	3:C:239:GLU:CB	2.59	0.49
3:C:597:SER:O	3:C:600:LEU:HB2	2.12	0.49
4:D:647:THR:O	4:D:649:ASN:N	2.42	0.49
8:H:446:ASP:O	8:H:450:ILE:CB	2.59	0.49
1:A:1045:VAL:O	1:A:1049:TYR:CB	2.60	0.49
2:B:263:LEU:O	2:B:267:ARG:N	2.43	0.49
7:G:109:ASP:HA	7:G:112:GLU:HB2	1.94	0.49
7:G:340:VAL:O	7:G:344:LEU:CB	2.60	0.49
3:C:362:LYS:O	3:C:366:SER:CB	2.60	0.49
7:G:334:THR:HA	7:G:337:VAL:HG12	1.94	0.49
7:G:388:GLY:O	7:G:392:ALA:CB	2.61	0.49
8:H:444:LYS:O	8:H:448:CYS:CB	2.61	0.49
1:A:1161:ILE:O	1:A:1165:VAL:CB	2.61	0.49
2:B:369:LEU:O	2:B:373:SER:CB	2.61	0.49
2:B:466:LEU:O	2:B:470:LYS:CB	2.60	0.49
3:C:503:GLN:HA	3:C:506:TRP:HD1	1.78	0.49
5:E:77:PHE:O	5:E:81:LEU:N	2.42	0.49
6:F:879:THR:O	6:F:883:ASP:CB	2.61	0.49
7:G:470:GLN:HE22	7:G:563:THR:HA	1.77	0.49
1:A:1198:VAL:O	1:A:1202:SER:CB	2.61	0.49
2:B:8:ASP:HA	3:C:142:LEU:HA	1.95	0.49
3:C:734:ILE:O	3:C:738:TYR:CB	2.60	0.49
6:F:144:GLU:O	6:F:148:LYS:CB	2.61	0.49
7:G:481:THR:O	7:G:485:GLN:HB2	2.13	0.49
7:G:539:SER:OG	7:G:541:ASP:O	2.31	0.49
8:H:527:SER:O	8:H:531:GLN:N	2.38	0.49
1:A:797:PHE:O	1:A:801:VAL:CB	2.61	0.49
2:B:501:ILE:O	2:B:505:LYS:CB	2.61	0.49
5:E:760:THR:O	5:E:764:LEU:CB	2.61	0.49
6:F:623:VAL:O	6:F:627:TYR:CB	2.60	0.49
7:G:142:GLU:HB3	7:G:146:ARG:HH12	1.77	0.49
4:D:719:ILE:O	4:D:723:LYS:CB	2.60	0.49
5:E:679:ILE:O	5:E:684:SER:N	2.44	0.49
6:F:115:GLU:O	6:F:119:ILE:CB	2.60	0.49
6:F:726:GLN:O	6:F:730:ILE:N	2.46	0.49
7:G:10:ALA:O	7:G:14:VAL:CB	2.61	0.49
7:G:209:LEU:HA	7:G:212:LYS:HD2	1.95	0.49
8:H:212:ILE:O	8:H:216:GLU:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:772:ILE:HA	4:D:773:ASP:HA	1.59	0.49
5:E:651:GLU:O	5:E:655:LEU:CB	2.61	0.49
7:G:525:ASN:HA	7:G:528:ASP:HB2	1.94	0.49
1:A:1165:VAL:O	1:A:1169:TRP:CB	2.60	0.48
1:A:699:MET:O	1:A:703:SER:CB	2.61	0.48
5:E:61:ARG:O	5:E:65:TRP:N	2.46	0.48
6:F:706:LEU:O	6:F:710:LEU:N	2.44	0.48
8:H:213:GLN:O	8:H:217:GLU:CB	2.61	0.48
3:C:52:GLU:O	3:C:56:LYS:CB	2.61	0.48
5:E:106:GLU:O	5:E:110:SER:CB	2.61	0.48
6:F:424:SER:O	6:F:428:PHE:CB	2.62	0.48
7:G:338:ARG:O	7:G:342:GLN:HB2	2.13	0.48
7:G:40:SER:O	7:G:44:SER:CB	2.61	0.48
7:G:51:LEU:O	7:G:55:ASN:CB	2.61	0.48
8:H:536:LEU:O	8:H:540:VAL:N	2.44	0.48
3:C:547:ALA:HA	3:C:550:ASN:HD22	1.79	0.48
5:E:333:SER:O	5:E:337:LYS:CB	2.61	0.48
5:E:353:GLN:O	5:E:357:ALA:CB	2.62	0.48
5:E:759:GLN:O	5:E:763:THR:CB	2.62	0.48
6:F:730:ILE:O	6:F:735:ASP:N	2.46	0.48
7:G:436:ASP:OD2	7:G:503:ARG:NH2	2.46	0.48
8:H:223:ASN:O	8:H:227:ASN:CB	2.61	0.48
8:H:328:LEU:O	8:H:332:VAL:CB	2.61	0.48
8:H:547:LEU:HD21	8:H:595:ILE:HG12	1.95	0.48
3:C:382:LEU:O	3:C:386:ALA:HB3	2.13	0.48
3:C:467:THR:O	3:C:471:MET:CB	2.62	0.48
3:C:735:TRP:CD1	3:C:772:ALA:HB1	2.48	0.48
4:D:111:VAL:O	4:D:115:MET:N	2.39	0.48
4:D:74:ARG:O	4:D:78:PHE:CB	2.62	0.48
5:E:252:ASN:O	5:E:256:ILE:CB	2.62	0.48
5:E:567:ASN:H	5:E:570:LEU:H	1.60	0.48
6:F:261:ILE:O	6:F:265:GLU:CB	2.61	0.48
7:G:249:PHE:O	7:G:253:GLU:HB3	2.14	0.48
3:C:269:TYR:O	3:C:274:GLY:N	2.47	0.48
5:E:652:ILE:O	5:E:656:LEU:CB	2.62	0.48
1:A:700:SER:O	1:A:704:ASN:CB	2.61	0.48
4:D:961:MET:O	4:D:965:SER:CB	2.62	0.48
7:G:231:PRO:O	7:G:301:PHE:N	2.39	0.48
7:G:542:LYS:HG2	7:G:545:ILE:HD12	1.95	0.48
8:H:739:TYR:OH	8:H:740:LYS:NZ	2.47	0.48
1:A:798:TYR:O	1:A:802:THR:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:O	2:B:329:ASN:CB	2.62	0.48
5:E:568:TYR:H	5:E:572:ASP:H	1.61	0.48
5:E:741:ILE:O	5:E:745:ILE:CB	2.62	0.48
7:G:18:GLU:O	7:G:22:THR:N	2.43	0.48
7:G:249:PHE:O	7:G:253:GLU:CB	2.61	0.48
8:H:266:LYS:O	8:H:270:LEU:CB	2.62	0.48
5:E:325:VAL:O	5:E:329:ILE:CB	2.62	0.48
6:F:672:ILE:O	6:F:676:ASP:CB	2.62	0.48
1:A:868:PRO:O	1:A:872:GLU:CB	2.62	0.47
2:B:824:LEU:O	2:B:827:THR:CB	2.61	0.47
5:E:180:VAL:HA	5:E:181:GLU:HA	1.66	0.47
7:G:433:ASP:OD1	7:G:503:ARG:NH2	2.35	0.47
1:A:670:ILE:O	1:A:674:ILE:N	2.46	0.47
2:B:155:PHE:O	2:B:159:VAL:N	2.44	0.47
2:B:351:GLU:O	2:B:355:LEU:N	2.47	0.47
3:C:597:SER:HA	3:C:600:LEU:HD22	1.95	0.47
4:D:825:PHE:O	4:D:829:ILE:CB	2.61	0.47
4:D:902:ASN:O	4:D:906:ILE:CB	2.62	0.47
5:E:87:LEU:O	5:E:91:THR:N	2.47	0.47
7:G:426:LEU:HA	7:G:429:CYS:HB3	1.96	0.47
7:G:591:ARG:HD3	7:G:595:ARG:HH22	1.79	0.47
1:A:856:GLN:O	1:A:860:GLU:N	2.47	0.47
1:A:928:GLU:O	1:A:932:THR:CB	2.62	0.47
3:C:148:LEU:O	3:C:152:ALA:N	2.47	0.47
3:C:193:ASP:O	3:C:197:TYR:CB	2.62	0.47
3:C:198:ASP:O	3:C:202:MET:N	2.47	0.47
3:C:723:LEU:HB3	3:C:753:ILE:HD13	1.95	0.47
4:D:288:GLN:O	4:D:292:ASP:CB	2.62	0.47
4:D:381:ASN:HA	4:D:382:ASP:HA	1.62	0.47
5:E:29:PHE:O	5:E:34:SER:N	2.40	0.47
8:H:218:VAL:O	8:H:222:ILE:CB	2.62	0.47
8:H:563:GLU:O	8:H:567:GLU:HB2	2.14	0.47
1:A:677:TYR:O	1:A:681:VAL:CB	2.62	0.47
2:B:74:GLU:O	2:B:78:TYR:CB	2.62	0.47
5:E:445:ALA:O	5:E:449:ASP:CB	2.63	0.47
5:E:577:LEU:O	5:E:581:VAL:CB	2.62	0.47
2:B:372:LEU:O	2:B:376:MET:CB	2.63	0.47
3:C:109:TYR:O	3:C:113:TYR:CB	2.62	0.47
4:D:327:GLY:O	4:D:331:LYS:CB	2.62	0.47
5:E:443:LEU:O	5:E:447:LEU:CB	2.63	0.47
7:G:104:VAL:O	7:G:108:ASP:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:312:ILE:HD12	7:G:315:VAL:HB	1.96	0.47
2:B:821:LYS:O	2:B:825:ARG:N	2.47	0.47
3:C:111:ARG:O	3:C:115:PHE:CB	2.62	0.47
3:C:775:MET:O	3:C:779:TYR:CB	2.63	0.47
4:D:119:GLU:O	4:D:124:LEU:N	2.48	0.47
6:F:497:PHE:O	6:F:500:GLU:N	2.43	0.47
8:H:227:ASN:O	8:H:231:THR:CB	2.63	0.47
8:H:253:LEU:O	8:H:257:LEU:N	2.43	0.47
3:C:196:THR:O	3:C:200:VAL:CB	2.63	0.47
4:D:218:HIS:O	4:D:222:ASN:CB	2.63	0.47
3:C:707:ASP:O	3:C:711:THR:N	2.48	0.47
6:F:560:THR:O	6:F:564:ALA:HB3	2.15	0.47
8:H:243:LEU:O	8:H:247:ARG:CB	2.63	0.47
1:A:1089:GLY:O	1:A:1093:SER:CB	2.62	0.47
2:B:19:THR:HA	2:B:20:ILE:HA	1.64	0.47
5:E:225:GLU:O	5:E:229:GLU:CB	2.63	0.47
5:E:447:LEU:O	5:E:451:THR:CB	2.63	0.47
5:E:76:THR:O	5:E:80:THR:N	2.44	0.47
4:D:190:ARG:O	4:D:194:LEU:CB	2.63	0.47
5:E:571:ASN:O	5:E:575:SER:N	2.48	0.47
8:H:172:SER:O	8:H:176:MET:CB	2.63	0.47
1:A:1294:CYS:O	1:A:1298:GLN:N	2.48	0.46
3:C:716:VAL:HG23	3:C:738:TYR:HE1	1.81	0.46
4:D:942:GLN:O	4:D:946:ARG:CB	2.63	0.46
6:F:705:ASP:O	6:F:709:PHE:N	2.43	0.46
7:G:374:ASP:O	7:G:378:ARG:CB	2.63	0.46
2:B:7:GLY:HA3	3:C:146:HIS:HA	1.98	0.46
3:C:37:GLU:O	3:C:41:ASN:CB	2.64	0.46
5:E:648:MET:O	5:E:652:ILE:CB	2.64	0.46
6:F:493:SER:HA	6:F:496:ALA:HB3	1.97	0.46
7:G:330:LEU:O	7:G:334:THR:OG1	2.29	0.46
1:A:676:PRO:O	1:A:680:LYS:CB	2.64	0.46
3:C:628:GLN:O	3:C:632:THR:CB	2.63	0.46
3:C:731:ILE:HG13	3:C:768:ILE:HG21	1.96	0.46
5:E:84:LEU:O	5:E:88:ASN:N	2.45	0.46
3:C:3:SER:O	3:C:7:GLN:N	2.41	0.46
3:C:735:TRP:O	3:C:739:LEU:HB2	2.15	0.46
4:D:252:ILE:HA	4:D:253:ILE:HA	1.61	0.46
5:E:253:GLU:O	5:E:257:ILE:CB	2.64	0.46
5:E:584:THR:O	5:E:588:MET:CB	2.64	0.46
6:F:112:SER:O	6:F:116:ILE:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:ASN:HA	7:G:390:LEU:HD12	1.97	0.46
8:H:358:ASN:N	8:H:363:LYS:O	2.47	0.46
8:H:475:PRO:HA	8:H:476:GLY:HA3	1.56	0.46
2:B:545:SER:O	2:B:549:ASN:CB	2.63	0.46
2:B:707:LEU:HA	7:G:604:ARG:HH21	1.79	0.46
2:B:961:LYS:HA	2:B:964:ALA:HB2	1.98	0.46
3:C:301:ILE:O	3:C:305:ILE:CB	2.64	0.46
3:C:308:MET:O	3:C:312:MET:CB	2.63	0.46
5:E:354:ARG:O	5:E:358:GLN:CB	2.64	0.46
5:E:746:PHE:O	5:E:751:LYS:N	2.48	0.46
7:G:267:SER:O	7:G:271:VAL:N	2.40	0.46
8:H:563:GLU:O	8:H:567:GLU:CB	2.62	0.46
1:A:1029:GLU:O	1:A:1033:LEU:N	2.46	0.46
2:B:881:GLN:O	2:B:885:ALA:CB	2.64	0.46
3:C:470:GLN:HG2	3:C:558:TYR:HE2	1.80	0.46
4:D:916:LEU:O	4:D:920:ALA:CB	2.63	0.46
8:H:383:SER:HA	8:H:384:ARG:HA	1.74	0.46
8:H:642:ASP:HA	8:H:645:LEU:HD13	1.98	0.46
2:B:421:LYS:HA	2:B:422:ASP:HA	1.70	0.46
2:B:461:ILE:O	2:B:465:TRP:CB	2.63	0.46
2:B:75:SER:O	2:B:79:ILE:CB	2.63	0.46
7:G:341:THR:OG1	7:G:342:GLN:N	2.49	0.46
2:B:462:ILE:O	2:B:466:LEU:CB	2.64	0.46
1:A:927:THR:O	1:A:931:GLN:N	2.38	0.46
2:B:254:GLU:HA	2:B:258:GLU:H	1.80	0.46
2:B:901:ASN:HA	2:B:902:ASP:HA	1.60	0.46
3:C:227:ARG:O	3:C:231:ILE:CB	2.64	0.46
3:C:265:LYS:HA	3:C:266:VAL:HA	1.57	0.46
3:C:303:ASN:O	3:C:307:GLU:CB	2.63	0.46
5:E:353:GLN:O	5:E:357:ALA:HB3	2.16	0.46
6:F:704:ILE:O	6:F:708:GLN:N	2.48	0.46
7:G:33:LEU:O	7:G:37:ALA:CB	2.56	0.46
7:G:459:ALA:HA	7:G:510:ARG:HD3	1.98	0.46
7:G:77:LEU:O	7:G:81:ALA:CB	2.64	0.46
1:A:689:ILE:O	1:A:693:SER:CB	2.64	0.46
1:A:795:LEU:O	1:A:799:GLU:CB	2.64	0.46
2:B:848:GLY:O	2:B:852:ILE:N	2.45	0.46
2:B:962:ARG:HA	2:B:963:THR:HA	1.75	0.46
3:C:620:TRP:HE1	3:C:626:ALA:HB2	1.80	0.46
4:D:858:PHE:HA	4:D:859:PHE:HA	1.81	0.46
5:E:573:VAL:O	5:E:577:LEU:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:CYS:H	2:B:183:ASP:HA	1.81	0.45
4:D:290:ILE:O	4:D:294:SER:CB	2.64	0.45
4:D:420:GLU:O	4:D:424:ILE:N	2.39	0.45
4:D:75:TYR:O	4:D:79:ASN:CB	2.65	0.45
5:E:345:THR:HA	5:E:346:HIS:HA	1.60	0.45
7:G:485:GLN:HA	7:G:488:GLU:HB2	1.99	0.45
2:B:76:LEU:O	2:B:80:ARG:CB	2.64	0.45
3:C:197:TYR:O	3:C:201:GLU:CB	2.64	0.45
4:D:210:ASN:O	4:D:214:GLU:CB	2.65	0.45
5:E:89:GLU:O	5:E:93:ASN:CB	2.65	0.45
7:G:574:LYS:O	7:G:578:LYS:HB2	2.15	0.45
1:A:831:ILE:O	1:A:835:THR:CB	2.63	0.45
1:A:863:ASN:O	1:A:867:GLN:N	2.49	0.45
3:C:258:ARG:HA	3:C:259:LEU:HA	1.68	0.45
3:C:469:PHE:HB3	3:C:558:TYR:CD2	2.51	0.45
5:E:659:SER:O	5:E:663:ILE:CB	2.64	0.45
6:F:569:SER:O	6:F:573:ALA:CB	2.64	0.45
6:F:601:ILE:O	6:F:603:ASN:N	2.49	0.45
7:G:247:LEU:HD11	7:G:314:ASP:HB3	1.98	0.45
8:H:259:GLN:O	8:H:263:ILE:N	2.49	0.45
1:A:810:VAL:O	1:A:814:GLN:CB	2.64	0.45
7:G:195:GLY:HA2	7:G:198:ILE:HG22	1.98	0.45
8:H:673:GLU:O	8:H:677:ASP:HB2	2.16	0.45
1:A:1022:LEU:O	1:A:1026:LEU:N	2.48	0.45
3:C:714:PHE:HA	3:C:717:MET:HB2	1.98	0.45
4:D:572:PRO:HA	4:D:573:SER:HA	1.50	0.45
4:D:931:ILE:O	4:D:935:LEU:CB	2.64	0.45
6:F:230:VAL:O	6:F:234:GLU:CB	2.65	0.45
6:F:602:VAL:O	6:F:606:ILE:N	2.48	0.45
7:G:135:GLU:HA	7:G:138:ILE:HD12	1.98	0.45
1:A:936:GLU:O	1:A:940:TYR:N	2.50	0.45
3:C:751:VAL:HA	3:C:765:ARG:HD2	1.98	0.45
5:E:649:SER:O	5:E:653:LEU:CB	2.64	0.45
8:H:417:PHE:HA	8:H:422:SER:HA	1.99	0.45
2:B:881:GLN:O	2:B:885:ALA:HB2	2.17	0.45
3:C:58:LEU:O	3:C:62:LYS:CB	2.64	0.45
6:F:195:LEU:O	6:F:199:ASP:CB	2.64	0.45
4:D:718:SER:O	4:D:722:PHE:CB	2.64	0.45
6:F:228:GLN:O	6:F:232:LYS:CB	2.65	0.45
8:H:585:SER:HA	8:H:588:ILE:HD12	1.98	0.45
8:H:614:SER:OG	8:H:615:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:506:TRP:HB3	3:C:510:ILE:HD12	1.97	0.45
7:G:211:LEU:O	7:G:215:ALA:CB	2.62	0.45
6:F:714:PHE:O	6:F:719:GLN:N	2.50	0.44
7:G:179:LEU:HD23	7:G:182:LEU:HD12	1.99	0.44
1:A:1009:VAL:HA	1:A:1108:ASP:HA	1.98	0.44
3:C:582:LEU:O	3:C:585:THR:OG1	2.33	0.44
4:D:1048:LYS:O	4:D:1052:LEU:CB	2.65	0.44
5:E:632:ASN:HA	5:E:707:LYS:HA	2.00	0.44
2:B:106:VAL:HA	2:B:107:ASN:HA	1.58	0.44
3:C:546:ILE:O	3:C:550:ASN:ND2	2.51	0.44
4:D:1059:VAL:H	4:D:1063:ASN:HA	1.83	0.44
7:G:105:HIS:O	7:G:109:ASP:CB	2.59	0.44
7:G:339:GLN:HA	7:G:342:GLN:HB3	1.98	0.44
1:A:659:LEU:O	1:A:663:ASN:CB	2.66	0.44
3:C:448:ARG:NH2	3:C:513:GLU:OE1	2.51	0.44
4:D:76:GLU:O	4:D:80:GLN:CB	2.66	0.44
1:A:655:GLU:O	1:A:659:LEU:CB	2.65	0.44
3:C:511:SER:HA	3:C:514:ILE:HD12	1.98	0.44
4:D:1042:LYS:O	4:D:1046:ARG:N	2.51	0.44
4:D:869:VAL:HA	4:D:870:GLY:HA2	1.70	0.44
6:F:622:LEU:O	6:F:626:ASP:N	2.37	0.44
7:G:203:VAL:O	7:G:207:SER:OG	2.27	0.44
7:G:203:VAL:O	7:G:207:SER:HB3	2.17	0.44
7:G:542:LYS:HB3	7:G:546:LYS:HZ3	1.82	0.44
6:F:220:ILE:O	6:F:224:ILE:CB	2.66	0.44
6:F:883:ASP:O	6:F:887:ILE:CB	2.66	0.44
7:G:538:LYS:NZ	7:G:598:ASP:O	2.50	0.44
3:C:591:GLU:O	3:C:594:GLN:HB2	2.17	0.44
4:D:684:HIS:HA	5:E:866:VAL:HA	2.00	0.44
6:F:310:ASP:O	6:F:314:ASP:CB	2.66	0.44
7:G:412:THR:O	7:G:503:ARG:NE	2.48	0.44
8:H:657:LEU:HD11	8:H:705:ILE:HG12	2.00	0.44
3:C:212:ILE:O	3:C:216:LYS:CB	2.66	0.44
3:C:681:PHE:O	3:C:684:ALA:HB3	2.17	0.44
5:E:761:PHE:O	5:E:765:ILE:CB	2.66	0.44
6:F:862:SER:HA	6:F:882:MET:HA	2.00	0.44
8:H:440:ILE:HA	8:H:443:ALA:HB3	1.99	0.44
1:A:1005:SER:O	1:A:1009:VAL:CB	2.66	0.44
2:B:575:SER:HA	2:B:576:ASN:HA	1.67	0.44
3:C:562:ILE:HA	3:C:565:LYS:HB3	2.00	0.44
5:E:693:ILE:O	5:E:697:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:733:GLU:O	6:F:737:LEU:N	2.51	0.44
2:B:322:SER:O	2:B:326:ASN:CB	2.66	0.43
4:D:398:ARG:O	4:D:402:TRP:CB	2.65	0.43
5:E:197:LYS:O	5:E:201:ASN:N	2.51	0.43
2:B:845:PHE:HA	2:B:846:ARG:HA	1.75	0.43
1:A:691:THR:O	1:A:695:PHE:CB	2.66	0.43
2:B:582:PRO:HA	2:B:583:LEU:HA	1.47	0.43
5:E:182:GLN:O	5:E:193:LEU:N	2.44	0.43
5:E:212:SER:H	6:F:67:PHE:HA	1.83	0.43
5:E:763:THR:O	5:E:767:GLU:CB	2.66	0.43
6:F:724:SER:O	6:F:726:GLN:N	2.51	0.43
7:G:312:ILE:HG13	7:G:316:LYS:HE2	2.00	0.43
8:H:252:ASP:O	8:H:256:VAL:N	2.50	0.43
1:A:1167:SER:O	1:A:1171:THR:N	2.49	0.43
3:C:510:ILE:HD11	3:C:548:VAL:HG21	2.00	0.43
3:C:768:ILE:O	3:C:772:ALA:HB2	2.18	0.43
7:G:77:LEU:HD22	7:G:110:MET:HG3	2.00	0.43
2:B:528:LYS:O	2:B:532:ILE:N	2.52	0.43
3:C:325:LEU:O	3:C:329:ASP:CB	2.66	0.43
3:C:657:ILE:HG22	3:C:713:ASN:HD22	1.84	0.43
4:D:202:THR:O	4:D:204:GLU:N	2.51	0.43
5:E:16:LYS:O	5:E:20:PHE:N	2.44	0.43
5:E:32:GLU:O	5:E:36:ASP:N	2.38	0.43
5:E:407:ASP:O	5:E:411:GLN:N	2.51	0.43
5:E:67:GLN:O	5:E:71:LYS:CB	2.66	0.43
6:F:155:ASN:O	6:F:159:SER:CB	2.67	0.43
6:F:89:GLU:O	6:F:93:GLN:CB	2.66	0.43
1:A:1157:TYR:O	1:A:1161:ILE:CB	2.67	0.43
4:D:836:LYS:O	4:D:840:ILE:CB	2.66	0.43
5:E:734:PRO:O	5:E:738:ILE:CB	2.67	0.43
7:G:153:LEU:HD23	7:G:153:LEU:HA	1.81	0.43
7:G:162:GLN:HA	7:G:165:ILE:HB	2.01	0.43
7:G:312:ILE:HD11	7:G:330:LEU:HB3	2.00	0.43
5:E:614:TYR:HA	5:E:618:ALA:HB3	2.01	0.43
7:G:17:GLN:O	7:G:21:LYS:N	2.41	0.43
7:G:573:LEU:HD23	7:G:573:LEU:HA	1.91	0.43
3:C:716:VAL:O	3:C:720:PHE:HB2	2.17	0.43
3:C:748:ASP:HB3	3:C:802:PHE:HB3	2.00	0.43
7:G:60:LEU:O	7:G:64:ILE:CB	2.67	0.43
3:C:621:TYR:HE2	3:C:675:LYS:HD3	1.83	0.43
3:C:724:SER:O	3:C:757:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:VAL:HA	4:D:70:GLY:HA2	1.77	0.43
6:F:227:LEU:O	6:F:231:THR:CB	2.67	0.43
6:F:571:ILE:O	6:F:575:LEU:N	2.52	0.43
8:H:711:ASN:OD1	8:H:711:ASN:N	2.52	0.43
2:B:620:ILE:HA	2:B:621:THR:HA	1.75	0.43
3:C:189:ASP:O	3:C:193:ASP:N	2.42	0.43
4:D:356:ASN:O	4:D:360:LYS:CB	2.67	0.43
5:E:436:PHE:O	5:E:440:LYS:N	2.47	0.43
7:G:349:ILE:HG23	7:G:437:THR:HG21	1.99	0.43
1:A:1292:TRP:O	1:A:1296:GLN:N	2.52	0.42
2:B:275:ALA:HA	2:B:276:SER:HA	1.62	0.42
3:C:451:PRO:HA	3:C:544:TYR:HE1	1.84	0.42
3:C:642:PRO:HG2	3:C:643:GLN:HG3	2.00	0.42
4:D:962:ASN:O	4:D:966:LEU:CB	2.67	0.42
7:G:491:GLU:O	7:G:495:MET:N	2.52	0.42
2:B:354:ILE:O	2:B:358:MET:N	2.39	0.42
3:C:750:LEU:O	3:C:754:LEU:N	2.50	0.42
3:C:735:TRP:HZ2	3:C:776:LEU:HD13	1.84	0.42
4:D:636:ARG:O	4:D:640:ASN:CB	2.67	0.42
6:F:251:LEU:O	6:F:255:GLY:N	2.38	0.42
5:E:213:SER:HA	6:F:73:ASP:H	1.83	0.42
7:G:176:ASP:HA	7:G:179:LEU:HB2	2.01	0.42
7:G:327:TYR:HA	7:G:330:LEU:HD12	2.00	0.42
7:G:368:VAL:HG13	7:G:479:ASN:HD22	1.84	0.42
7:G:98:LYS:O	7:G:102:GLN:HB2	2.19	0.42
6:F:431:GLY:O	6:F:435:ARG:CB	2.67	0.42
7:G:155:SER:O	7:G:157:LYS:NZ	2.50	0.42
3:C:775:MET:O	3:C:779:TYR:HB3	2.19	0.42
7:G:137:LEU:HD13	7:G:140:ARG:HH21	1.84	0.42
7:G:67:THR:OG1	8:H:178:ALA:O	2.37	0.42
2:B:209:LYS:O	2:B:213:LEU:N	2.52	0.42
2:B:67:SER:HA	2:B:68:ARG:HA	1.72	0.42
6:F:503:ILE:O	6:F:507:ASP:N	2.50	0.42
6:F:663:SER:O	6:F:667:ALA:HB2	2.19	0.42
7:G:426:LEU:O	7:G:430:PHE:HB3	2.19	0.42
3:C:149:LEU:HA	3:C:152:ALA:HB3	2.02	0.42
3:C:382:LEU:O	3:C:386:ALA:CB	2.67	0.42
3:C:441:GLU:OE2	3:C:465:THR:N	2.53	0.42
3:C:654:ASP:HB2	3:C:709:LEU:HD13	2.02	0.42
5:E:98:PHE:O	5:E:101:GLN:N	2.52	0.42
6:F:520:LEU:O	6:F:524:VAL:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:569:SER:O	6:F:573:ALA:HB2	2.19	0.42
2:B:188:ASN:HA	2:B:189:GLN:HA	1.88	0.42
2:B:682:GLU:HA	2:B:683:TYR:HA	1.77	0.42
5:E:382:ILE:O	5:E:386:LEU:CB	2.68	0.42
5:E:772:LEU:O	5:E:776:HIS:N	2.48	0.42
6:F:560:THR:O	6:F:564:ALA:CB	2.67	0.42
6:F:646:GLN:HA	6:F:647:ASN:HA	1.83	0.42
7:G:519:TRP:CZ2	7:G:559:LEU:HB3	2.55	0.42
1:A:1036:SER:O	1:A:1038:HIS:N	2.47	0.42
1:A:969:PRO:HA	1:A:970:PRO:HA	1.70	0.42
7:G:165:ILE:HD11	7:G:245:ALA:HB2	2.02	0.42
7:G:276:LEU:O	7:G:280:ILE:N	2.35	0.42
7:G:428:SER:HA	7:G:496:LEU:HD22	2.02	0.42
1:A:1030:ILE:HA	1:A:1034:GLU:H	1.84	0.42
2:B:379:LYS:O	2:B:382:HIS:C	2.58	0.42
3:C:560:VAL:HG22	3:C:583:GLU:HA	2.01	0.42
3:C:545:LEU:HD13	3:C:596:SER:HB2	2.00	0.42
3:C:750:LEU:HA	3:C:753:ILE:HB	2.01	0.42
7:G:338:ARG:O	7:G:342:GLN:CB	2.68	0.42
7:G:366:ASN:HD21	7:G:471:ARG:HH21	1.67	0.42
7:G:398:ARG:HG2	7:G:402:LEU:HD11	2.00	0.42
1:A:768:LEU:O	1:A:772:GLN:N	2.50	0.42
2:B:299:ILE:O	2:B:303:LEU:CB	2.68	0.42
3:C:237:LYS:O	3:C:241:GLU:CB	2.68	0.42
3:C:441:GLU:OE2	3:C:465:THR:OG1	2.32	0.42
4:D:794:GLU:O	4:D:798:LEU:N	2.53	0.42
7:G:402:LEU:HD13	7:G:406:TYR:CZ	2.54	0.42
7:G:484:GLU:O	7:G:488:GLU:N	2.53	0.42
7:G:546:LYS:HD3	7:G:606:HIS:HD2	1.85	0.42
8:H:662:VAL:O	8:H:666:GLN:HB3	2.20	0.42
1:A:903:TRP:HA	1:A:905:THR:H	1.85	0.41
1:A:932:THR:O	1:A:936:GLU:N	2.53	0.41
2:B:900:SER:O	2:B:904:SER:N	2.43	0.41
3:C:420:LYS:HA	3:C:423:LEU:HD12	2.02	0.41
4:D:597:LYS:O	4:D:601:THR:CB	2.68	0.41
5:E:157:ASN:O	5:E:161:SER:CB	2.68	0.41
7:G:181:ALA:O	7:G:185:ILE:HB	2.20	0.41
7:G:547:GLU:O	7:G:551:LYS:HB2	2.19	0.41
7:G:574:LYS:O	7:G:578:LYS:CB	2.68	0.41
1:A:723:LYS:N	4:D:94:ASN:O	2.53	0.41
8:H:338:PHE:N	8:H:339:ILE:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ASN:O	2:B:257:ILE:N	2.36	0.41
2:B:594:GLY:O	2:B:596:SER:N	2.51	0.41
8:H:662:VAL:O	8:H:666:GLN:CB	2.68	0.41
4:D:389:VAL:HA	4:D:391:ASP:N	2.35	0.41
7:G:343:SER:O	7:G:347:ASP:CB	2.69	0.41
1:A:1088:VAL:O	1:A:1092:ASN:CB	2.69	0.41
7:G:179:LEU:HD22	7:G:260:LEU:HD11	2.03	0.41
7:G:379:LEU:HD23	7:G:379:LEU:HA	1.90	0.41
5:E:448:VAL:O	5:E:452:SER:CB	2.68	0.41
6:F:342:LYS:HA	6:F:343:LEU:HA	1.75	0.41
2:B:874:HIS:O	2:B:878:ILE:CB	2.67	0.41
7:G:195:GLY:O	7:G:199:GLN:HB3	2.20	0.41
7:G:412:THR:HB	7:G:506:ARG:HE	1.86	0.41
2:B:250:ASN:H	2:B:251:ASP:C	2.24	0.41
3:C:447:GLU:O	3:C:449:SER:N	2.52	0.41
7:G:476:ILE:HG21	7:G:511:TYR:CZ	2.56	0.41
7:G:548:LYS:O	7:G:552:PHE:CB	2.68	0.41
2:B:520:SER:HA	2:B:521:TYR:HA	1.59	0.41
3:C:455:ASP:H	3:C:460:LEU:HD23	1.84	0.41
4:D:1050:GLY:O	4:D:1054:SER:N	2.54	0.41
4:D:589:TYR:HA	4:D:593:SER:H	1.86	0.41
7:G:344:LEU:HA	7:G:347:ASP:HB3	2.02	0.41
5:E:324:ASP:O	5:E:328:VAL:CB	2.69	0.41
5:E:766:GLY:HA3	5:E:808:SER:H	1.86	0.41
6:F:241:ASN:O	6:F:245:LEU:N	2.51	0.41
2:B:390:ASN:HA	2:B:391:ASN:HA	1.73	0.41
2:B:838:PRO:HA	2:B:903:GLY:N	2.36	0.41
3:C:290:PRO:HA	3:C:291:ARG:HA	1.56	0.41
7:G:173:TYR:HA	7:G:256:LEU:HD22	2.01	0.41
8:H:657:LEU:HD12	8:H:657:LEU:HA	1.88	0.41
1:A:811:GLU:O	1:A:815:LYS:CB	2.69	0.40
2:B:565:LEU:HA	2:B:566:LYS:HA	1.80	0.40
4:D:817:LEU:O	4:D:820:LYS:N	2.54	0.40
7:G:465:LYS:HE2	7:G:465:LYS:HB2	1.90	0.40
2:B:26:TRP:HA	2:B:27:ALA:HA	1.79	0.40
3:C:637:LEU:HA	3:C:637:LEU:HD23	1.93	0.40
3:C:683:GLU:O	3:C:687:ARG:N	2.53	0.40
7:G:172:PRO:HD2	7:G:249:PHE:HE1	1.86	0.40
8:H:702:PHE:HA	8:H:705:ILE:HD12	2.03	0.40
1:A:951:SER:HA	1:A:952:SER:HA	1.92	0.40
4:D:96:HIS:O	4:D:98:GLN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:736:SER:O	6:F:740:GLN:CB	2.68	0.40
7:G:105:HIS:HA	7:G:108:ASP:HB3	2.03	0.40
1:A:924:SER:O	1:A:928:GLU:N	2.54	0.40
3:C:428:VAL:O	3:C:431:THR:OG1	2.24	0.40
3:C:779:TYR:O	3:C:783:MET:N	2.39	0.40
3:C:794:LEU:HG	3:C:795:MET:HG2	2.04	0.40
3:C:9:VAL:O	3:C:13:ILE:N	2.55	0.40
5:E:237:GLU:O	5:E:242:ALA:N	2.44	0.40
6:F:477:PRO:O	6:F:481:ILE:CB	2.70	0.40
7:G:309:VAL:HA	7:G:312:ILE:HG22	2.03	0.40
8:H:715:LEU:N	8:H:751:LYS:HE2	2.36	0.40
8:H:682:LEU:HA	8:H:682:LEU:HD13	1.85	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	662/1336 (50%)	518 (78%)	143 (22%)	1 (0%)	51	85
2	B	922/971 (95%)	707 (77%)	202 (22%)	13 (1%)	13	54
3	C	788/805 (98%)	673 (85%)	114 (14%)	1 (0%)	55	89
4	D	944/1065 (89%)	718 (76%)	213 (23%)	13 (1%)	13	54
5	E	770/871 (88%)	641 (83%)	127 (16%)	2 (0%)	44	81
6	F	715/910 (79%)	578 (81%)	130 (18%)	7 (1%)	18	61
7	G	609/623 (98%)	555 (91%)	52 (8%)	2 (0%)	44	81
8	H	506/753 (67%)	431 (85%)	73 (14%)	2 (0%)	38	77
All	All	5916/7334 (81%)	4821 (82%)	1054 (18%)	41 (1%)	30	68

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	349	SER
2	B	350	ASN
2	B	590	PRO
2	B	762	SER
4	D	97	SER
6	F	453	ASP
7	G	231	PRO
8	H	337	LYS
4	D	203	VAL
6	F	725	VAL
1	A	751	PRO
4	D	245	THR
4	D	553	MET
4	D	588	ASP
4	D	783	ALA
4	D	803	PRO
6	F	344	MET
6	F	452	GLU
6	F	589	ILE
2	B	348	SER
2	B	497	TYR
2	B	589	PRO
4	D	648	ALA
4	D	738	SER
4	D	796	MET
4	D	800	TYR
6	F	644	ILE
6	F	724	SER
7	G	230	ALA
8	H	315	LEU
2	B	666	VAL
2	B	837	TRP
2	B	920	PRO
4	D	427	PRO
2	B	412	LEU
4	D	625	HIS
2	B	185	PRO
2	B	684	GLY
5	E	362	PRO
3	C	528	PRO
5	E	70	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	
3	C	300/740 (40%)	300 (100%)	0	100	100
7	G	480/570 (84%)	478 (100%)	2 (0%)	93	95
8	H	202/697 (29%)	200 (99%)	2 (1%)	80	90
All	All	982/2007 (49%)	978 (100%)	4 (0%)	93	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	320	ARG
7	G	623	ARG
8	H	579	MET
8	H	753	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	475	GLN
3	C	505	ASN
3	C	550	ASN
3	C	594	GLN
3	C	625	GLN
3	C	627	GLN
3	C	655	ASN
3	C	694	GLN
7	G	105	HIS
7	G	190	HIS
7	G	199	GLN
7	G	313	ASN
7	G	395	ASN
7	G	424	ASN
7	G	470	GLN
7	G	606	HIS
8	H	638	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.