



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

Aug 14, 2017 – 05:33 PM EDT

PDB ID : 5VHQ  
EMDB ID: : EMD-8682  
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle  
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.  
Deposited on : unknown  
Resolution : 8.90 Å(reported)

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

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

---

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-20029824

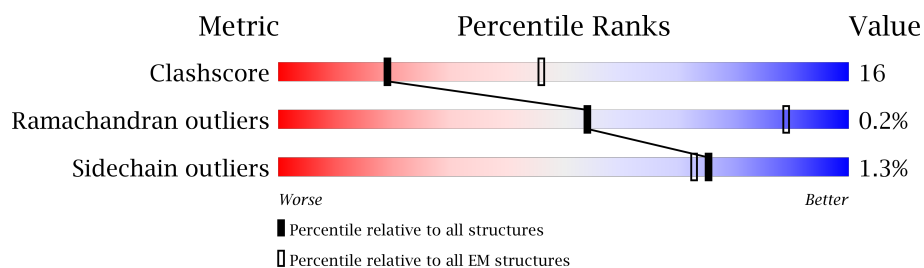
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.90 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	G	223	67% 32% .
2	A	266	68% 29% ..
3	B	267	61% 27% 13%
4	D	262	65% 25% 10%
5	E	262	54% 26% 20%
6	F	267	63% 27% 11%
7	C	266	61% 27% 12%
8	f	848	79% . 19%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18058 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 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	220	Total	C	N	O	S	0	0
			1670	1040	296	325	9		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	261	Total	C	N	O	S	0	0
			2050	1292	368	375	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	233	Total	C	N	O	S	0	0
			1843	1163	318	354	8		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	236	Total	C	N	O	S	0	0
			1873	1184	332	348	9		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1644	1032	294	306	12		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1848	1161	327	347	13		

- Molecule 7 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	234	Total	C	N	O	S	0	0
			1826	1150	329	335	12		

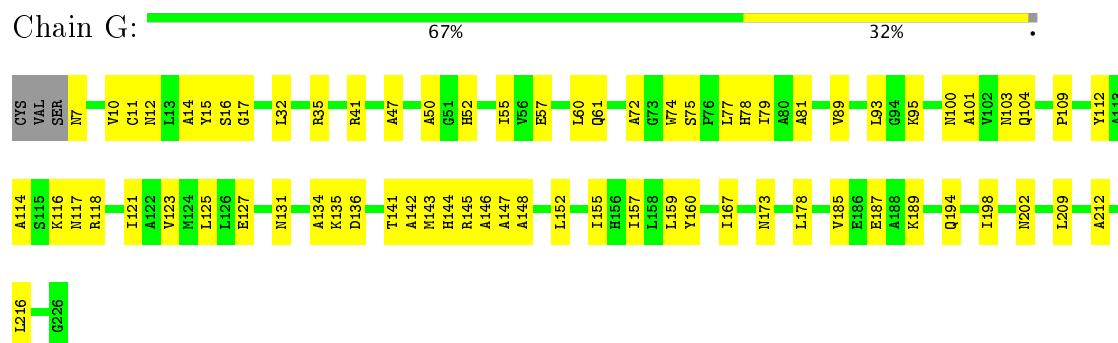
- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	686	Total	C	N	O	S	0	0
			5304	3335	901	1033	35		

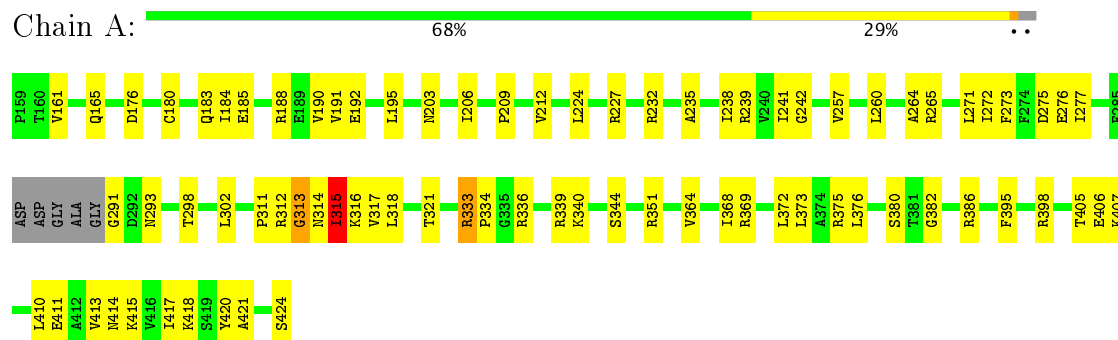
### 3 Residue-property plots

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.

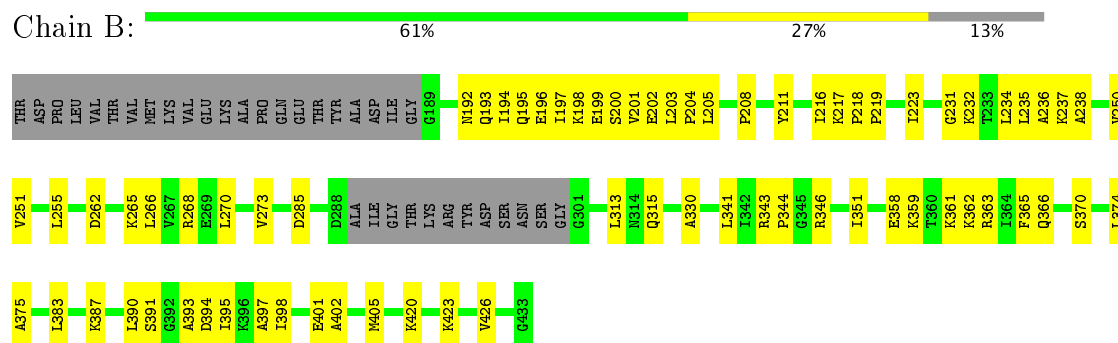
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10



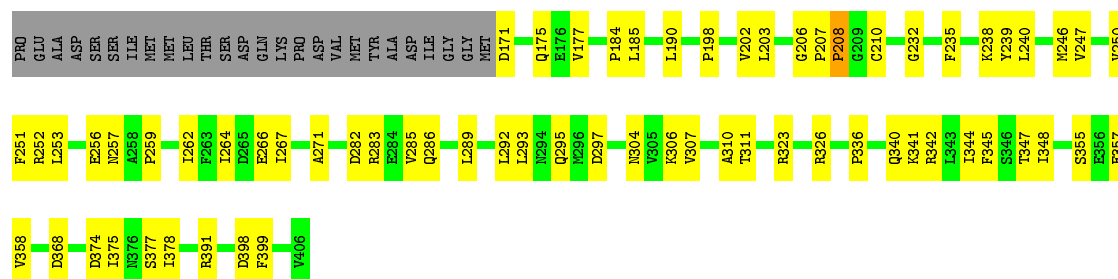
- Molecule 2: 26S proteasome regulatory subunit 7



- Molecule 3: 26S proteasome regulatory subunit 4

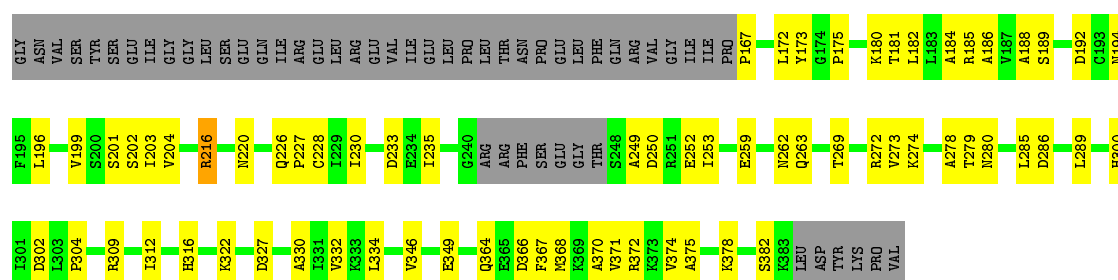


Chain D: 



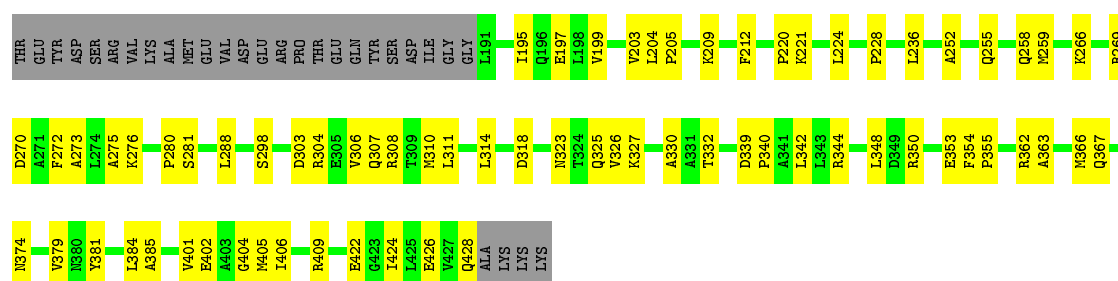
- Molecule 5: 26S proteasome regulatory subunit 10B

Chain E: 



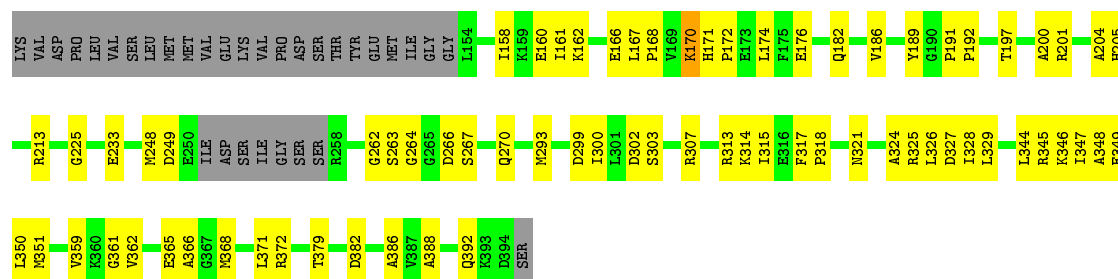
- Molecule 6: 26S proteasome regulatory subunit 6A

Chain F: 



- Molecule 7: 26S proteasome regulatory subunit 8

Chain C: 

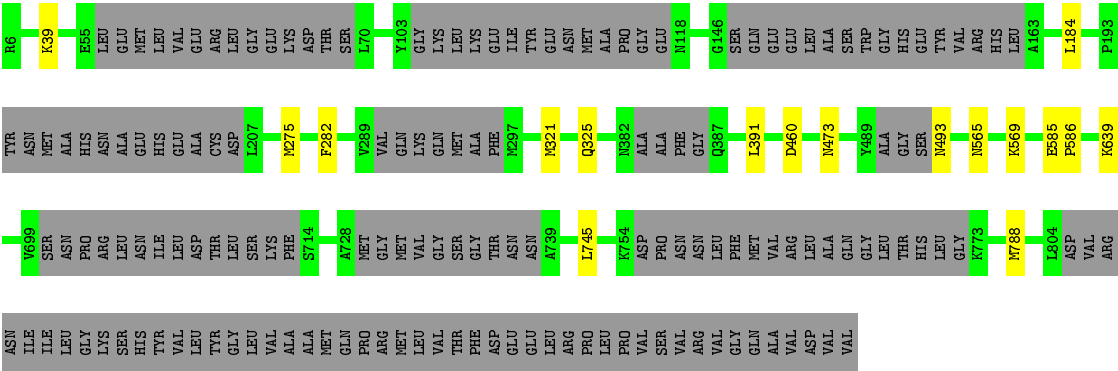


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 

79%

19%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	11610	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	G	0.23	0/1695	0.37	0/2290
2	A	0.23	0/2082	0.49	2/2799 (0.1%)
3	B	0.24	0/1868	0.42	0/2513
4	D	0.24	0/1903	0.43	0/2568
5	E	0.23	0/1669	0.40	0/2244
6	F	0.24	0/1874	0.40	0/2525
7	C	0.25	0/1851	0.43	0/2485
8	f	0.24	0/5377	0.44	1/7248 (0.0%)
All	All	0.24	0/18319	0.43	3/24672 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	313	GLY	N-CA-C	-9.76	88.70	113.10
2	A	315	ILE	N-CA-C	5.80	126.65	111.00
8	f	585	GLU	C-N-CD	-5.46	108.58	120.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1670	0	1673	46	0
2	A	2050	0	2102	73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1843	0	1895	57	0
4	D	1873	0	1912	45	0
5	E	1644	0	1667	56	0
6	F	1848	0	1889	58	0
7	C	1826	0	1891	48	0
8	f	5304	0	5315	0	0
All	All	18058	0	18344	362	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:271:LEU:HG	2:A:315:ILE:CD1	1.76	1.14
2:A:271:LEU:CG	2:A:315:ILE:HD13	1.86	1.05
2:A:271:LEU:HA	2:A:315:ILE:HD11	1.36	1.03
5:E:216:ARG:O	5:E:220:ASN:HB2	1.62	0.99
6:F:314:LEU:O	6:F:318:ASP:HB2	1.62	0.99
7:C:344:LEU:O	7:C:348:ALA:HB3	1.66	0.95
7:C:263:SER:O	7:C:267:SER:HB2	1.67	0.94
2:A:271:LEU:HG	2:A:315:ILE:HD13	0.96	0.93
3:B:198:LYS:O	3:B:202:GLU:HB2	1.66	0.93
7:C:345:ARG:O	7:C:349:GLU:HB2	1.68	0.92
5:E:367:PHE:O	5:E:371:VAL:HB	1.70	0.90
7:C:346:LYS:O	7:C:350:LEU:HB2	1.72	0.89
4:D:246:MET:O	4:D:250:VAL:HB	1.74	0.88
5:E:378:LYS:O	5:E:382:SER:HB3	1.75	0.86
4:D:247:VAL:O	4:D:251:PHE:HB2	1.76	0.85
6:F:266:LYS:O	6:F:270:ASP:HB2	1.77	0.84
5:E:366:ASP:O	5:E:370:ALA:HB3	1.79	0.83
4:D:289:LEU:O	4:D:293:LEU:HB2	1.81	0.81
5:E:330:ALA:O	5:E:334:LEU:HB2	1.85	0.76
3:B:231:GLY:O	3:B:235:LEU:HB3	1.86	0.76
2:A:271:LEU:HA	2:A:315:ILE:CD1	2.13	0.76
7:C:318:PRO:HG2	7:C:324:ALA:HB2	1.68	0.75
4:D:171:ASP:O	4:D:175:GLN:HB2	1.88	0.74
2:A:315:ILE:HD12	2:A:316:LYS:CB	2.17	0.73
2:A:382:GLY:O	2:A:386:ARG:HB2	1.90	0.71
2:A:414:ASN:O	2:A:418:LYS:HB2	1.92	0.70
5:E:199:VAL:HB	5:E:202:SER:HB2	1.72	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:362:VAL:O	7:C:366:ALA:HB2	1.92	0.70
2:A:351:ARG:HH11	2:A:380:SER:H	1.39	0.69
6:F:381:TYR:O	6:F:385:ALA:HB2	1.92	0.69
7:C:361:GLY:O	7:C:365:GLU:HB2	1.93	0.69
6:F:269:ARG:O	6:F:273:ALA:HB2	1.93	0.68
1:G:100:ASN:HD21	1:G:131:ASN:H	1.39	0.68
7:C:262:GLY:O	7:C:266:ASP:HB3	1.94	0.68
2:A:180:CYS:HB3	2:A:183:GLN:HB2	1.75	0.68
5:E:184:ALA:O	5:E:188:ALA:HB3	1.94	0.68
7:C:158:ILE:HA	7:C:161:ILE:HG22	1.76	0.68
5:E:181:THR:O	5:E:185:ARG:HB2	1.94	0.68
7:C:263:SER:O	7:C:267:SER:CB	2.41	0.67
2:A:224:LEU:HB3	2:A:227:ARG:HH11	1.59	0.67
1:G:10:VAL:O	1:G:14:ALA:HB3	1.94	0.66
6:F:363:ALA:O	6:F:367:GLN:HB2	1.94	0.66
6:F:304:ARG:O	6:F:308:ARG:HB2	1.95	0.66
1:G:152:LEU:HD23	1:G:187:GLU:HG2	1.78	0.66
1:G:89:VAL:HG11	1:G:121:ILE:HG23	1.77	0.66
6:F:381:TYR:O	6:F:385:ALA:CB	2.44	0.66
2:A:315:ILE:HD12	2:A:316:LYS:HB3	1.76	0.66
1:G:41:ARG:NH2	4:D:357:GLU:OE1	2.29	0.66
3:B:361:LYS:O	3:B:365:PHE:CB	2.44	0.65
6:F:303:ASP:O	6:F:307:GLN:HB2	1.96	0.65
5:E:181:THR:O	5:E:185:ARG:CB	2.44	0.65
2:A:165:GLN:HB3	2:A:238:ILE:HG23	1.78	0.65
2:A:232:ARG:NE	2:A:235:ALA:O	2.29	0.65
5:E:202:SER:OG	6:F:304:ARG:NH1	2.30	0.65
6:F:224:LEU:HD13	6:F:348:LEU:HD13	1.79	0.65
5:E:194:ASN:ND2	5:E:227:PRO:O	2.30	0.64
6:F:272:PHE:O	6:F:276:LYS:HB2	1.97	0.64
7:C:362:VAL:O	7:C:366:ALA:CB	2.46	0.64
5:E:199:VAL:HG22	6:F:311:LEU:HD12	1.79	0.64
2:A:165:GLN:NE2	2:A:239:ARG:O	2.31	0.64
3:B:398:ILE:HA	3:B:401:GLU:HG2	1.79	0.64
2:A:417:ILE:O	2:A:421:ALA:CB	2.45	0.64
5:E:216:ARG:O	5:E:220:ASN:CB	2.43	0.63
5:E:185:ARG:O	5:E:189:SER:CB	2.47	0.63
2:A:191:VAL:HG13	2:A:192:GLU:HG3	1.79	0.63
3:B:194:ILE:O	3:B:198:LYS:HB2	1.99	0.63
3:B:358:GLU:O	3:B:362:LYS:CB	2.48	0.62
5:E:304:PRO:HG3	5:E:309:ARG:HH21	1.64	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:293:ASN:HD21	6:F:258:GLN:HB3	1.63	0.62
2:A:364:VAL:HG13	2:A:368:ILE:HD12	1.81	0.62
4:D:355:SER:HB3	4:D:358:VAL:HG23	1.82	0.62
5:E:259:GLU:O	5:E:263:GLN:HB2	2.00	0.62
2:A:190:VAL:HG23	2:A:209:PRO:HB2	1.82	0.61
3:B:358:GLU:O	3:B:362:LYS:HB2	2.00	0.61
1:G:17:GLY:HA2	1:G:52:HIS:HE1	1.65	0.61
5:E:322:LYS:HD2	5:E:364:GLN:HE21	1.65	0.61
2:A:417:ILE:O	2:A:421:ALA:HB2	1.99	0.61
4:D:203:LEU:HD12	4:D:310:ALA:HA	1.83	0.60
6:F:272:PHE:O	6:F:276:LYS:CB	2.50	0.60
2:A:180:CYS:SG	2:A:344:SER:OG	2.59	0.59
3:B:205:LEU:HA	3:B:208:PRO:HB3	1.84	0.59
3:B:234:LEU:O	3:B:238:ALA:HB2	2.03	0.59
2:A:184:ILE:O	2:A:188:ARG:HB2	2.03	0.59
2:A:317:VAL:HG11	2:A:336:ARG:HH22	1.66	0.59
7:C:213:ARG:HH22	7:C:249:ASP:HB3	1.68	0.59
3:B:361:LYS:O	3:B:365:PHE:HB2	2.03	0.58
7:C:321:ASN:O	7:C:325:ARG:NH1	2.37	0.58
5:E:235:ILE:HG22	5:E:279:THR:HB	1.86	0.58
3:B:197:ILE:HD13	3:B:237:LYS:HD3	1.86	0.58
2:A:398:ARG:HH12	3:B:196:GLU:HA	1.68	0.58
2:A:375:ARG:HG3	2:A:376:LEU:HD12	1.85	0.58
7:C:262:GLY:O	7:C:266:ASP:CB	2.52	0.58
1:G:78:HIS:HE1	1:G:101:ALA:HB3	1.67	0.58
4:D:323:ARG:HE	4:D:326:ARG:HE	1.52	0.57
5:E:185:ARG:HH11	6:F:344:ARG:HD2	1.69	0.57
1:G:185:VAL:HG12	1:G:189:LYS:HE2	1.86	0.57
5:E:184:ALA:O	5:E:188:ALA:CB	2.52	0.57
2:A:339:ARG:NH2	6:F:402:GLU:OE1	2.38	0.57
5:E:185:ARG:O	5:E:189:SER:OG	2.18	0.57
1:G:143:MET:O	1:G:147:ALA:HB3	2.05	0.57
7:C:346:LYS:HA	7:C:350:LEU:HD13	1.86	0.57
5:E:185:ARG:NE	6:F:318:ASP:OD1	2.38	0.57
1:G:77:LEU:O	1:G:81:ALA:HB3	2.05	0.57
6:F:266:LYS:O	6:F:270:ASP:CB	2.51	0.57
6:F:281:SER:H	6:F:326:VAL:HG22	1.70	0.57
1:G:72:ALA:HB1	1:G:104:GLN:HB2	1.86	0.57
1:G:60:LEU:HD22	1:G:95:LYS:HG3	1.87	0.56
5:E:199:VAL:HG12	5:E:201:SER:H	1.70	0.56
2:A:407:LYS:HA	2:A:410:LEU:HD23	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:242:GLY:H	2:A:276:GLU:HB2	1.71	0.56
5:E:173:TYR:O	5:E:175:PRO:HD3	2.04	0.56
5:E:279:THR:HG21	5:E:285:LEU:HD11	1.88	0.56
3:B:255:LEU:HD13	3:B:266:LEU:HD22	1.86	0.56
4:D:340:GLN:O	4:D:344:ILE:HB	2.06	0.56
7:C:344:LEU:O	7:C:348:ALA:CB	2.48	0.56
5:E:366:ASP:O	5:E:370:ALA:CB	2.54	0.56
1:G:11:CYS:O	1:G:15:TYR:HB3	2.06	0.56
1:G:77:LEU:O	1:G:81:ALA:CB	2.54	0.56
3:B:383:LEU:HB3	3:B:387:LYS:HE2	1.89	0.55
2:A:265:ARG:HH21	2:A:311:PRO:HA	1.69	0.55
7:C:162:LYS:O	7:C:166:GLU:HB2	2.05	0.55
1:G:141:THR:H	1:G:144:HIS:HD2	1.52	0.55
5:E:185:ARG:O	5:E:189:SER:HB3	2.05	0.55
6:F:330:ALA:HB3	6:F:348:LEU:HD21	1.89	0.55
4:D:344:ILE:HA	4:D:347:THR:HG22	1.89	0.55
4:D:391:ARG:NH2	4:D:398:ASP:OD2	2.39	0.55
3:B:361:LYS:O	3:B:365:PHE:HB3	2.07	0.55
3:B:313:LEU:HD22	3:B:341:LEU:HD23	1.88	0.55
5:E:249:ALA:HA	6:F:298:SER:HB3	1.87	0.55
3:B:203:LEU:HG	3:B:211:TYR:HB2	1.88	0.55
5:E:196:LEU:HD22	5:E:230:ILE:HG12	1.89	0.55
2:A:185:GLU:OE1	2:A:188:ARG:NH2	2.39	0.55
1:G:103:ASN:ND2	1:G:112:TYR:OH	2.39	0.55
3:B:217:LYS:O	3:B:219:PRO:HD3	2.07	0.55
3:B:393:ALA:O	3:B:397:ALA:HB2	2.07	0.54
4:D:259:PRO:HG3	4:D:304:ASN:HB3	1.89	0.54
1:G:136:ASP:OD2	1:G:145:ARG:NH2	2.40	0.54
3:B:231:GLY:O	3:B:235:LEU:CB	2.54	0.54
2:A:368:ILE:HD11	2:A:405:THR:HA	1.89	0.54
1:G:7:ASN:N	1:G:11:CYS:HG	2.06	0.54
1:G:11:CYS:O	1:G:15:TYR:CB	2.56	0.54
2:A:398:ARG:HG2	3:B:199:GLU:HG2	1.88	0.54
6:F:252:ALA:HB3	6:F:255:GLN:HG2	1.90	0.54
5:E:167:PRO:O	5:E:274:LYS:NZ	2.39	0.53
5:E:309:ARG:HD2	5:E:332:VAL:HG13	1.90	0.53
3:B:390:LEU:HD22	3:B:426:VAL:HG13	1.89	0.53
4:D:203:LEU:HD11	4:D:311:THR:HG22	1.89	0.53
2:A:203:ASN:O	6:F:374:ASN:ND2	2.38	0.53
6:F:197:GLU:OE2	6:F:350:ARG:NH2	2.41	0.53
6:F:228:PRO:HD2	6:F:354:PHE:HB2	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:270:LEU:HA	3:B:273:VAL:HG12	1.89	0.53
4:D:297:ASP:OD2	4:D:326:ARG:NH2	2.35	0.52
5:E:327:ASP:N	5:E:364:GLN:OE1	2.41	0.52
1:G:123:VAL:O	1:G:127:GLU:HB2	2.10	0.52
2:A:239:ARG:HA	2:A:273:PHE:HB3	1.91	0.52
7:C:201:ARG:O	7:C:205:HIS:HB2	2.10	0.52
4:D:190:LEU:HB3	7:C:371:LEU:HD12	1.92	0.52
7:C:167:LEU:O	7:C:171:HIS:ND1	2.42	0.52
4:D:289:LEU:HD12	4:D:292:LEU:HD11	1.92	0.52
3:B:387:LYS:HG2	3:B:426:VAL:HG11	1.92	0.52
1:G:57:GLU:O	1:G:61:GLN:HB2	2.10	0.52
2:A:188:ARG:HA	2:A:191:VAL:HG12	1.92	0.52
2:A:313:GLY:HA2	2:A:336:ARG:HH11	1.75	0.52
1:G:109:PRO:HA	1:G:112:TYR:HD2	1.75	0.52
4:D:207:PRO:N	4:D:208:PRO:HD2	2.25	0.52
5:E:286:ASP:O	5:E:289:LEU:N	2.39	0.52
7:C:299:ASP:O	7:C:303:SER:OG	2.21	0.51
7:C:186:VAL:HG21	7:C:315:ILE:HD12	1.92	0.51
5:E:300:HIS:ND1	5:E:302:ASP:OD2	2.43	0.51
7:C:170:LYS:HD2	7:C:170:LYS:H	1.75	0.51
4:D:336:PRO:HB3	4:D:368:ASP:HA	1.92	0.51
2:A:277:ILE:HG22	2:A:321:THR:HB	1.91	0.51
2:A:373:LEU:HD11	2:A:413:VAL:HG21	1.93	0.51
1:G:32:LEU:HD23	1:G:35:ARG:HE	1.76	0.51
4:D:232:GLY:HA3	4:D:266:GLU:HB2	1.93	0.51
2:A:298:THR:O	2:A:302:LEU:HB2	2.11	0.51
3:B:398:ILE:O	3:B:402:ALA:HB2	2.10	0.51
5:E:188:ALA:HA	5:E:192:ASP:HB2	1.93	0.51
2:A:333:ARG:HG3	2:A:334:PRO:HD3	1.92	0.51
3:B:358:GLU:HG3	3:B:359:LYS:HG3	1.93	0.51
1:G:131:ASN:HB3	1:G:134:ALA:HB2	1.92	0.51
7:C:313:ARG:NH1	7:C:314:LYS:O	2.44	0.50
6:F:204:LEU:HG	6:F:205:PRO:HD3	1.93	0.50
3:B:374:LEU:HG	3:B:375:ALA:H	1.76	0.50
4:D:235:PHE:HE2	4:D:285:VAL:HB	1.76	0.50
1:G:147:ALA:HA	1:G:155:ILE:HD11	1.94	0.50
3:B:232:LYS:O	3:B:236:ALA:CB	2.59	0.50
5:E:203:ILE:HG21	5:E:253:ILE:HA	1.94	0.50
6:F:422:GLU:O	6:F:426:GLU:HB2	2.12	0.50
5:E:312:ILE:HG13	5:E:316:HIS:HD2	1.76	0.50
2:A:420:TYR:O	2:A:424:SER:OG	2.29	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:203:LEU:N	3:B:204:PRO:HD2	2.26	0.50
5:E:201:SER:OG	6:F:307:GLN:OE1	2.28	0.50
5:E:233:ASP:HA	5:E:278:ALA:HB3	1.92	0.50
5:E:368:MET:O	5:E:372:ARG:HB2	2.12	0.50
6:F:379:VAL:HG13	6:F:384:LEU:HD21	1.92	0.50
1:G:144:HIS:HB3	1:G:178:LEU:HD22	1.93	0.50
2:A:184:ILE:O	2:A:188:ARG:CB	2.59	0.50
3:B:223:ILE:HD12	3:B:346:ARG:HB2	1.93	0.50
1:G:159:LEU:HD21	1:G:194:GLN:HG3	1.94	0.50
5:E:252:GLU:OE2	6:F:298:SER:OG	2.23	0.49
7:C:200:ALA:O	7:C:204:ALA:CB	2.60	0.49
5:E:371:VAL:O	5:E:375:ALA:CB	2.59	0.49
6:F:195:ILE:HD12	6:F:236:LEU:HD11	1.93	0.49
1:G:157:ILE:HA	1:G:160:TYR:HD2	1.76	0.49
4:D:262:ILE:HG22	4:D:264:ILE:HG13	1.94	0.49
6:F:205:PRO:HB3	6:F:220:PRO:HD2	1.92	0.49
6:F:221:LYS:NZ	6:F:325:GLN:O	2.46	0.49
4:D:267:ILE:O	4:D:271:ALA:HB2	2.12	0.49
2:A:369:ARG:HH11	2:A:372:LEU:HD22	1.78	0.49
4:D:177:VAL:HG22	4:D:202:VAL:HG11	1.93	0.49
1:G:52:HIS:HB3	1:G:55:ILE:HB	1.94	0.49
2:A:411:GLU:O	2:A:415:LYS:CB	2.61	0.49
7:C:176:GLU:OE1	7:C:182:GLN:NE2	2.45	0.49
2:A:314:ASN:OD1	2:A:315:ILE:HG23	2.13	0.49
7:C:303:SER:O	7:C:307:ARG:N	2.41	0.49
2:A:206:ILE:HD13	6:F:404:GLY:HA3	1.95	0.49
6:F:424:ILE:O	6:F:428:GLN:C	2.51	0.49
7:C:327:ASP:OD1	7:C:328:ILE:N	2.46	0.48
1:G:141:THR:HG23	1:G:167:ILE:HG21	1.95	0.48
1:G:173:ASN:OD1	1:G:202:ASN:ND2	2.44	0.48
3:B:395:ILE:HA	3:B:398:ILE:HG12	1.96	0.48
5:E:312:ILE:HG13	5:E:316:HIS:CD2	2.48	0.48
2:A:315:ILE:HD12	2:A:316:LYS:N	2.29	0.48
2:A:271:LEU:HD23	2:A:316:LYS:HD2	1.95	0.48
3:B:313:LEU:HD21	3:B:344:PRO:HG2	1.95	0.48
3:B:196:GLU:O	3:B:200:SER:HB2	2.13	0.48
4:D:252:ARG:O	4:D:256:GLU:CB	2.61	0.48
4:D:208:PRO:O	4:D:210:CYS:N	2.46	0.47
7:C:362:VAL:HA	7:C:386:ALA:HB1	1.95	0.47
6:F:325:GLN:HG2	6:F:326:VAL:H	1.79	0.47
2:A:271:LEU:CG	2:A:315:ILE:CD1	2.67	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:411:GLU:O	2:A:415:LYS:HB2	2.13	0.47
4:D:247:VAL:O	4:D:251:PHE:CB	2.55	0.47
4:D:262:ILE:HD12	4:D:307:VAL:HG22	1.95	0.47
1:G:10:VAL:O	1:G:14:ALA:CB	2.61	0.47
3:B:198:LYS:HD3	3:B:202:GLU:HG3	1.96	0.47
5:E:250:ASP:HA	5:E:253:ILE:HD12	1.96	0.47
5:E:346:VAL:HG12	5:E:371:VAL:HG22	1.95	0.47
1:G:93:LEU:HD21	1:G:125:LEU:HD23	1.96	0.47
4:D:267:ILE:O	4:D:271:ALA:CB	2.63	0.47
2:A:241:ILE:HA	2:A:275:ASP:HB3	1.98	0.46
2:A:368:ILE:HG12	2:A:406:GLU:H	1.80	0.46
3:B:197:ILE:HA	3:B:200:SER:HB3	1.96	0.46
3:B:192:ASN:HA	3:B:195:GLN:HG2	1.97	0.46
3:B:234:LEU:HD22	3:B:330:ALA:HB1	1.97	0.46
7:C:368:MET:O	7:C:372:ARG:HB2	2.16	0.46
4:D:374:ASP:HB2	4:D:377:SER:HB2	1.97	0.46
2:A:382:GLY:O	2:A:386:ARG:CB	2.60	0.46
4:D:239:TYR:O	4:D:240:LEU:HG	2.14	0.46
3:B:234:LEU:O	3:B:238:ALA:CB	2.63	0.46
5:E:182:LEU:O	5:E:186:ALA:HB2	2.16	0.46
6:F:304:ARG:O	6:F:308:ARG:CB	2.63	0.46
2:A:273:PHE:HE1	2:A:318:LEU:HD22	1.81	0.46
7:C:267:SER:HA	7:C:270:GLN:HB2	1.97	0.46
4:D:253:LEU:O	4:D:257:ASN:HB3	2.16	0.46
4:D:282:ASP:HA	4:D:285:VAL:HG22	1.97	0.46
5:E:228:CYS:HB3	5:E:273:VAL:HG23	1.98	0.46
6:F:307:GLN:HA	6:F:310:MET:HB3	1.97	0.46
6:F:306:VAL:O	6:F:310:MET:HB2	2.16	0.46
4:D:345:PHE:HA	4:D:348:ILE:HG22	1.98	0.45
1:G:135:LYS:HE2	1:G:167:ILE:HG23	1.98	0.45
3:B:390:LEU:HD23	3:B:394:ASP:HB3	1.97	0.45
3:B:251:VAL:HG22	3:B:285:ASP:HB3	1.99	0.45
6:F:362:ARG:O	6:F:366:MET:CB	2.65	0.45
3:B:194:ILE:HA	3:B:197:ILE:HG22	1.98	0.45
3:B:358:GLU:O	3:B:362:LYS:HB3	2.16	0.45
1:G:74:TRP:HB3	1:G:79:ILE:HD11	1.99	0.45
2:A:257:VAL:HA	2:A:260:LEU:HG	1.99	0.45
2:A:312:ARG:HB3	2:A:314:ASN:HB2	1.97	0.45
5:E:204:VAL:HG12	6:F:298:SER:HA	1.99	0.45
2:A:195:LEU:HD13	2:A:232:ARG:HH12	1.82	0.45
5:E:181:THR:O	5:E:185:ARG:HB3	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:SER:OG	1:G:78:HIS:ND1	2.40	0.45
6:F:406:ILE:HG22	6:F:409:ARG:HH11	1.82	0.44
3:B:232:LYS:O	3:B:236:ALA:HB2	2.17	0.44
3:B:387:LYS:HZ1	3:B:395:ILE:HD12	1.82	0.44
1:G:212:ALA:HB1	1:G:216:LEU:HB3	2.00	0.44
2:A:291:GLY:N	6:F:259:MET:SD	2.90	0.44
2:A:333:ARG:NH1	2:A:340:LYS:HB3	2.32	0.44
3:B:197:ILE:O	3:B:201:VAL:HG22	2.18	0.44
6:F:209:LYS:HD3	6:F:212:PHE:HD2	1.81	0.44
6:F:280:PRO:HA	6:F:326:VAL:HG22	1.99	0.44
2:A:293:ASN:ND2	6:F:258:GLN:OE1	2.51	0.43
7:C:167:LEU:HB3	7:C:168:PRO:HD3	1.99	0.43
7:C:344:LEU:HA	7:C:347:ILE:HG22	2.00	0.43
5:E:280:ASN:HD21	6:F:340:PRO:HG2	1.83	0.43
1:G:198:ILE:HD12	1:G:209:LEU:HD11	2.00	0.43
2:A:161:VAL:O	2:A:165:GLN:HG2	2.18	0.43
2:A:264:ALA:HB2	2:A:272:ILE:HD11	2.01	0.43
3:B:366:GLN:O	3:B:370:SER:OG	2.30	0.43
7:C:197:THR:O	7:C:201:ARG:CB	2.66	0.43
6:F:353:GLU:O	6:F:355:PRO:HD3	2.18	0.43
1:G:12:ASN:O	1:G:16:SER:OG	2.24	0.43
7:C:172:PRO:HG2	7:C:174:LEU:HG	2.01	0.43
6:F:199:VAL:O	6:F:203:VAL:HB	2.19	0.43
1:G:114:ALA:HB1	1:G:146:ALA:HB2	2.01	0.43
3:B:232:LYS:HB2	3:B:391:SER:HA	2.01	0.43
2:A:185:GLU:OE2	6:F:409:ARG:NH2	2.52	0.43
4:D:283:ARG:HA	4:D:286:GLN:HG2	2.01	0.43
1:G:144:HIS:O	1:G:148:ALA:HB2	2.19	0.43
4:D:341:LYS:O	4:D:344:ILE:HG22	2.19	0.43
6:F:272:PHE:HA	6:F:275:ALA:HB3	2.01	0.43
6:F:288:LEU:HD22	6:F:330:ALA:HB1	2.01	0.42
2:A:414:ASN:HA	2:A:417:ILE:HG12	2.01	0.42
3:B:401:GLU:O	3:B:405:MET:HB2	2.20	0.42
7:C:351:MET:HE3	7:C:359:VAL:HG22	2.01	0.42
4:D:292:LEU:HA	4:D:295:GLN:HB2	2.01	0.42
5:E:172:LEU:HD13	5:E:180:LYS:HB2	2.01	0.42
2:A:191:VAL:HG23	2:A:316:LYS:HD2	2.01	0.42
2:A:395:PHE:HD1	2:A:398:ARG:HD3	1.83	0.42
7:C:200:ALA:O	7:C:204:ALA:HB3	2.19	0.42
7:C:189:TYR:O	7:C:317:PHE:HB3	2.20	0.42
6:F:401:VAL:O	6:F:405:MET:HG2	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:349:GLU:HG2	5:E:374:VAL:HG11	2.01	0.42
6:F:205:PRO:HB2	6:F:327:LYS:HE2	2.02	0.42
7:C:191:PRO:HA	7:C:192:PRO:HD3	1.86	0.42
7:C:225:GLY:HA3	7:C:233:GLU:HG3	2.01	0.42
6:F:269:ARG:O	6:F:273:ALA:CB	2.65	0.42
4:D:171:ASP:O	4:D:175:GLN:CB	2.63	0.42
2:A:314:ASN:CG	2:A:315:ILE:H	2.22	0.42
2:A:417:ILE:O	2:A:421:ALA:HB3	2.18	0.42
7:C:160:GLU:HB3	7:C:315:ILE:HG12	2.01	0.42
7:C:264:GLY:HA2	7:C:267:SER:HB3	2.00	0.42
4:D:185:LEU:HB2	4:D:306:LYS:NZ	2.34	0.42
3:B:262:ASP:OD2	3:B:265:LYS:HB2	2.20	0.41
1:G:116:LYS:O	1:G:118:ARG:NH1	2.52	0.41
3:B:351:ILE:HG13	3:B:351:ILE:H	1.76	0.41
1:G:148:ALA:HB1	4:D:342:ARG:HH22	1.85	0.41
5:E:226:GLN:HB3	5:E:272:ARG:HD3	2.01	0.41
1:G:50:ALA:HB3	1:G:52:HIS:CD2	2.56	0.41
3:B:420:LYS:HA	3:B:423:LYS:HB3	2.01	0.41
4:D:184:PRO:HG3	4:D:198:PRO:HB2	2.02	0.41
3:B:216:ILE:HG22	3:B:218:PRO:HD3	2.03	0.41
7:C:299:ASP:HA	7:C:302:ASP:HB3	2.03	0.41
7:C:326:LEU:HD11	7:C:349:GLU:HG3	2.03	0.41
7:C:388:ALA:O	7:C:392:GLN:HG2	2.20	0.41
2:A:212:VAL:HG12	2:A:339:ARG:HB3	2.02	0.41
3:B:343:ARG:HB2	3:B:344:PRO:HD3	2.02	0.41
3:B:193:GLN:HE21	3:B:351:ILE:HD13	1.85	0.41
7:C:325:ARG:O	7:C:329:LEU:HB2	2.20	0.41
6:F:362:ARG:O	6:F:366:MET:HB2	2.20	0.41
1:G:142:ALA:O	1:G:146:ALA:CB	2.69	0.41
7:C:379:THR:HG23	7:C:382:ASP:H	1.85	0.41
4:D:206:GLY:C	4:D:208:PRO:HD2	2.41	0.41
3:B:250:VAL:O	3:B:285:ASP:N	2.47	0.41
4:D:358:VAL:HG13	4:D:399:PHE:HE2	1.86	0.41
5:E:192:ASP:C	5:E:194:ASN:H	2.23	0.41
6:F:339:ASP:HB3	6:F:342:LEU:HG	2.02	0.41
2:A:273:PHE:CE1	2:A:318:LEU:HD22	2.56	0.41
2:A:413:VAL:O	2:A:417:ILE:HG12	2.21	0.41
4:D:185:LEU:HD11	4:D:259:PRO:HB3	2.03	0.41
5:E:371:VAL:O	5:E:375:ALA:HB2	2.21	0.41
3:B:268:ARG:HA	3:B:315:GLN:HE22	1.86	0.40
4:D:252:ARG:O	4:D:256:GLU:HB2	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:322:LYS:HG2	5:E:367:PHE:HE2	1.86	0.40
4:D:375:ILE:HD13	4:D:378:ILE:HD12	2.03	0.40
3:B:359:LYS:O	3:B:363:ARG:CB	2.70	0.40
7:C:300:ILE:HA	7:C:300:ILE:HD12	1.98	0.40
6:F:288:LEU:HB3	6:F:332:THR:HG22	2.03	0.40
1:G:47:ALA:HA	1:G:52:HIS:HD2	1.87	0.40
2:A:312:ARG:HG3	2:A:313:GLY:O	2.21	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	G	218/223 (98%)	211 (97%)	7 (3%)	0	100	100
2	A	257/266 (97%)	225 (88%)	31 (12%)	1 (0%)	38	77
3	B	229/267 (86%)	212 (93%)	17 (7%)	0	100	100
4	D	234/262 (89%)	217 (93%)	16 (7%)	1 (0%)	38	77
5	E	206/262 (79%)	189 (92%)	17 (8%)	0	100	100
6	F	236/267 (88%)	220 (93%)	16 (7%)	0	100	100
7	C	230/266 (86%)	213 (93%)	17 (7%)	0	100	100
8	f	664/848 (78%)	602 (91%)	60 (9%)	2 (0%)	44	81
All	All	2274/2661 (86%)	2089 (92%)	181 (8%)	4 (0%)	54	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	f	586	PRO
2	A	315	ILE
8	f	325	GLN

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	208	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	G	175/178 (98%)	174 (99%)	1 (1%)	89	94
2	A	222/224 (99%)	220 (99%)	2 (1%)	82	91
3	B	203/231 (88%)	203 (100%)	0	100	100
4	D	202/224 (90%)	201 (100%)	1 (0%)	91	95
5	E	178/225 (79%)	175 (98%)	3 (2%)	66	84
6	F	197/222 (89%)	196 (100%)	1 (0%)	91	95
7	C	196/225 (87%)	193 (98%)	3 (2%)	70	85
8	f	579/714 (81%)	565 (98%)	14 (2%)	54	78
All	All	1952/2243 (87%)	1927 (99%)	25 (1%)	75	87

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	117	ASN
2	A	176	ASP
2	A	333	ARG
4	D	238	LYS
5	E	216	ARG
5	E	262	ASN
5	E	269	THR
6	F	323	ASN
7	C	170	LYS
7	C	248	MET
7	C	293	MET
8	f	39	LYS
8	f	184	LEU
8	f	275	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	f	282	PHE
8	f	321	MET
8	f	391	LEU
8	f	460	ASP
8	f	473	ASN
8	f	493	ASN
8	f	565	ASN
8	f	569	LYS
8	f	639	LYS
8	f	745	LEU
8	f	788	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	52	HIS
1	G	100	ASN
1	G	117	ASN
1	G	144	HIS
2	A	197	HIS
3	B	193	GLN
3	B	315	GLN
4	D	286	GLN
5	E	262	ASN
5	E	280	ASN
5	E	316	HIS
5	E	339	ASN
5	E	345	ASN
6	F	323	ASN
6	F	417	HIS
6	F	428	GLN
7	C	377	HIS
8	f	102	HIS
8	f	213	GLN
8	f	325	GLN
8	f	475	ASN
8	f	493	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.