



## Full wwPDB EM Validation Report ⓘ

Nov 10, 2025 – 02:07 PM EST

PDB ID : 9PDL / pdb\_00009pdl  
EMDB ID : EMD-71537  
Title : Nub1/Fat10-processing human 26S proteasome with Rpt5 at top of spiral staircase (AAA+ locally refined)  
Authors : Arkinson, C.; Gee, C.L.; Martin, A.  
Deposited on : 2025-06-30  
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

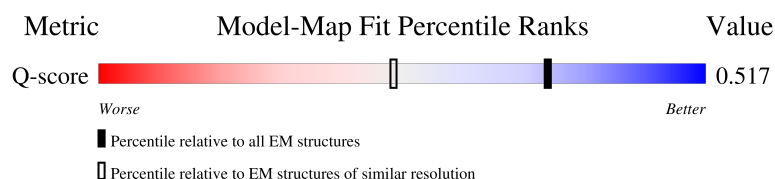
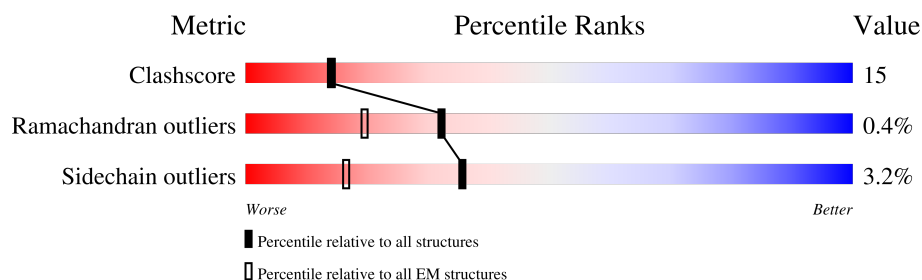
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 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 2.76 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.



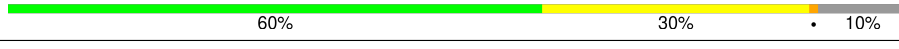
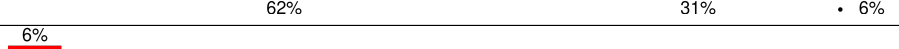




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10642 ( 2.26 - 3.26 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	406	 71% 24% 5%
2	G	246	 66% 29% 5%
3	H	234	 66% 33% 1%
4	I	261	 62% 33% 5%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	J	248	
6	L	263	
7	M	255	
8	c	424	
9	v	12	
10	A	433	
11	B	440	
12	D	418	
13	E	389	
14	F	439	
15	K	241	

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33269 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 protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	386	Total	C	N	O	S	0	0
			3051	1919	547	567	18		

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	239	Total	C	N	O	S	0	0
			1831	1164	306	348	13		

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	248	Total	C	N	O	S	0	0
			1908	1205	325	369	9		

- Molecule 5 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	239	Total	C	N	O	S	0	0
			1813	1136	320	352	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	230	VAL	ALA	conflict	UNP O14818

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	237	Total	C	N	O	S	0	0
			1845	1156	333	345	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	288	Total	C	N	O	S	0	0
			2264	1433	390	422	19		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	expression tag	UNP O00487
c	312	ILE	-	expression tag	UNP O00487
c	313	ASN	-	expression tag	UNP O00487
c	314	HIS	-	expression tag	UNP O00487
c	315	HIS	-	expression tag	UNP O00487
c	316	HIS	-	expression tag	UNP O00487
c	317	HIS	-	expression tag	UNP O00487
c	318	HIS	-	expression tag	UNP O00487
c	319	HIS	-	expression tag	UNP O00487
c	320	ASP	-	expression tag	UNP O00487
c	321	TYR	-	expression tag	UNP O00487
c	322	ASP	-	expression tag	UNP O00487
c	323	ILE	-	expression tag	UNP O00487
c	324	PRO	-	expression tag	UNP O00487
c	325	THR	-	expression tag	UNP O00487
c	326	THR	-	expression tag	UNP O00487
c	327	ALA	-	expression tag	UNP O00487
c	328	SER	-	expression tag	UNP O00487
c	329	GLU	-	expression tag	UNP O00487
c	330	ASN	-	expression tag	UNP O00487
c	331	LEU	-	expression tag	UNP O00487
c	332	TYR	-	expression tag	UNP O00487
c	333	PHE	-	expression tag	UNP O00487
c	334	GLN	-	expression tag	UNP O00487
c	335	GLY	-	expression tag	UNP O00487

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
c	336	GLU	-	expression tag	UNP O00487
c	337	LEU	-	expression tag	UNP O00487
c	338	GLY	-	expression tag	UNP O00487
c	339	MET	-	expression tag	UNP O00487
c	340	ARG	-	expression tag	UNP O00487
c	341	GLY	-	expression tag	UNP O00487
c	342	SER	-	expression tag	UNP O00487
c	343	ALA	-	expression tag	UNP O00487
c	344	GLY	-	expression tag	UNP O00487
c	345	LYS	-	expression tag	UNP O00487
c	346	ALA	-	expression tag	UNP O00487
c	347	GLY	-	expression tag	UNP O00487
c	348	GLU	-	expression tag	UNP O00487
c	349	GLY	-	expression tag	UNP O00487
c	350	GLU	-	expression tag	UNP O00487
c	351	ILE	-	expression tag	UNP O00487
c	352	PRO	-	expression tag	UNP O00487
c	353	ALA	-	expression tag	UNP O00487
c	354	PRO	-	expression tag	UNP O00487
c	355	LEU	-	expression tag	UNP O00487
c	356	ALA	-	expression tag	UNP O00487
c	357	GLY	-	expression tag	UNP O00487
c	358	THR	-	expression tag	UNP O00487
c	359	VAL	-	expression tag	UNP O00487
c	360	SER	-	expression tag	UNP O00487
c	361	LYS	-	expression tag	UNP O00487
c	362	ILE	-	expression tag	UNP O00487
c	363	LEU	-	expression tag	UNP O00487
c	364	VAL	-	expression tag	UNP O00487
c	365	LYS	-	expression tag	UNP O00487
c	366	GLU	-	expression tag	UNP O00487
c	367	GLY	-	expression tag	UNP O00487
c	368	ASP	-	expression tag	UNP O00487
c	369	THR	-	expression tag	UNP O00487
c	370	VAL	-	expression tag	UNP O00487
c	371	LYS	-	expression tag	UNP O00487
c	372	ALA	-	expression tag	UNP O00487
c	373	GLY	-	expression tag	UNP O00487
c	374	GLN	-	expression tag	UNP O00487
c	375	THR	-	expression tag	UNP O00487
c	376	VAL	-	expression tag	UNP O00487
c	377	LEU	-	expression tag	UNP O00487

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
c	378	VAL	-	expression tag	UNP O00487
c	379	LEU	-	expression tag	UNP O00487
c	380	GLU	-	expression tag	UNP O00487
c	381	ALA	-	expression tag	UNP O00487
c	382	MET	-	expression tag	UNP O00487
c	383	LYS	-	expression tag	UNP O00487
c	384	MET	-	expression tag	UNP O00487
c	385	GLU	-	expression tag	UNP O00487
c	386	THR	-	expression tag	UNP O00487
c	387	GLU	-	expression tag	UNP O00487
c	388	ILE	-	expression tag	UNP O00487
c	389	ASN	-	expression tag	UNP O00487
c	390	ALA	-	expression tag	UNP O00487
c	391	PRO	-	expression tag	UNP O00487
c	392	THR	-	expression tag	UNP O00487
c	393	ASP	-	expression tag	UNP O00487
c	394	GLY	-	expression tag	UNP O00487
c	395	LYS	-	expression tag	UNP O00487
c	396	VAL	-	expression tag	UNP O00487
c	397	GLU	-	expression tag	UNP O00487
c	398	LYS	-	expression tag	UNP O00487
c	399	VAL	-	expression tag	UNP O00487
c	400	LEU	-	expression tag	UNP O00487
c	401	VAL	-	expression tag	UNP O00487
c	402	LYS	-	expression tag	UNP O00487
c	403	GLU	-	expression tag	UNP O00487
c	404	ARG	-	expression tag	UNP O00487
c	405	ASP	-	expression tag	UNP O00487
c	406	ALA	-	expression tag	UNP O00487
c	407	VAL	-	expression tag	UNP O00487
c	408	GLN	-	expression tag	UNP O00487
c	409	GLY	-	expression tag	UNP O00487
c	410	GLY	-	expression tag	UNP O00487
c	411	GLN	-	expression tag	UNP O00487
c	412	GLY	-	expression tag	UNP O00487
c	413	LEU	-	expression tag	UNP O00487
c	414	ILE	-	expression tag	UNP O00487
c	415	LYS	-	expression tag	UNP O00487
c	416	ILE	-	expression tag	UNP O00487
c	417	GLY	-	expression tag	UNP O00487
c	418	VAL	-	expression tag	UNP O00487
c	419	HIS	-	expression tag	UNP O00487

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
c	420	HIS	-	expression tag	UNP O00487
c	421	HIS	-	expression tag	UNP O00487
c	422	HIS	-	expression tag	UNP O00487
c	423	HIS	-	expression tag	UNP O00487
c	424	HIS	-	expression tag	UNP O00487

- Molecule 9 is a protein called Substrate polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	v	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 10 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	401	Total	C	N	O	S	0	0
			3163	1995	557	593	18		

- Molecule 11 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	395	Total	C	N	O	S	0	0
			3104	1956	528	605	15		

- Molecule 12 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	377	Total	C	N	O	S	0	0
			3018	1911	521	573	13		

- Molecule 13 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	347	Total	C	N	O	S	0	0
			2750	1736	487	511	16		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	364	Total	C	N	O	S	0	0
			2850	1803	492	538	17		



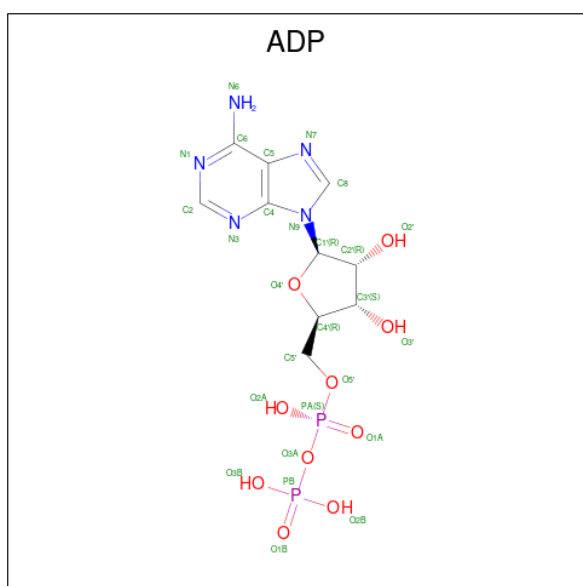
- Molecule 15 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	231	1763	1106	292	355	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	83	LYS	ALA	conflict	UNP P28066

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
16	C	1	27	10	5	10	2	0
16	D	1	27	10	5	10	2	0
16	E	1	27	10	5	10	2	0

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	C	1	Total	Mg	0
			1	1	

*Continued on next page...*

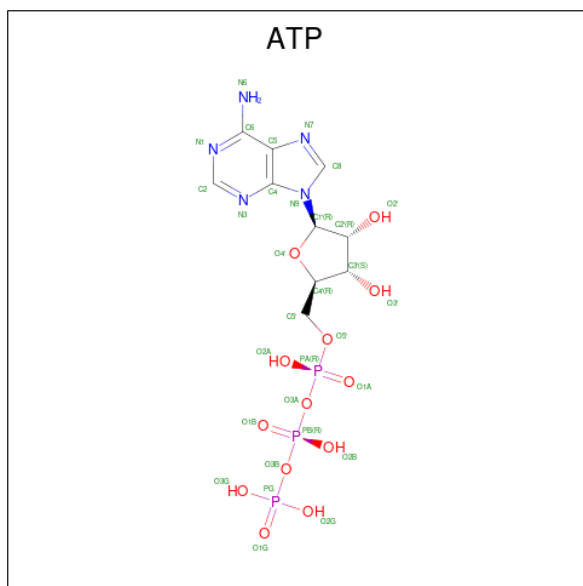
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	
17	B	1	Total	Mg	0
			1	1	
17	D	1	Total	Mg	0
			1	1	
17	F	1	Total	Mg	0
			1	1	

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	c	1	Total	Zn	0
			1	1	

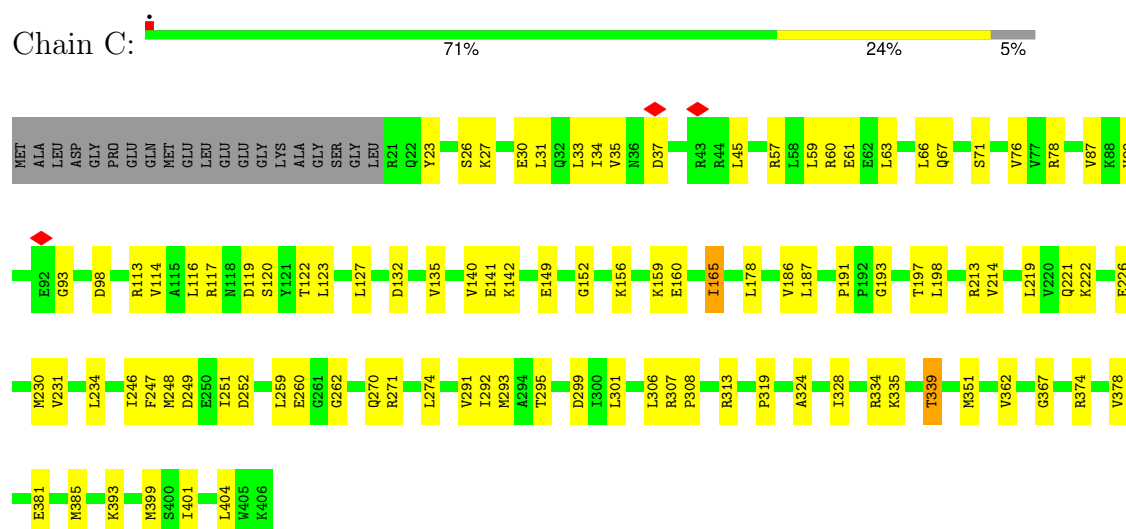
- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



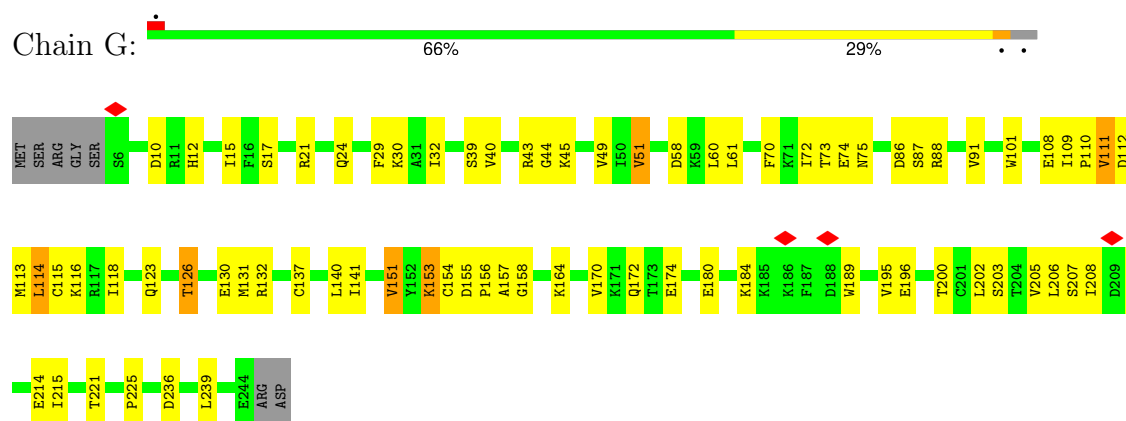
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 protease regulatory subunit 8

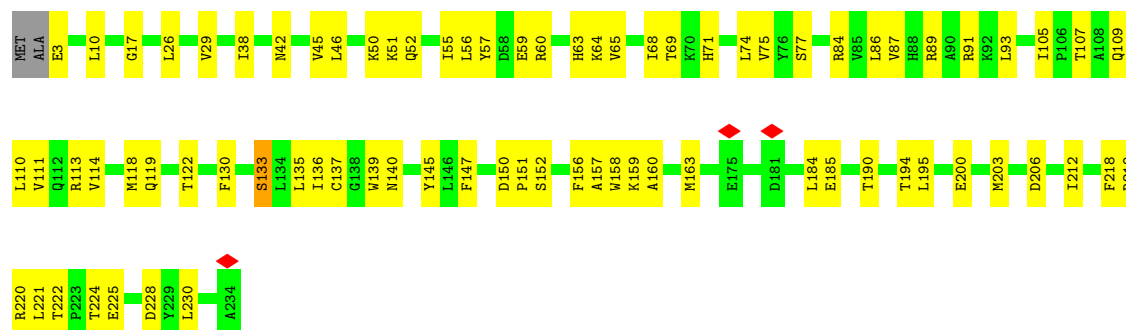


#### • Molecule 2: Proteasome subunit alpha type-6

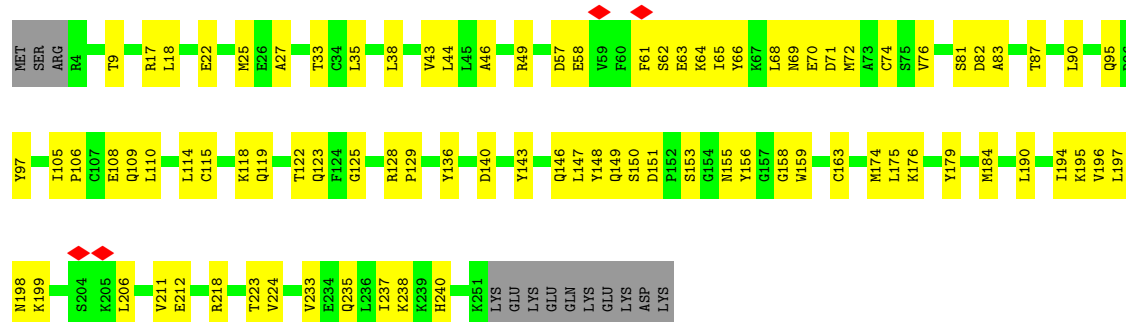


#### • Molecule 3: Proteasome subunit alpha type-2

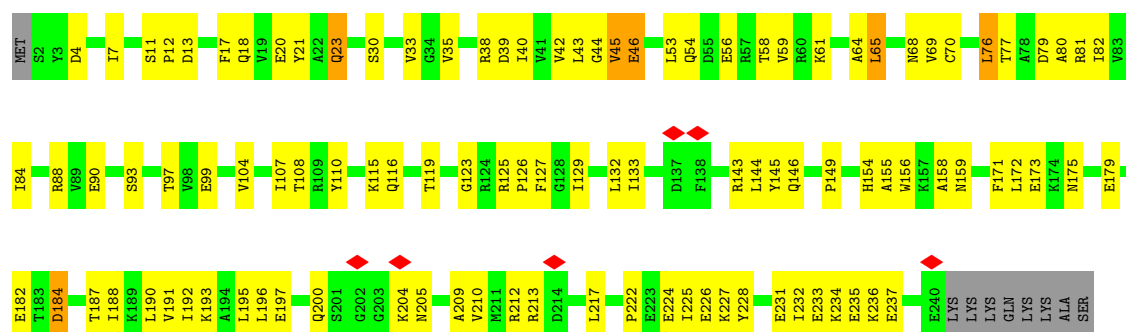




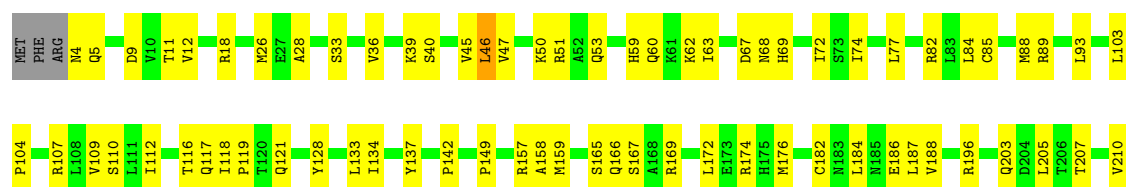
• Molecule 4: Proteasome subunit alpha type-4



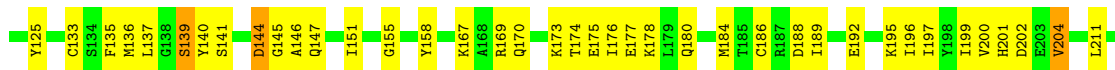
• Molecule 5: Proteasome subunit alpha type-7



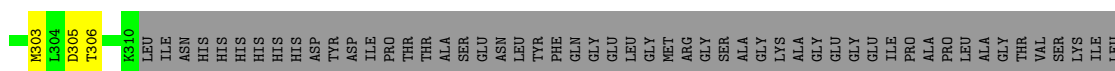
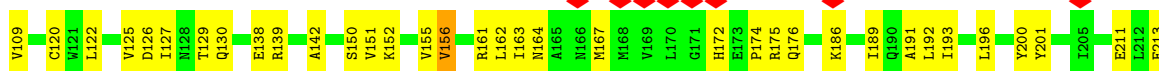
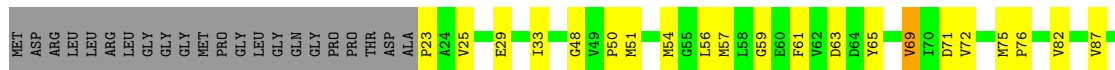
• Molecule 6: Proteasome subunit alpha type-1



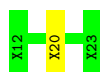
- Molecule 7: Proteasome subunit alpha type-3



- Molecule 8: 26S proteasome non-ATPase regulatory subunit 14

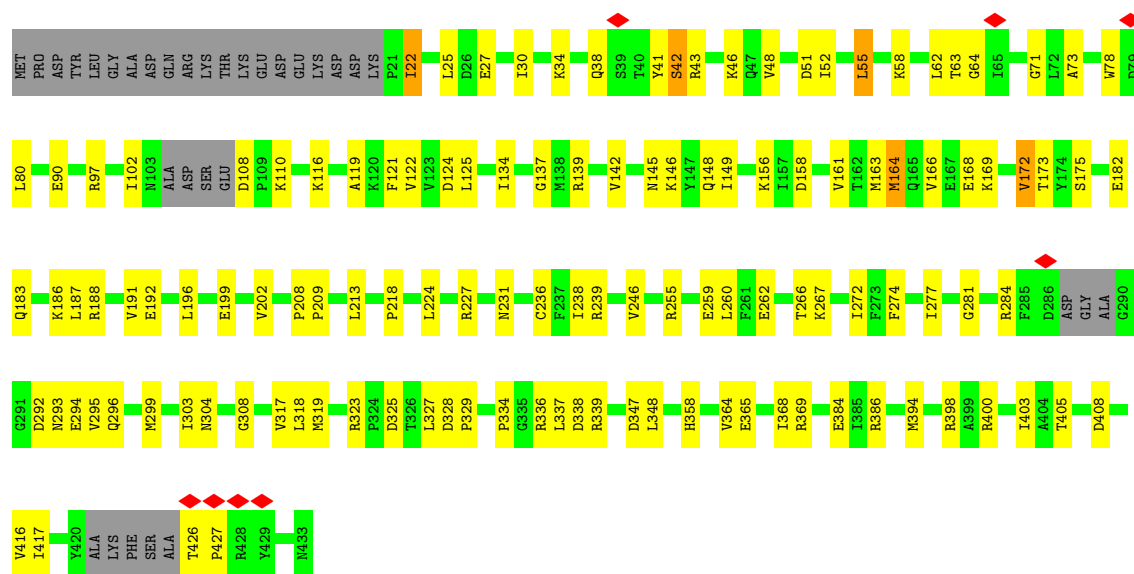


- Molecule 9: Substrate polypeptide

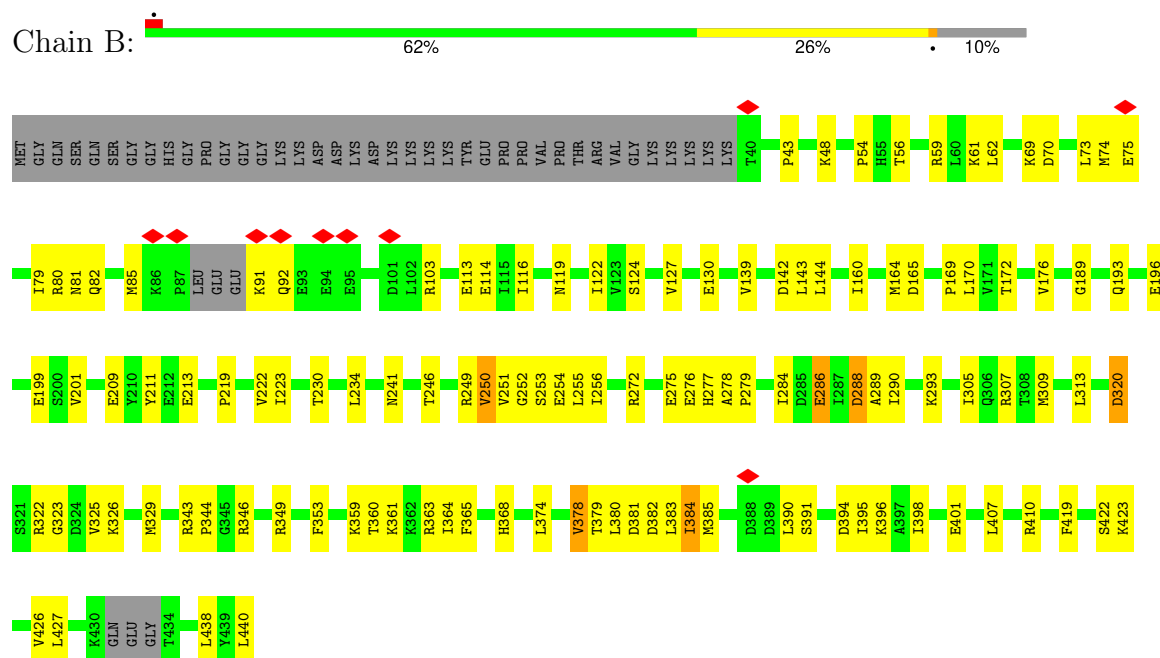


- Molecule 10: 26S proteasome regulatory subunit 7

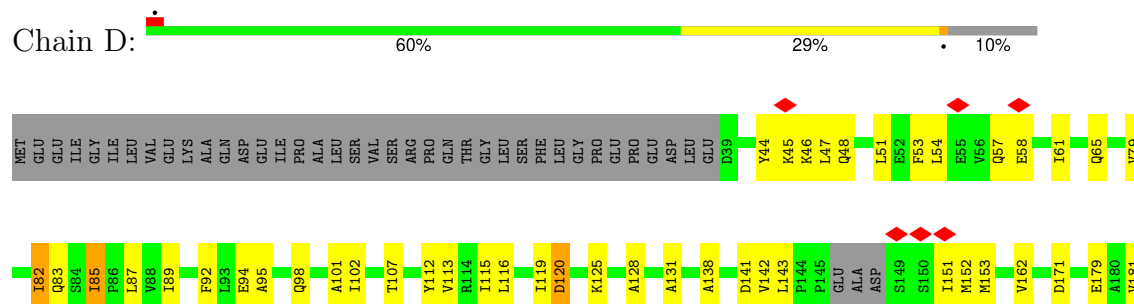




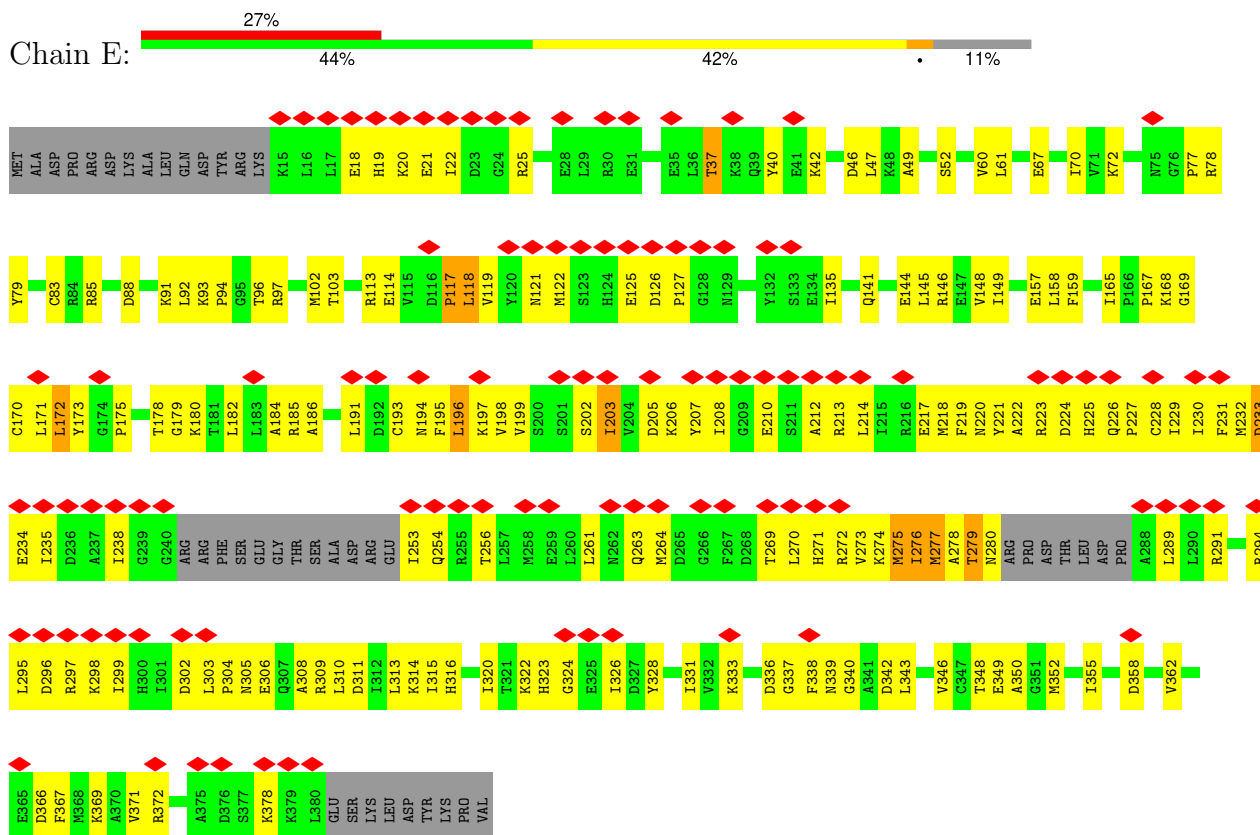
- Molecule 11: 26S proteasome regulatory subunit 4



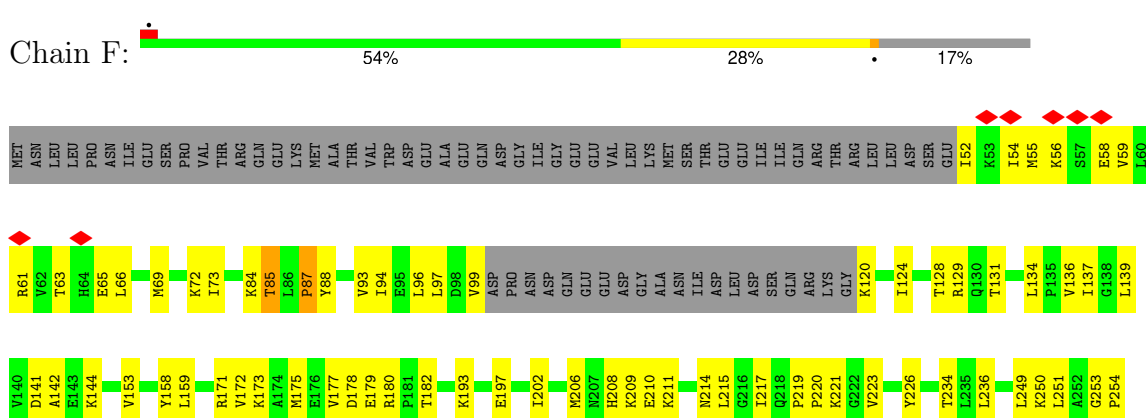
- Molecule 12: 26S proteasome regulatory subunit 6B

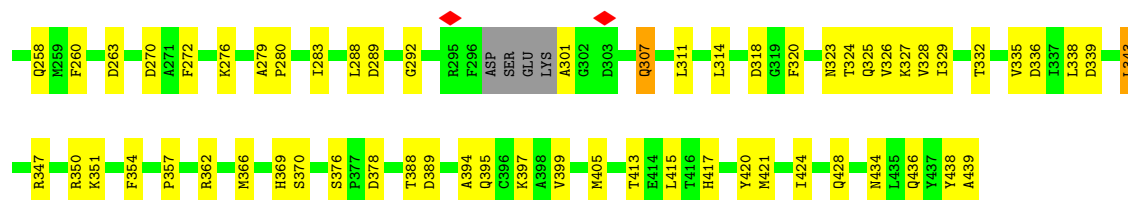


- Molecule 13: 26S protease regulatory subunit 10B

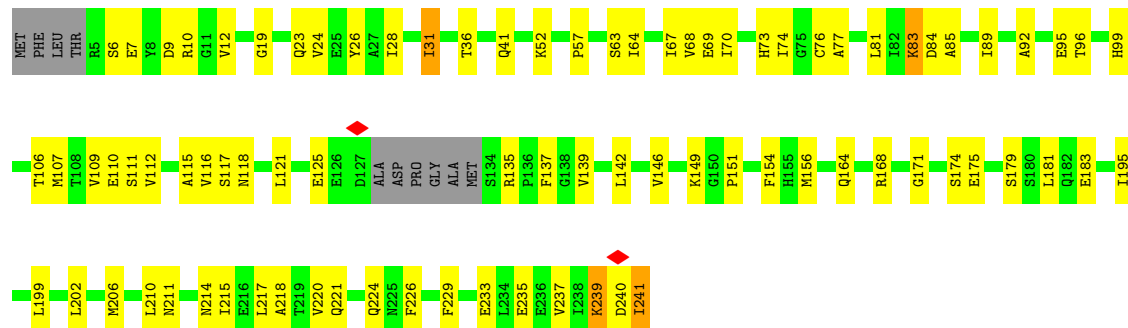


- Molecule 14: 26S proteasome regulatory subunit 6A





• Molecule 15: Proteasome subunit alpha type-5





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.276	Depositor
Minimum map value	-0.557	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.048, 1.048, 1.048	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.20	0/3092	0.42	1/4154 (0.0%)
2	G	0.16	0/1864	0.45	3/2527 (0.1%)
3	H	0.14	0/1852	0.35	0/2507
4	I	0.18	0/1938	0.40	0/2622
5	J	0.15	0/1838	0.38	0/2493
6	L	0.16	0/1880	0.35	1/2545 (0.0%)
7	M	0.16	0/1891	0.39	1/2552 (0.0%)
8	c	0.17	0/2306	0.48	1/3117 (0.0%)
10	A	0.16	0/3213	0.36	0/4333
11	B	0.19	0/3148	0.39	0/4244
12	D	0.18	0/3067	0.44	0/4135
13	E	0.32	0/2789	0.64	2/3751 (0.1%)
14	F	0.18	0/2888	0.38	0/3889
15	K	0.16	0/1789	0.32	0/2417
All	All	0.19	0/33555	0.42	9/45286 (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
2	G	0	1
13	E	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	114	LEU	CA-C-N	-7.52	109.62	122.56
2	G	114	LEU	C-N-CA	-7.52	109.62	122.56
8	c	23	PRO	N-CA-CB	6.72	110.39	103.00
1	C	262	GLY	CA-C-O	-5.67	117.51	122.16
7	M	204	VAL	N-CA-C	-5.44	108.20	113.53
2	G	184	LYS	N-CA-C	-5.35	108.01	114.75
13	E	276	ILE	N-CA-C	5.21	120.17	109.34
13	E	277	MET	N-CA-CB	5.05	117.07	109.34
6	L	226	ASP	CB-CA-C	-5.00	110.42	117.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	E	113	ARG	Sidechain
2	G	154	CYS	Peptide

## 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	C	3051	0	3165	76	0
2	G	1831	0	1813	50	0
3	H	1813	0	1804	60	0
4	I	1908	0	1864	76	0
5	J	1813	0	1751	85	0
6	L	1845	0	1820	64	0
7	M	1856	0	1814	58	0
8	c	2264	0	2278	67	0
9	v	60	0	15	1	0
10	A	3163	0	3226	83	0
11	B	3104	0	3170	88	0
12	D	3018	0	3059	88	0
13	E	2750	0	2832	176	0
14	F	2850	0	2944	89	0
15	K	1763	0	1723	63	0
16	C	27	0	12	3	0
16	D	27	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	E	27	0	12	2	0
17	A	1	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
17	F	1	0	0	0	0
18	c	1	0	0	0	0
19	A	31	0	12	2	0
19	B	31	0	12	2	0
19	F	31	0	12	3	0
All	All	33269	0	33350	1023	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 (1023) 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)
13:E:114:GLU:OE2	14:F:94:ILE:HD13	1.56	1.05
13:E:114:GLU:OE2	14:F:94:ILE:CD1	2.07	1.03
13:E:229:ILE:HG21	13:E:276:ILE:HD12	1.55	0.87
13:E:199:VAL:HG23	13:E:233:ASP:HB2	1.61	0.83
8:c:130:GLN:HE21	8:c:142:ALA:HB2	1.41	0.82
6:L:33:SER:HB2	6:L:51:ARG:HD2	1.63	0.79
3:H:159:LYS:HG3	4:I:57:ASP:HB2	1.62	0.79
13:E:229:ILE:HG22	13:E:231:PHE:HB2	1.65	0.79
13:E:213:ARG:HH12	13:E:217:GLU:HB3	1.48	0.78
3:H:107:THR:HB	3:H:145:TYR:HD2	1.49	0.78
1:C:367:GLY:HA3	12:D:196:ILE:HG21	1.64	0.78
10:A:239:ARG:NH1	11:B:320:ASP:OD2	2.17	0.78
11:B:222:VAL:HG12	11:B:349:ARG:HB2	1.67	0.76
3:H:75:VAL:HG23	3:H:135:LEU:HB3	1.67	0.76
11:B:359:LYS:HE2	11:B:359:LYS:H	1.49	0.76
10:A:292:ASP:HB3	10:A:295:VAL:HB	1.68	0.76
11:B:251:VAL:HG12	11:B:254:GLU:HG2	1.66	0.75
14:F:220:PRO:HG2	14:F:350:ARG:HD3	1.69	0.75
4:I:25:MET:HE3	4:I:153:SER:HB3	1.69	0.74
14:F:438:TYR:OH	15:K:19:GLY:O	2.06	0.74
5:J:77:THR:HG22	11:B:440:LEU:HB2	1.69	0.73
13:E:218:MET:HA	13:E:221:TYR:CE2	2.24	0.73
12:D:153:MET:SD	12:D:257:ASN:ND2	2.60	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:309:ARG:HE	13:E:343:LEU:HD21	1.54	0.72
14:F:175:MET:HE3	14:F:251:LEU:HB3	1.70	0.72
7:M:108:LEU:HD23	7:M:147:GLN:HB2	1.72	0.72
5:J:99:GLU:N	5:J:99:GLU:OE1	2.23	0.71
11:B:251:VAL:HG13	11:B:253:SER:H	1.55	0.71
4:I:155:ASN:ND2	5:J:77:THR:OG1	2.24	0.71
5:J:200:GLN:O	5:J:200:GLN:NE2	2.23	0.71
13:E:277:MET:SD	13:E:279:THR:HG22	2.30	0.71
2:G:208:ILE:HG22	2:G:210:PHE:H	1.56	0.71
2:G:32:ILE:HD13	2:G:137:CYS:HB2	1.73	0.71
6:L:109:VAL:HG22	6:L:134:ILE:HD12	1.73	0.70
11:B:256:ILE:HD12	11:B:305:ILE:HG12	1.73	0.70
1:C:127:LEU:HD13	12:D:102:ILE:HD11	1.74	0.70
12:D:98:GLN:OE1	12:D:98:GLN:N	2.25	0.70
7:M:192:GLU:O	7:M:196:ILE:HG13	1.92	0.70
8:c:270:LEU:HA	8:c:273:LYS:HG2	1.74	0.70
15:K:210:LEU:HD11	15:K:215:ILE:HD13	1.72	0.70
6:L:47:VAL:HG12	6:L:212:ILE:HG12	1.74	0.70
13:E:97:ARG:NH1	13:E:114:GLU:HB2	2.06	0.70
7:M:218:GLU:N	7:M:218:GLU:OE2	2.24	0.69
4:I:63:GLU:N	4:I:63:GLU:OE1	2.24	0.69
13:E:276:ILE:HG22	13:E:276:ILE:O	1.91	0.69
13:E:121:ASN:ND2	13:E:197:LYS:O	2.24	0.69
13:E:146:ARG:HE	13:E:146:ARG:HA	1.57	0.69
4:I:119:GLN:NE2	4:I:123:GLN:OE1	2.25	0.69
4:I:118:LYS:NZ	4:I:150:SER:OG	2.26	0.69
10:A:369:ARG:NH2	15:K:206:MET:O	2.25	0.69
13:E:254:GLN:CD	13:E:254:GLN:H	2.00	0.69
7:M:234:GLU:OE1	7:M:234:GLU:N	2.24	0.68
1:C:87:VAL:HG21	1:C:116:LEU:HD11	1.76	0.68
5:J:209:ALA:HB1	5:J:217:LEU:HD11	1.76	0.67
14:F:54:ILE:HD12	14:F:55:MET:N	2.10	0.67
2:G:70:PHE:HD2	2:G:91:VAL:HG11	1.58	0.67
6:L:85:CYS:SG	6:L:89:ARG:NH2	2.67	0.67
3:H:68:ILE:HD11	3:H:74:LEU:HD22	1.76	0.67
8:c:164:ASN:HB2	8:c:167:MET:HG2	1.77	0.67
11:B:391:SER:OG	11:B:394:ASP:OD1	2.13	0.67
2:G:75:ASN:ND2	2:G:225:PRO:O	2.28	0.66
1:C:271:ARG:NH1	11:B:289:ALA:O	2.28	0.66
7:M:197:ILE:HG21	7:M:211:LEU:HD13	1.77	0.66
13:E:127:PRO:HG3	13:E:193:CYS:HB3	1.75	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:256:ASN:O	8:c:260:GLU:HG3	1.95	0.66
1:C:178:LEU:HD11	11:B:407:LEU:HG	1.77	0.66
10:A:246:VAL:HG21	11:B:307:ARG:HD3	1.78	0.66
14:F:141:ASP:HB2	14:F:144:LYS:HG2	1.78	0.66
2:G:153:LYS:NZ	2:G:172:GLN:OE1	2.29	0.66
4:I:68:LEU:HD11	4:I:74:CYS:HB3	1.78	0.66
6:L:220:GLU:OE1	6:L:220:GLU:N	2.20	0.66
13:E:117:PRO:O	13:E:119:VAL:N	2.29	0.66
6:L:166:GLN:OE1	6:L:169:ARG:NH1	2.29	0.65
6:L:45:VAL:HG23	6:L:214:ILE:HG12	1.79	0.65
5:J:143:ARG:HH11	5:J:143:ARG:HG3	1.62	0.65
10:A:73:ALA:HB3	10:A:78:TRP:HD1	1.62	0.65
13:E:213:ARG:HA	13:E:213:ARG:NH1	2.10	0.65
8:c:63:ASP:O	8:c:139:ARG:NH2	2.29	0.65
8:c:284:LEU:O	8:c:286:GLU:N	2.30	0.65
4:I:106:PRO:HD2	4:I:109:GLN:HG3	1.78	0.65
4:I:153:SER:OG	4:I:155:ASN:OD1	2.14	0.65
13:E:362:VAL:HG13	13:E:366:ASP:HB3	1.77	0.65
12:D:203:LEU:HB2	12:D:327:LEU:HD13	1.79	0.64
15:K:77:ALA:HB3	15:K:142:LEU:HB2	1.79	0.64
4:I:218:ARG:NH1	4:I:223:THR:OG1	2.30	0.64
13:E:195:PHE:H	13:E:228:CYS:HB2	1.63	0.64
3:H:46:LEU:HD11	3:H:137:CYS:HB3	1.79	0.64
12:D:53:PHE:O	12:D:57:GLN:HG2	1.98	0.64
13:E:149:ILE:HG23	13:E:274:LYS:HD3	1.79	0.64
12:D:284:GLU:OE2	12:D:287:ARG:NH2	2.29	0.64
5:J:11:SER:OG	5:J:13:ASP:OD1	2.13	0.64
6:L:45:VAL:HG21	6:L:188:VAL:HG22	1.80	0.64
8:c:215:LYS:HA	8:c:218:LEU:HD12	1.80	0.64
13:E:234:GLU:HA	13:E:279:THR:HB	1.79	0.64
13:E:309:ARG:HH22	13:E:337:GLY:H	1.43	0.64
2:G:58:ASP:HB3	2:G:61:LEU:HD23	1.80	0.64
6:L:157:ARG:NH2	7:M:60:GLU:OE1	2.31	0.64
11:B:246:THR:HG21	11:B:277:HIS:HB2	1.80	0.63
2:G:87:SER:O	2:G:91:VAL:HG13	1.98	0.63
6:L:33:SER:H	6:L:62:LYS:HZ3	1.46	0.63
11:B:374:LEU:HD12	11:B:378:VAL:HG11	1.80	0.63
7:M:170:GLN:O	7:M:174:THR:HG23	1.98	0.63
10:A:55:LEU:HD21	11:B:73:LEU:HD23	1.81	0.63
1:C:60:ARG:HG3	1:C:60:ARG:HH11	1.64	0.63
10:A:281:GLY:HA2	10:A:299:MET:HG3	1.81	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:209:PRO:HB3	10:A:338:ASP:HB2	1.81	0.63
11:B:401:GLU:HB3	11:B:422:SER:HB2	1.80	0.63
10:A:255:ARG:O	10:A:259:GLU:HG2	1.97	0.63
12:D:153:MET:HE2	12:D:153:MET:HA	1.80	0.62
15:K:95:GLU:HG2	15:K:115:ALA:HB1	1.80	0.62
7:M:214:SER:OG	7:M:224:HIS:NE2	2.32	0.62
3:H:212:ILE:HG13	3:H:221:LEU:HD21	1.80	0.62
4:I:158:GLY:H	5:J:58:THR:HG1	1.47	0.62
6:L:103:LEU:HD12	6:L:104:PRO:HD2	1.82	0.62
11:B:361:LYS:HD3	11:B:390:LEU:HB3	1.81	0.62
7:M:108:LEU:HD22	7:M:139:SER:HB3	1.81	0.62
12:D:141:ASP:OD1	12:D:142:VAL:N	2.33	0.62
3:H:17:GLY:HA3	4:I:27:ALA:HB2	1.82	0.62
12:D:411:GLU:HB3	12:D:412:GLN:OE1	2.00	0.62
13:E:114:GLU:OE2	14:F:94:ILE:HD12	1.98	0.62
15:K:146:VAL:HG13	15:K:220:VAL:HG12	1.82	0.62
6:L:72:ILE:HG21	6:L:88:MET:HE1	1.81	0.62
13:E:367:PHE:O	13:E:371:VAL:HG22	2.00	0.61
14:F:324:THR:HG23	14:F:326:VAL:H	1.64	0.61
1:C:35:VAL:HG22	12:D:51:LEU:HD23	1.83	0.61
13:E:25:ARG:HH22	14:F:55:MET:HE1	1.64	0.61
13:E:305:ASN:O	13:E:309:ARG:N	2.33	0.61
3:H:10:LEU:HD21	3:H:122:THR:HA	1.81	0.61
12:D:267:ILE:HG21	12:D:309:MET:HB3	1.82	0.61
7:M:97:ASN:O	7:M:101:ASN:ND2	2.33	0.61
8:c:265:MET:HG3	8:c:265:MET:O	2.01	0.61
13:E:144:GLU:HG3	13:E:299:ILE:HG21	1.83	0.61
10:A:284:ARG:NH2	14:F:289:ASP:OD1	2.33	0.61
13:E:314:LYS:HG3	13:E:328:TYR:HD2	1.65	0.61
2:G:12:HIS:HB2	2:G:15:ILE:HD12	1.82	0.61
1:C:66:LEU:HD11	12:D:116:LEU:HD13	1.83	0.60
5:J:30:SER:HB3	5:J:46:GLU:HG2	1.80	0.60
6:L:51:ARG:HD3	6:L:60:GLN:HE22	1.66	0.60
3:H:45:VAL:HG22	3:H:212:ILE:HG22	1.83	0.60
2:G:158:GLY:O	3:H:84:ARG:NH1	2.26	0.60
3:H:50:LYS:HZ1	3:H:64:LYS:H	1.50	0.60
7:M:236:GLU:O	7:M:240:LYS:HG2	2.01	0.60
4:I:174:MET:HE1	4:I:199:LYS:HD2	1.83	0.60
8:c:61:PHE:HB3	8:c:139:ARG:HH21	1.65	0.60
10:A:166:VAL:HG12	10:A:168:GLU:H	1.65	0.60
15:K:221:GLN:HG3	15:K:224:GLN:HB2	1.82	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:118:LYS:O	4:I:122:THR:HG23	2.02	0.60
13:E:227:PRO:HD3	13:E:271:HIS:NE2	2.17	0.60
3:H:111:VAL:HG22	3:H:136:ILE:HD13	1.83	0.60
6:L:69:HIS:NE2	6:L:103:LEU:O	2.29	0.59
13:E:352:MET:HA	13:E:355:ILE:HG12	1.84	0.59
15:K:110:GLU:HG2	15:K:154:PHE:CZ	2.37	0.59
5:J:231:GLU:O	5:J:235:GLU:HG2	2.03	0.59
1:C:113:ARG:O	1:C:127:LEU:HB2	2.02	0.59
10:A:97:ARG:HA	10:A:139:ARG:HA	1.84	0.59
15:K:199:LEU:HB3	15:K:241:ILE:HD13	1.84	0.59
8:c:57:MET:HA	8:c:72:VAL:HG23	1.85	0.59
15:K:69:GLU:HG3	15:K:226:PHE:HD2	1.68	0.59
10:A:158:ASP:HB3	10:A:161:VAL:HB	1.84	0.59
13:E:219:PHE:HB3	13:E:270:LEU:HD12	1.86	0.58
15:K:107:MET:HG2	15:K:111:SER:HB2	1.86	0.58
1:C:57:ARG:O	1:C:61:GLU:HG3	2.03	0.58
6:L:9:ASP:OD1	6:L:11:THR:OG1	2.22	0.58
6:L:67:ASP:OD1	6:L:68:ASN:N	2.34	0.58
19:A:501:ATP:O1G	11:B:346:ARG:NH1	2.34	0.58
13:E:135:ILE:HG21	13:E:186:ALA:HB2	1.85	0.58
14:F:172:VAL:HG21	14:F:270:ASP:HB2	1.85	0.58
1:C:198:LEU:HD22	16:C:501:ADP:H2'	1.86	0.58
6:L:159:MET:HE2	6:L:159:MET:HA	1.84	0.58
8:c:236:GLU:OE2	8:c:236:GLU:N	2.31	0.58
2:G:236:ASP:HA	2:G:239:LEU:HD12	1.85	0.58
1:C:222:LYS:HD3	12:D:239:TYR:HB3	1.84	0.58
8:c:291:LEU:O	8:c:295:ASN:ND2	2.33	0.58
13:E:40:TYR:HB2	14:F:73:ILE:HD11	1.85	0.58
11:B:164:MET:HA	11:B:164:MET:HE3	1.85	0.58
7:M:41:CYS:N	7:M:44:GLY:O	2.32	0.58
14:F:311:LEU:HA	14:F:314:LEU:HD12	1.85	0.58
13:E:171:LEU:HG	13:E:277:MET:HE1	1.85	0.57
13:E:180:LYS:HD2	13:E:278:ALA:HB1	1.85	0.57
6:L:36:VAL:HG13	6:L:172:LEU:HD11	1.86	0.57
7:M:108:LEU:HD11	7:M:137:LEU:HB3	1.86	0.57
13:E:305:ASN:OD1	13:E:306:GLU:N	2.37	0.57
14:F:221:LYS:HD2	14:F:320:PHE:HB2	1.86	0.57
3:H:93:LEU:HD13	3:H:113:ARG:HB3	1.86	0.57
6:L:26:MET:HA	6:L:149:PRO:HG2	1.85	0.57
12:D:412:GLN:OE1	12:D:412:GLN:N	2.37	0.57
13:E:202:SER:HB3	13:E:214:LEU:HD12	1.86	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:HD23	12:D:47:LEU:HB3	1.85	0.57
4:I:17:ARG:NH2	4:I:22:GLU:OE1	2.37	0.57
1:C:156:LYS:O	1:C:160:GLU:HG3	2.05	0.57
4:I:25:MET:HE2	4:I:151:ASP:HB3	1.86	0.57
8:c:285:GLU:HA	8:c:288:VAL:HB	1.85	0.57
5:J:115:LYS:O	5:J:119:THR:HG23	2.05	0.57
6:L:82:ARG:NH2	15:K:118:ASN:OD1	2.38	0.57
13:E:207:TYR:O	13:E:208:ILE:HD13	2.04	0.57
10:A:173:THR:HG23	10:A:175:SER:H	1.69	0.57
11:B:272:ARG:NH1	11:B:276:GLU:OE2	2.37	0.57
10:A:292:ASP:O	10:A:294:GLU:N	2.38	0.56
11:B:116:ILE:HD11	11:B:122:ILE:HD12	1.87	0.56
12:D:234:GLU:HG2	13:E:208:ILE:HG13	1.87	0.56
15:K:9:ASP:O	15:K:23:GLN:NE2	2.38	0.56
12:D:179:GLU:O	12:D:191:TYR:OH	2.23	0.56
13:E:171:LEU:HD13	13:E:298:LYS:HB3	1.86	0.56
14:F:318:ASP:OD2	14:F:347:ARG:NH1	2.38	0.56
4:I:106:PRO:O	4:I:108:GLU:N	2.35	0.56
4:I:174:MET:SD	4:I:196:VAL:HG22	2.46	0.56
11:B:252:GLY:HA2	11:B:255:LEU:HD12	1.87	0.56
5:J:79:ASP:HB3	5:J:127:PHE:HD2	1.70	0.56
14:F:61:ARG:O	14:F:65:GLU:HG2	2.05	0.56
13:E:118:LEU:H	13:E:118:LEU:HD22	1.70	0.56
10:A:145:ASN:OD1	10:A:146:LYS:N	2.39	0.56
10:A:323:ARG:NH1	10:A:325:ASP:OD1	2.39	0.56
10:A:139:ARG:NH1	11:B:114:GLU:OE2	2.28	0.56
14:F:307:GLN:O	14:F:311:LEU:HD23	2.05	0.56
7:M:34:SER:OG	7:M:65:ARG:NH1	2.37	0.56
13:E:272:ARG:HB3	13:E:274:LYS:NZ	2.21	0.56
13:E:309:ARG:NE	13:E:343:LEU:HD21	2.20	0.56
14:F:357:PRO:O	14:F:362:ARG:NH1	2.38	0.56
14:F:366:MET:HE1	14:F:388:THR:HG21	1.88	0.56
10:A:384:GLU:HG2	11:B:344:PRO:HG2	1.88	0.56
1:C:141:GLU:OE1	1:C:141:GLU:N	2.29	0.55
1:C:186:VAL:HG12	1:C:313:ARG:HB3	1.88	0.55
1:C:248:MET:HB2	1:C:293:MET:HG2	1.88	0.55
11:B:219:PRO:HG2	11:B:349:ARG:HE	1.71	0.55
6:L:117:GLN:NE2	6:L:121:GLN:OE1	2.37	0.55
5:J:158:ALA:HB1	5:J:172:LEU:HD13	1.88	0.55
10:A:124:ASP:OD1	10:A:148:GLN:NE2	2.38	0.55
11:B:278:ALA:HB3	11:B:279:PRO:HD3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:141:GLN:OE1	13:E:141:GLN:N	2.30	0.55
13:E:313:LEU:HD12	13:E:328:TYR:HB3	1.87	0.55
4:I:83:ALA:O	4:I:87:THR:HG23	2.06	0.55
11:B:343:ARG:NH1	11:B:344:PRO:O	2.38	0.55
13:E:182:LEU:HA	13:E:185:ARG:HB3	1.87	0.55
5:J:90:GLU:HG2	5:J:110:TYR:CG	2.42	0.55
5:J:190:LEU:HA	5:J:193:LYS:HD3	1.88	0.55
5:J:108:THR:HG21	5:J:145:TYR:HB3	1.89	0.55
6:L:174:ARG:NH2	14:F:378:ASP:OD1	2.38	0.55
13:E:92:LEU:HA	13:E:96:THR:HG21	1.89	0.55
3:H:119:GLN:HG3	4:I:81:SER:HB2	1.87	0.55
6:L:165:SER:OG	6:L:169:ARG:NH2	2.39	0.55
8:c:257:LYS:HA	8:c:260:GLU:OE1	2.07	0.55
15:K:24:VAL:O	15:K:28:ILE:HG12	2.07	0.55
15:K:224:GLN:N	15:K:224:GLN:OE1	2.40	0.55
2:G:115:CYS:HA	2:G:118:ILE:HB	1.89	0.54
4:I:49:ARG:NH1	4:I:212:GLU:OE1	2.39	0.54
8:c:130:GLN:NE2	8:c:142:ALA:HB2	2.18	0.54
8:c:192:LEU:HD13	8:c:196:LEU:HB3	1.89	0.54
3:H:222:THR:N	3:H:225:GLU:OE1	2.36	0.54
12:D:366:ARG:NH2	12:D:400:GLU:OE1	2.37	0.54
13:E:88:ASP:HB3	13:E:91:LYS:HE2	1.89	0.54
7:M:117:MET:HE2	7:M:117:MET:HA	1.88	0.54
12:D:409:LYS:HE2	12:D:409:LYS:HA	1.90	0.54
4:I:143:TYR:HB2	4:I:146:GLN:NE2	2.22	0.54
10:A:156:LYS:NZ	11:B:113:GLU:OE1	2.40	0.54
12:D:113:VAL:HB	12:D:138:ALA:HA	1.90	0.54
13:E:263:GLN:HG3	13:E:264:MET:H	1.73	0.54
5:J:119:THR:HG22	5:J:126:PRO:HB3	1.89	0.54
14:F:370:SER:OG	14:F:420:TYR:OH	2.13	0.54
8:c:255:TYR:O	8:c:259:VAL:HG12	2.07	0.54
8:c:54:MET:HB3	8:c:82:VAL:HG12	1.90	0.54
8:c:163:ILE:HG12	8:c:174:PRO:HG2	1.89	0.54
13:E:207:TYR:CG	13:E:208:ILE:N	2.74	0.54
13:E:314:LYS:HZ2	13:E:328:TYR:HB2	1.72	0.54
14:F:223:VAL:HG22	14:F:350:ARG:HB2	1.89	0.54
15:K:36:THR:HA	15:K:171:GLY:HA3	1.90	0.54
1:C:339:THR:OG1	1:C:378:VAL:O	2.22	0.54
3:H:3:GLU:N	3:H:3:GLU:OE2	2.40	0.54
10:A:27:GLU:OE1	10:A:27:GLU:N	2.40	0.54
5:J:187:THR:O	5:J:191:VAL:HG23	2.07	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:29:PHE:HE2	2:G:157:ALA:HB2	1.72	0.53
6:L:157:ARG:HD2	6:L:176:MET:HE3	1.90	0.53
6:L:184:LEU:HD11	6:L:214:ILE:HD13	1.89	0.53
7:M:31:GLU:OE1	7:M:169:ARG:NH1	2.40	0.53
10:A:364:VAL:HB	10:A:368:ILE:HD12	1.90	0.53
12:D:89:ILE:HD13	13:E:78:ARG:HB3	1.89	0.53
15:K:7:GLU:OE1	15:K:7:GLU:N	2.39	0.53
2:G:60:LEU:HD11	7:M:177:GLU:HG2	1.91	0.53
12:D:231:VAL:HB	12:D:234:GLU:HG3	1.91	0.53
13:E:355:ILE:HA	14:F:211:LYS:NZ	2.22	0.53
8:c:224:SER:O	8:c:227:GLU:HG3	2.09	0.53
10:A:303:ILE:HG23	10:A:336:ARG:CZ	2.38	0.53
10:A:336:ARG:NH2	19:F:501:ATP:O1G	2.41	0.53
6:L:137:TYR:CE1	6:L:217:LYS:HA	2.43	0.53
13:E:122:MET:SD	13:E:122:MET:N	2.82	0.53
10:A:213:LEU:HB2	10:A:337:LEU:HD13	1.89	0.53
13:E:222:ALA:HB1	13:E:273:VAL:HG21	1.91	0.53
15:K:240:ASP:OD1	15:K:240:ASP:N	2.38	0.53
5:J:173:GLU:HG2	15:K:57:PRO:HD2	1.90	0.53
6:L:88:MET:HG3	6:L:112:ILE:HD11	1.91	0.53
11:B:365:PHE:HB3	11:B:380:LEU:HD13	1.91	0.53
13:E:171:LEU:HD12	13:E:295:LEU:HD13	1.91	0.53
13:E:272:ARG:HB3	13:E:274:LYS:HZ2	1.74	0.53
13:E:303:LEU:HD21	13:E:338:PHE:HB3	1.91	0.53
3:H:190:THR:O	3:H:194:THR:OG1	2.24	0.53
15:K:69:GLU:HG3	15:K:226:PHE:CD2	2.44	0.53
8:c:69:VAL:HG12	8:c:109:VAL:HG21	1.91	0.53
12:D:107:THR:HG22	13:E:77:PRO:HG3	1.91	0.53
14:F:323:ASN:O	14:F:323:ASN:ND2	2.42	0.53
3:H:200:GLU:OE1	3:H:200:GLU:N	2.42	0.52
12:D:337:ASP:OD1	12:D:337:ASP:N	2.43	0.52
13:E:37:THR:HA	14:F:69:MET:HE1	1.91	0.52
1:C:214:VAL:HG13	1:C:248:MET:HE3	1.92	0.52
2:G:174:GLU:HB2	2:G:205:VAL:HG23	1.90	0.52
5:J:104:VAL:HG11	5:J:143:ARG:HB2	1.91	0.52
7:M:173:LYS:HA	7:M:176:ILE:HG22	1.91	0.52
1:C:381:GLU:O	1:C:385:MET:HG3	2.10	0.52
10:A:186:LYS:HB3	10:A:339:ARG:HD3	1.91	0.52
10:A:238:ILE:HG21	10:A:260:LEU:HD11	1.90	0.52
12:D:189:GLU:HG2	12:D:190:LEU:N	2.24	0.52
13:E:97:ARG:HH12	13:E:114:GLU:HB2	1.75	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:222:PRO:O	5:J:226:GLU:HG2	2.09	0.52
8:c:167:MET:HE2	8:c:167:MET:N	2.24	0.52
13:E:291:ARG:CZ	13:E:294:ARG:HH12	2.23	0.52
1:C:301:LEU:HD12	1:C:306:LEU:HD21	1.92	0.52
2:G:51:VAL:HG23	2:G:202:LEU:HD22	1.91	0.52
5:J:179:GLU:OE2	5:J:179:GLU:N	2.38	0.52
12:D:317:LEU:HD12	12:D:322:LEU:HD21	1.91	0.52
15:K:149:LYS:HB2	15:K:149:LYS:NZ	2.25	0.52
2:G:112:ASP:O	2:G:116:LYS:HB3	2.08	0.52
3:H:42:ASN:HD21	3:H:184:LEU:HB2	1.74	0.52
7:M:186:CYS:HA	7:M:189:ILE:HG22	1.92	0.52
8:c:71:ASP:OD1	8:c:72:VAL:N	2.43	0.52
14:F:211:LYS:O	14:F:215:LEU:HD12	2.09	0.52
8:c:151:VAL:HG13	8:c:152:LYS:HG2	1.91	0.52
13:E:158:LEU:HD12	13:E:159:PHE:N	2.25	0.52
5:J:146:GLN:OE1	5:J:159:ASN:ND2	2.43	0.52
7:M:180:GLN:O	7:M:184:MET:HG3	2.10	0.52
7:M:233:GLU:O	7:M:237:LYS:HG2	2.10	0.52
11:B:54:PRO:O	11:B:56:THR:N	2.40	0.52
6:L:36:VAL:HB	6:L:47:VAL:HG23	1.92	0.52
12:D:410:ASP:OD1	12:D:411:GLU:N	2.42	0.52
2:G:86:ASP:OD1	2:G:132:ARG:NH2	2.40	0.51
13:E:225:HIS:CG	13:E:226:GLN:H	2.28	0.51
4:I:235:GLN:O	4:I:238:LYS:HG3	2.11	0.51
12:D:189:GLU:O	12:D:193:GLN:HG3	2.10	0.51
12:D:241:GLY:O	12:D:245:ARG:HB2	2.10	0.51
14:F:283:ILE:HB	14:F:328:VAL:HG22	1.93	0.51
2:G:73:THR:HG22	2:G:74:GLU:H	1.74	0.51
3:H:59:GLU:HG3	3:H:206:ASP:HB3	1.91	0.51
8:c:138:GLU:OE2	8:c:138:GLU:N	2.37	0.51
10:A:73:ALA:HB3	10:A:78:TRP:CD1	2.44	0.51
13:E:91:LYS:HA	13:E:93:LYS:NZ	2.25	0.51
13:E:207:TYR:C	13:E:208:ILE:HD13	2.35	0.51
5:J:155:ALA:N	15:K:63:SER:OG	2.32	0.51
5:J:93:SER:O	5:J:97:THR:HG23	2.10	0.51
13:E:182:LEU:O	13:E:186:ALA:N	2.39	0.51
1:C:221:GLN:NE2	1:C:230:MET:SD	2.83	0.51
4:I:71:ASP:HB2	4:I:223:THR:HG21	1.92	0.51
6:L:137:TYR:HE2	6:L:142:PRO:HD3	1.76	0.51
12:D:204:MET:HB3	12:D:333:PHE:CE1	2.46	0.51
7:M:86:SER:O	7:M:90:ILE:HG12	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:383:LEU:O	11:B:423:LYS:NZ	2.44	0.51
11:B:423:LYS:O	11:B:427:LEU:HG	2.11	0.51
12:D:381:GLU:HB3	12:D:402:ALA:HB1	1.93	0.51
13:E:169:GLY:HA3	13:E:296:ASP:H	1.76	0.51
13:E:310:LEU:HB2	13:E:314:LYS:HZ3	1.76	0.51
5:J:33:VAL:O	5:J:44:GLY:N	2.42	0.50
6:L:220:GLU:H	6:L:220:GLU:CD	2.15	0.50
8:c:299:CYS:O	8:c:303:MET:HG2	2.10	0.50
10:A:97:ARG:NH2	10:A:137:GLY:O	2.44	0.50
10:A:187:LEU:O	10:A:191:VAL:HG22	2.11	0.50
3:H:65:VAL:O	3:H:220:ARG:NH1	2.31	0.50
4:I:72:MET:HE2	4:I:110:LEU:HD23	1.92	0.50
10:A:41:TYR:HE2	11:B:59:ARG:HB2	1.75	0.50
15:K:142:LEU:HD21	15:K:168:ARG:HB3	1.93	0.50
1:C:259:LEU:N	1:C:270:GLN:OE1	2.42	0.50
4:I:206:LEU:HD11	4:I:211:VAL:HG21	1.94	0.50
14:F:202:ILE:HD12	14:F:327:LYS:HB3	1.94	0.50
4:I:90:LEU:HD11	4:I:136:TYR:HE2	1.76	0.50
4:I:143:TYR:HB2	4:I:146:GLN:HE21	1.75	0.50
13:E:331:ILE:HG23	13:E:371:VAL:HG11	1.93	0.50
5:J:90:GLU:HG2	5:J:110:TYR:CD1	2.46	0.50
12:D:151:ILE:HD12	12:D:152:MET:N	2.27	0.50
13:E:46:ASP:OD2	13:E:47:LEU:N	2.45	0.50
13:E:117:PRO:O	13:E:118:LEU:C	2.55	0.50
13:E:294:ARG:HB2	13:E:294:ARG:CZ	2.42	0.50
2:G:101:TRP:CG	2:G:109:ILE:HB	2.47	0.50
4:I:233:VAL:O	4:I:237:ILE:HG12	2.11	0.50
5:J:4:ASP:O	5:J:18:GLN:NE2	2.44	0.50
5:J:143:ARG:HG3	5:J:143:ARG:NH1	2.25	0.50
7:M:33:SER:O	7:M:167:LYS:N	2.45	0.50
1:C:246:ILE:HB	1:C:291:VAL:HG12	1.94	0.50
12:D:116:LEU:O	12:D:119:ILE:HD12	2.12	0.50
3:H:59:GLU:HG2	3:H:60:ARG:HG2	1.94	0.49
10:A:262:GLU:O	10:A:266:THR:HG23	2.12	0.49
13:E:18:GLU:O	13:E:21:GLU:HG3	2.12	0.49
4:I:66:TYR:CD2	4:I:87:THR:HG21	2.47	0.49
5:J:104:VAL:HG22	5:J:145:TYR:HD2	1.76	0.49
6:L:53:GLN:OE1	14:F:436:GLN:HA	2.11	0.49
12:D:323:ARG:HH21	12:D:326:ARG:CZ	2.25	0.49
12:D:352:MET:HE1	12:D:379:CYS:HB3	1.94	0.49
13:E:217:GLU:HA	13:E:220:ASN:OD1	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:261:LEU:HD11	13:E:294:ARG:NE	2.28	0.49
15:K:85:ALA:HB2	15:K:139:VAL:HG21	1.94	0.49
1:C:45:LEU:HB3	12:D:61:ILE:HG21	1.93	0.49
1:C:404:LEU:HD11	3:H:26:LEU:HD11	1.94	0.49
4:I:35:LEU:HG	4:I:46:ALA:HB3	1.94	0.49
4:I:115:CYS:SG	4:I:156:TYR:HB3	2.52	0.49
4:I:105:ILE:HG21	4:I:110:LEU:HB2	1.95	0.49
8:c:25:VAL:HG23	8:c:175:ARG:HD2	1.95	0.49
11:B:176:VAL:HG23	11:B:249:ARG:HG2	1.95	0.49
1:C:271:ARG:HG2	11:B:289:ALA:HB1	1.95	0.49
13:E:276:ILE:O	13:E:276:ILE:CG2	2.60	0.49
14:F:72:LYS:HB3	14:F:72:LYS:HZ2	1.78	0.49
15:K:68:VAL:HG21	15:K:89:ILE:HD13	1.93	0.49
2:G:44:GLY:HA2	2:G:189:TRP:HB3	1.94	0.49
3:H:65:VAL:HG12	3:H:218:PHE:HZ	1.77	0.49
3:H:157:ALA:O	4:I:57:ASP:HB3	2.13	0.49
10:A:274:PHE:HB2	10:A:319:MET:HG3	1.95	0.49
13:E:294:ARG:HB2	13:E:294:ARG:NH1	2.27	0.49
15:K:84:ASP:OD2	15:K:135:ARG:NH1	2.37	0.49
4:I:18:LEU:HD11	5:J:125:ARG:HD3	1.94	0.49
6:L:51:ARG:NH2	14:F:434:ASN:OD1	2.46	0.49
8:c:127:ILE:HG23	8:c:162:LEU:HD22	1.95	0.49
11:B:81:ASN:O	11:B:85:MET:HB3	2.13	0.49
12:D:44:TYR:O	12:D:48:GLN:HG3	2.12	0.49
13:E:91:LYS:HA	13:E:93:LYS:HZ3	1.78	0.49
15:K:84:ASP:HB3	15:K:137:PHE:HD1	1.77	0.49
3:H:135:LEU:HD22	3:H:163:MET:HE2	1.94	0.49
13:E:289:LEU:HD12	13:E:294:ARG:HD3	1.94	0.49
1:C:135:VAL:HG22	1:C:230:MET:HE3	1.95	0.48
5:J:233:GLU:HA	5:J:236:LYS:HG2	1.95	0.48
11:B:189:GLY:HA3	11:B:360:THR:HG23	1.95	0.48
11:B:196:GLU:OE1	11:B:349:ARG:NH1	2.45	0.48
13:E:323:HIS:CD2	13:E:324:GLY:H	2.30	0.48
6:L:50:LYS:HB3	6:L:59:HIS:HB3	1.93	0.48
11:B:82:GLN:OE1	11:B:82:GLN:HA	2.12	0.48
7:M:47:PHE:CE2	7:M:136:MET:HG3	2.47	0.48
10:A:48:VAL:O	10:A:52:ILE:HG13	2.13	0.48
1:C:251:ILE:HG22	1:C:295:THR:HB	1.95	0.48
2:G:17:SER:HB3	2:G:21:ARG:H	1.78	0.48
2:G:131:MET:HG2	7:M:125:TYR:CE2	2.48	0.48
3:H:109:GLN:HB3	3:H:113:ARG:NH1	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:40:ILE:HD13	5:J:212:ARG:HG3	1.95	0.48
6:L:133:LEU:HD21	6:L:159:MET:HB3	1.95	0.48
8:c:277:LYS:HA	8:c:282:ARG:HD2	1.96	0.48
10:A:122:VAL:HB	14:F:88:TYR:HB2	1.93	0.48
12:D:378:ILE:HD13	12:D:403:TYR:HD1	1.78	0.48
13:E:221:TYR:HA	13:E:224:ASP:OD2	2.13	0.48
14:F:58:GLU:HA	14:F:61:ARG:HG2	1.94	0.48
4:I:114:LEU:HD12	4:I:114:LEU:HA	1.69	0.48
8:c:151:VAL:O	8:c:152:LYS:HD3	2.13	0.48
11:B:124:SER:HA	11:B:130:GLU:HA	1.95	0.48
2:G:196:GLU:O	2:G:200:THR:HG23	2.13	0.48
2:G:202:LEU:O	2:G:206:LEU:HB2	2.13	0.48
4:I:140:ASP:OD2	4:I:146:GLN:NE2	2.34	0.48
7:M:200:VAL:HG23	7:M:200:VAL:O	2.14	0.48
13:E:311:ASP:O	13:E:315:ILE:HG13	2.14	0.48
15:K:99:HIS:CD2	15:K:107:MET:HG3	2.48	0.48
3:H:225:GLU:HA	3:H:228:ASP:OD2	2.13	0.48
5:J:17:PHE:HA	5:J:20:GLU:HG3	1.96	0.48
6:L:4:ASN:HB3	6:L:5:GLN:H	1.54	0.48
7:M:199:ILE:HA	7:M:244:LYS:HG3	1.94	0.48
8:c:191:ALA:HB1	8:c:196:LEU:HB2	1.95	0.48
14:F:394:ALA:HB2	19:F:501:ATP:H5'2	1.96	0.48
5:J:144:LEU:HD22	5:J:156:TRP:HB2	1.95	0.48
5:J:184:ASP:OD1	5:J:184:ASP:N	2.47	0.48
10:A:400:ARG:HA	10:A:400:ARG:HD3	1.66	0.48
12:D:85:ILE:O	12:D:87:LEU:N	2.47	0.48
13:E:233:ASP:O	13:E:234:GLU:C	2.57	0.48
14:F:93:VAL:HG22	14:F:124:ILE:HD11	1.95	0.48
4:I:95:GLN:OE1	4:I:95:GLN:HA	2.12	0.48
12:D:398:ASP:OD1	12:D:399:PHE:N	2.47	0.48
14:F:211:LYS:HA	14:F:214:ASN:HB3	1.95	0.48
14:F:369:HIS:CE1	14:F:397:LYS:HD2	2.49	0.48
3:H:118:MET:HE2	3:H:151:PRO:HA	1.95	0.48
5:J:38:ARG:O	5:J:213:ARG:NH2	2.47	0.48
6:L:9:ASP:HB3	6:L:12:VAL:HG13	1.96	0.48
8:c:56:LEU:HD11	8:c:87:VAL:HG13	1.96	0.48
10:A:284:ARG:HG3	10:A:296:GLN:HG2	1.95	0.48
12:D:345:PHE:O	12:D:349:THR:OG1	2.29	0.48
13:E:49:ALA:HB1	14:F:136:VAL:HG21	1.96	0.48
1:C:76:VAL:HG22	1:C:87:VAL:HG12	1.96	0.47
5:J:64:ALA:O	5:J:88:ARG:NH1	2.46	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:87:LEU:HD12	7:M:133:CYS:SG	2.53	0.47
8:c:186:LYS:HD3	8:c:186:LYS:C	2.39	0.47
13:E:179:GLY:HA2	13:E:182:LEU:HD23	1.96	0.47
13:E:184:ALA:HB2	13:E:276:ILE:HG21	1.96	0.47
14:F:59:VAL:O	14:F:63:THR:HG23	2.14	0.47
3:H:130:PHE:O	3:H:151:PRO:HB3	2.15	0.47
13:E:67:GLU:OE1	13:E:67:GLU:N	2.47	0.47
13:E:125:GLU:HA	13:E:194:ASN:HA	1.95	0.47
13:E:229:ILE:HG21	13:E:276:ILE:CD1	2.35	0.47
13:E:316:HIS:NE2	16:E:501:ADP:N3	2.61	0.47
13:E:323:HIS:HD2	13:E:324:GLY:H	1.62	0.47
6:L:39:LYS:HD2	6:L:142:PRO:HG2	1.96	0.47
6:L:196:ARG:NH1	6:L:237:GLU:O	2.30	0.47
14:F:129:ARG:NH2	14:F:260:PHE:HB3	2.29	0.47
2:G:112:ASP:OD1	2:G:113:MET:N	2.46	0.47
5:J:30:SER:H	11:B:440:LEU:C	2.22	0.47
5:J:56:GLU:O	5:J:59:VAL:HG12	2.14	0.47
8:c:150:SER:HB3	8:c:156:VAL:HG12	1.97	0.47
11:B:230:THR:HG21	11:B:353:PHE:HB3	1.96	0.47
12:D:354:LEU:HD22	12:D:358:VAL:HG11	1.95	0.47
1:C:31:LEU:O	1:C:35:VAL:HG23	2.15	0.47
3:H:185:GLU:N	3:H:185:GLU:OE1	2.48	0.47
4:I:198:ASN:C	4:I:198:ASN:HD22	2.21	0.47
6:L:205:LEU:HG	6:L:210:VAL:HG21	1.96	0.47
15:K:171:GLY:O	15:K:174:SER:OG	2.32	0.47
2:G:174:GLU:CD	2:G:174:GLU:H	2.22	0.47
6:L:82:ARG:NH1	15:K:117:SER:OG	2.29	0.47
7:M:33:SER:OG	7:M:34:SER:N	2.47	0.47
12:D:267:ILE:HG12	12:D:309:MET:SD	2.53	0.47
14:F:289:ASP:OD2	14:F:332:THR:OG1	2.15	0.47
5:J:38:ARG:HD2	5:J:182:GLU:HA	1.97	0.47
5:J:79:ASP:OD2	5:J:125:ARG:NH1	2.47	0.47
6:L:77:LEU:HG	14:F:438:TYR:CE1	2.49	0.47
6:L:203:GLN:O	6:L:239:ARG:NH2	2.48	0.47
7:M:47:PHE:N	7:M:214:SER:O	2.38	0.47
10:A:102:ILE:HB	10:A:110:LYS:HB2	1.96	0.47
13:E:326:ILE:HD11	13:E:367:PHE:CD2	2.49	0.47
14:F:178:ASP:OD2	14:F:179:GLU:N	2.48	0.47
14:F:226:TYR:CE2	14:F:351:LYS:HB3	2.50	0.47
1:C:140:VAL:HG22	1:C:213:ARG:HH11	1.79	0.47
4:I:136:TYR:HB2	4:I:148:TYR:HB2	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:70:ASP:OD2	7:M:99:ARG:NH2	2.48	0.47
15:K:195:ILE:HD12	15:K:217:LEU:HD11	1.96	0.47
1:C:152:GLY:O	16:C:501:ADP:N6	2.44	0.47
3:H:59:GLU:CD	3:H:59:GLU:H	2.23	0.47
8:c:50:PRO:HG3	13:E:102:MET:SD	2.55	0.47
11:B:394:ASP:O	11:B:398:ILE:HG13	2.15	0.47
12:D:101:ALA:HB2	12:D:115:ILE:HD11	1.97	0.47
13:E:172:LEU:HD22	13:E:299:ILE:HD11	1.97	0.47
15:K:28:ILE:O	15:K:31:ILE:HG12	2.15	0.47
1:C:31:LEU:HA	1:C:34:ILE:HG22	1.97	0.47
5:J:64:ALA:HA	5:J:70:CYS:HA	1.96	0.47
8:c:236:GLU:HA	8:c:239:LYS:HE2	1.97	0.47
8:c:266:THR:OG1	8:c:269:GLN:HB3	2.15	0.47
12:D:292:LEU:HD21	12:D:309:MET:HE1	1.97	0.47
13:E:19:HIS:HA	13:E:22:ILE:HD12	1.95	0.47
13:E:217:GLU:OE2	13:E:217:GLU:N	2.46	0.47
13:E:339:ASN:O	13:E:342:ASP:HB3	2.15	0.47
1:C:187:LEU:HD11	1:C:295:THR:HG22	1.97	0.46
6:L:4:ASN:HD22	6:L:5:GLN:HE22	1.63	0.46
7:M:69:VAL:HG11	7:M:111:LEU:HD21	1.97	0.46
8:c:150:SER:HB3	8:c:156:VAL:H	1.80	0.46
11:B:54:PRO:HB2	11:B:61:LYS:HB2	1.97	0.46
13:E:217:GLU:HG2	13:E:221:TYR:CE1	2.50	0.46
13:E:279:THR:HG23	13:E:280:ASN:N	2.30	0.46
14:F:208:HIS:O	14:F:210:GLU:N	2.48	0.46
4:I:71:ASP:OD1	4:I:72:MET:HG2	2.16	0.46
1:C:247:PHE:CE2	1:C:249:ASP:HB2	2.51	0.46
5:J:39:ASP:OD1	5:J:213:ARG:NH2	2.41	0.46
5:J:224:GLU:O	5:J:227:LYS:HG2	2.14	0.46
10:A:62:LEU:HD12	11:B:80:ARG:HH21	1.80	0.46
10:A:416:VAL:HG12	10:A:417:ILE:HD12	1.97	0.46
13:E:333:LYS:HD2	13:E:333:LYS:O	2.14	0.46
8:c:242:GLU:O	8:c:246:LYS:HG3	2.15	0.46
11:B:288:ASP:OD2	11:B:288:ASP:N	2.44	0.46
15:K:195:ILE:CD1	15:K:217:LEU:HD11	2.45	0.46
1:C:374:ARG:HD2	1:C:374:ARG:HA	1.69	0.46
1:C:401:ILE:HA	1:C:404:LEU:HD13	1.96	0.46
3:H:68:ILE:HD11	3:H:87:VAL:HG23	1.97	0.46
7:M:47:PHE:HB2	7:M:214:SER:HB3	1.97	0.46
7:M:175:GLU:O	7:M:178:LYS:HG2	2.16	0.46
10:A:236:CYS:SG	10:A:267:LYS:HD3	2.55	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:248:ARG:HG2	12:D:252:ARG:HH21	1.81	0.46
13:E:378:LYS:HB3	13:E:378:LYS:HE3	1.59	0.46
3:H:111:VAL:HG21	3:H:147:PHE:HB2	1.97	0.46
11:B:193:GLN:OE1	11:B:193:GLN:N	2.44	0.46
13:E:303:LEU:HD11	13:E:338:PHE:CD1	2.50	0.46
14:F:376:SER:HB2	14:F:415:LEU:O	2.15	0.46
7:M:140:TYR:HD2	7:M:146:ALA:HB2	1.80	0.46
10:A:125:LEU:HD22	10:A:134:ILE:HG13	1.98	0.46
12:D:204:MET:HE3	12:D:212:LYS:HB3	1.97	0.46
12:D:389:GLU:OE2	12:D:391:ARG:NH1	2.46	0.46
13:E:72:LYS:HD2	13:E:78:ARG:HD2	1.98	0.46
13:E:253:ILE:O	13:E:256:THR:OG1	2.26	0.46
1:C:113:ARG:HH22	12:D:94:GLU:CD	2.24	0.46
3:H:152:SER:O	4:I:81:SER:HB3	2.15	0.46
7:M:175:GLU:OE1	7:M:196:ILE:HG12	2.15	0.46
8:c:122:LEU:HD22	8:c:126:ASP:HB3	1.98	0.46
10:A:38:GLN:HG3	10:A:42:SER:OG	2.16	0.46
14:F:236:LEU:HD23	14:F:354:PHE:HZ	1.80	0.46
10:A:30:ILE:O	10:A:34:LYS:HG3	2.16	0.46
10:A:71:GLY:O	11:B:139:VAL:HA	2.16	0.46
11:B:379:THR:OG1	11:B:382:ASP:OD2	2.34	0.46
13:E:180:LYS:CD	13:E:278:ALA:HB1	2.45	0.46
13:E:304:PRO:HB2	13:E:309:ARG:HD3	1.97	0.46
3:H:65:VAL:HG22	3:H:75:VAL:HG12	1.98	0.46
13:E:172:LEU:HD11	13:E:276:ILE:HG23	1.97	0.46
14:F:85:THR:HG22	14:F:87:PRO:HD2	1.97	0.46
1:C:399:MET:HE2	1:C:399:MET:HB2	1.79	0.45
2:G:43:ARG:HH21	2:G:164:LYS:HG3	1.81	0.45
13:E:333:LYS:HD2	13:E:333:LYS:C	2.41	0.45
14:F:52:ILE:O	14:F:56:LYS:NZ	2.49	0.45
15:K:179:SER:O	15:K:183:GLU:HG2	2.17	0.45
4:I:97:TYR:CD1	4:I:105:ILE:HG13	2.51	0.45
5:J:4:ASP:OD1	5:J:4:ASP:N	2.49	0.45
8:c:211:GLU:N	8:c:211:GLU:OE2	2.45	0.45
2:G:202:LEU:HB3	2:G:210:PHE:CE2	2.50	0.45
5:J:104:VAL:HG23	5:J:133:ILE:HG22	1.98	0.45
11:B:43:PRO:HA	11:B:277:HIS:HB3	1.98	0.45
13:E:203:ILE:HG21	13:E:232:MET:SD	2.56	0.45
13:E:343:LEU:HA	13:E:346:VAL:HG12	1.97	0.45
3:H:52:GLN:HB3	3:H:57:TYR:CD2	2.51	0.45
4:I:69:ASN:OD1	4:I:70:GLU:N	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:211:GLU:C	8:c:213:GLU:H	2.24	0.45
8:c:285:GLU:O	8:c:289:ASP:N	2.41	0.45
12:D:92:PHE:HZ	12:D:95:ALA:HB2	1.81	0.45
12:D:231:VAL:HG12	12:D:233:SER:H	1.81	0.45
14:F:202:ILE:HG21	14:F:329:ILE:HD11	1.97	0.45
5:J:204:LYS:HD2	5:J:204:LYS:HA	1.70	0.45
8:c:267:PRO:HA	8:c:270:LEU:HD12	1.99	0.45
13:E:102:MET:HE1	14:F:158:TYR:HD2	1.82	0.45
14:F:226:TYR:CD1	14:F:335:VAL:HG21	2.51	0.45
14:F:279:ALA:HB3	14:F:280:PRO:HD3	1.99	0.45
15:K:217:LEU:HD13	15:K:218:ALA:N	2.32	0.45
1:C:324:ALA:O	1:C:328:ILE:HG13	2.17	0.45
2:G:130:GLU:HG3	2:G:131:MET:HG3	1.99	0.45
3:H:38:ILE:HG23	3:H:160:ALA:HB2	1.98	0.45
3:H:105:ILE:HD13	3:H:110:LEU:HD23	1.99	0.45
7:M:195:LYS:O	7:M:199:ILE:HG12	2.16	0.45
11:B:201:VAL:HA	11:B:326:LYS:HD3	1.99	0.45
12:D:46:LYS:N	12:D:46:LYS:HE2	2.32	0.45
13:E:77:PRO:HG2	13:E:79:TYR:CZ	2.51	0.45
13:E:170:CYS:H	13:E:296:ASP:CB	2.30	0.45
15:K:41:GLN:OE1	15:K:164:GLN:NE2	2.50	0.45
15:K:146:VAL:HA	15:K:151:PRO:HA	1.99	0.45
10:A:347:ASP:OD1	10:A:347:ASP:N	2.45	0.45
13:E:20:LYS:HA	13:E:20:LYS:HD3	1.65	0.45
13:E:148:VAL:HG12	13:E:149:ILE:HD13	1.98	0.45
15:K:218:ALA:HB1	15:K:226:PHE:CE1	2.52	0.45
4:I:44:LEU:HD22	4:I:190:LEU:HD23	1.99	0.45
5:J:45:VAL:N	5:J:195:LEU:HD11	2.31	0.45
8:c:150:SER:HB2	8:c:155:VAL:HA	1.99	0.45
10:A:51:ASP:OD2	11:B:69:LYS:HE3	2.16	0.45
13:E:303:LEU:HD22	13:E:304:PRO:HD2	1.99	0.45
4:I:175:LEU:CD1	4:I:196:VAL:HG21	2.47	0.45
6:L:93:LEU:HD23	6:L:93:LEU:HA	1.84	0.45
3:H:60:ARG:O	3:H:63:HIS:NE2	2.49	0.45
4:I:9:THR:HG21	4:I:129:PRO:HD3	1.98	0.45
12:D:257:ASN:OD1	12:D:257:ASN:N	2.50	0.45
14:F:215:LEU:HB2	14:F:217:ILE:HG22	1.99	0.45
15:K:6:SER:O	15:K:10:ARG:NH2	2.49	0.45
1:C:119:ASP:OD1	1:C:120:SER:N	2.46	0.44
1:C:127:LEU:HD21	12:D:112:TYR:CE2	2.52	0.44
2:G:180:GLU:OE2	3:H:55:ILE:HG22	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:203:SER:O	2:G:207:SER:N	2.50	0.44
4:I:158:GLY:N	5:J:58:THR:OG1	2.37	0.44
5:J:53:LEU:HD12	5:J:53:LEU:HA	1.76	0.44
5:J:76:LEU:HD12	5:J:76:LEU:H	1.82	0.44
8:c:291:LEU:HD12	8:c:291:LEU:HA	1.88	0.44
10:A:272:ILE:O	10:A:318:LEU:N	2.48	0.44
12:D:190:LEU:O	12:D:194:ILE:HG13	2.16	0.44
1:C:274:LEU:HD22	11:B:286:GLU:HG2	1.98	0.44
2:G:210:PHE:CE1	2:G:215:ILE:HD11	2.52	0.44
8:c:33:ILE:HA	8:c:69:VAL:HG22	1.98	0.44
10:A:25:LEU:HD12	11:B:410:ARG:HH12	1.82	0.44
12:D:264:ILE:HG21	12:D:267:ILE:HD13	1.99	0.44
1:C:226:GLU:O	1:C:230:MET:HG3	2.17	0.44
1:C:230:MET:HE2	1:C:230:MET:HB3	1.79	0.44
2:G:72:ILE:HG21	2:G:114:LEU:HD21	1.99	0.44
2:G:110:PRO:HB2	2:G:112:ASP:OD1	2.18	0.44
2:G:123:GLN:O	2:G:126:THR:HG22	2.17	0.44
3:H:222:THR:HG23	3:H:224:THR:H	1.82	0.44
4:I:136:TYR:HE1	4:I:150:SER:HB2	1.82	0.44
6:L:18:ARG:NH1	14:F:389:ASP:OD2	2.45	0.44
6:L:62:LYS:HE3	6:L:74:ILE:O	2.17	0.44
10:A:43:ARG:HB3	10:A:43:ARG:CZ	2.47	0.44
10:A:58:LYS:HB2	10:A:58:LYS:HE3	1.54	0.44
12:D:143:LEU:HD13	13:E:70:ILE:HD11	1.99	0.44
13:E:275:MET:HE3	13:E:277:MET:H	1.82	0.44
14:F:219:PRO:HA	14:F:220:PRO:HD3	1.89	0.44
1:C:193:GLY:HA3	12:D:323:ARG:HD2	1.99	0.44
1:C:351:MET:SD	1:C:362:VAL:HG21	2.58	0.44
4:I:125:GLY:HA3	5:J:123:GLY:HA2	1.98	0.44
5:J:77:THR:HG23	11:B:438:LEU:O	2.17	0.44
6:L:84:LEU:HD23	6:L:84:LEU:HA	1.87	0.44
7:M:141:SER:O	7:M:145:GLY:N	2.51	0.44
8:c:175:ARG:HD3	8:c:201:TYR:CD1	2.53	0.44
10:A:169:LYS:HD3	10:A:231:ASN:O	2.16	0.44
11:B:309:MET:O	11:B:313:LEU:HG	2.17	0.44
13:E:205:ASP:HB2	13:E:210:GLU:HG2	2.00	0.44
13:E:213:ARG:HA	13:E:213:ARG:HH11	1.78	0.44
15:K:202:LEU:HD23	15:K:202:LEU:HA	1.83	0.44
2:G:45:LYS:HG2	2:G:189:TRP:HB2	1.98	0.44
2:G:101:TRP:CD1	2:G:109:ILE:HB	2.51	0.44
3:H:69:THR:OG1	3:H:71:HIS:ND1	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:40:SER:HB3	6:L:187:LEU:HD13	1.98	0.44
12:D:185:LEU:HD22	12:D:185:LEU:H	1.82	0.44
15:K:233:GLU:O	15:K:237:VAL:HG22	2.18	0.44
1:C:114:VAL:HG11	1:C:123:LEU:HD11	2.00	0.44
1:C:393:LYS:HA	1:C:393:LYS:HD3	1.73	0.44
4:I:179:TYR:CD1	5:J:53:LEU:HD11	2.53	0.44
11:B:75:GLU:O	11:B:79:ILE:HG23	2.18	0.44
12:D:345:PHE:HB3	12:D:360:LEU:HD13	2.00	0.44
13:E:146:ARG:HA	13:E:146:ARG:NE	2.30	0.44
15:K:220:VAL:HG22	15:K:226:PHE:HA	1.99	0.44
2:G:49:VAL:HG11	2:G:195:VAL:HG22	1.99	0.44
8:c:29:GLU:HA	8:c:65:TYR:O	2.17	0.44
10:A:119:ALA:HB2	14:F:128:THR:HG22	2.00	0.44
10:A:394:MET:SD	11:B:211:TYR:HE2	2.41	0.44
10:A:398:ARG:NH2	11:B:199:GLU:OE1	2.51	0.44
7:M:135:PHE:CZ	7:M:151:ILE:HD12	2.53	0.44
9:v:20:UNK:O	14:F:301:ALA:N	2.51	0.44
1:C:98:ASP:OD1	1:C:98:ASP:N	2.48	0.44
2:G:86:ASP:OD2	2:G:86:ASP:N	2.51	0.44
3:H:139:TRP:C	3:H:140:ASN:HD22	2.26	0.44
5:J:145:TYR:CE1	5:J:155:ALA:HB2	2.53	0.44
5:J:224:GLU:O	5:J:228:TYR:HD1	2.01	0.44
8:c:125:VAL:O	8:c:129:THR:HG22	2.17	0.44
3:H:29:VAL:HG11	3:H:133:SER:HB2	1.99	0.43
4:I:199:LYS:HE2	4:I:199:LYS:HB3	1.70	0.43
6:L:128:TYR:O	6:L:149:PRO:HB3	2.18	0.43
7:M:71:ARG:NH2	7:M:105:ASN:OD1	2.49	0.43
12:D:45:LYS:HD2	12:D:48:GLN:OE1	2.18	0.43
13:E:309:ARG:HH12	13:E:336:ASP:HA	1.83	0.43
15:K:81:LEU:HD23	15:K:81:LEU:HA	1.85	0.43
1:C:30:GLU:O	1:C:33:LEU:HG	2.18	0.43
1:C:313:ARG:NH2	11:B:401:GLU:OE1	2.45	0.43
3:H:203:MET:HE2	3:H:230:LEU:HD21	1.99	0.43
4:I:25:MET:HE1	11:B:438:LEU:HD21	1.99	0.43
10:A:172:VAL:HG11	10:A:227:ARG:HH21	1.83	0.43
10:A:224:LEU:HD22	19:A:501:ATP:H2'	2.00	0.43
12:D:131:ALA:HB3	12:D:141:ASP:HB3	2.00	0.43
12:D:313:ARG:HA	12:D:313:ARG:NE	2.33	0.43
12:D:378:ILE:HD13	12:D:403:TYR:CD1	2.53	0.43
13:E:275:MET:HE2	13:E:275:MET:HB3	1.74	0.43
13:E:303:LEU:HD11	13:E:338:PHE:CG	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:159:TRP:HA	5:J:54:GLN:HA	2.01	0.43
7:M:69:VAL:HB	7:M:73:VAL:HB	1.99	0.43
10:A:405:THR:N	10:A:408:ASP:OD2	2.50	0.43
11:B:144:LEU:HD23	11:B:144:LEU:HA	1.75	0.43
13:E:72:LYS:HB2	13:E:78:ARG:HG3	2.00	0.43
14:F:99:VAL:HG12	14:F:120:LYS:HD3	1.99	0.43
4:I:82:ASP:OD2	4:I:128:ARG:NH1	2.26	0.43
6:L:196:ARG:CZ	6:L:239:ARG:HG3	2.48	0.43
12:D:125:LYS:HB2	12:D:128:ALA:HB2	2.00	0.43
13:E:308:ALA:HA	13:E:311:ASP:OD1	2.18	0.43
14:F:137:ILE:HG13	14:F:142:ALA:HB2	1.99	0.43
15:K:73:HIS:CE1	15:K:106:THR:HB	2.53	0.43
15:K:156:MET:HE2	15:K:156:MET:HB3	1.85	0.43
6:L:166:GLN:HG2	14:F:417:HIS:CE1	2.53	0.43
7:M:81:LEU:HG	7:M:85:ARG:NH2	2.33	0.43
10:A:119:ALA:HB3	10:A:121:PHE:CE2	2.54	0.43
10:A:164:MET:HG2	10:A:239:ARG:O	2.19	0.43
10:A:182:GLU:HG3	10:A:183:GLN:N	2.32	0.43
13:E:340:GLY:HA3	16:E:501:ADP:N7	2.33	0.43
14:F:258:GLN:HB2	14:F:263:ASP:HB3	2.00	0.43
15:K:84:ASP:OD1	15:K:84:ASP:N	2.52	0.43
1:C:26:SER:O	1:C:30:GLU:HG2	2.18	0.43
4:I:176:LYS:HA	5:J:53:LEU:HD22	1.99	0.43
5:J:116:GLN:HG3	15:K:83:LYS:HB3	2.01	0.43
10:A:308:GLY:HA2	14:F:234:THR:HG21	2.00	0.43
11:B:209:GLU:O	11:B:213:GLU:HG3	2.17	0.43
13:E:235:ILE:HA	13:E:238:ILE:HG23	2.01	0.43
1:C:399:MET:HE3	3:H:158:TRP:HH2	1.83	0.43
4:I:151:ASP:N	4:I:151:ASP:OD2	2.52	0.43
6:L:207:THR:OG1	6:L:226:ASP:O	2.36	0.43
8:c:280:PRO:O	8:c:281:LYS:HD3	2.18	0.43
13:E:169:GLY:HA3	13:E:296:ASP:HB2	2.00	0.43
13:E:261:LEU:HD13	13:E:294:ARG:HA	2.00	0.43
13:E:305:ASN:O	13:E:309:ARG:HG2	2.18	0.43
13:E:326:ILE:HD12	13:E:326:ILE:HA	1.85	0.43
19:F:501:ATP:H5'1	19:F:501:ATP:H8	1.84	0.43
1:C:252:ASP:OD1	1:C:295:THR:OG1	2.25	0.43
2:G:180:GLU:HG2	3:H:56:LEU:HD13	2.00	0.43
5:J:7:ILE:HG13	5:J:18:GLN:HG2	1.99	0.43
10:A:218:PRO:HB2	11:B:343:ARG:HD3	1.99	0.43
13:E:168:LYS:HE2	13:E:269:THR:HG23	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:141:ILE:HG22	2:G:151:VAL:HB	1.99	0.43
4:I:184:MET:HE3	4:I:184:MET:HB3	1.81	0.43
12:D:296:MET:HE2	12:D:326:ARG:HB3	2.01	0.43
13:E:165:ILE:O	13:E:167:PRO:HD3	2.19	0.43
1:C:334:ARG:HG3	1:C:335:LYS:HG3	2.00	0.43
2:G:155:ASP:HB2	2:G:156:PRO:HD2	2.01	0.43
5:J:42:VAL:HB	5:J:191:VAL:HG21	2.00	0.43
5:J:115:LYS:NZ	5:J:129:ILE:O	2.52	0.43
7:M:81:LEU:HD12	7:M:81:LEU:HA	1.86	0.43
8:c:219:ASN:HA	8:c:222:LYS:HB2	2.00	0.43
13:E:279:THR:HG23	13:E:280:ASN:H	1.83	0.43
15:K:229:PHE:HE2	15:K:237:VAL:HG11	1.84	0.43
1:C:165:ILE:HG12	1:C:292:ILE:HD11	2.00	0.42
3:H:133:SER:OG	3:H:150:ASP:OD2	2.32	0.42
4:I:58:GLU:HG3	4:I:61:PHE:CD1	2.54	0.42
5:J:192:ILE:O	5:J:196:LEU:HG	2.19	0.42
8:c:266:THR:OG1	8:c:266:THR:O	2.30	0.42
13:E:93:LYS:H	13:E:93:LYS:HD2	1.83	0.42
13:E:114:GLU:CD	14:F:94:ILE:HD13	2.39	0.42
13:E:141:GLN:NE2	13:E:302:ASP:OD1	2.52	0.42
13:E:182:LEU:HD22	13:E:182:LEU:H	1.84	0.42
14:F:134:LEU:HD23	14:F:134:LEU:HA	1.85	0.42
1:C:34:ILE:HD12	1:C:37:ASP:OD1	2.19	0.42
4:I:38:LEU:HA	4:I:43:VAL:HG23	2.02	0.42
5:J:234:LYS:HB3	5:J:234:LYS:HE3	1.70	0.42
7:M:51:LYS:HE2	7:M:51:LYS:HB3	1.91	0.42
10:A:46:LYS:HE3	10:A:46:LYS:HB2	1.78	0.42
12:D:116:LEU:HB3	12:D:119:ILE:CD1	2.49	0.42
12:D:374:ASP:O	12:D:378:ILE:HG13	2.19	0.42
12:D:384:MET:O	12:D:387:VAL:HG12	2.18	0.42
13:E:173:TYR:HB2	13:E:280:ASN:HA	2.00	0.42
13:E:191:LEU:HD12	13:E:227:PRO:HD2	2.01	0.42
13:E:322:LYS:HD2	13:E:328:TYR:OH	2.19	0.42
14:F:343:LEU:H	14:F:343:LEU:HD22	1.84	0.42
15:K:74:ILE:HG12	15:K:109:VAL:HG22	2.01	0.42
15:K:210:LEU:HD12	15:K:211:ASN:N	2.34	0.42
3:H:65:VAL:HG13	3:H:75:VAL:HG13	2.01	0.42
5:J:13:ASP:OD1	5:J:13:ASP:N	2.43	0.42
5:J:197:GLU:H	5:J:197:GLU:HG3	1.61	0.42
10:A:163:MET:HE2	10:A:163:MET:HB2	1.85	0.42
10:A:208:PRO:HA	14:F:405:MET:HE3	2.00	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:277:ILE:HG23	10:A:327:LEU:HD21	2.02	0.42
12:D:187:HIS:HB3	12:D:190:LEU:HD13	2.01	0.42
13:E:61:LEU:HD11	13:E:72:LYS:HB2	2.01	0.42
13:E:254:GLN:CD	13:E:254:GLN:N	2.75	0.42
14:F:84:LYS:HD3	14:F:139:LEU:HD12	2.01	0.42
4:I:33:THR:HG23	4:I:163:CYS:SG	2.60	0.42
5:J:171:PHE:CE1	5:J:175:ASN:ND2	2.84	0.42
11:B:361:LYS:HG2	11:B:395:ILE:HD11	2.00	0.42
13:E:145:LEU:O	13:E:149:ILE:HG12	2.19	0.42
13:E:227:PRO:HD3	13:E:271:HIS:CE1	2.53	0.42
13:E:279:THR:OG1	13:E:280:ASN:N	2.48	0.42
15:K:70:ILE:HD12	15:K:92:ALA:HB3	2.01	0.42
4:I:115:CYS:HB3	5:J:81:ARG:NH2	2.34	0.42
11:B:223:ILE:HD12	11:B:329:MET:HE2	2.00	0.42
11:B:383:LEU:HD21	11:B:419:PHE:HB3	2.00	0.42
13:E:117:PRO:C	13:E:119:VAL:N	2.77	0.42
13:E:223:ARG:NH1	13:E:271:HIS:HB2	2.34	0.42
14:F:288:LEU:HD23	14:F:338:LEU:HD21	2.00	0.42
1:C:197:THR:HB	16:C:501:ADP:O2A	2.18	0.42
4:I:72:MET:HE3	4:I:72:MET:HB3	1.79	0.42
4:I:105:ILE:H	4:I:105:ILE:HD12	1.85	0.42
4:I:195:LYS:HA	4:I:240:HIS:CE1	2.54	0.42
4:I:197:LEU:HD23	4:I:197:LEU:HA	1.84	0.42
10:A:348:LEU:HD13	15:K:175:GLU:HB3	2.01	0.42
12:D:54:LEU:O	12:D:58:GLU:HG2	2.19	0.42
13:E:196:LEU:H	13:E:196:LEU:HD22	1.85	0.42
1:C:307:ARG:NH1	1:C:308:PRO:O	2.51	0.42
5:J:23:GLN:NE2	5:J:149:PRO:HG2	2.34	0.42
5:J:154:HIS:CE1	15:K:64:ILE:HG22	2.55	0.42
7:M:50:GLU:OE2	7:M:201:HIS:ND1	2.53	0.42
7:M:173:LYS:O	7:M:177:GLU:HG3	2.19	0.42
12:D:191:TYR:CD1	12:D:198:PRO:HB3	2.54	0.42
13:E:157:GLU:CD	13:E:157:GLU:H	2.28	0.42
14:F:193:LYS:O	14:F:197:GLU:HG3	2.19	0.42
15:K:64:ILE:HD12	15:K:64:ILE:O	2.20	0.42
1:C:119:ASP:OD2	8:c:189:ILE:HD13	2.20	0.42
3:H:86:LEU:HD23	3:H:86:LEU:HA	1.86	0.42
4:I:218:ARG:HA	4:I:218:ARG:HD2	1.81	0.42
7:M:116:ALA:HB1	7:M:155:GLY:O	2.20	0.42
8:c:48:GLY:O	8:c:51:MET:HG2	2.19	0.42
12:D:120:ASP:OD1	12:D:120:ASP:C	2.63	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:289:LEU:O	12:D:293:LEU:HG	2.20	0.42
1:C:63:LEU:O	1:C:67:GLN:HG2	2.20	0.42
2:G:30:LYS:HE2	2:G:30:LYS:HB2	1.81	0.42
3:H:212:ILE:HD11	3:H:219:ARG:NE	2.34	0.42
4:I:71:ASP:OD1	4:I:71:ASP:C	2.63	0.42
5:J:222:PRO:O	5:J:225:ILE:HG13	2.19	0.42
5:J:234:LYS:O	5:J:237:GLU:HG2	2.19	0.42
6:L:62:LYS:NZ	14:F:439:ALA:OXT	2.43	0.42
11:B:391:SER:O	11:B:395:ILE:HG13	2.19	0.42
13:E:326:ILE:HD11	13:E:367:PHE:HD2	1.84	0.42
15:K:112:VAL:O	15:K:116:VAL:HG23	2.20	0.42
2:G:214:GLU:HG3	2:G:215:ILE:HD13	2.01	0.42
6:L:104:PRO:HG2	6:L:107:ARG:HD3	2.01	0.42
8:c:130:GLN:HG3	8:c:162:LEU:HG	2.01	0.42
8:c:163:ILE:HG23	8:c:174:PRO:HG3	2.02	0.42
11:B:364:ILE:HG12	19:B:501:ATP:N1	2.35	0.42
12:D:376:ASN:O	12:D:380:GLN:HG2	2.20	0.42
13:E:261:LEU:HD11	13:E:294:ARG:HE	1.84	0.42
15:K:52:LYS:HB2	15:K:214:ASN:C	2.44	0.42
1:C:132:ASP:HB3	1:C:135:VAL:HG23	2.00	0.41
1:C:159:LYS:HB3	10:A:22:ILE:HD11	2.02	0.41
4:I:122:THR:HG22	4:I:129:PRO:HB3	2.02	0.41
5:J:42:VAL:HG13	5:J:210:VAL:HG22	2.02	0.41
5:J:132:LEU:HD23	5:J:132:LEU:HA	1.88	0.41
7:M:41:CYS:SG	7:M:189:ILE:HG21	2.60	0.41
7:M:80:LEU:HD23	7:M:80:LEU:HA	1.77	0.41
11:B:48:LYS:HE2	11:B:241:ASN:O	2.20	0.41
13:E:296:ASP:OD1	13:E:297:ARG:HG3	2.20	0.41
13:E:337:GLY:HA3	13:E:342:ASP:OD1	2.20	0.41
13:E:358:ASP:OD1	13:E:358:ASP:C	2.63	0.41
15:K:67:ILE:HA	15:K:76:CYS:O	2.20	0.41
1:C:27:LYS:HD3	1:C:27:LYS:HA	1.79	0.41
3:H:107:THR:HB	3:H:145:TYR:CD2	2.40	0.41
5:J:228:TYR:O	5:J:232:ILE:HG12	2.19	0.41
11:B:234:LEU:HD22	19:B:501:ATP:H2'	2.02	0.41
12:D:186:THR:OG1	12:D:187:HIS:N	2.53	0.41
14:F:272:PHE:O	14:F:276:LYS:HG2	2.20	0.41
14:F:279:ALA:O	14:F:325:GLN:HB3	2.20	0.41
1:C:219:LEU:HD13	1:C:231:VAL:HG22	2.03	0.41
3:H:68:ILE:HD12	3:H:91:ARG:HG3	2.02	0.41
4:I:194:ILE:HD13	4:I:194:ILE:HA	1.89	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:80:ALA:O	5:J:84:ILE:HG13	2.20	0.41
6:L:88:MET:CG	6:L:112:ILE:HD11	2.50	0.41
6:L:158:ALA:HB1	6:L:172:LEU:HD22	2.02	0.41
7:M:144:ASP:OD1	7:M:144:ASP:N	2.53	0.41
8:c:59:GLY:HA3	8:c:69:VAL:HA	2.03	0.41
11:B:250:VAL:HG22	11:B:284:ILE:HA	2.02	0.41
13:E:289:LEU:HA	13:E:294:ARG:HD2	2.01	0.41
1:C:34:ILE:HD12	1:C:34:ILE:HA	1.92	0.41
1:C:71:SER:HB2	1:C:116:LEU:O	2.20	0.41
1:C:89:VAL:N	1:C:93:GLY:O	2.53	0.41
1:C:117:ARG:HG3	1:C:122:THR:HB	2.02	0.41
5:J:7:ILE:H	5:J:7:ILE:HD12	1.84	0.41
5:J:65:LEU:HB2	5:J:69:VAL:HG13	2.02	0.41
8:c:269:GLN:OE1	8:c:273:LYS:HB3	2.21	0.41
11:B:256:ILE:HD11	11:B:290:ILE:HG22	2.03	0.41
11:B:380:LEU:C	11:B:384:ILE:HD12	2.46	0.41
13:E:122:MET:HG3	13:E:198:VAL:HG12	2.02	0.41
13:E:280:ASN:O	13:E:280:ASN:ND2	2.30	0.41
13:E:350:ALA:HB1	13:E:362:VAL:HG11	2.01	0.41
14:F:137:ILE:HD13	14:F:137:ILE:HA	1.84	0.41
15:K:83:LYS:H	15:K:83:LYS:HD3	1.86	0.41
1:C:191:PRO:HG2	1:C:319:PRO:HG3	2.02	0.41
3:H:114:VAL:O	3:H:118:MET:HG3	2.19	0.41
6:L:50:LYS:HG2	6:L:60:GLN:O	2.20	0.41
6:L:82:ARG:HH12	15:K:117:SER:HG	1.60	0.41
8:c:196:LEU:HD12	8:c:200:TYR:O	2.21	0.41
10:A:328:ASP:OD2	10:A:329:PRO:HD2	2.21	0.41
11:B:275:GLU:OE1	11:B:323:GLY:HA3	2.20	0.41
12:D:82:ILE:HD13	12:D:82:ILE:HA	1.95	0.41
14:F:177:VAL:HG22	14:F:250:LYS:HD3	2.02	0.41
2:G:88:ARG:O	2:G:91:VAL:HG22	2.20	0.41
4:I:38:LEU:O	4:I:179:TYR:OH	2.25	0.41
6:L:46:LEU:HD13	6:L:63:ILE:HG12	2.03	0.41
10:A:334:PRO:HG2	14:F:395:GLN:HG2	2.03	0.41
11:B:230:THR:CG2	11:B:353:PHE:HB3	2.51	0.41
12:D:264:ILE:HD12	12:D:309:MET:HE2	2.01	0.41
12:D:274:ARG:NH1	12:D:318:ASP:OD1	2.54	0.41
13:E:297:ARG:HG3	13:E:297:ARG:H	1.71	0.41
13:E:349:GLU:HA	13:E:352:MET:HB2	2.02	0.41
14:F:399:VAL:HG22	14:F:424:ILE:HA	2.01	0.41
3:H:195:LEU:HD23	3:H:195:LEU:HA	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:184:ASP:O	5:J:188:ILE:HG13	2.20	0.41
6:L:116:THR:O	6:L:119:PRO:HD2	2.21	0.41
8:c:303:MET:HA	8:c:306:THR:HG22	2.03	0.41
14:F:253:GLY:N	14:F:254:PRO:HD2	2.36	0.41
14:F:292:GLY:O	14:F:339:ASP:N	2.54	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.92	0.41
2:G:101:TRP:CD1	2:G:101:TRP:C	2.98	0.41
4:I:147:LEU:HB3	4:I:159:TRP:O	2.21	0.41
5:J:4:ASP:HB2	5:J:21:TYR:CE2	2.56	0.41
10:A:142:VAL:HG12	10:A:149:ILE:HA	2.03	0.41
11:B:169:PRO:HA	11:B:172:THR:HG22	2.03	0.41
11:B:363:ARG:HD2	11:B:363:ARG:HA	1.67	0.41
12:D:397:LYS:HG3	12:D:398:ASP:N	2.36	0.41
13:E:202:SER:HA	13:E:210:GLU:HG3	2.02	0.41
14:F:180:ARG:HE	14:F:180:ARG:HB2	1.71	0.41
2:G:40:VAL:HG12	2:G:202:LEU:HD13	2.02	0.41
5:J:12:PRO:HA	15:K:26:TYR:CD1	2.56	0.41
5:J:107:ILE:HD12	5:J:107:ILE:HA	1.87	0.41
7:M:36:ALA:HB1	7:M:49:VAL:HG12	2.02	0.41
7:M:135:PHE:CE2	7:M:151:ILE:HD12	2.55	0.41
7:M:188:ASP:O	7:M:192:GLU:HG2	2.21	0.41
10:A:63:THR:OG1	10:A:64:GLY:N	2.54	0.41
10:A:319:MET:SD	10:A:337:LEU:HD21	2.61	0.41
11:B:70:ASP:O	11:B:74:MET:HG3	2.20	0.41
11:B:293:LYS:HB2	11:B:293:LYS:HE2	1.89	0.41
11:B:368:HIS:CE1	11:B:396:LYS:HB2	2.56	0.41
12:D:162:VAL:O	12:D:218:ALA:HA	2.21	0.41
13:E:60:VAL:O	13:E:94:PRO:HA	2.20	0.41
13:E:122:MET:HB3	13:E:221:TYR:OH	2.21	0.41
13:E:218:MET:HB3	13:E:230:ILE:HD12	2.01	0.41
13:E:348:THR:HG23	14:F:217:ILE:HD11	2.02	0.41
14:F:173:LYS:HB2	14:F:173:LYS:HE2	1.82	0.41
14:F:249:LEU:HD23	14:F:249:LEU:HA	1.84	0.41
2:G:10:ASP:O	2:G:24:GLN:NE2	2.51	0.41
3:H:77:SER:OG	3:H:163:MET:HB3	2.20	0.41
5:J:82:ILE:HD13	5:J:82:ILE:HA	1.90	0.41
6:L:28:ALA:HB1	14:F:438:TYR:CE1	2.55	0.41
6:L:188:VAL:HG11	6:L:232:PHE:CD2	2.56	0.41
10:A:292:ASP:OD2	10:A:292:ASP:N	2.53	0.41
11:B:103:ARG:HG2	11:B:160:ILE:HB	2.02	0.41
13:E:369:LYS:HA	13:E:372:ARG:HG2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:171:ARG:H	14:F:171:ARG:HD3	1.85	0.41
14:F:421:MET:HA	14:F:424:ILE:HD12	2.03	0.41
1:C:59:LEU:HD23	1:C:59:LEU:HA	1.81	0.40
4:I:68:LEU:HD13	4:I:90:LEU:HD13	2.02	0.40
5:J:61:LYS:HZ1	11:B:440:LEU:C	2.29	0.40
6:L:118:ILE:HB	6:L:119:PRO:HD3	2.03	0.40
10:A:196:LEU:HD23	10:A:196:LEU:HA	1.82	0.40
10:A:199:GLU:HA	10:A:202:VAL:HG12	2.03	0.40
11:B:322:ARG:NH1	11:B:325:VAL:O	2.50	0.40
12:D:313:ARG:NH2	12:D:315:ASP:OD1	2.53	0.40
12:D:403:TYR:O	12:D:407:ILE:HG12	2.21	0.40
13:E:336:ASP:HB3	13:E:338:PHE:CE1	2.56	0.40
1:C:399:MET:HE3	3:H:158:TRP:CH2	2.56	0.40
3:H:74:LEU:HD12	3:H:74:LEU:HA	1.86	0.40
7:M:184:MET:HE2	7:M:184:MET:HB3	1.88	0.40
8:c:189:ILE:O	8:c:193:ILE:HG12	2.21	0.40
10:A:426:THR:HB	10:A:427:PRO:HD3	2.03	0.40
11:B:143:LEU:HD22	11:B:164:MET:SD	2.61	0.40
12:D:355:SER:O	12:D:358:VAL:HG12	2.21	0.40
14:F:428:GLN:H	14:F:428:GLN:HG2	1.64	0.40
2:G:111:VAL:CG1	2:G:140:LEU:HB3	2.51	0.40
3:H:89:ARG:HA	3:H:89:ARG:HD2	1.87	0.40
4:I:62:SER:HB2	4:I:65:ILE:O	2.21	0.40
4:I:175:LEU:HD12	4:I:196:VAL:HG21	2.03	0.40
6:L:236:LEU:HD23	6:L:236:LEU:HA	1.82	0.40
7:M:28:LYS:HB2	7:M:28:LYS:HE3	1.83	0.40
8:c:120:CYS:SG	8:c:156:VAL:HG22	2.62	0.40
8:c:161:ARG:HD2	8:c:201:TYR:OH	2.20	0.40
8:c:196:LEU:HD12	8:c:196:LEU:HA	1.86	0.40
10:A:188:ARG:NH1	10:A:192:GLU:OE2	2.54	0.40
10:A:358:HIS:CE1	10:A:386:ARG:HB2	2.56	0.40
11:B:91:LYS:HB2	11:B:92:GLN:H	1.71	0.40
11:B:103:ARG:HG2	11:B:160:ILE:HD12	2.03	0.40
12:D:279:THR:OG1	12:D:282:ASP:HB2	2.20	0.40
12:D:342:ARG:HB2	12:D:364:VAL:HG11	2.04	0.40
12:D:357:GLU:OE1	12:D:395:LEU:HB3	2.22	0.40
13:E:93:LYS:H	13:E:93:LYS:CD	2.34	0.40
15:K:235:GLU:O	15:K:239:LYS:HG3	2.21	0.40
4:I:69:ASN:OD1	4:I:71:ASP:N	2.41	0.40
7:M:202:ASP:OD1	7:M:204:VAL:HG22	2.21	0.40
7:M:230:ASP:OD1	7:M:231:ILE:HG23	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:80:LEU:HD23	10:A:80:LEU:HA	1.95	0.40
10:A:365:GLU:HG3	10:A:405:THR:HA	2.04	0.40
13:E:175:PRO:HG2	13:E:178:THR:HG21	2.02	0.40
13:E:280:ASN:HD22	13:E:280:ASN:C	2.16	0.40
14:F:96:LEU:HD23	14:F:96:LEU:HA	1.85	0.40
15:K:125:GLU:OE2	15:K:125:GLU:N	2.54	0.40
1:C:78:ARG:NH2	11:B:165:ASP:HB3	2.35	0.40
2:G:74:GLU:OE1	2:G:74:GLU:HA	2.21	0.40
7:M:87:LEU:HD13	7:M:135:PHE:CE1	2.57	0.40
8:c:75:MET:SD	8:c:76:PRO:HD2	2.61	0.40
8:c:138:GLU:H	8:c:138:GLU:CD	2.24	0.40
11:B:381:ASP:O	11:B:385:MET:HG2	2.22	0.40
13:E:126:ASP:N	13:E:193:CYS:O	2.43	0.40
13:E:225:HIS:CD2	13:E:226:GLN:H	2.40	0.40
13:E:337:GLY:HA2	13:E:378:LYS:HE2	2.04	0.40
15:K:109:VAL:HA	15:K:112:VAL:HG12	2.04	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	C	384/406 (95%)	380 (99%)	4 (1%)	0	100	100
2	G	237/246 (96%)	230 (97%)	7 (3%)	0	100	100
3	H	230/234 (98%)	224 (97%)	6 (3%)	0	100	100
4	I	246/261 (94%)	238 (97%)	8 (3%)	0	100	100
5	J	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
6	L	235/263 (89%)	230 (98%)	5 (2%)	0	100	100
7	M	238/255 (93%)	225 (94%)	13 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c	286/424 (68%)	268 (94%)	16 (6%)	2 (1%)	19	32
10	A	393/433 (91%)	373 (95%)	18 (5%)	2 (0%)	25	41
11	B	389/440 (88%)	368 (95%)	20 (5%)	1 (0%)	37	55
12	D	373/418 (89%)	341 (91%)	29 (8%)	3 (1%)	16	29
13	E	341/389 (88%)	299 (88%)	36 (11%)	6 (2%)	7	12
14	F	358/439 (82%)	339 (95%)	18 (5%)	1 (0%)	37	55
15	K	227/241 (94%)	219 (96%)	8 (4%)	0	100	100
All	All	4174/4697 (89%)	3964 (95%)	195 (5%)	15 (0%)	32	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	c	285	GLU
12	D	85	ILE
13	E	117	PRO
13	E	118	LEU
10	A	116	LYS
10	A	293	ASN
12	D	339	ARG
13	E	85	ARG
13	E	279	THR
14	F	209	LYS
13	E	212	ALA
8	c	172	HIS
12	D	303	VAL
11	B	320	ASP
13	E	206	LYS

### 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	C	338/352 (96%)	330 (98%)	8 (2%)	44	65

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	195/210 (93%)	186 (95%)	9 (5%)	23	41
3	H	190/191 (100%)	187 (98%)	3 (2%)	58	75
4	I	195/221 (88%)	191 (98%)	4 (2%)	48	69
5	J	183/212 (86%)	173 (94%)	10 (6%)	18	33
6	L	198/224 (88%)	193 (98%)	5 (2%)	42	64
7	M	192/212 (91%)	187 (97%)	5 (3%)	41	63
8	c	252/359 (70%)	245 (97%)	7 (3%)	38	60
10	A	347/372 (93%)	337 (97%)	10 (3%)	37	59
11	B	349/385 (91%)	338 (97%)	11 (3%)	34	55
12	D	331/366 (90%)	319 (96%)	12 (4%)	30	51
13	E	303/341 (89%)	292 (96%)	11 (4%)	30	51
14	F	311/379 (82%)	298 (96%)	13 (4%)	25	44
15	K	192/204 (94%)	184 (96%)	8 (4%)	25	44
All	All	3576/4028 (89%)	3460 (97%)	116 (3%)	36	55

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	TYR
1	C	142	LYS
1	C	149	GLU
1	C	165	ILE
1	C	234	LEU
1	C	260	GLU
1	C	299	ASP
1	C	339	THR
2	G	39	SER
2	G	51	VAL
2	G	108	GLU
2	G	111	VAL
2	G	126	THR
2	G	151	VAL
2	G	153	LYS
2	G	170	VAL
2	G	221	THR
3	H	51	LYS
3	H	133	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	H	156	PHE
4	I	64	LYS
4	I	76	VAL
4	I	149	GLN
4	I	224	VAL
5	J	23	GLN
5	J	35	VAL
5	J	43	LEU
5	J	45	VAL
5	J	46	GLU
5	J	65	LEU
5	J	68	ASN
5	J	76	LEU
5	J	184	ASP
5	J	205	ASN
6	L	46	LEU
6	L	110	SER
6	L	167	SER
6	L	182	CYS
6	L	186	GLU
7	M	27	MET
7	M	139	SER
7	M	144	ASP
7	M	158	TYR
7	M	243	LEU
8	c	69	VAL
8	c	156	VAL
8	c	176	GLN
8	c	284	LEU
8	c	288	VAL
8	c	294	SER
8	c	305	ASP
10	A	22	ILE
10	A	42	SER
10	A	55	LEU
10	A	90	GLU
10	A	108	ASP
10	A	164	MET
10	A	172	VAL
10	A	304	ASN
10	A	317	VAL
10	A	403	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
11	B	62	LEU
11	B	119	ASN
11	B	127	VAL
11	B	142	ASP
11	B	170	LEU
11	B	250	VAL
11	B	286	GLU
11	B	288	ASP
11	B	378	VAL
11	B	384	ILE
11	B	426	VAL
12	D	65	GLN
12	D	79	VAL
12	D	82	ILE
12	D	83	GLN
12	D	120	ASP
12	D	171	ASP
12	D	181	VAL
12	D	240	LEU
12	D	282	ASP
12	D	305	VAL
12	D	357	GLU
12	D	399	PHE
13	E	37	THR
13	E	42	LYS
13	E	52	SER
13	E	83	CYS
13	E	103	THR
13	E	172	LEU
13	E	196	LEU
13	E	203	ILE
13	E	233	ASP
13	E	275	MET
13	E	320	ILE
14	F	66	LEU
14	F	85	THR
14	F	87	PRO
14	F	97	LEU
14	F	131	THR
14	F	153	VAL
14	F	159	LEU
14	F	182	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	F	206	MET
14	F	307	GLN
14	F	336	ASP
14	F	343	LEU
14	F	413	THR
15	K	12	VAL
15	K	31	ILE
15	K	83	LYS
15	K	96	THR
15	K	121	LEU
15	K	181	LEU
15	K	239	LYS
15	K	241	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	106	ASN
1	C	171	HIS
2	G	92	GLN
4	I	240	HIS
5	J	23	GLN
5	J	92	GLN
5	J	116	GLN
5	J	175	ASN
5	J	200	GLN
6	L	5	GLN
7	M	101	ASN
10	A	94	GLN
10	A	103	ASN
10	A	358	HIS
11	B	257	GLN
12	D	83	GLN
12	D	278	GLN
12	D	295	GLN
12	D	301	GLN
13	E	55	GLN
13	E	226	GLN
13	E	300	HIS
13	E	364	GLN
14	F	92	ASN
14	F	316	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	F	333	ASN
15	K	164	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	ATP	F	501	17	28,33,33	0.74	0	34,52,52	0.63	1 (2%)
19	ATP	A	501	17	28,33,33	0.70	0	34,52,52	0.61	1 (2%)
16	ADP	D	501	17	24,29,29	0.88	0	29,45,45	1.19	2 (6%)
16	ADP	C	501	17	24,29,29	0.86	0	29,45,45	1.24	2 (6%)
19	ATP	B	501	17	28,33,33	0.72	0	34,52,52	0.62	1 (2%)
16	ADP	E	501	-	24,29,29	0.89	0	29,45,45	1.23	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ATP	F	501	17	-	1/18/38/38	0/3/3/3
19	ATP	A	501	17	-	6/18/38/38	0/3/3/3
16	ADP	D	501	17	-	5/12/32/32	0/3/3/3
16	ADP	C	501	17	-	0/12/32/32	0/3/3/3
19	ATP	B	501	17	-	3/18/38/38	0/3/3/3
16	ADP	E	501	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	ADP	N3-C2-N1	-3.54	123.87	128.67
16	E	501	ADP	N3-C2-N1	-3.49	123.93	128.67
16	C	501	ADP	N3-C2-N1	-3.47	123.96	128.67
16	E	501	ADP	C4-C5-N7	-2.48	106.72	109.34
16	C	501	ADP	C4-C5-N7	-2.44	106.76	109.34
16	D	501	ADP	C4-C5-N7	-2.40	106.80	109.34
19	B	501	ATP	C5-C6-N6	2.34	123.88	120.31
19	A	501	ATP	C5-C6-N6	2.31	123.83	120.31
19	F	501	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	D	501	ADP	C5'-O5'-PA-O1A
16	D	501	ADP	C5'-O5'-PA-O3A
16	E	501	ADP	C5'-O5'-PA-O3A
19	A	501	ATP	PB-O3B-PG-O2G
19	A	501	ATP	C5'-O5'-PA-O1A
19	A	501	ATP	C5'-O5'-PA-O3A
19	B	501	ATP	C5'-O5'-PA-O1A
19	B	501	ATP	C5'-O5'-PA-O3A
19	F	501	ATP	O4'-C4'-C5'-O5'
16	D	501	ADP	O4'-C4'-C5'-O5'
16	E	501	ADP	C5'-O5'-PA-O1A
19	A	501	ATP	C5'-O5'-PA-O2A
19	B	501	ATP	C5'-O5'-PA-O2A
16	D	501	ADP	PB-O3A-PA-O2A

*Continued on next page...*

*Continued from previous page...*

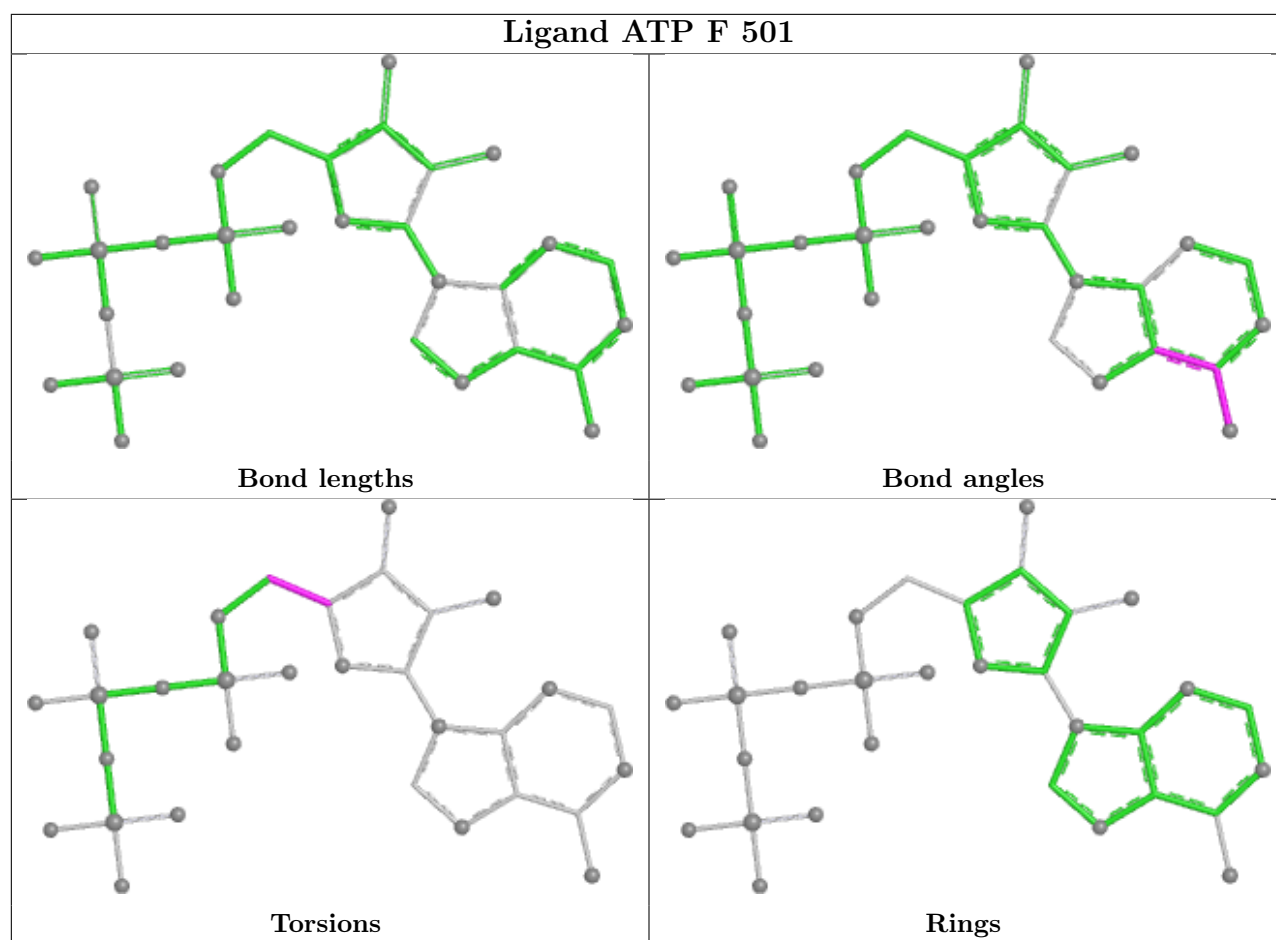
Mol	Chain	Res	Type	Atoms
16	D	501	ADP	C3'-C4'-C5'-O5'
19	A	501	ATP	PB-O3B-PG-O3G
19	A	501	ATP	PG-O3B-PB-O2B

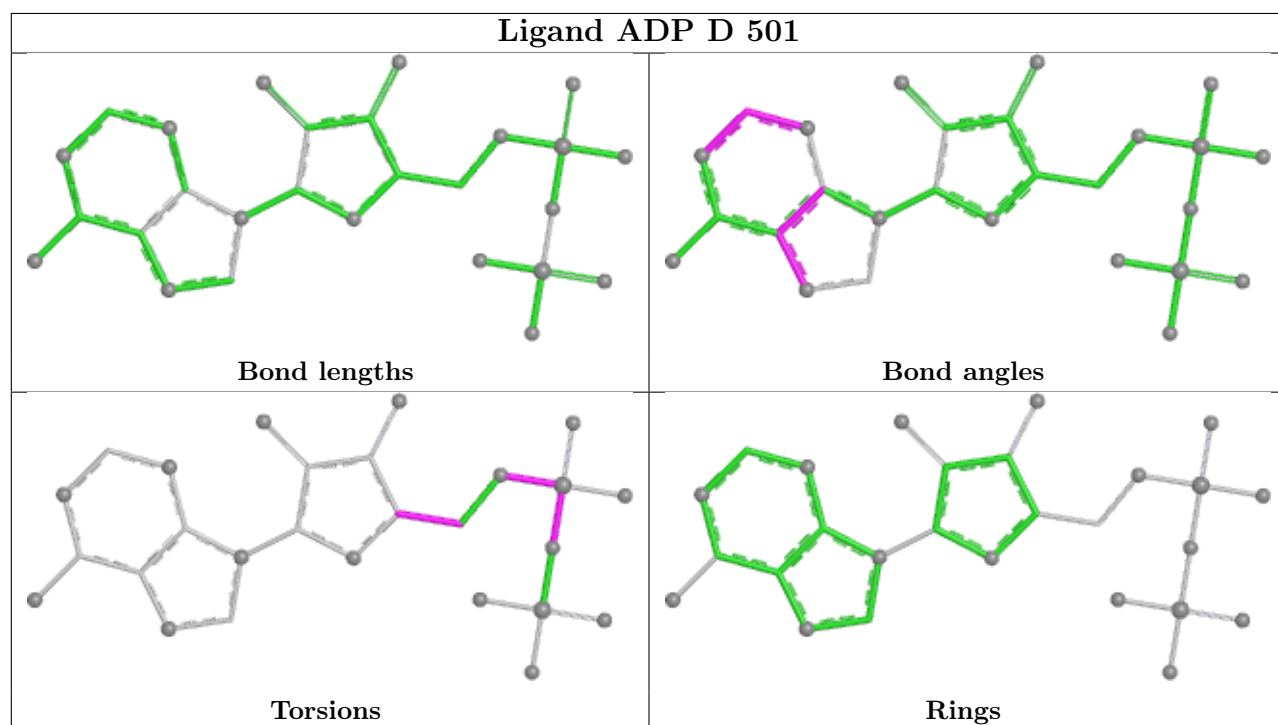
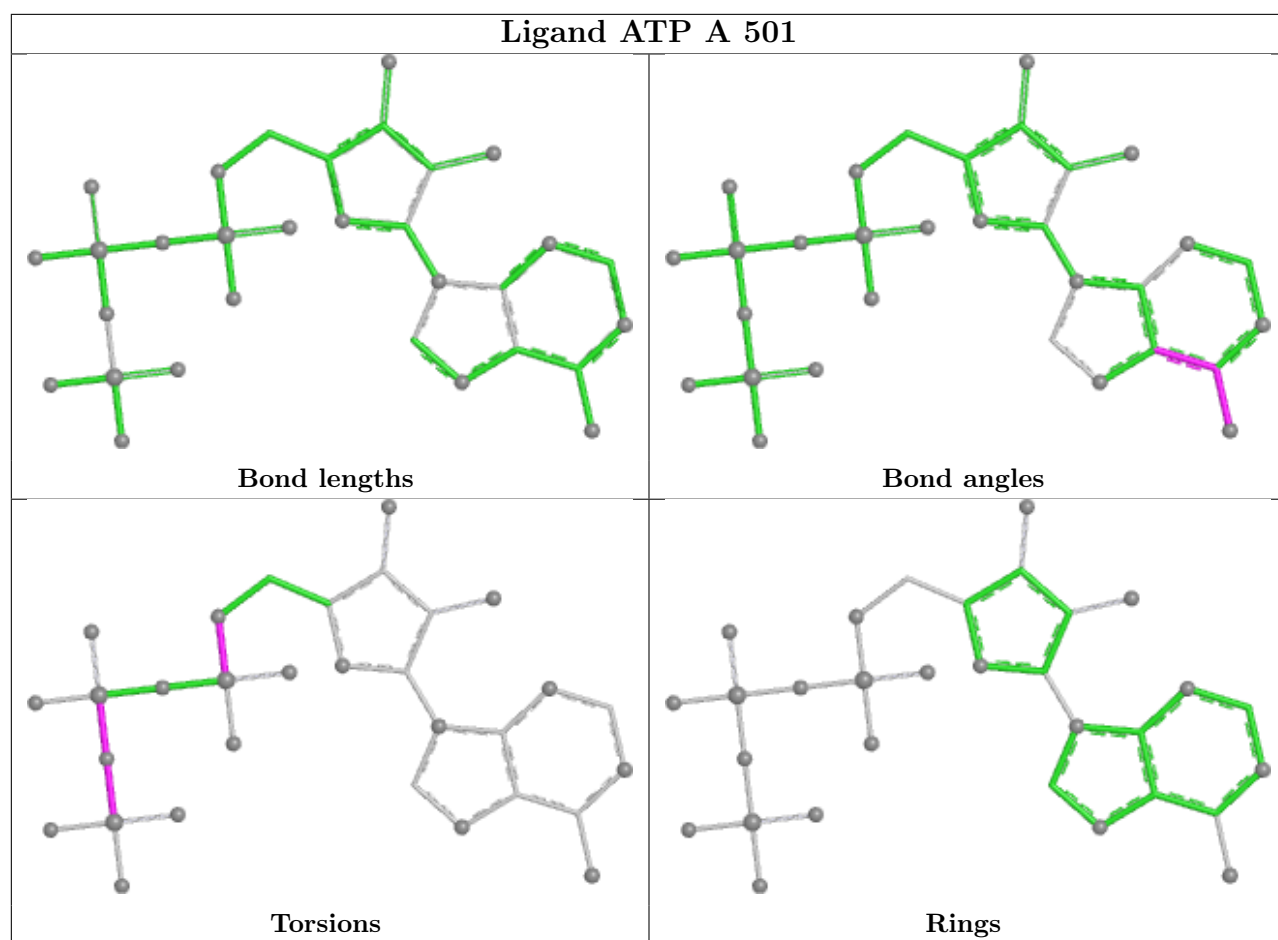
There are no ring outliers.

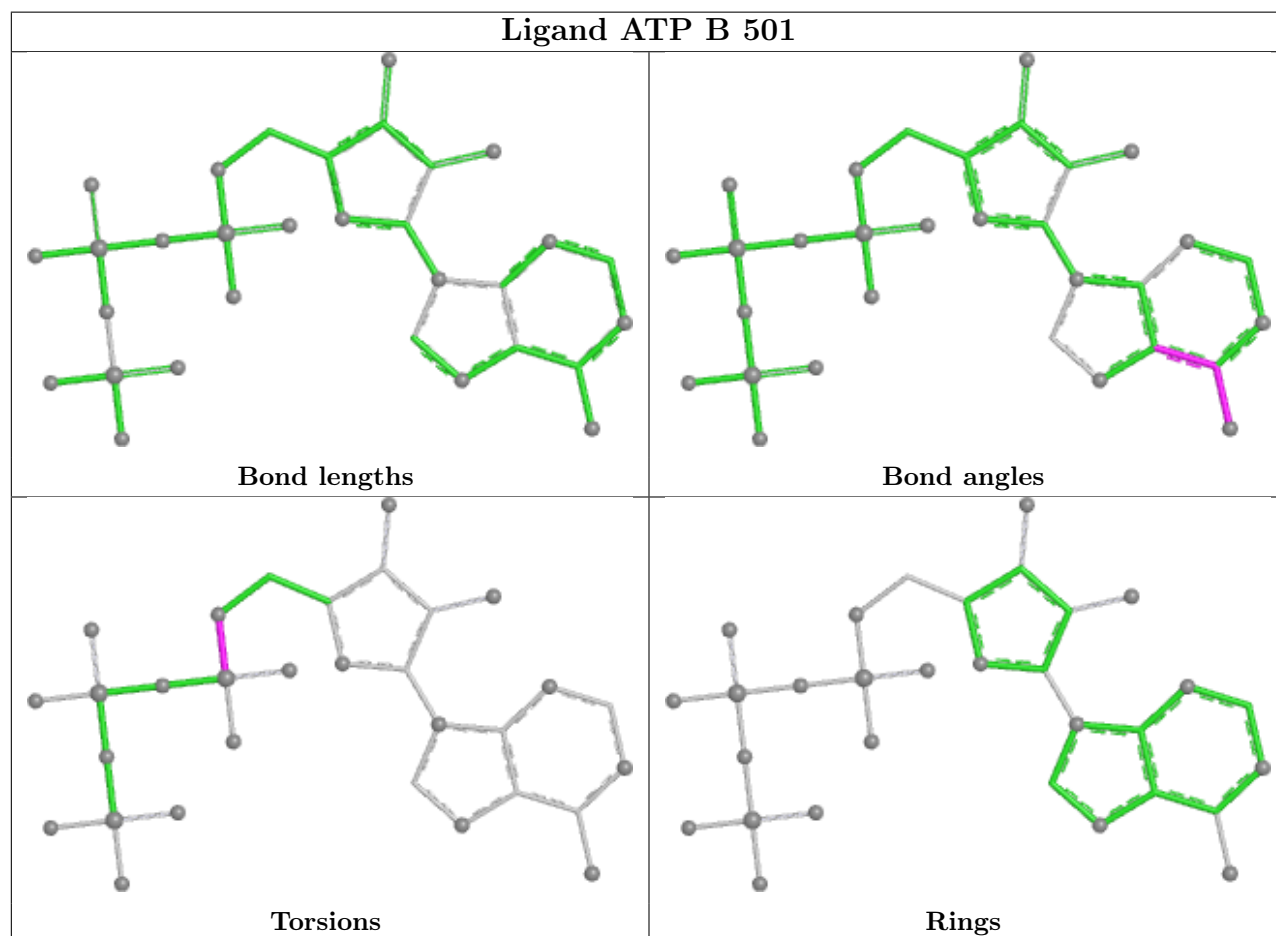
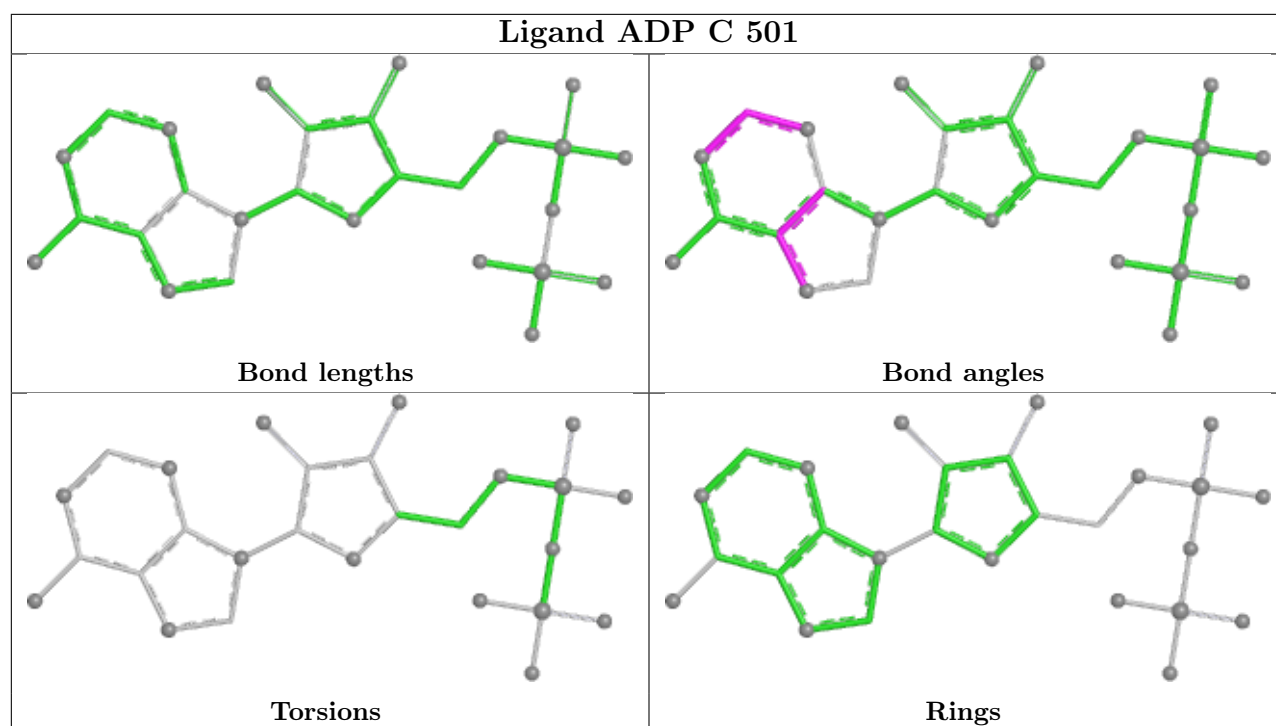
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F	501	ATP	3	0
19	A	501	ATP	2	0
16	C	501	ADP	3	0
19	B	501	ATP	2	0
16	E	501	ADP	2	0

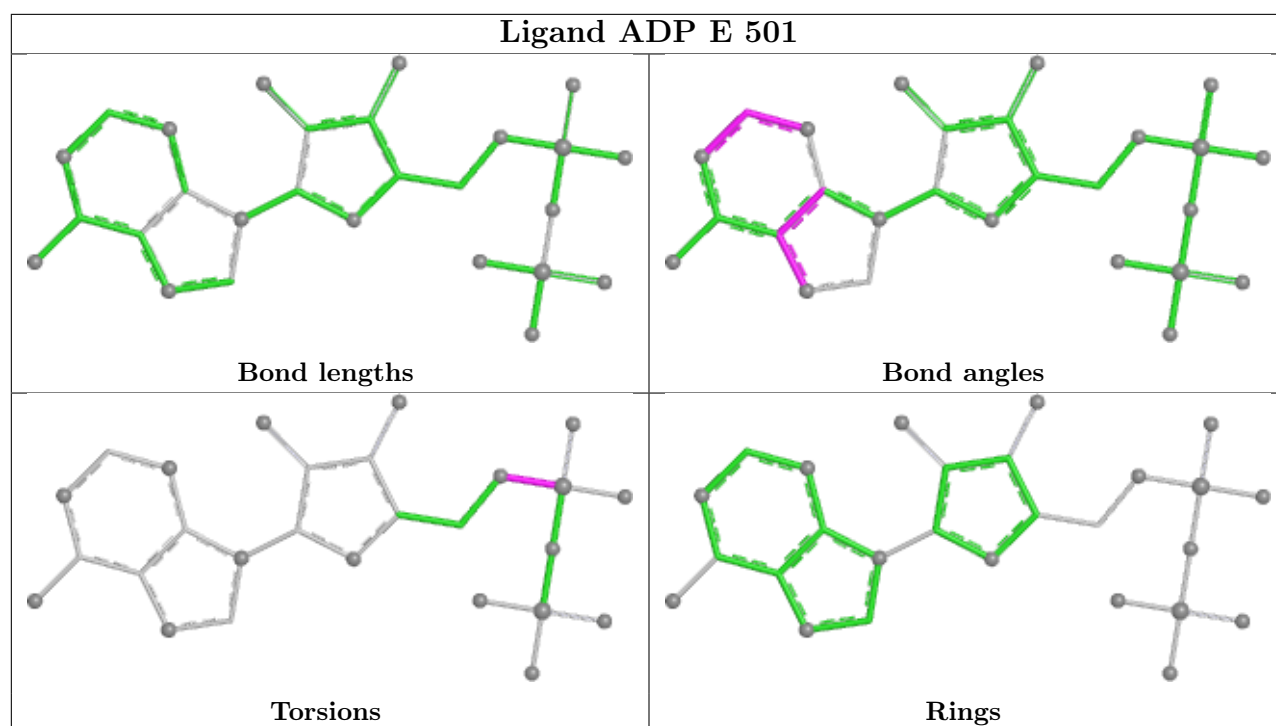
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

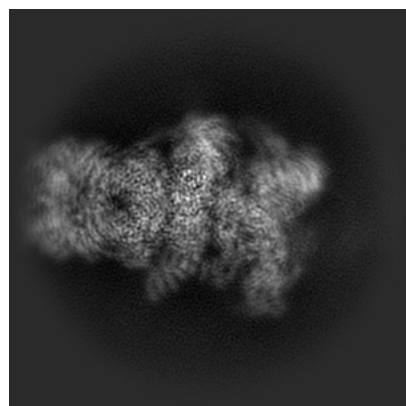
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71537. These allow visual inspection of the internal detail of the map and identification of artifacts.

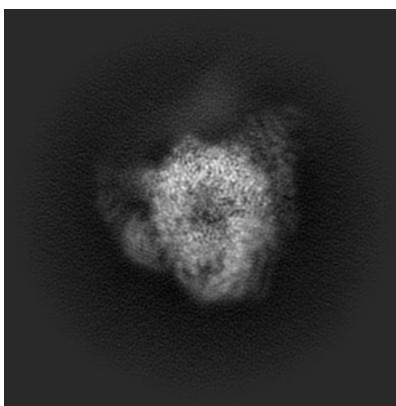
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

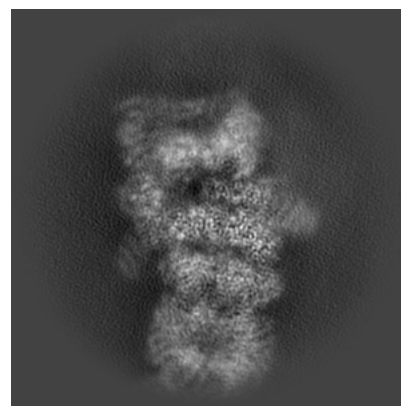
#### 6.1.1 Primary map



X

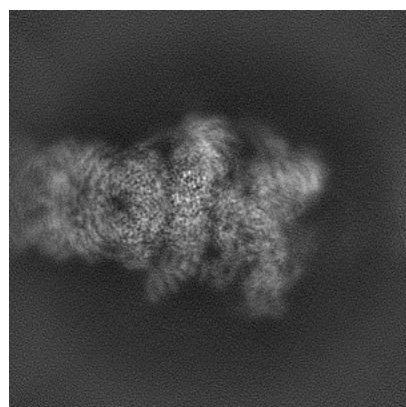


Y

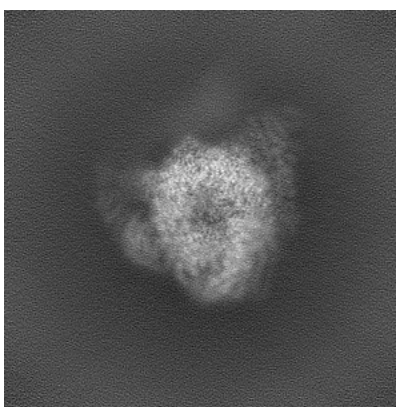


Z

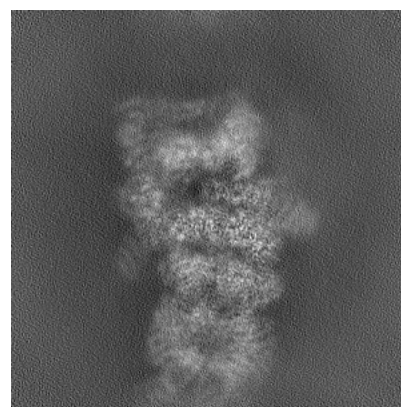
#### 6.1.2 Raw map



X



Y

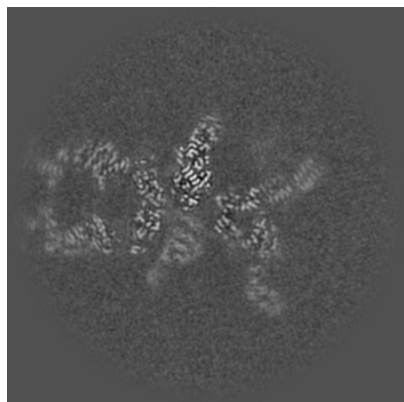


Z

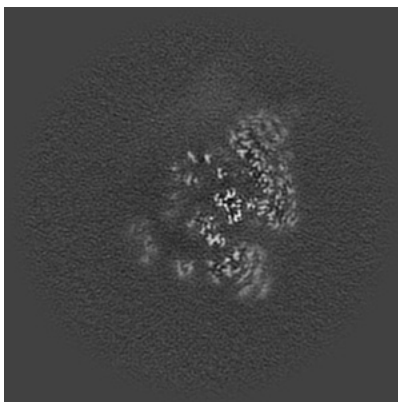
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

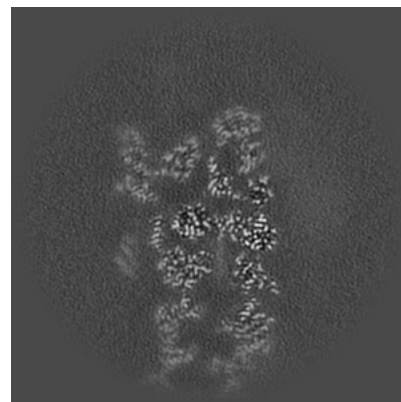
### 6.2.1 Primary map



X Index: 170

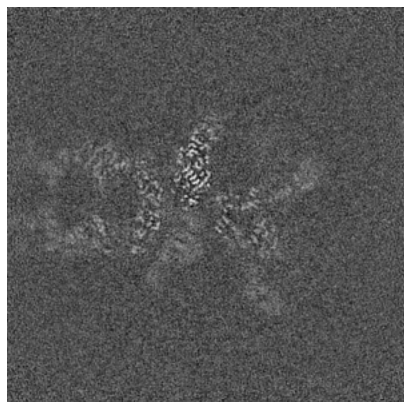


Y Index: 170

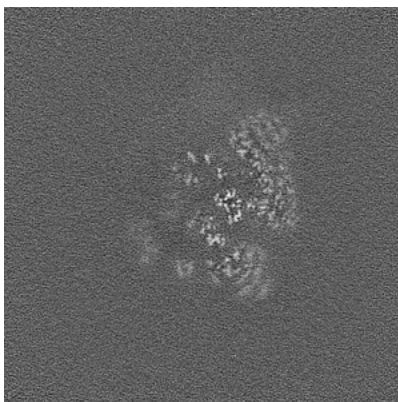


Z Index: 170

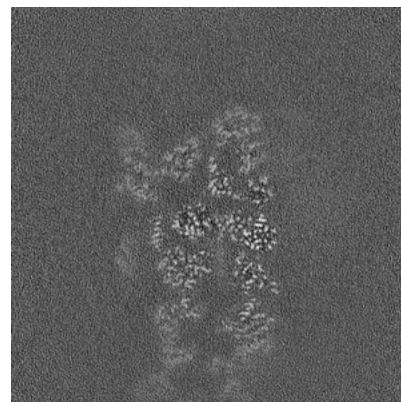
### 6.2.2 Raw map



X Index: 170



Y Index: 170

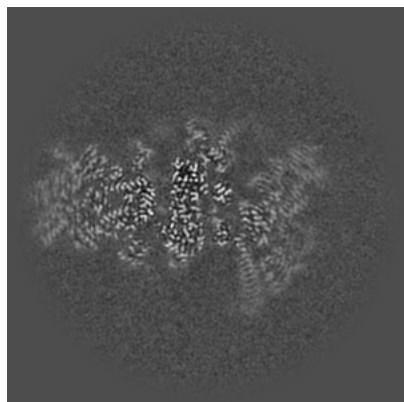


Z Index: 170

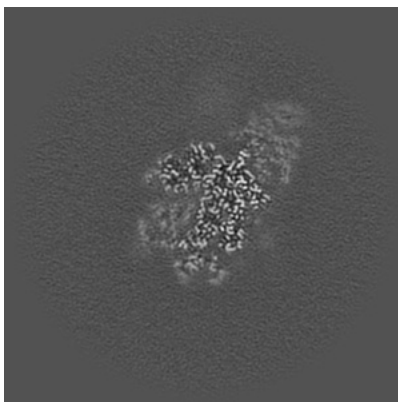
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

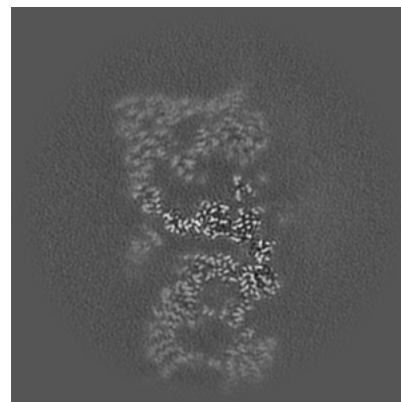
### 6.3.1 Primary map



X Index: 198

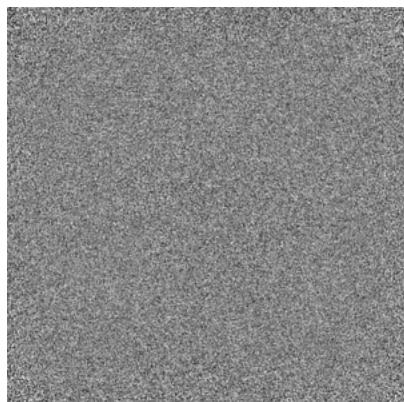


Y Index: 153

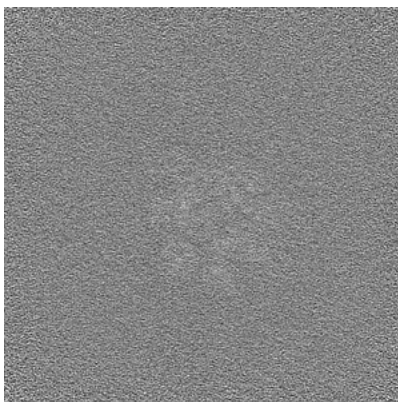


Z Index: 190

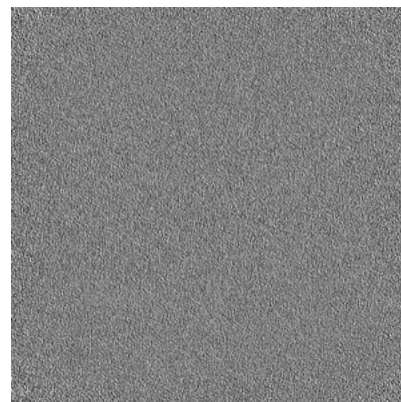
### 6.3.2 Raw map



X Index: 0



Y Index: 0



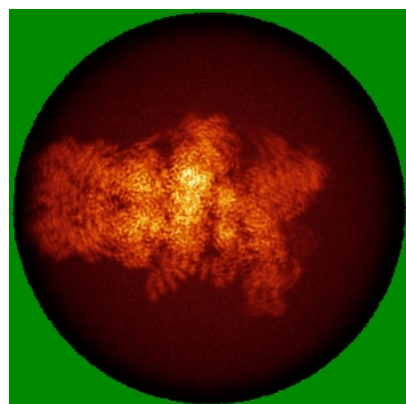
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

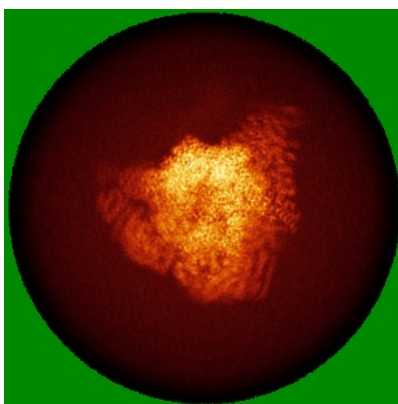


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

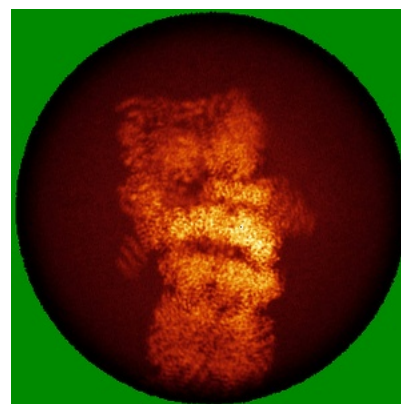
### 6.4.1 Primary map



X

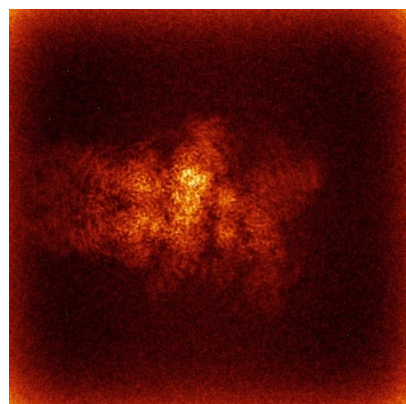


Y

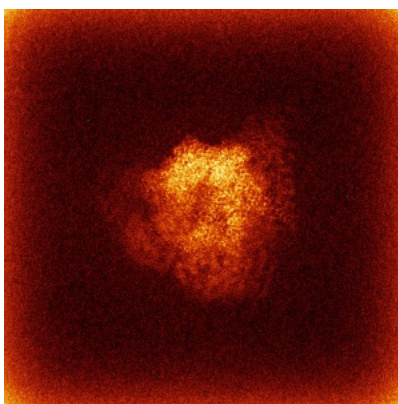


Z

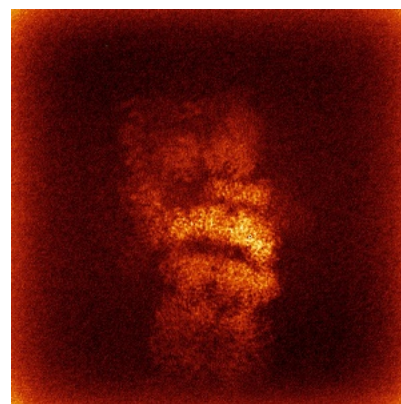
### 6.4.2 Raw map



X



Y

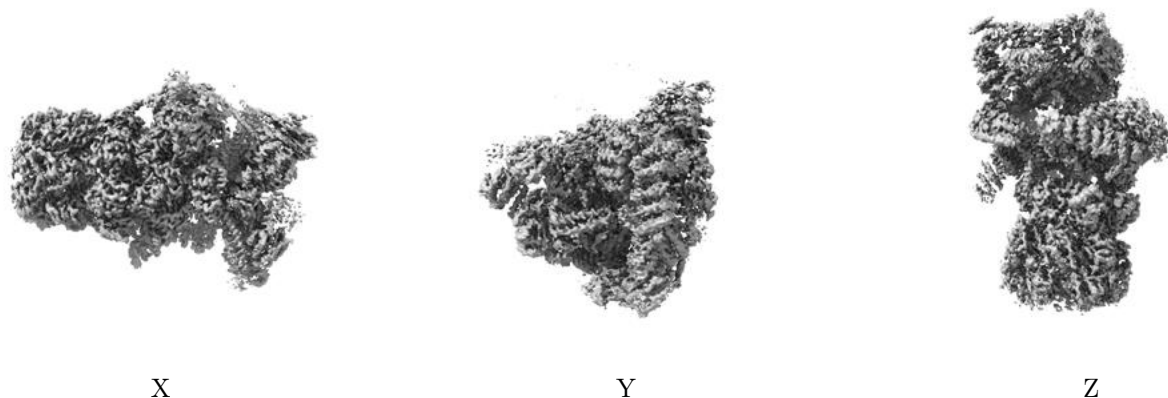


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

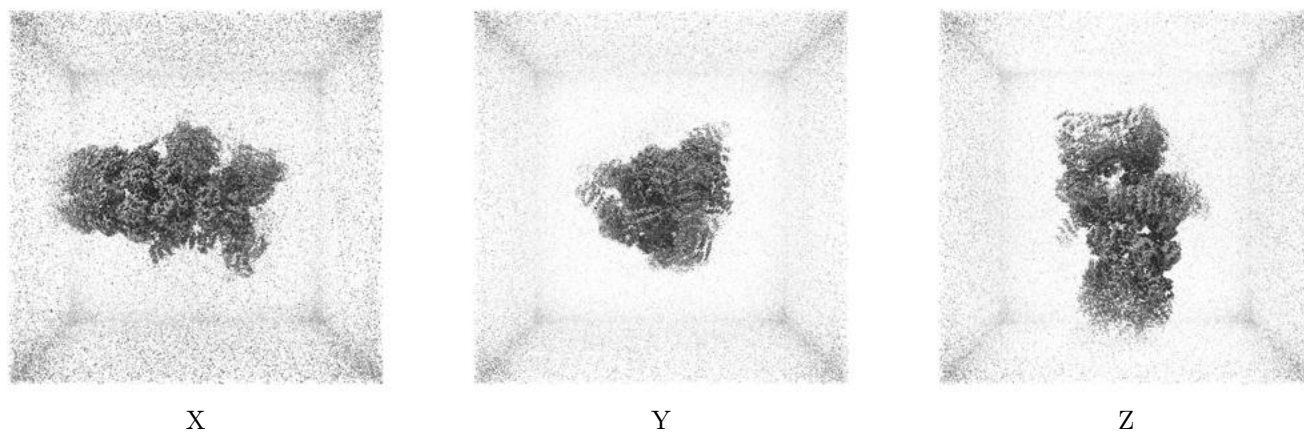
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

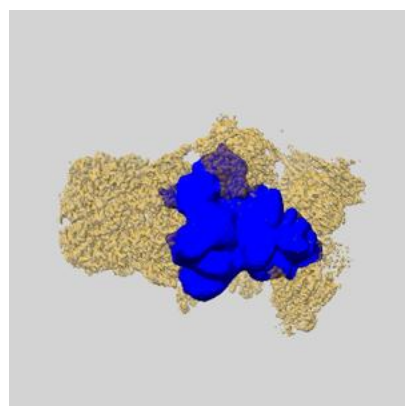
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

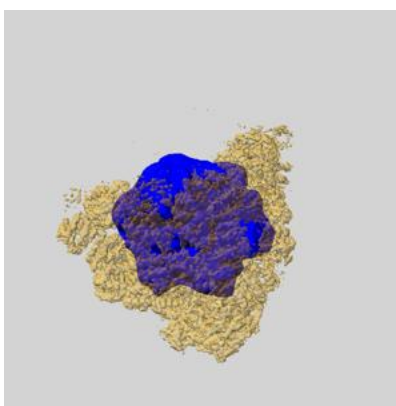
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

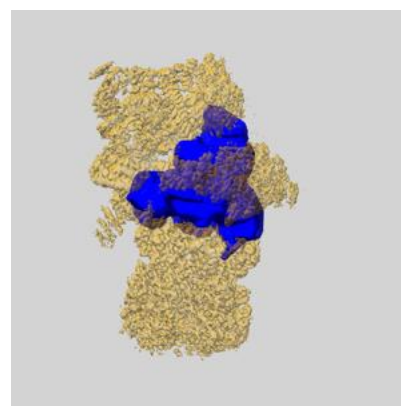
### 6.6.1 emd\_71537\_msk\_1.map [i](#)



X



Y

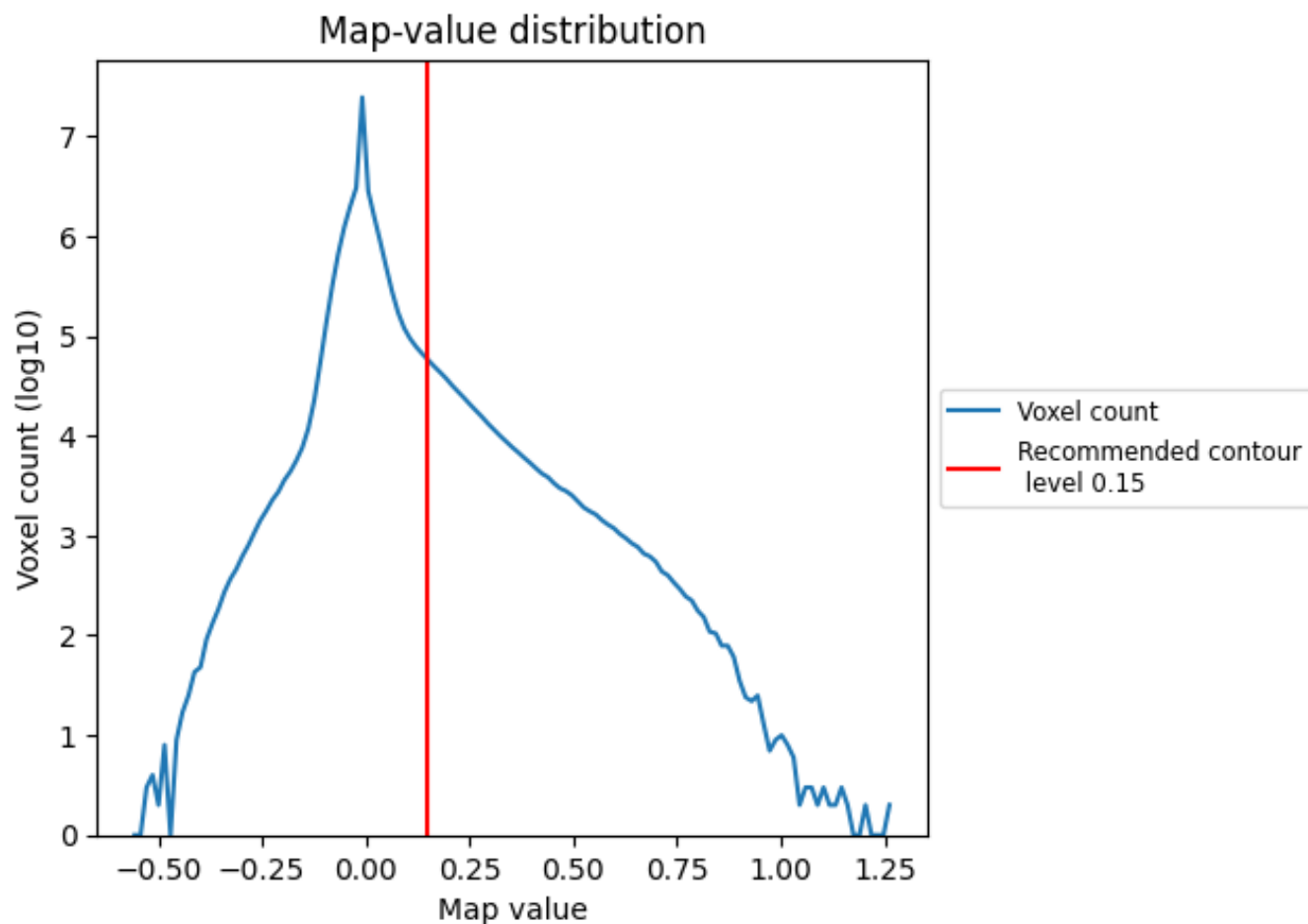


Z

## 7 Map analysis [i](#)

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

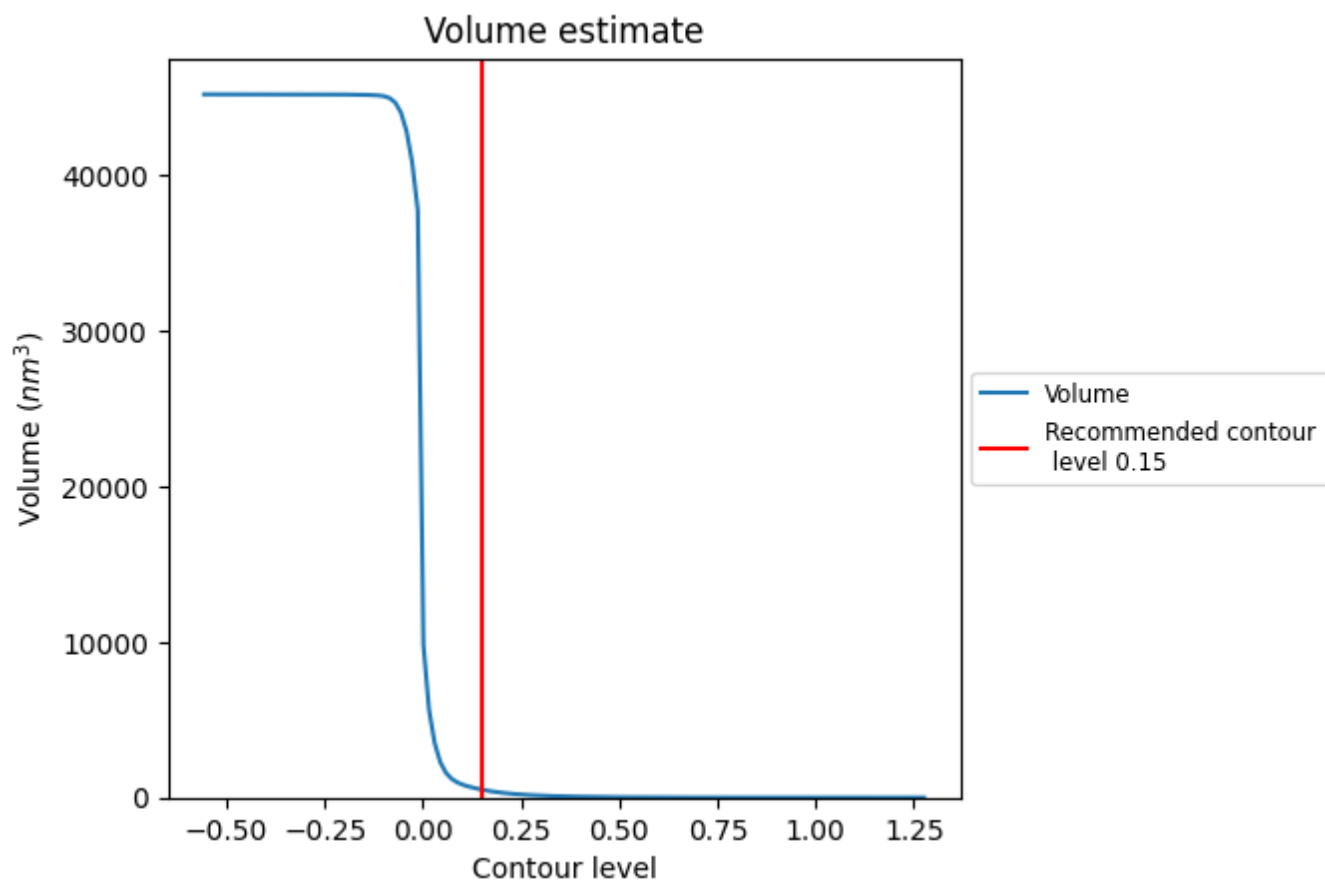
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



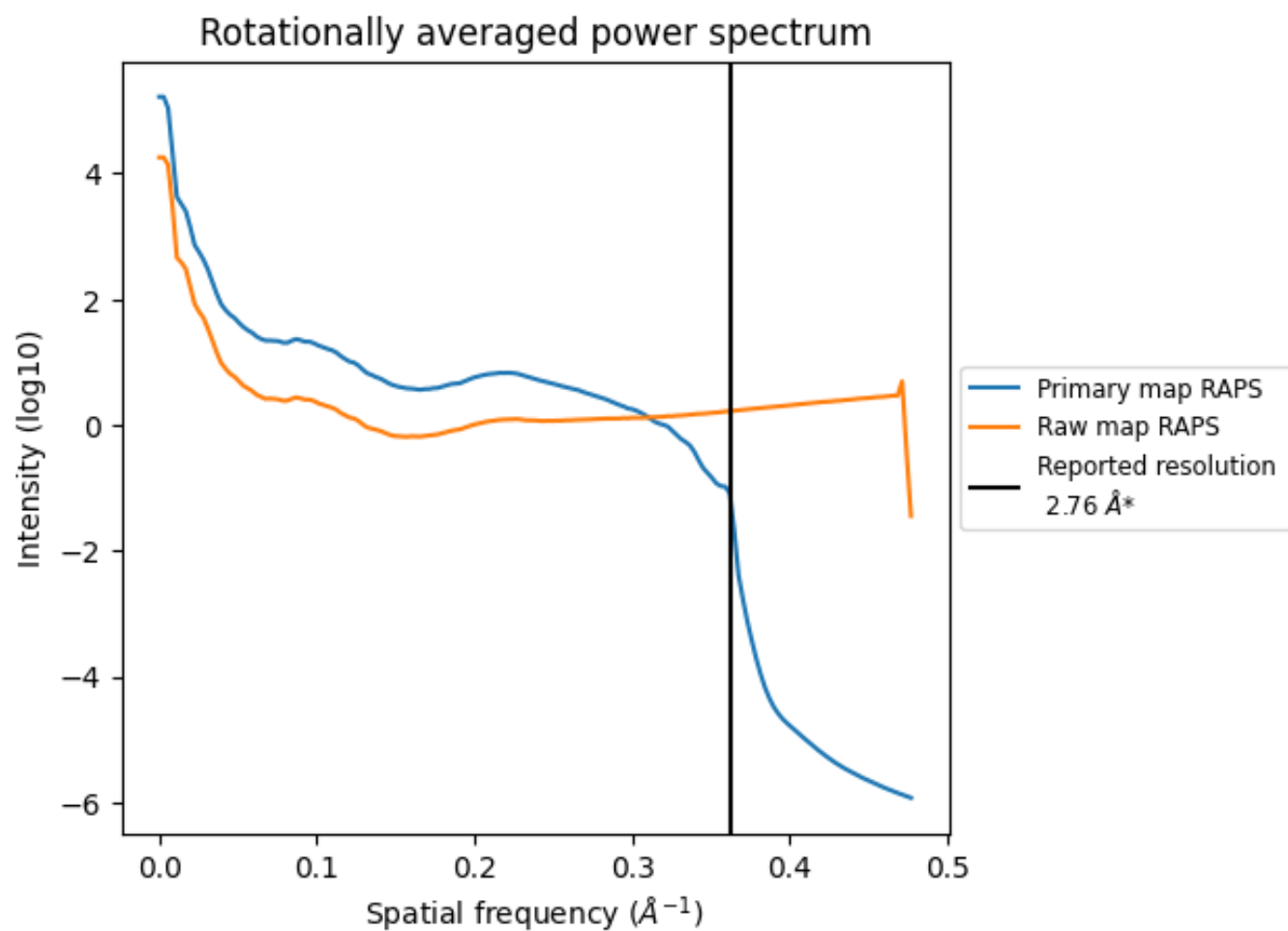
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 507 nm<sup>3</sup>; this corresponds to an approximate mass of 458 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

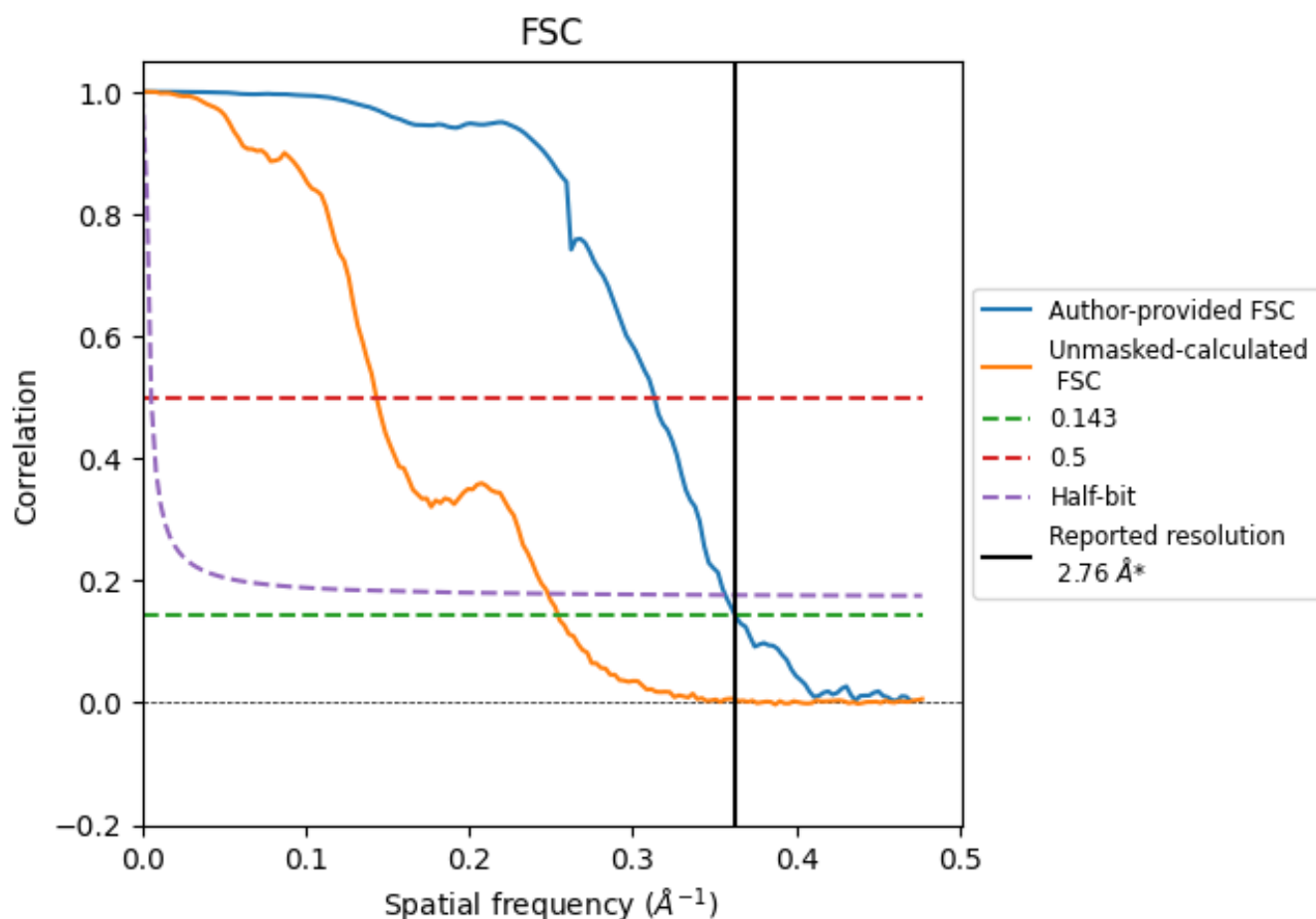


\*Reported resolution corresponds to spatial frequency of 0.362  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.362  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

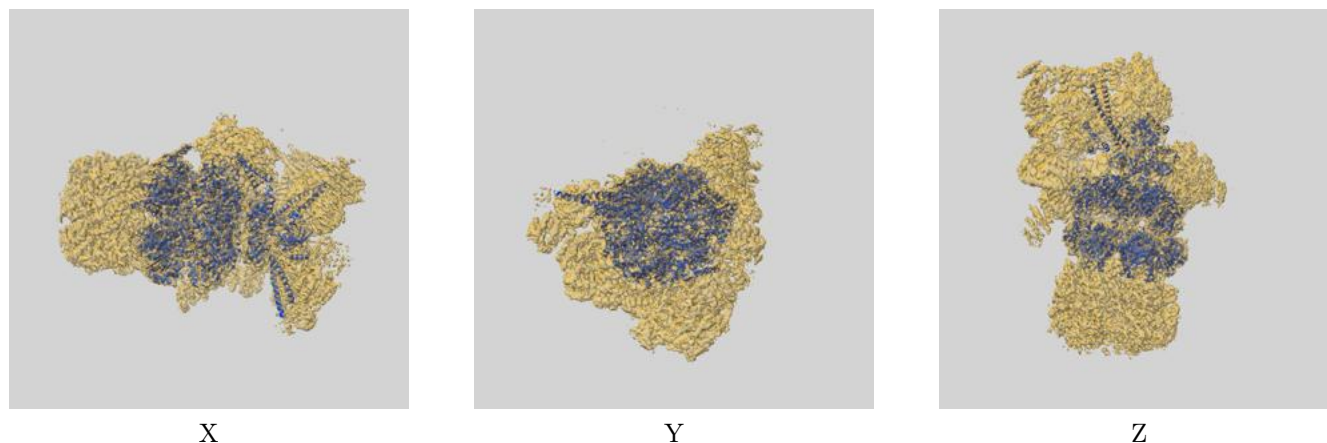
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.19	2.80
Unmasked-calculated*	3.93	6.98	4.03

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 2.76 by more than 10 %

## 9 Map-model fit [i](#)

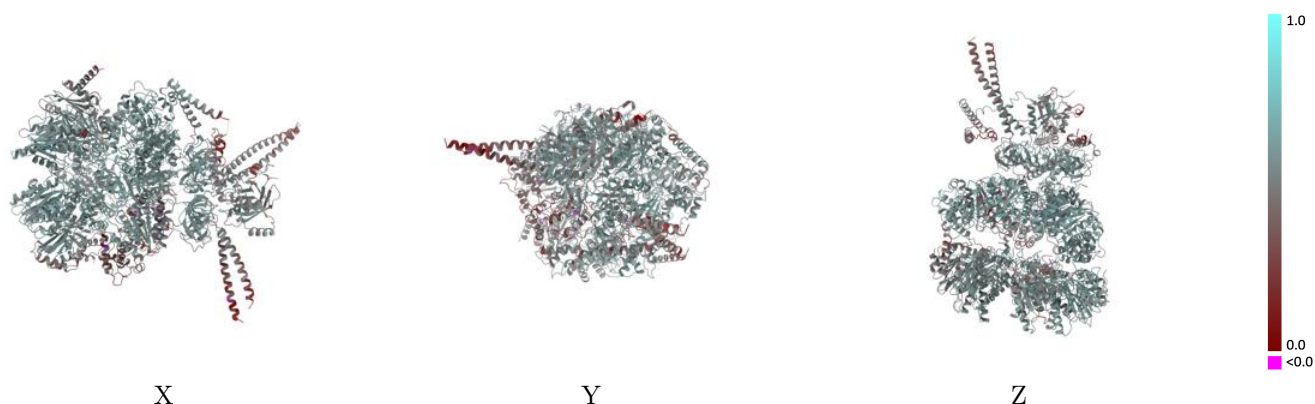
This section contains information regarding the fit between EMDB map EMD-71537 and PDB model 9PDL. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [i](#)



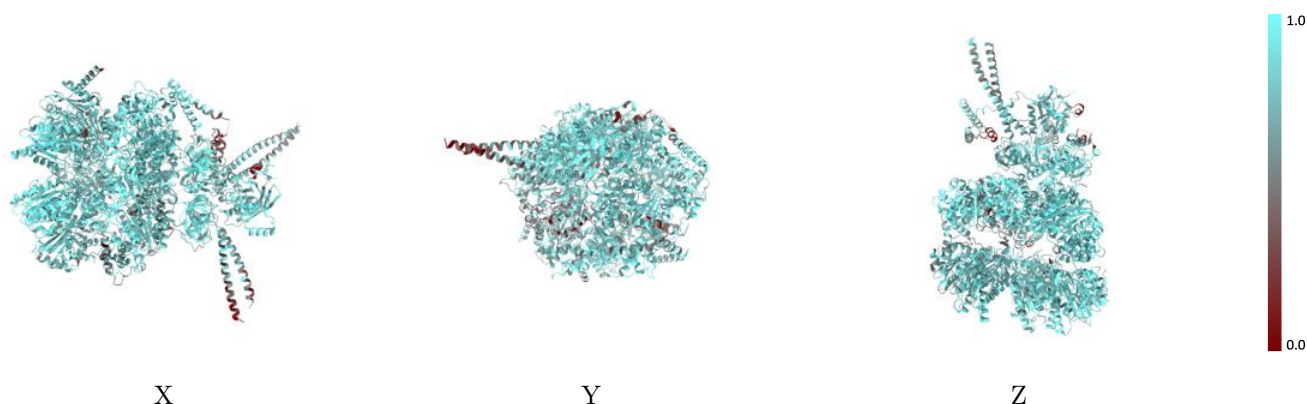
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



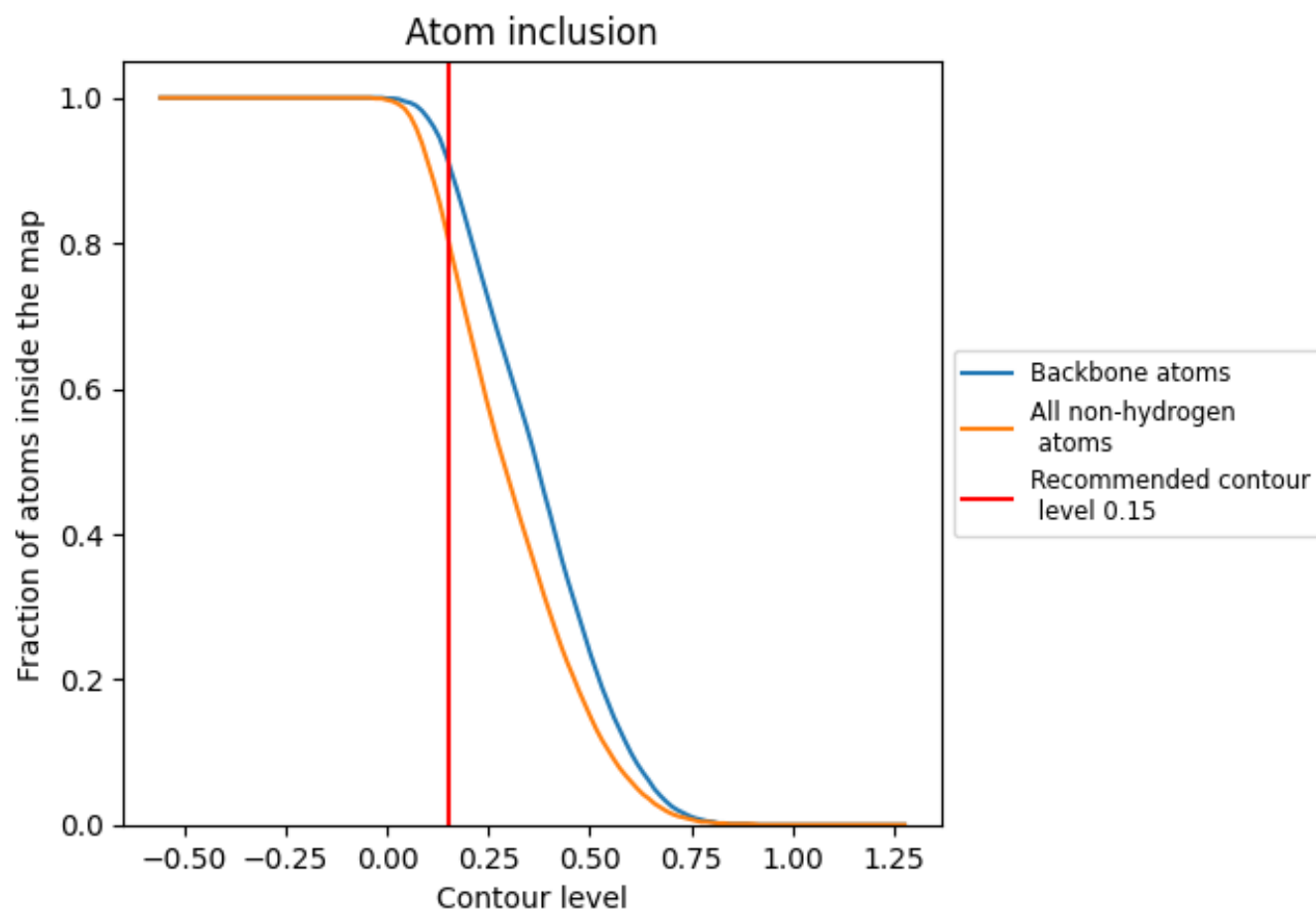
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8090	<div></div> 0.5170
A	<div></div> 0.8620	<div></div> 0.5490
B	<div></div> 0.8560	<div></div> 0.5490
C	<div></div> 0.8710	<div></div> 0.5660
D	<div></div> 0.8190	<div></div> 0.5230
E	<div></div> 0.5560	<div></div> 0.3400
F	<div></div> 0.8240	<div></div> 0.5250
G	<div></div> 0.8170	<div></div> 0.5220
H	<div></div> 0.8140	<div></div> 0.5320
I	<div></div> 0.7880	<div></div> 0.5120
J	<div></div> 0.8140	<div></div> 0.5190
K	<div></div> 0.8740	<div></div> 0.5630
L	<div></div> 0.9000	<div></div> 0.5690
M	<div></div> 0.8390	<div></div> 0.5280
c	<div></div> 0.7080	<div></div> 0.4600
v	<div></div> 0.9170	<div></div> 0.5610

