



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 07:55 AM UTC

PDB ID : 8CO1 / pdb_00008co1
EMDB ID : EMD-16770
Title : Type II Secretion System
Authors : Farci, D.; Piano, D.
Deposited on : 2023-02-26
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

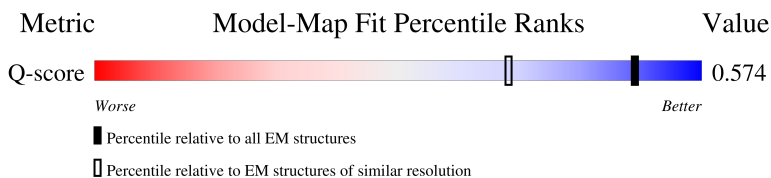
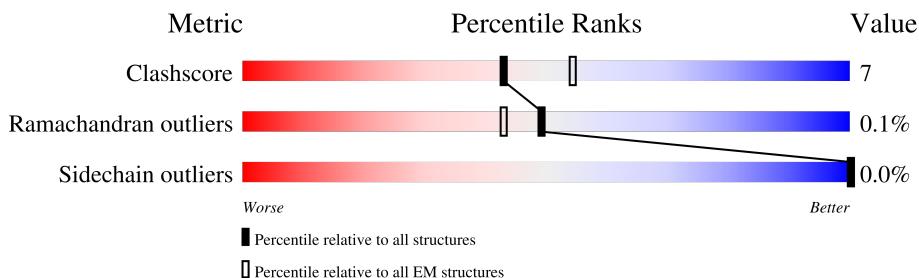
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.56 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.



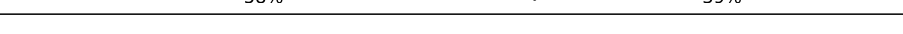
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7558 (2.06 - 3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A1	740	
1	B1	740	
1	C1	740	
1	D1	740	

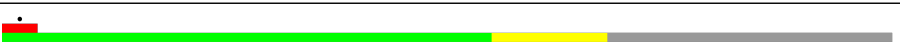
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Mol	Chain	Length	Quality of chain
1	E1	740	
1	F1	740	
1	G1	740	
1	H1	740	
1	I1	740	
1	L1	740	
1	M1	740	
1	N1	740	
1	O1	740	
1	P1	740	
1	Q1	740	
2	A2	155	
2	B2	155	
2	C2	155	
2	D2	155	
2	E2	155	
2	F2	155	
2	G2	155	
2	H2	155	
2	I2	155	
2	L2	155	
2	M2	155	
2	N2	155	
2	O2	155	
2	P2	155	

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Mol	Chain	Length	Quality of chain
2	Q2	155	
3	A3	208	
3	B3	208	
3	C3	208	
3	D3	208	
3	E3	208	
3	F3	208	
3	G3	208	
3	H3	208	
3	I3	208	
3	L3	208	
3	M3	208	
3	N3	208	
3	O3	208	
3	P3	208	
3	Q3	208	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 94677 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 Probable type IV piliation system protein DR_0774.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	P1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	O1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	N1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	M1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	L1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	A1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	I1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	H1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	F1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	G1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	E1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	D1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	C1	609	Total	C	N	O	S	0	0
			4589	2901	802	883	3		
1	B1	609	Total	C	N	O	S	0	0
			4587	2899	802	883	3		

- Molecule 2 is a protein called IPT/TIG domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	P2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	O2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	N2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	M2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	L2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	A2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	I2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	H2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	F2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	G2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	E2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	D2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	C2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		
2	B2	95	Total	C	N	O	S	0	0
			683	428	121	133	1		

- Molecule 3 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	P3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	O3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	N3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	M3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		

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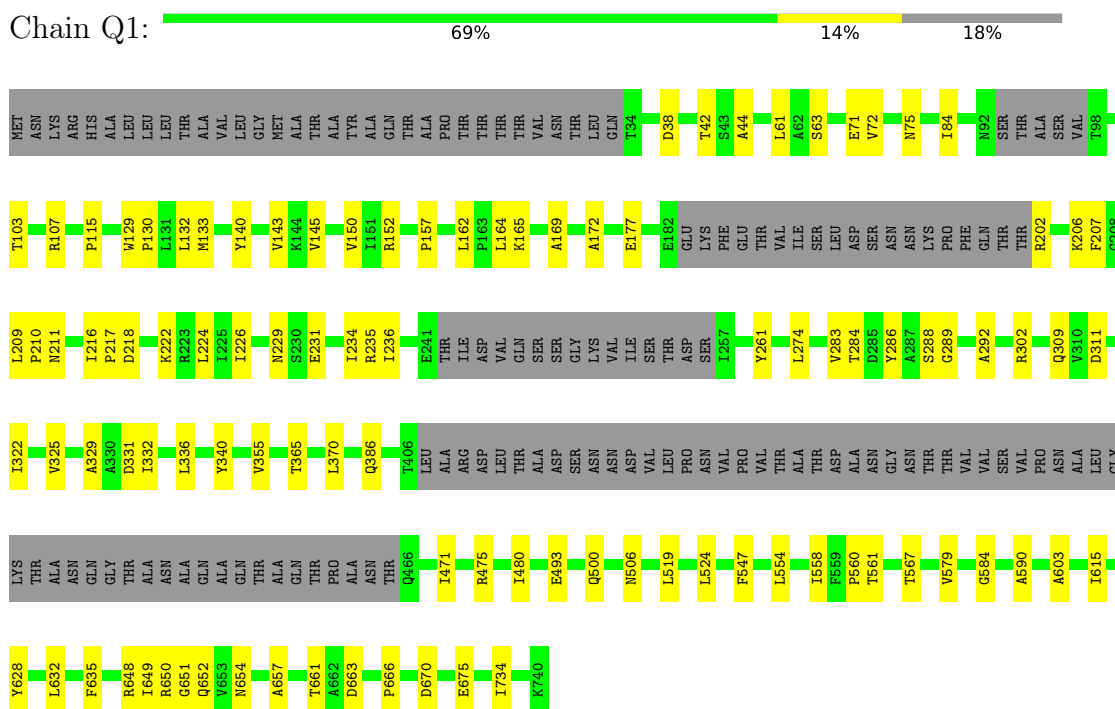
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	A3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	I3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	H3	142	Total	C	N	O	S	0	0
			1039	646	184	206	3		
3	F3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	G3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	E3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	D3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	C3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		
3	B3	142	Total	C	N	O	S	0	0
			1040	646	184	207	3		

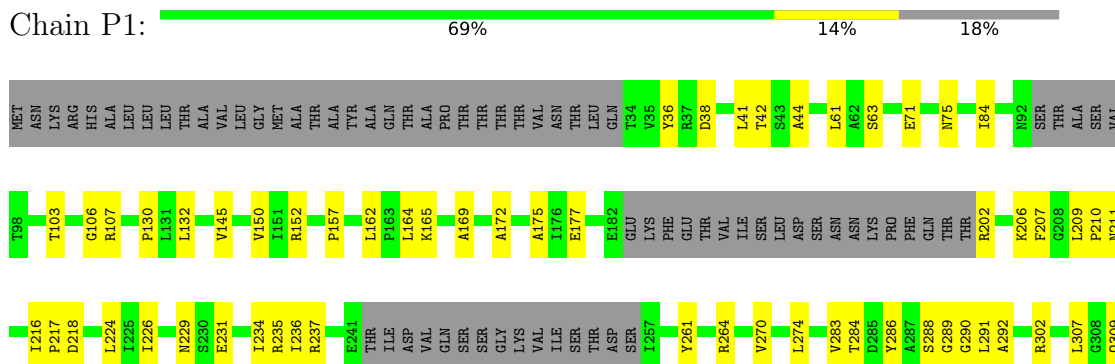
3 Residue-property plots

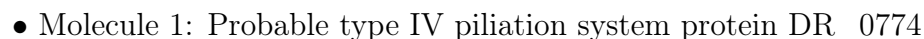
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Probable type IV piliation system protein DR_0774

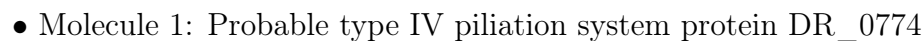


- Molecule 1: Probable type IV piliation system protein DR_0774

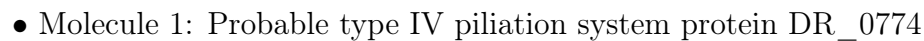




Response	Percentage
Yes	68%
No	15%
Don't know	18%

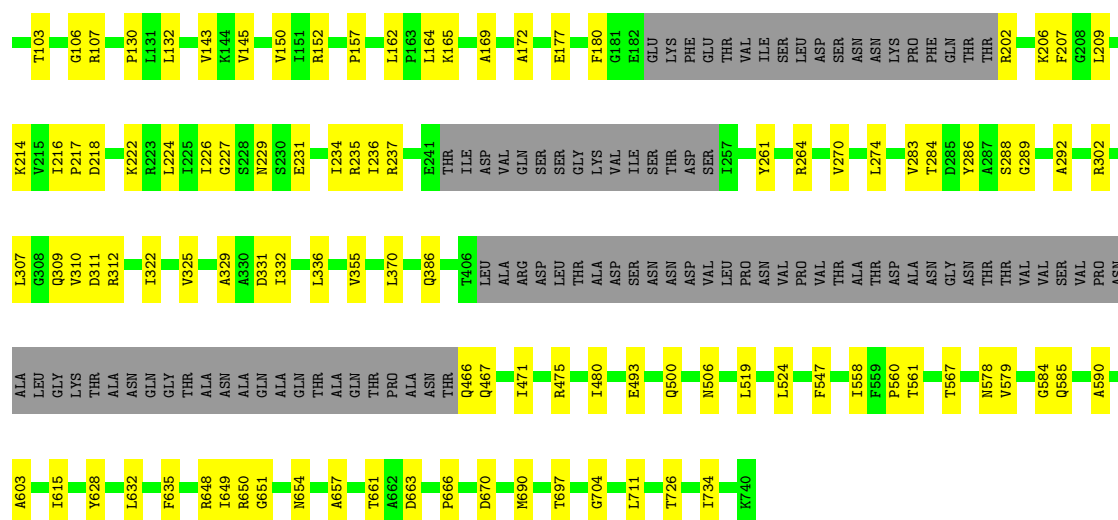


App Type	Percentage
Shopping app	68%
Social media app	14%
Productivity app	18%



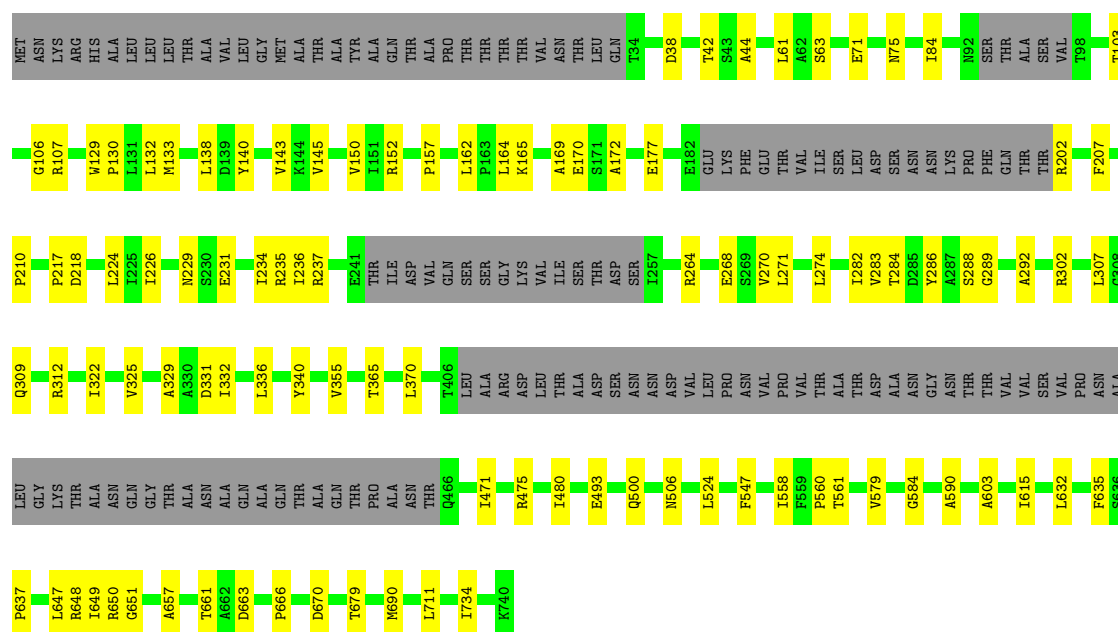
Response	Percentage
Doing a good job	67%
Not doing a good job	15%
Don't know	18%





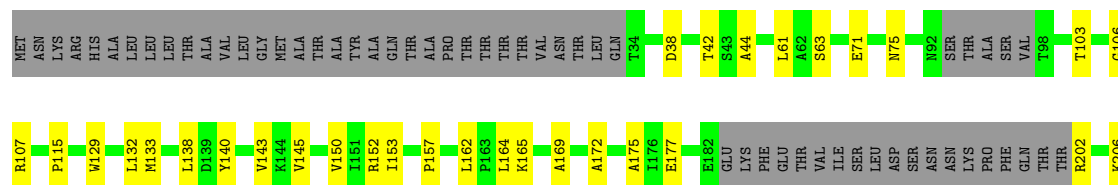
- Molecule 1: Probable type IV piliation system protein DR_0774

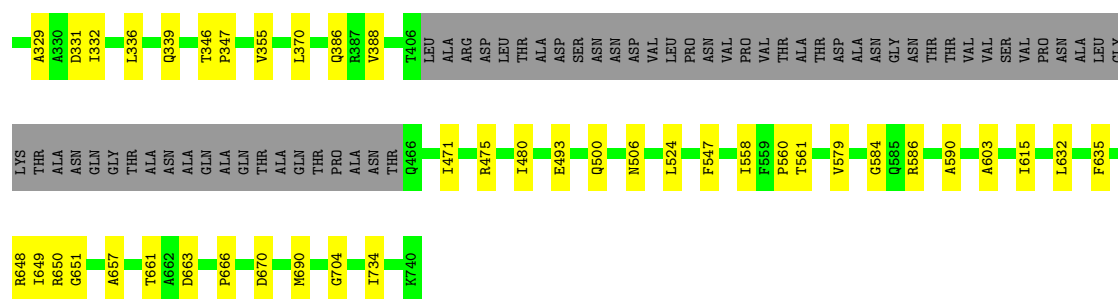
Chain E1: 69% 14% 18%



- Molecule 1: Probable type IV piliation system protein DR_0774

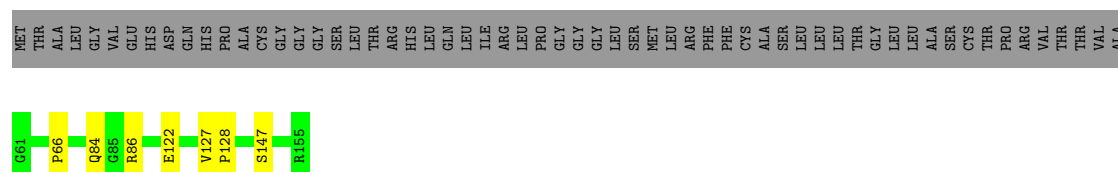
Chain D1: 69% 14% 18%





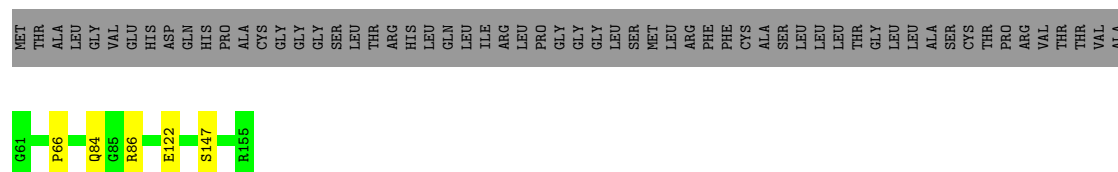
- Molecule 2: IPT/TIG domain-containing protein

Chain Q2: 57% 5% 39%



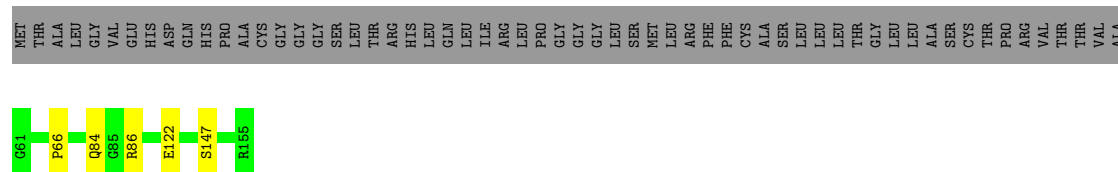
- Molecule 2: IPT/TIG domain-containing protein

Chain P2: 58% . 39%



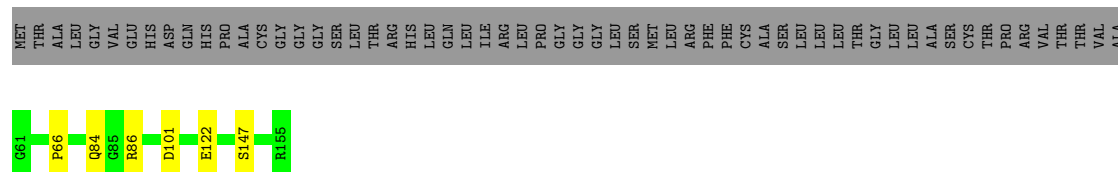
- Molecule 2: IPT/TIG domain-containing protein

Chain O2: 58% . 39%



- Molecule 2: IPT/TIG domain-containing protein

Chain N2: 57% . 39%



- Molecule 2: IPT/TIG domain-containing protein

Chain M2:  57% 39%

MET THR ALA LEU VAL GLU HIS ASP GLN HIS PRO PRO CYS GLY GLY SER LEU THR ARG ARG HIS LEU LEU LEU ILE ARG ARG LEU PRO PRO GLY GLY GLY LEU SER MET MET LEU ARG PHE PHE CYS CYS ALA SER SER LEU LEU LEU THR GLY LEU LEU ALA SER CYS THR PRO ARG VAL THR THR VAL ALA

G61 V62 T63 P66 Q84 G85 R86 E122 S147 R155

- Molecule 2: IPT/TIG domain-containing protein

Chain L2:  58% 39%

MET THR ALA LEU VAL GLU HIS ASP GLN HIS PRO PRO CYS GLY GLY SER LEU THR ARG ARG HIS LEU LEU LEU ILE ARG ARG LEU PRO PRO GLY GLY GLY LEU SER MET MET LEU ARG PHE PHE CYS CYS ALA SER SER LEU LEU LEU THR GLY LEU LEU ALA SER CYS THR PRO ARG VAL THR THR VAL ALA

G61 P66 Q84 G85 R86 E122 S147 R155

- Molecule 2: IPT/TIG domain-containing protein

Chain A2:  58% 39%

MET THR ALA LEU VAL GLU HIS ASP GLN HIS PRO PRO CYS GLY GLY SER LEU THR ARG ARG HIS LEU LEU LEU ILE ARG ARG LEU PRO PRO GLY GLY GLY LEU SER MET MET LEU ARG PHE PHE CYS CYS ALA SER SER LEU LEU LEU THR GLY LEU LEU ALA SER CYS THR PRO ARG VAL THR THR VAL ALA

G61 P66 Q84 G85 R86 E122 S147 R155

- Molecule 2: IPT/TIG domain-containing protein

Chain I2:  58% 39%

MET THR ALA LEU VAL GLU HIS ASP GLN HIS PRO PRO CYS GLY GLY SER LEU THR ARG ARG HIS LEU LEU LEU ILE ARG ARG LEU PRO PRO GLY GLY GLY LEU SER MET MET LEU ARG PHE PHE CYS CYS ALA SER SER LEU LEU LEU THR GLY LEU LEU ALA SER CYS THR PRO ARG VAL THR THR VAL ALA

G61 P66 Q84 G85 R86 E122 S147 R155

- Molecule 2: IPT/TIG domain-containing protein

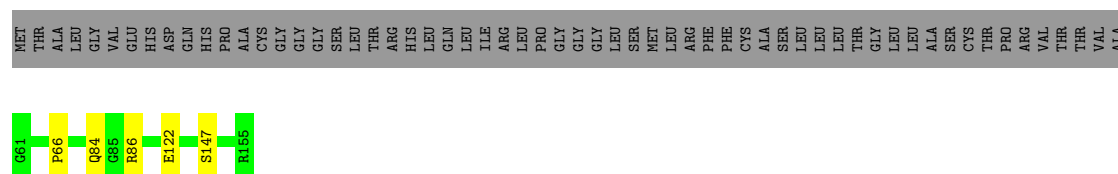
Chain H2:  57% 5% 39%

MET THR ALA LEU VAL GLU HIS ASP GLN HIS PRO PRO CYS GLY GLY SER LEU THR ARG ARG HIS LEU LEU LEU ILE ARG ARG LEU PRO PRO GLY GLY GLY LEU SER MET MET LEU ARG PHE PHE CYS CYS ALA SER SER LEU LEU LEU THR GLY LEU LEU ALA SER CYS THR PRO ARG VAL THR THR VAL ALA

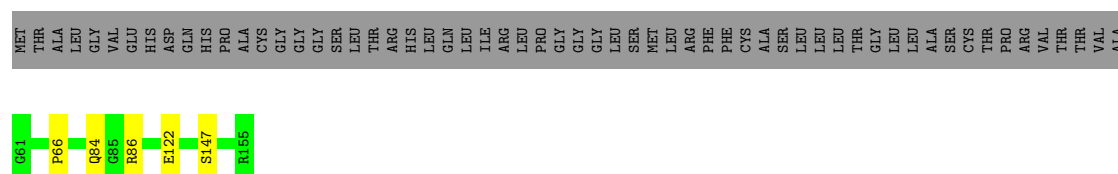
G61 P66 Q84 G85 R86 E122 V127 P128 S147 R155

- Molecule 2: IPT/TIG domain-containing protein

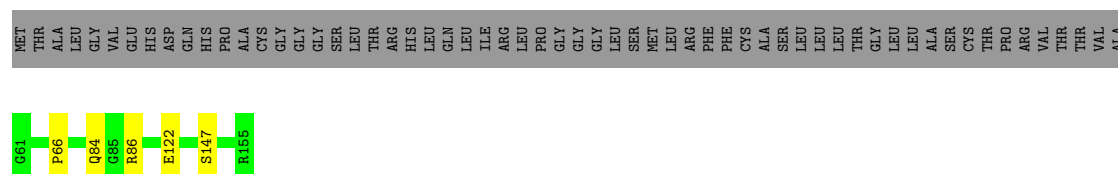
Chain F2:  58% 39%



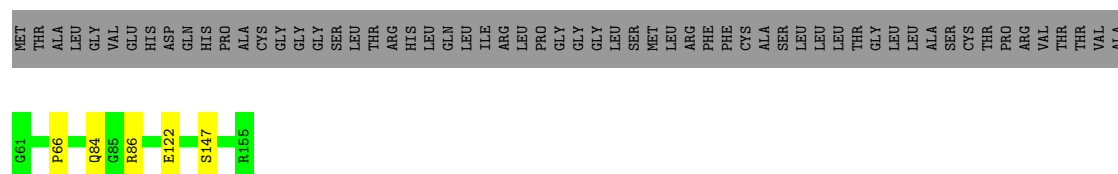
- Molecule 2: IPT/TIG domain-containing protein



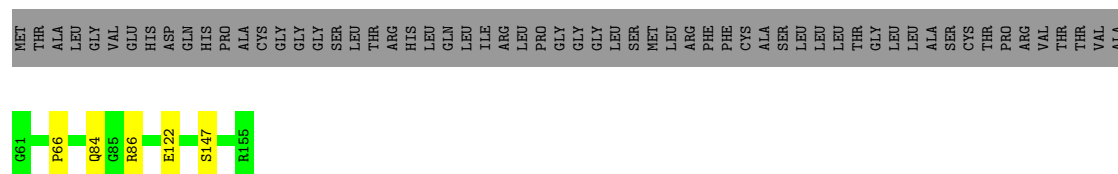
- Molecule 2: IPT/TIG domain-containing protein



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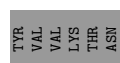


- Molecule 2: IPT/TIG domain-containing protein

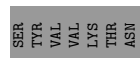
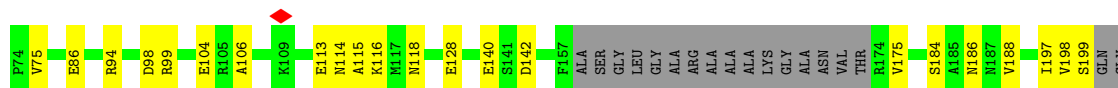




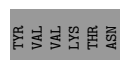
● Molecule 3: Lipoprotein



● Molecule 3: Lipoprotein

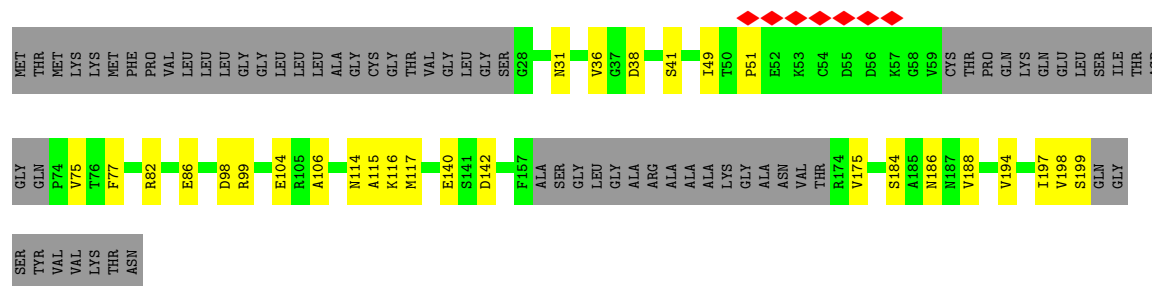


● Molecule 3: Lipoprotein

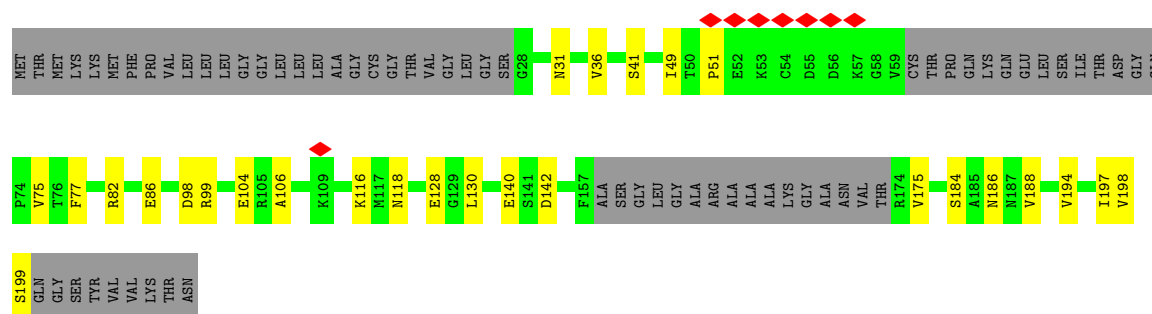


● Molecule 3: Lipoprotein

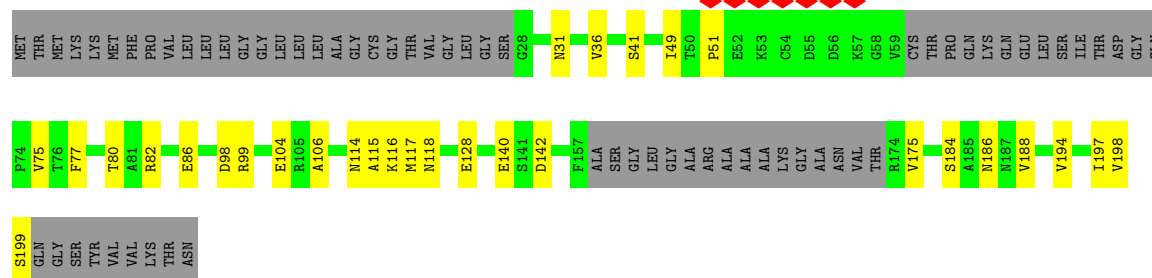




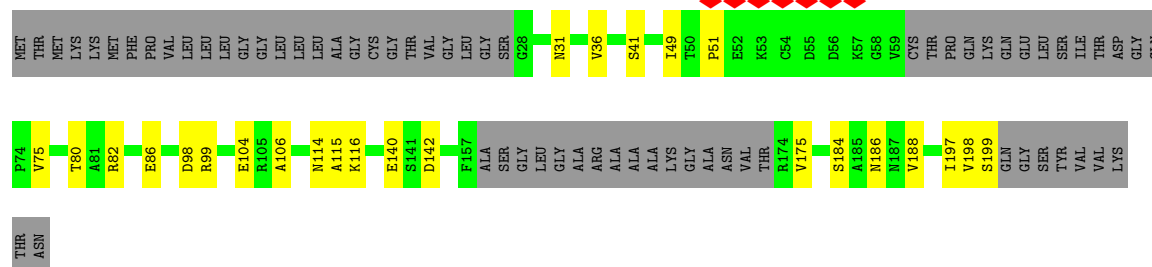
- Molecule 3: Lipoprotein



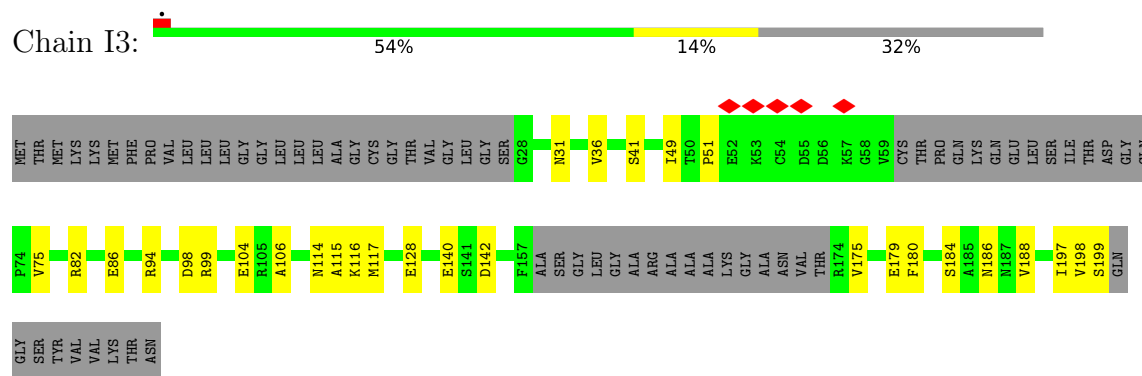
- Molecule 3: Lipoprotein



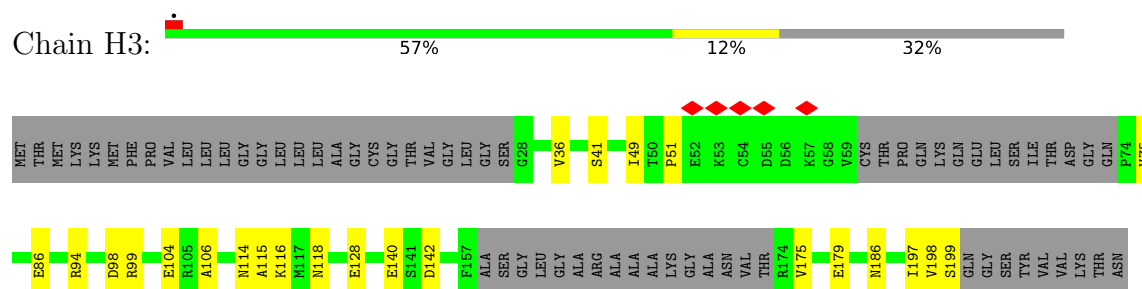
- Molecule 3: Lipoprotein



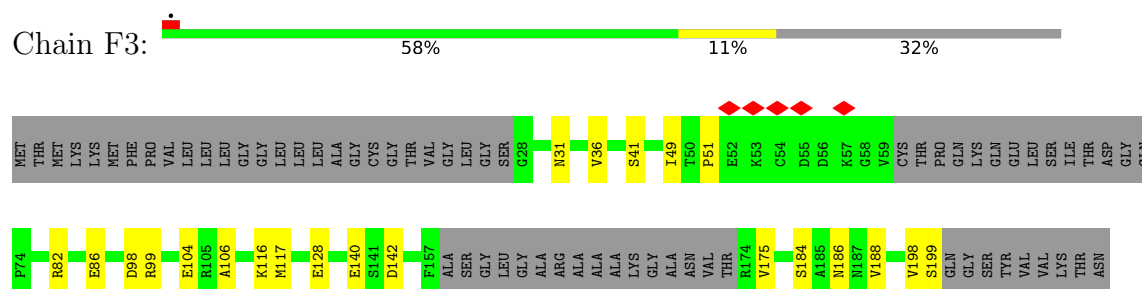
- Molecule 3: Lipoprotein



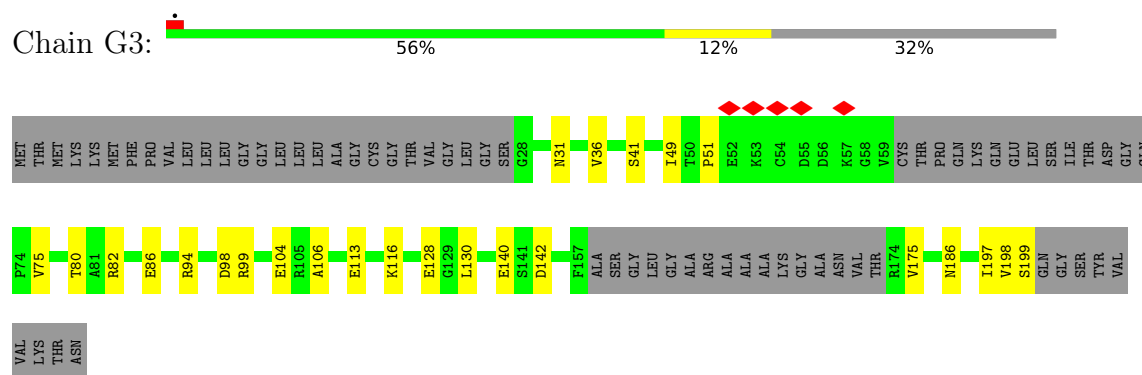
- Molecule 3: Lipoprotein



- Molecule 3: Lipoprotein

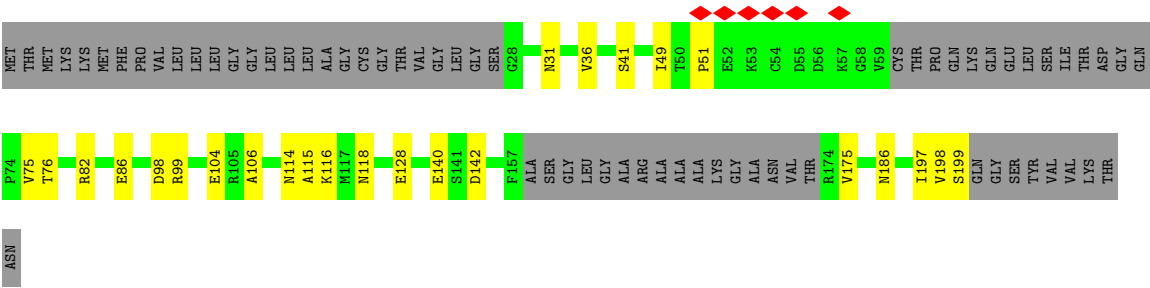


- Molecule 3: Lipoprotein

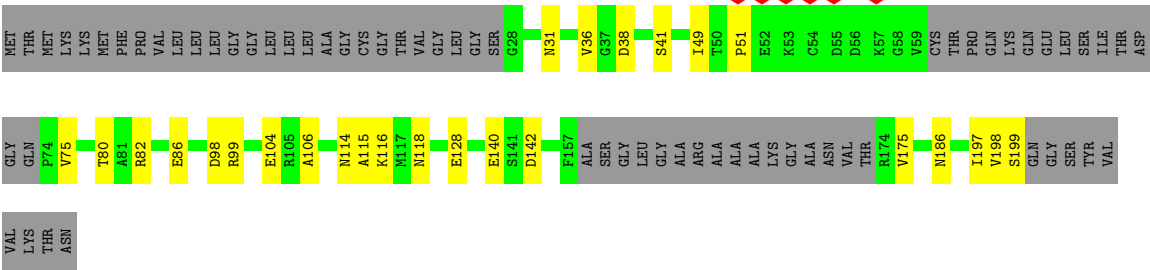


- Molecule 3: Lipoprotein

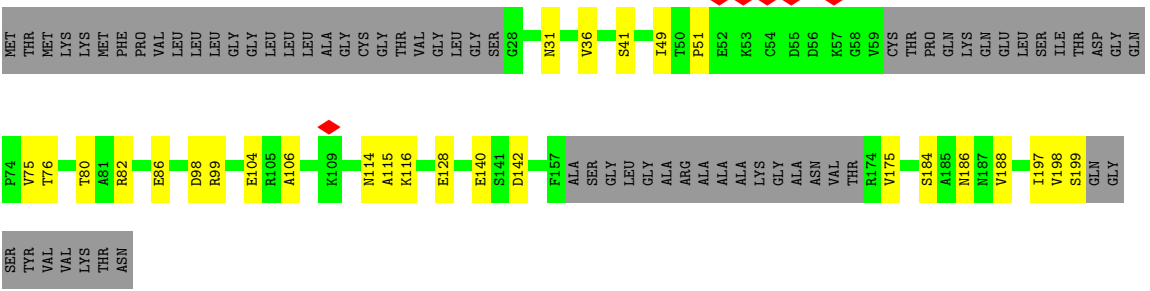




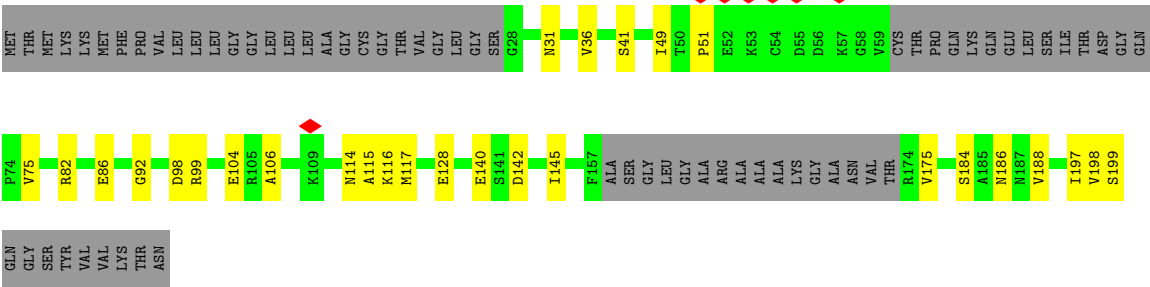
• Molecule 3: Lipoprotein



• Molecule 3: Lipoprotein



• Molecule 3: Lipoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C15	Depositor
Number of particles used	11000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.504	Depositor
Minimum map value	-4.908	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	600.0, 600.0, 600.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A1	0.31	0/4661	0.45	1/6343 (0.0%)
1	B1	0.31	0/4659	0.44	1/6340 (0.0%)
1	C1	0.31	0/4661	0.44	1/6343 (0.0%)
1	D1	0.31	0/4661	0.45	1/6343 (0.0%)
1	E1	0.31	0/4661	0.46	1/6343 (0.0%)
1	F1	0.30	0/4661	0.44	1/6343 (0.0%)
1	G1	0.31	0/4661	0.44	1/6343 (0.0%)
1	H1	0.31	0/4661	0.45	1/6343 (0.0%)
1	I1	0.31	0/4661	0.44	0/6343
1	L1	0.31	0/4661	0.46	2/6343 (0.0%)
1	M1	0.31	0/4661	0.44	1/6343 (0.0%)
1	N1	0.31	0/4661	0.45	2/6343 (0.0%)
1	O1	0.31	0/4661	0.45	0/6343
1	P1	0.31	0/4661	0.44	1/6343 (0.0%)
1	Q1	0.31	0/4661	0.45	0/6343
2	A2	0.29	0/694	0.40	0/944
2	B2	0.29	0/694	0.40	0/944
2	C2	0.29	0/694	0.40	0/944
2	D2	0.29	0/694	0.39	0/944
2	E2	0.29	0/694	0.40	0/944
2	F2	0.29	0/694	0.40	0/944
2	G2	0.29	0/694	0.40	0/944
2	H2	0.29	0/694	0.40	0/944
2	I2	0.29	0/694	0.39	0/944
2	L2	0.29	0/694	0.40	0/944
2	M2	0.29	0/694	0.40	0/944
2	N2	0.29	0/694	0.40	0/944
2	O2	0.29	0/694	0.40	0/944
2	P2	0.29	0/694	0.40	0/944
2	Q2	0.29	0/694	0.40	0/944
3	A3	0.17	0/1056	0.44	1/1434 (0.1%)
3	B3	0.17	0/1056	0.45	1/1434 (0.1%)
3	C3	0.17	0/1056	0.45	1/1434 (0.1%)
3	D3	0.17	0/1056	0.45	1/1434 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	E3	0.17	0/1056	0.45	1/1434 (0.1%)
3	F3	0.18	0/1056	0.45	1/1434 (0.1%)
3	G3	0.17	0/1056	0.44	1/1434 (0.1%)
3	H3	0.17	0/1055	0.45	1/1433 (0.1%)
3	I3	0.18	0/1056	0.46	1/1434 (0.1%)
3	L3	0.17	0/1056	0.44	1/1434 (0.1%)
3	M3	0.17	0/1056	0.45	1/1434 (0.1%)
3	N3	0.17	0/1056	0.45	1/1434 (0.1%)
3	O3	0.17	0/1056	0.44	1/1434 (0.1%)
3	P3	0.18	0/1056	0.45	1/1434 (0.1%)
3	Q3	0.17	0/1056	0.44	1/1434 (0.1%)
All	All	0.29	0/96162	0.44	29/130811 (0.0%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O3	51	PRO	N-CA-CB	6.58	110.29	102.60
3	C3	51	PRO	N-CA-CB	6.58	110.29	102.60
3	D3	51	PRO	N-CA-CB	6.57	110.28	102.60
3	N3	51	PRO	N-CA-CB	6.57	110.28	102.60
1	D1	671	PHE	N-CA-C	6.56	118.59	110.91
3	L3	51	PRO	N-CA-CB	6.55	110.27	102.60
3	P3	51	PRO	N-CA-CB	6.55	110.27	102.60
3	E3	51	PRO	N-CA-CB	6.55	110.26	102.60
3	B3	51	PRO	N-CA-CB	6.55	110.26	102.60
3	Q3	51	PRO	N-CA-CB	6.54	110.25	102.60
3	I3	51	PRO	N-CA-CB	6.54	110.25	102.60
3	F3	51	PRO	N-CA-CB	6.53	110.24	102.60
3	H3	51	PRO	N-CA-CB	6.51	110.22	102.60
3	A3	51	PRO	N-CA-CB	6.50	110.21	102.60
3	G3	51	PRO	N-CA-CB	6.50	110.20	102.60
3	M3	51	PRO	N-CA-CB	6.47	110.17	102.60
1	L1	671	PHE	N-CA-C	6.45	118.45	110.91
1	F1	671	PHE	N-CA-C	6.43	118.44	110.91
1	H1	213	ILE	N-CA-C	-6.36	107.67	113.71
1	N1	671	PHE	N-CA-C	6.30	118.28	110.91
1	M1	170	GLU	N-CA-C	-5.95	107.84	114.62
1	E1	170	GLU	N-CA-C	-5.86	107.94	114.62
1	L1	170	GLU	N-CA-C	-5.71	108.11	114.62
1	N1	704	GLY	N-CA-C	5.21	117.08	110.20
1	P1	704	GLY	N-CA-C	5.11	116.94	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B1	704	GLY	N-CA-C	5.03	116.84	110.20
1	G1	704	GLY	N-CA-C	5.02	116.82	110.20
1	C1	704	GLY	N-CA-C	5.01	116.82	110.20
1	A1	704	GLY	N-CA-C	5.01	116.81	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	4589	0	4667	87	0
1	B1	4587	0	4660	80	0
1	C1	4589	0	4667	93	0
1	D1	4589	0	4667	80	0
1	E1	4589	0	4667	81	0
1	F1	4589	0	4667	85	0
1	G1	4589	0	4667	86	0
1	H1	4589	0	4667	84	0
1	I1	4589	0	4667	83	0
1	L1	4589	0	4667	78	0
1	M1	4589	0	4667	88	0
1	N1	4589	0	4667	87	0
1	O1	4589	0	4667	82	0
1	P1	4589	0	4667	78	0
1	Q1	4589	0	4667	77	0
2	A2	683	0	690	3	0
2	B2	683	0	690	3	0
2	C2	683	0	690	3	0
2	D2	683	0	690	3	0
2	E2	683	0	690	3	0
2	F2	683	0	690	4	0
2	G2	683	0	690	3	0
2	H2	683	0	690	4	0
2	I2	683	0	690	3	0
2	L2	683	0	690	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M2	683	0	690	4	0
2	N2	683	0	690	4	0
2	O2	683	0	690	3	0
2	P2	683	0	690	3	0
2	Q2	683	0	690	4	0
3	A3	1040	0	975	13	0
3	B3	1040	0	975	15	0
3	C3	1040	0	975	15	0
3	D3	1040	0	975	15	0
3	E3	1040	0	975	16	0
3	F3	1040	0	975	13	0
3	G3	1040	0	975	14	0
3	H3	1039	0	972	13	0
3	I3	1040	0	975	16	0
3	L3	1040	0	975	17	0
3	M3	1040	0	975	16	0
3	N3	1040	0	975	16	0
3	O3	1040	0	975	15	0
3	P3	1040	0	975	18	0
3	Q3	1040	0	975	13	0
All	All	94677	0	94970	1257	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 7.

All (1257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F3:116:LYS:HG3	3:E3:36:VAL:HB	1.53	0.91
3:F3:36:VAL:HB	3:G3:116:LYS:HG3	1.54	0.90
3:D3:116:LYS:HG3	3:C3:36:VAL:HB	1.54	0.90
3:H3:116:LYS:HG3	3:G3:36:VAL:HB	1.54	0.90
3:Q3:36:VAL:HB	3:B3:116:LYS:HG3	1.54	0.89
3:M3:116:LYS:HG3	3:L3:36:VAL:HB	1.54	0.88
3:I3:116:LYS:HG3	3:H3:36:VAL:HB	1.55	0.88
1:L1:270:VAL:HG13	1:L1:307:LEU:HD11	1.63	0.80
1:G1:202:ARG:HH21	1:G1:206:LYS:HB3	1.47	0.79
1:M1:270:VAL:HG13	1:M1:307:LEU:HD11	1.64	0.78
1:B1:558:ILE:HG23	1:B1:560:PRO:HD3	1.67	0.77
3:A3:116:LYS:HB3	3:I3:36:VAL:HB	1.66	0.77
1:I1:558:ILE:HG23	1:I1:560:PRO:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O1:558:ILE:HG23	1:O1:560:PRO:HD3	1.68	0.76
1:I1:42:THR:HG22	1:I1:44:ALA:H	1.50	0.76
1:F1:558:ILE:HG23	1:F1:560:PRO:HD3	1.68	0.76
1:G1:558:ILE:HG23	1:G1:560:PRO:HD3	1.67	0.76
1:M1:558:ILE:HG23	1:M1:560:PRO:HD3	1.68	0.76
1:P1:558:ILE:HG23	1:P1:560:PRO:HD3	1.68	0.76
1:L1:42:THR:HG22	1:L1:44:ALA:H	1.51	0.76
1:C1:558:ILE:HG23	1:C1:560:PRO:HD3	1.69	0.76
1:H1:539:GLY:HA3	1:H1:720:GLU:HG3	1.67	0.75
1:A1:558:ILE:HG23	1:A1:560:PRO:HD3	1.67	0.75
1:Q1:558:ILE:HG23	1:Q1:560:PRO:HD3	1.68	0.75
1:P1:42:THR:HG22	1:P1:44:ALA:H	1.52	0.75
1:D1:558:ILE:HG23	1:D1:560:PRO:HD3	1.68	0.75
1:O1:270:VAL:HG13	1:O1:307:LEU:HD11	1.67	0.75
1:O1:302:ARG:NH2	1:N1:286:TYR:OH	2.19	0.75
1:E1:558:ILE:HG23	1:E1:560:PRO:HD3	1.68	0.75
1:C1:42:THR:HG22	1:C1:44:ALA:H	1.51	0.75
1:I1:506:ASN:OD1	2:H2:86:ARG:NH2	2.19	0.75
1:H1:558:ILE:HG23	1:H1:560:PRO:HD3	1.69	0.75
1:C1:357:ASN:ND2	1:B1:339:GLN:HE22	1.85	0.75
1:L1:558:ILE:HG23	1:L1:560:PRO:HD3	1.68	0.75
1:H1:42:THR:HG22	1:H1:44:ALA:H	1.51	0.74
1:A1:42:THR:HG22	1:A1:44:ALA:H	1.51	0.74
3:L3:116:LYS:HB3	3:A3:36:VAL:HB	1.70	0.74
1:F1:42:THR:HG22	1:F1:44:ALA:H	1.51	0.74
1:E1:42:THR:HG22	1:E1:44:ALA:H	1.51	0.74
1:M1:42:THR:HG22	1:M1:44:ALA:H	1.53	0.74
1:Q1:286:TYR:OH	1:B1:302:ARG:NH2	2.18	0.73
1:N1:558:ILE:HG23	1:N1:560:PRO:HD3	1.71	0.73
1:D1:475:ARG:NH2	1:C1:500:GLN:O	2.21	0.73
1:N1:42:THR:HG22	1:N1:44:ALA:H	1.53	0.72
1:G1:42:THR:HG22	1:G1:44:ALA:H	1.51	0.72
1:P1:506:ASN:OD1	2:O2:86:ARG:NH2	2.23	0.72
1:D1:506:ASN:OD1	2:C2:86:ARG:NH2	2.22	0.72
1:D1:42:THR:HG22	1:D1:44:ALA:H	1.52	0.72
1:H1:214:LYS:HD2	1:G1:237:ARG:HH12	1.55	0.72
1:E1:336:LEU:HD11	1:E1:370:LEU:HD11	1.72	0.72
1:Q1:506:ASN:OD1	2:P2:86:ARG:NH2	2.22	0.71
1:E1:506:ASN:OD1	2:D2:86:ARG:NH2	2.22	0.71
1:A1:506:ASN:OD1	2:I2:86:ARG:NH2	2.24	0.71
3:C3:116:LYS:HB3	3:B3:36:VAL:HB	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E3:116:LYS:HB3	3:D3:36:VAL:HB	1.70	0.71
3:N3:116:LYS:HB3	3:M3:36:VAL:HB	1.72	0.71
1:G1:270:VAL:HG13	1:G1:307:LEU:HD11	1.72	0.71
1:L1:506:ASN:OD1	2:A2:86:ARG:NH2	2.24	0.71
1:P1:475:ARG:NH2	1:O1:500:GLN:O	2.24	0.70
1:F1:500:GLN:O	1:G1:475:ARG:NH2	2.24	0.70
1:D1:214:LYS:HD2	1:C1:237:ARG:HH12	1.56	0.70
1:Q1:475:ARG:NH2	1:P1:500:GLN:O	2.24	0.70
1:M1:475:ARG:NH2	1:L1:500:GLN:O	2.24	0.70
1:Q1:336:LEU:HD11	1:Q1:370:LEU:HD11	1.73	0.70
3:P3:116:LYS:HB3	3:O3:36:VAL:HB	1.74	0.70
1:L1:336:LEU:HD11	1:L1:370:LEU:HD11	1.71	0.70
1:D1:336:LEU:HD11	1:D1:370:LEU:HD11	1.73	0.69
1:L1:475:ARG:NH2	1:A1:500:GLN:O	2.25	0.69
1:Q1:42:THR:HG22	1:Q1:44:ALA:H	1.58	0.69
1:A1:336:LEU:HD11	1:A1:370:LEU:HD11	1.73	0.69
1:C1:506:ASN:OD1	2:B2:86:ARG:NH2	2.25	0.69
1:O1:165:LYS:HD3	1:O1:236:ILE:HG21	1.74	0.69
1:C1:302:ARG:NH2	1:B1:286:TYR:OH	2.23	0.69
1:H1:475:ARG:NH2	1:G1:500:GLN:O	2.25	0.68
1:H1:177:GLU:HG2	1:H1:202:ARG:HD3	1.75	0.68
1:I1:475:ARG:NH2	1:H1:500:GLN:O	2.25	0.68
1:P1:165:LYS:HD3	1:P1:236:ILE:HG21	1.76	0.68
1:M1:539:GLY:HA3	1:M1:720:GLU:HG3	1.74	0.68
1:C1:320:GLN:HG3	1:C1:357:ASN:OD1	1.94	0.68
1:N1:475:ARG:NH2	1:M1:500:GLN:O	2.26	0.68
1:M1:336:LEU:HD11	1:M1:370:LEU:HD11	1.74	0.68
1:A1:302:ARG:NH2	1:I1:286:TYR:OH	2.25	0.68
1:F1:286:TYR:OH	1:G1:302:ARG:NH2	2.26	0.68
1:P1:150:VAL:HG12	1:O1:71:GLU:HB2	1.75	0.68
1:A1:475:ARG:NH2	1:I1:500:GLN:O	2.26	0.67
1:O1:302:ARG:HH12	1:N1:286:TYR:HE2	1.43	0.67
1:H1:336:LEU:HD11	1:H1:370:LEU:HD11	1.77	0.67
1:C1:165:LYS:HD3	1:C1:236:ILE:HG21	1.77	0.67
1:Q1:500:GLN:O	1:B1:475:ARG:NH2	2.26	0.67
1:E1:475:ARG:NH2	1:D1:500:GLN:O	2.26	0.67
1:C1:336:LEU:HD11	1:C1:370:LEU:HD11	1.76	0.67
1:C1:475:ARG:NH2	1:B1:500:GLN:O	2.27	0.67
1:N1:506:ASN:OD1	2:M2:86:ARG:NH2	2.27	0.67
1:O1:475:ARG:NH2	1:N1:500:GLN:O	2.26	0.66
1:E1:133:MET:HE3	1:E1:138:LEU:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O3:116:LYS:HB3	3:N3:36:VAL:HB	1.76	0.66
1:B1:42:THR:HG22	1:B1:44:ALA:H	1.60	0.66
2:F2:86:ARG:NH2	1:G1:506:ASN:OD1	2.28	0.66
1:G1:165:LYS:HD3	1:G1:236:ILE:HG21	1.78	0.66
1:F1:214:LYS:HD2	1:E1:237:ARG:HH12	1.61	0.66
1:M1:506:ASN:OD1	2:L2:86:ARG:NH2	2.29	0.65
3:D3:118:ASN:ND2	3:C3:80:THR:OG1	2.29	0.65
1:O1:214:LYS:HD2	1:N1:237:ARG:HH12	1.60	0.65
1:F1:336:LEU:HD11	1:F1:370:LEU:HD11	1.79	0.65
1:F1:475:ARG:NH2	1:E1:500:GLN:O	2.27	0.65
2:Q2:86:ARG:NH2	1:B1:506:ASN:OD1	2.29	0.65
1:P1:336:LEU:HD11	1:P1:370:LEU:HD11	1.77	0.65
1:F1:133:MET:HE3	1:F1:138:LEU:HB2	1.78	0.65
1:O1:336:LEU:HD11	1:O1:370:LEU:HD11	1.78	0.65
1:M1:560:PRO:HD2	1:L1:547:PHE:HB3	1.79	0.64
1:L1:560:PRO:HD2	1:A1:547:PHE:HB3	1.80	0.64
1:H1:506:ASN:OD1	2:G2:86:ARG:NH2	2.30	0.64
1:F1:237:ARG:HH12	1:G1:214:LYS:HD2	1.62	0.64
3:M3:118:ASN:ND2	3:L3:80:THR:OG1	2.31	0.64
1:I1:336:LEU:HD11	1:I1:370:LEU:HD11	1.78	0.64
1:C1:357:ASN:HD22	1:B1:339:GLN:HE22	1.45	0.64
1:M1:214:LYS:HD2	1:L1:237:ARG:HH12	1.63	0.64
1:N1:270:VAL:HG13	1:N1:307:LEU:HD11	1.80	0.63
1:A1:103:THR:OG1	1:A1:107:ARG:NH2	2.31	0.63
1:O1:506:ASN:OD1	2:N2:86:ARG:NH2	2.31	0.63
1:N1:162:LEU:HD12	1:N1:217:PRO:HG2	1.80	0.63
3:L3:118:ASN:ND2	3:A3:80:THR:OG1	2.32	0.63
1:F1:286:TYR:HE2	1:G1:302:ARG:HH12	1.45	0.63
1:H1:332:ILE:HD11	1:H1:370:LEU:HD22	1.81	0.63
1:F1:270:VAL:HG13	1:F1:307:LEU:HD11	1.81	0.63
1:F1:506:ASN:OD1	2:E2:86:ARG:NH2	2.31	0.63
1:Q1:560:PRO:HD2	1:P1:547:PHE:HB3	1.80	0.62
1:O1:103:THR:OG1	1:O1:107:ARG:NH2	2.32	0.62
3:N3:77:PHE:HE1	3:N3:194:VAL:HG11	1.64	0.62
1:O1:177:GLU:HG2	1:O1:202:ARG:HD3	1.80	0.62
1:O1:133:MET:HE3	1:O1:138:LEU:HB2	1.82	0.62
1:A1:270:VAL:HG13	1:A1:307:LEU:HD11	1.82	0.62
1:Q1:547:PHE:HB3	1:B1:560:PRO:HD2	1.81	0.62
1:O1:560:PRO:HD2	1:N1:547:PHE:HB3	1.81	0.62
1:L1:302:ARG:NH2	1:A1:286:TYR:OH	2.32	0.62
1:H1:560:PRO:HD2	1:G1:547:PHE:HB3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E1:560:PRO:HD2	1:D1:547:PHE:HB3	1.81	0.62
1:N1:336:LEU:HD11	1:N1:370:LEU:HD11	1.80	0.62
1:G1:336:LEU:HD11	1:G1:370:LEU:HD11	1.82	0.62
1:C1:177:GLU:HG2	1:C1:202:ARG:HD3	1.82	0.62
1:B1:336:LEU:HD11	1:B1:370:LEU:HD11	1.81	0.62
1:Q1:286:TYR:HE2	1:B1:302:ARG:HH12	1.47	0.62
3:P3:118:ASN:ND2	3:O3:80:THR:OG1	2.33	0.62
1:N1:560:PRO:HD2	1:M1:547:PHE:HB3	1.82	0.62
1:M1:286:TYR:HE2	1:M1:292:ALA:HB2	1.65	0.62
1:A1:560:PRO:HD2	1:I1:547:PHE:HB3	1.81	0.62
3:H3:118:ASN:ND2	3:G3:80:THR:OG1	2.32	0.62
1:F1:214:LYS:HZ2	1:E1:237:ARG:HH22	1.48	0.62
1:C1:560:PRO:HD2	1:B1:547:PHE:HB3	1.82	0.62
1:D1:560:PRO:HD2	1:C1:547:PHE:HB3	1.82	0.62
1:N1:133:MET:HE3	1:N1:138:LEU:HB2	1.82	0.61
1:Q1:177:GLU:HA	1:Q1:202:ARG:HD3	1.83	0.61
1:D1:165:LYS:HD3	1:D1:236:ILE:HG21	1.83	0.61
1:O1:214:LYS:HZ2	1:N1:237:ARG:HH22	1.48	0.61
1:M1:214:LYS:HZ2	1:L1:237:ARG:HH22	1.49	0.61
1:C1:211:ASN:O	1:C1:211:ASN:ND2	2.33	0.61
1:I1:635:PHE:HB2	1:I1:648:ARG:HB2	1.83	0.61
1:E1:332:ILE:HD11	1:E1:370:LEU:HD22	1.82	0.60
3:P3:86:GLU:OE1	3:P3:186:ASN:ND2	2.34	0.60
1:O1:635:PHE:HB2	1:O1:648:ARG:HB2	1.83	0.60
1:I1:560:PRO:HD2	1:H1:547:PHE:HB3	1.82	0.60
1:H1:579:VAL:HG11	1:H1:603:ALA:HB1	1.83	0.60
1:E1:309:GLN:NE2	1:D1:288:SER:O	2.35	0.60
1:Q1:165:LYS:HD3	1:Q1:236:ILE:HG21	1.84	0.60
1:P1:579:VAL:HG11	1:P1:603:ALA:HB1	1.83	0.60
1:L1:635:PHE:HB2	1:L1:648:ARG:HB3	1.84	0.60
1:A1:635:PHE:HB2	1:A1:648:ARG:HB2	1.84	0.60
1:Q1:579:VAL:HG11	1:Q1:603:ALA:HB1	1.84	0.60
1:A1:177:GLU:HA	1:A1:202:ARG:HD3	1.84	0.60
1:A1:302:ARG:HH12	1:I1:286:TYR:HE2	1.49	0.60
1:G1:164:LEU:HD22	1:G1:236:ILE:HD11	1.82	0.60
1:M1:207:PHE:HB2	1:M1:218:ASP:HB2	1.84	0.60
1:L1:177:GLU:HA	1:L1:202:ARG:HD3	1.83	0.60
1:F1:214:LYS:NZ	1:E1:237:ARG:HH22	2.00	0.60
1:F1:635:PHE:HB2	1:F1:648:ARG:HB2	1.83	0.60
1:A1:579:VAL:HG11	1:A1:603:ALA:HB1	1.84	0.59
3:M3:86:GLU:OE1	3:M3:186:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:214:LYS:HE2	1:B1:237:ARG:NH1	2.16	0.59
1:B1:177:GLU:HA	1:B1:202:ARG:HD3	1.83	0.59
3:Q3:86:GLU:OE1	3:Q3:186:ASN:ND2	2.36	0.59
3:A3:86:GLU:OE1	3:A3:186:ASN:ND2	2.34	0.59
1:F1:237:ARG:HH22	1:G1:214:LYS:HZ2	1.51	0.59
1:F1:332:ILE:HD11	1:F1:370:LEU:HD22	1.84	0.59
3:C3:86:GLU:OE1	3:C3:186:ASN:ND2	2.34	0.59
1:B1:332:ILE:HD11	1:B1:370:LEU:HD22	1.84	0.59
3:N3:86:GLU:OE1	3:N3:186:ASN:ND2	2.36	0.59
1:I1:309:GLN:NE2	1:H1:288:SER:O	2.36	0.59
3:G3:94:ARG:HG2	3:G3:113:GLU:HG2	1.84	0.59
1:Q1:332:ILE:HD11	1:Q1:370:LEU:HD22	1.83	0.59
1:P1:211:ASN:O	1:P1:211:ASN:ND2	2.35	0.59
1:G1:207:PHE:HB2	1:G1:218:ASP:HB2	1.85	0.59
1:D1:133:MET:HE3	1:D1:138:LEU:HB2	1.85	0.59
1:Q1:302:ARG:NH1	1:P1:286:TYR:OH	2.35	0.59
1:M1:261:TYR:OH	1:M1:311:ASP:OD2	2.21	0.59
1:G1:177:GLU:HA	1:G1:202:ARG:HD3	1.85	0.59
1:N1:164:LEU:HD22	1:N1:236:ILE:HD11	1.85	0.59
1:P1:560:PRO:HD2	1:O1:547:PHE:HB3	1.84	0.59
1:M1:214:LYS:NZ	1:L1:237:ARG:HH22	2.00	0.59
1:M1:331:ASP:OD1	1:M1:332:ILE:N	2.36	0.59
1:L1:309:GLN:NE2	1:A1:288:SER:O	2.36	0.59
1:P1:164:LEU:HD22	1:P1:236:ILE:HD11	1.86	0.58
1:M1:177:GLU:HG2	1:M1:202:ARG:HD3	1.84	0.58
1:H1:309:GLN:NE2	1:G1:288:SER:O	2.36	0.58
1:O1:42:THR:HG22	1:O1:44:ALA:H	1.68	0.58
1:F1:560:PRO:HD2	1:E1:547:PHE:HB3	1.84	0.58
1:Q1:331:ASP:OD1	1:Q1:332:ILE:N	2.36	0.58
1:P1:309:GLN:NE2	1:O1:288:SER:O	2.36	0.58
1:N1:635:PHE:HB2	1:N1:648:ARG:HB3	1.86	0.58
1:M1:309:GLN:NE2	1:L1:288:SER:O	2.35	0.58
1:G1:635:PHE:HB2	1:G1:648:ARG:HB3	1.86	0.58
1:M1:635:PHE:HB2	1:M1:648:ARG:HB3	1.86	0.58
1:Q1:309:GLN:NE2	1:P1:288:SER:O	2.36	0.58
1:O1:579:VAL:HG11	1:O1:603:ALA:HB1	1.85	0.58
1:H1:302:ARG:NH1	1:G1:286:TYR:OH	2.35	0.58
3:Q3:116:LYS:HB3	3:P3:36:VAL:HB	1.83	0.58
1:L1:579:VAL:HG11	1:L1:603:ALA:HB1	1.85	0.58
1:B1:579:VAL:HG11	1:B1:603:ALA:HB1	1.84	0.58
1:M1:75:ASN:HB3	1:M1:222:LYS:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I1:207:PHE:HB2	1:I1:218:ASP:HB2	1.86	0.58
1:H1:270:VAL:HG13	1:H1:307:LEU:HD11	1.85	0.58
1:F1:288:SER:O	1:G1:309:GLN:NE2	2.37	0.58
1:P1:635:PHE:HB2	1:P1:648:ARG:HB3	1.86	0.58
3:O3:86:GLU:OE1	3:O3:186:ASN:ND2	2.36	0.58
1:F1:331:ASP:OD1	1:F1:332:ILE:N	2.37	0.58
1:I1:332:ILE:HD11	1:I1:370:LEU:HD22	1.84	0.58
1:D1:309:GLN:NE2	1:C1:288:SER:O	2.37	0.58
1:C1:635:PHE:HB2	1:C1:648:ARG:HB3	1.85	0.58
1:P1:332:ILE:HD11	1:P1:370:LEU:HD22	1.85	0.58
1:M1:302:ARG:NH1	1:L1:286:TYR:OH	2.36	0.58
1:F1:237:ARG:HH22	1:G1:214:LYS:NZ	2.02	0.58
1:E1:579:VAL:HG11	1:E1:603:ALA:HB1	1.85	0.58
1:Q1:288:SER:O	1:B1:309:GLN:NE2	2.36	0.57
3:P3:38:ASP:OD1	3:P3:197:ILE:HG13	2.03	0.57
1:O1:214:LYS:NZ	1:N1:237:ARG:HH22	2.01	0.57
1:L1:103:THR:OG1	1:L1:107:ARG:NH2	2.36	0.57
3:L3:86:GLU:OE1	3:L3:186:ASN:ND2	2.34	0.57
1:I1:103:THR:OG1	1:I1:107:ARG:NH2	2.37	0.57
1:D1:332:ILE:HD11	1:D1:370:LEU:HD22	1.87	0.57
1:A1:309:GLN:NE2	1:I1:288:SER:O	2.37	0.57
3:F3:86:GLU:OE1	3:F3:186:ASN:ND2	2.35	0.57
3:B3:86:GLU:OE1	3:B3:186:ASN:ND2	2.37	0.57
1:M1:332:ILE:HD11	1:M1:370:LEU:HD22	1.85	0.57
1:L1:207:PHE:HB2	1:L1:218:ASP:HB2	1.86	0.57
1:F1:579:VAL:HG11	1:F1:603:ALA:HB1	1.86	0.57
1:I1:579:VAL:HG11	1:I1:603:ALA:HB1	1.85	0.57
1:P1:302:ARG:NH2	1:O1:286:TYR:OH	2.37	0.57
1:O1:309:GLN:NE2	1:N1:288:SER:O	2.37	0.57
1:I1:177:GLU:HA	1:I1:202:ARG:HD3	1.86	0.57
1:F1:309:GLN:NE2	1:E1:288:SER:O	2.38	0.57
1:F1:547:PHE:HB3	1:G1:560:PRO:HD2	1.85	0.57
1:N1:332:ILE:HD11	1:N1:370:LEU:HD22	1.86	0.57
3:H3:86:GLU:OE1	3:H3:186:ASN:ND2	2.34	0.57
1:F1:261:TYR:OH	1:F1:311:ASP:OD2	2.21	0.57
1:E1:177:GLU:HA	1:E1:202:ARG:HD3	1.85	0.57
1:A1:331:ASP:OD1	1:A1:332:ILE:N	2.38	0.57
1:D1:177:GLU:HG2	1:D1:202:ARG:HD3	1.86	0.57
1:D1:635:PHE:HB2	1:D1:648:ARG:HB3	1.86	0.57
1:D1:207:PHE:HB2	1:D1:218:ASP:HB2	1.86	0.57
1:C1:164:LEU:HD22	1:C1:236:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H1:635:PHE:HB2	1:H1:648:ARG:HB3	1.87	0.57
1:C1:331:ASP:OD1	1:C1:332:ILE:N	2.38	0.57
1:O1:164:LEU:HD22	1:O1:236:ILE:HD11	1.87	0.56
1:E1:164:LEU:HD22	1:E1:236:ILE:HD11	1.86	0.56
1:D1:164:LEU:HD22	1:D1:236:ILE:HD11	1.85	0.56
1:C1:386:GLN:NE2	1:B1:493:GLU:OE2	2.38	0.56
1:L1:331:ASP:OD1	1:L1:332:ILE:N	2.36	0.56
1:F1:286:TYR:O	1:F1:289:GLY:N	2.37	0.56
1:N1:177:GLU:HA	1:N1:202:ARG:HD3	1.87	0.56
1:F1:493:GLU:OE2	1:G1:386:GLN:NE2	2.39	0.56
1:G1:331:ASP:OD1	1:G1:332:ILE:N	2.37	0.56
1:D1:302:ARG:NH2	1:C1:286:TYR:OH	2.35	0.56
1:C1:309:GLN:NE2	1:B1:288:SER:O	2.38	0.56
1:C1:579:VAL:HG11	1:C1:603:ALA:HB1	1.87	0.56
1:B1:635:PHE:HB2	1:B1:648:ARG:HB3	1.86	0.56
1:O1:332:ILE:HD11	1:O1:370:LEU:HD22	1.87	0.56
1:N1:286:TYR:O	1:N1:289:GLY:N	2.36	0.56
1:E1:331:ASP:OD1	1:E1:332:ILE:N	2.39	0.56
1:D1:331:ASP:OD1	1:D1:332:ILE:N	2.38	0.56
1:Q1:164:LEU:HD22	1:Q1:236:ILE:HD11	1.88	0.56
1:F1:164:LEU:HD22	1:F1:236:ILE:HD11	1.86	0.56
3:G3:86:GLU:OE1	3:G3:186:ASN:ND2	2.36	0.56
3:E3:86:GLU:OE1	3:E3:186:ASN:ND2	2.35	0.56
1:O1:261:TYR:OH	1:O1:311:ASP:OD2	2.20	0.56
1:I1:162:LEU:HD12	1:I1:217:PRO:HG2	1.88	0.56
1:F1:177:GLU:HA	1:F1:202:ARG:HD3	1.87	0.56
1:B1:331:ASP:OD1	1:B1:332:ILE:N	2.39	0.56
1:N1:586:ARG:O	1:M1:648:ARG:NH2	2.39	0.56
1:P1:331:ASP:OD1	1:P1:332:ILE:N	2.38	0.56
1:O1:331:ASP:OD1	1:O1:332:ILE:N	2.38	0.56
1:D1:475:ARG:HA	1:C1:584:GLY:HA3	1.87	0.56
1:M1:579:VAL:HG11	1:M1:603:ALA:HB1	1.89	0.55
3:I3:86:GLU:OE1	3:I3:186:ASN:ND2	2.37	0.55
1:E1:635:PHE:HB2	1:E1:648:ARG:HB2	1.87	0.55
3:M3:99:ARG:NE	3:M3:104:GLU:OE1	2.38	0.55
1:H1:331:ASP:OD1	1:H1:332:ILE:N	2.39	0.55
1:I1:302:ARG:NH1	1:H1:286:TYR:OH	2.40	0.55
1:G1:579:VAL:HG11	1:G1:603:ALA:HB1	1.87	0.55
3:D3:99:ARG:NE	3:D3:104:GLU:OE1	2.38	0.55
1:A1:207:PHE:HB2	1:A1:218:ASP:HB2	1.88	0.55
1:I1:331:ASP:OD1	1:I1:332:ILE:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N1:331:ASP:OD1	1:N1:332:ILE:N	2.39	0.55
1:N1:579:VAL:HG11	1:N1:603:ALA:HB1	1.88	0.55
1:L1:475:ARG:HA	1:A1:584:GLY:HA3	1.89	0.55
1:F1:207:PHE:HB2	1:F1:218:ASP:HB2	1.89	0.55
1:Q1:635:PHE:HB2	1:Q1:648:ARG:HB3	1.89	0.55
1:A1:386:GLN:NE2	1:I1:493:GLU:OE2	2.39	0.55
1:H1:153:ILE:HD12	1:G1:72:VAL:HG13	1.89	0.55
1:L1:332:ILE:HD11	1:L1:370:LEU:HD22	1.88	0.55
1:C1:325:VAL:HG11	1:C1:329:ALA:HB2	1.89	0.55
1:A1:332:ILE:HD11	1:A1:370:LEU:HD22	1.88	0.55
1:O1:648:ARG:HG2	1:O1:679:THR:OG1	2.07	0.54
1:G1:332:ILE:HD11	1:G1:370:LEU:HD22	1.88	0.54
1:M1:162:LEU:HD12	1:M1:217:PRO:HG2	1.89	0.54
1:L1:164:LEU:HD22	1:L1:236:ILE:HD11	1.89	0.54
1:L1:261:TYR:OH	1:L1:311:ASP:OD2	2.19	0.54
1:N1:207:PHE:HB2	1:N1:218:ASP:HB2	1.89	0.54
1:A1:129:TRP:CZ2	1:A1:133:MET:HE3	2.43	0.54
1:H1:164:LEU:HD22	1:H1:236:ILE:HD11	1.89	0.54
1:P1:475:ARG:HA	1:O1:584:GLY:HA3	1.88	0.54
3:A3:41:SER:OG	3:A3:199:SER:O	2.25	0.54
1:H1:180:PHE:CZ	1:H1:227:GLY:HA2	2.42	0.54
1:C1:162:LEU:HD12	1:C1:217:PRO:HG2	1.90	0.54
3:P3:41:SER:OG	3:P3:199:SER:O	2.25	0.54
1:L1:649:ILE:HD13	1:L1:734:ILE:HG12	1.90	0.54
1:F1:162:LEU:HD12	1:F1:217:PRO:HG2	1.90	0.54
1:E1:152:ARG:NH2	1:D1:75:ASN:OD1	2.39	0.54
3:C3:99:ARG:NE	3:C3:104:GLU:OE1	2.40	0.54
1:P1:152:ARG:NH2	1:O1:75:ASN:OD1	2.39	0.54
1:F1:152:ARG:NH2	1:E1:75:ASN:OD1	2.38	0.54
1:E1:38:ASP:OD2	1:E1:140:TYR:OH	2.17	0.54
1:Q1:261:TYR:OH	1:Q1:311:ASP:OD2	2.23	0.54
1:M1:164:LEU:HD22	1:M1:236:ILE:HD11	1.90	0.54
3:I3:41:SER:OG	3:I3:199:SER:O	2.25	0.54
1:E1:302:ARG:NH1	1:D1:286:TYR:OH	2.40	0.54
1:E1:322:ILE:HG12	1:E1:355:VAL:HG22	1.89	0.54
1:B1:164:LEU:HD22	1:B1:236:ILE:HD11	1.90	0.54
3:Q3:99:ARG:NE	3:Q3:104:GLU:OE1	2.39	0.54
3:L3:41:SER:OG	3:L3:199:SER:O	2.25	0.54
1:A1:162:LEU:HD12	1:A1:217:PRO:HG2	1.90	0.54
1:B1:38:ASP:OD2	1:B1:140:TYR:OH	2.18	0.54
1:F1:648:ARG:HG2	1:F1:679:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:386:GLN:NE2	1:C1:493:GLU:OE2	2.40	0.54
1:P1:386:GLN:NE2	1:O1:493:GLU:OE2	2.39	0.54
3:D3:86:GLU:OE1	3:D3:186:ASN:ND2	2.38	0.54
1:N1:309:GLN:NE2	1:M1:288:SER:O	2.41	0.53
1:G1:325:VAL:HG11	1:G1:329:ALA:HB2	1.90	0.53
1:E1:648:ARG:HG2	1:E1:679:THR:OG1	2.09	0.53
1:M1:180:PHE:CZ	1:M1:227:GLY:HA2	2.43	0.53
1:H1:475:ARG:HA	1:G1:584:GLY:HA3	1.88	0.53
3:E3:118:ASN:ND2	3:D3:80:THR:OG1	2.41	0.53
1:A1:164:LEU:HD22	1:A1:236:ILE:HD11	1.91	0.53
1:B1:162:LEU:HD12	1:B1:217:PRO:HG2	1.90	0.53
1:H1:286:TYR:CE2	1:H1:292:ALA:HB2	2.43	0.53
1:G1:162:LEU:HD12	1:G1:217:PRO:HG2	1.91	0.53
1:C1:202:ARG:HH21	1:C1:206:LYS:HE3	1.74	0.53
3:B3:99:ARG:NE	3:B3:104:GLU:OE1	2.40	0.53
1:Q1:286:TYR:O	1:Q1:289:GLY:N	2.33	0.53
3:H3:99:ARG:NE	3:H3:104:GLU:OE1	2.39	0.53
1:E1:286:TYR:O	1:E1:289:GLY:N	2.39	0.53
1:D1:152:ARG:NH2	1:C1:75:ASN:OD1	2.40	0.53
1:C1:475:ARG:HA	1:B1:584:GLY:HA3	1.90	0.53
1:Q1:584:GLY:HA3	1:B1:475:ARG:HA	1.90	0.53
1:A1:648:ARG:HG2	1:A1:679:THR:OG1	2.08	0.53
1:G1:103:THR:OG1	1:G1:107:ARG:NH2	2.42	0.53
1:D1:38:ASP:OD2	1:D1:140:TYR:OH	2.19	0.53
3:M3:41:SER:OG	3:M3:199:SER:O	2.25	0.53
1:H1:162:LEU:HD12	1:H1:217:PRO:HG2	1.91	0.53
1:D1:214:LYS:NZ	1:C1:237:ARG:HH22	2.07	0.53
1:Q1:493:GLU:OE2	1:B1:386:GLN:NE2	2.41	0.53
3:Q3:41:SER:OG	3:Q3:199:SER:O	2.25	0.53
1:I1:648:ARG:HG2	1:I1:679:THR:OG1	2.08	0.53
1:H1:150:VAL:HG23	1:G1:71:GLU:O	2.09	0.53
1:P1:177:GLU:HA	1:P1:202:ARG:HD3	1.89	0.53
1:N1:153:ILE:HD12	1:M1:72:VAL:HG13	1.91	0.53
3:N3:41:SER:OG	3:N3:199:SER:O	2.24	0.53
1:H1:207:PHE:HB2	1:H1:218:ASP:HB2	1.91	0.53
1:F1:475:ARG:HA	1:E1:584:GLY:HA3	1.90	0.53
1:C1:332:ILE:HD11	1:C1:370:LEU:HD22	1.89	0.53
1:N1:322:ILE:HG12	1:N1:355:VAL:HG22	1.91	0.52
1:E1:207:PHE:HB2	1:E1:218:ASP:HB2	1.91	0.52
1:B1:103:THR:OG1	1:B1:107:ARG:NH2	2.42	0.52
1:Q1:162:LEU:HD12	1:Q1:217:PRO:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O1:207:PHE:HB2	1:O1:218:ASP:HB2	1.90	0.52
1:Q1:172:ALA:HA	1:Q1:235:ARG:NH2	2.24	0.52
1:H1:386:GLN:NE2	1:G1:493:GLU:OE2	2.40	0.52
1:D1:579:VAL:HG11	1:D1:603:ALA:HB1	1.90	0.52
1:C1:207:PHE:HB2	1:C1:218:ASP:HB2	1.91	0.52
1:Q1:475:ARG:HA	1:P1:584:GLY:HA3	1.90	0.52
1:P1:286:TYR:CE2	1:P1:292:ALA:HB2	2.45	0.52
1:I1:386:GLN:NE2	1:H1:493:GLU:OE2	2.41	0.52
1:D1:286:TYR:CE2	1:D1:292:ALA:HB2	2.44	0.52
1:B1:286:TYR:O	1:B1:289:GLY:N	2.36	0.52
1:N1:261:TYR:OH	1:N1:311:ASP:OD2	2.23	0.52
1:M1:307:LEU:HA	1:M1:310:VAL:HG22	1.91	0.52
1:I1:475:ARG:HA	1:H1:584:GLY:HA3	1.89	0.52
1:G1:261:TYR:OH	1:G1:311:ASP:OD2	2.24	0.52
1:O1:657:ALA:HB3	1:O1:670:ASP:HB3	1.91	0.52
3:I3:94:ARG:NH2	3:I3:179:GLU:OE1	2.43	0.52
3:I3:99:ARG:NE	3:I3:104:GLU:OE1	2.40	0.52
1:C1:152:ARG:NH2	1:B1:75:ASN:OD1	2.40	0.52
1:B1:207:PHE:HB2	1:B1:218:ASP:HB2	1.91	0.52
1:M1:475:ARG:HA	1:L1:584:GLY:HA3	1.91	0.52
1:L1:162:LEU:HD12	1:L1:217:PRO:HG2	1.92	0.52
1:L1:307:LEU:HA	1:L1:310:VAL:HG22	1.92	0.52
1:H1:202:ARG:HH21	1:H1:206:LYS:HE3	1.74	0.52
3:F3:99:ARG:NE	3:F3:104:GLU:OE1	2.40	0.52
1:N1:475:ARG:HA	1:M1:584:GLY:HA3	1.91	0.52
1:M1:286:TYR:O	1:M1:289:GLY:N	2.39	0.52
1:A1:261:TYR:OH	1:A1:311:ASP:OD2	2.25	0.52
1:P1:657:ALA:HB3	1:P1:670:ASP:HB3	1.91	0.52
1:O1:150:VAL:HG23	1:N1:71:GLU:O	2.09	0.52
1:L1:286:TYR:CE2	1:L1:292:ALA:HB2	2.45	0.52
1:H1:223:ARG:O	1:H1:227:GLY:HA3	2.10	0.52
1:F1:615:ILE:HD11	1:F1:666:PRO:HG2	1.92	0.52
1:B1:211:ASN:O	1:B1:211:ASN:ND2	2.42	0.52
1:Q1:152:ARG:NH2	1:P1:75:ASN:OD1	2.39	0.51
1:P1:649:ILE:HD13	1:P1:734:ILE:HG12	1.92	0.51
1:H1:261:TYR:OH	1:H1:311:ASP:OD2	2.26	0.51
3:E3:99:ARG:NE	3:E3:104:GLU:OE1	2.41	0.51
1:P1:103:THR:OG1	1:P1:107:ARG:NH2	2.43	0.51
1:H1:133:MET:HE3	1:H1:138:LEU:HB2	1.92	0.51
1:O1:325:VAL:HG11	1:O1:329:ALA:HB2	1.93	0.51
1:N1:129:TRP:O	1:N1:133:MET:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H1:214:LYS:NZ	1:G1:237:ARG:HH22	2.07	0.51
1:F1:71:GLU:O	1:G1:150:VAL:HG23	2.10	0.51
1:F1:103:THR:OG1	1:F1:107:ARG:NH2	2.43	0.51
1:D1:150:VAL:HG23	1:C1:71:GLU:O	2.10	0.51
1:Q1:38:ASP:OD2	1:Q1:140:TYR:OH	2.19	0.51
3:L3:99:ARG:NE	3:L3:104:GLU:OE1	2.41	0.51
1:G1:649:ILE:HD13	1:G1:734:ILE:HG12	1.91	0.51
1:E1:162:LEU:HD12	1:E1:217:PRO:HG2	1.92	0.51
1:O1:475:ARG:HA	1:N1:584:GLY:HA3	1.91	0.51
1:L1:519:LEU:HB3	1:L1:567:THR:HB	1.92	0.51
3:A3:99:ARG:NE	3:A3:104:GLU:OE1	2.41	0.51
1:F1:150:VAL:HG23	1:E1:71:GLU:O	2.11	0.51
1:A1:165:LYS:HD3	1:A1:236:ILE:HG21	1.91	0.51
3:H3:94:ARG:NH2	3:H3:179:GLU:OE1	2.43	0.51
1:Q1:202:ARG:HH21	1:Q1:206:LYS:HB3	1.75	0.51
1:I1:152:ARG:NH2	1:H1:75:ASN:OD1	2.37	0.51
1:D1:162:LEU:HD12	1:D1:217:PRO:HG2	1.93	0.51
1:B1:165:LYS:HD3	1:B1:236:ILE:HG21	1.93	0.51
3:Q3:94:ARG:HG2	3:Q3:113:GLU:HG2	1.92	0.51
1:O1:284:THR:HB	1:O1:292:ALA:HB3	1.92	0.51
1:L1:150:VAL:HG23	1:A1:71:GLU:O	2.11	0.51
1:D1:615:ILE:HD11	1:D1:666:PRO:HG2	1.92	0.51
1:C1:322:ILE:HG12	1:C1:355:VAL:HG22	1.92	0.51
1:M1:649:ILE:HD13	1:M1:734:ILE:HG12	1.93	0.51
1:L1:302:ARG:HH12	1:A1:286:TYR:HE2	1.57	0.51
1:I1:150:VAL:HG23	1:H1:71:GLU:O	2.11	0.51
3:G3:99:ARG:NE	3:G3:104:GLU:OE1	2.40	0.51
1:D1:172:ALA:HA	1:D1:235:ARG:NH2	2.26	0.51
1:O1:649:ILE:HD13	1:O1:734:ILE:HG12	1.93	0.51
1:N1:38:ASP:OD2	1:N1:140:TYR:OH	2.21	0.51
1:A1:475:ARG:HA	1:I1:584:GLY:HA3	1.92	0.51
1:A1:519:LEU:HB3	1:A1:567:THR:HB	1.92	0.51
1:F1:386:GLN:NE2	1:E1:493:GLU:OE2	2.44	0.51
1:P1:325:VAL:HG11	1:P1:329:ALA:HB2	1.93	0.50
1:N1:165:LYS:HD3	1:N1:236:ILE:HG21	1.92	0.50
1:M1:322:ILE:HG12	1:M1:355:VAL:HG22	1.93	0.50
3:A3:140:GLU:C	3:A3:142:ASP:H	2.19	0.50
1:E1:284:THR:HB	1:E1:292:ALA:HB3	1.93	0.50
3:E3:41:SER:OG	3:E3:199:SER:O	2.26	0.50
1:C1:657:ALA:HB3	1:C1:670:ASP:HB3	1.92	0.50
3:B3:41:SER:OG	3:B3:199:SER:O	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:657:ALA:HB3	1:L1:670:ASP:HB3	1.92	0.50
1:I1:322:ILE:HG12	1:I1:355:VAL:HG22	1.92	0.50
1:G1:657:ALA:HB3	1:G1:670:ASP:HB3	1.92	0.50
1:C1:286:TYR:O	1:C1:289:GLY:N	2.37	0.50
1:Q1:386:GLN:NE2	1:P1:493:GLU:OE2	2.43	0.50
1:P1:209:LEU:HB2	1:P1:216:ILE:HB	1.93	0.50
3:P3:94:ARG:HG2	3:P3:113:GLU:HG2	1.92	0.50
3:M3:75:VAL:HG21	3:M3:197:ILE:HD11	1.93	0.50
1:B1:284:THR:HB	1:B1:292:ALA:HB3	1.91	0.50
1:I1:164:LEU:HD22	1:I1:236:ILE:HD11	1.92	0.50
1:F1:584:GLY:HA3	1:G1:475:ARG:HA	1.92	0.50
1:P1:322:ILE:HG12	1:P1:355:VAL:HG22	1.94	0.50
1:P1:615:ILE:HD11	1:P1:666:PRO:HG2	1.92	0.50
1:N1:519:LEU:HB3	1:N1:567:THR:HB	1.93	0.50
1:F1:165:LYS:HD3	1:F1:236:ILE:HG21	1.92	0.50
1:D1:103:THR:OG1	1:D1:107:ARG:NH2	2.44	0.50
1:D1:177:GLU:HA	1:D1:202:ARG:HD3	1.94	0.50
1:D1:657:ALA:HB3	1:D1:670:ASP:HB3	1.93	0.50
3:Q3:140:GLU:C	3:Q3:142:ASP:H	2.19	0.50
1:I1:202:ARG:HH21	1:I1:206:LYS:HB3	1.76	0.50
1:I1:270:VAL:HG13	1:I1:307:LEU:HD11	1.94	0.50
1:F1:129:TRP:O	1:F1:133:MET:HG2	2.12	0.50
1:C1:175:ALA:HB3	1:C1:235:ARG:HH21	1.77	0.50
3:P3:140:GLU:C	3:P3:142:ASP:H	2.19	0.50
1:N1:218:ASP:OD2	1:M1:179:PHE:CD1	2.64	0.50
1:L1:325:VAL:HG11	1:L1:329:ALA:HB2	1.94	0.50
3:I3:75:VAL:HG21	3:I3:197:ILE:HD11	1.94	0.50
3:I3:140:GLU:C	3:I3:142:ASP:H	2.20	0.50
1:H1:471:ILE:HB	1:H1:480:ILE:HB	1.94	0.50
1:F1:284:THR:HB	1:F1:292:ALA:HB3	1.93	0.50
3:P3:99:ARG:NE	3:P3:104:GLU:OE1	2.41	0.50
1:O1:172:ALA:HA	1:O1:235:ARG:NH2	2.26	0.50
1:O1:307:LEU:HA	1:O1:310:VAL:HG22	1.94	0.50
1:O1:615:ILE:HD11	1:O1:666:PRO:HG2	1.94	0.50
1:N1:152:ARG:NH2	1:M1:75:ASN:OD1	2.38	0.50
1:M1:152:ARG:NH2	1:L1:75:ASN:OD1	2.39	0.50
3:M3:140:GLU:C	3:M3:142:ASP:H	2.19	0.50
1:D1:214:LYS:HZ2	1:C1:237:ARG:HH22	1.60	0.50
3:B3:140:GLU:C	3:B3:142:ASP:H	2.20	0.50
3:O3:140:GLU:C	3:O3:142:ASP:H	2.19	0.50
1:H1:103:THR:OG1	1:H1:107:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F3:41:SER:OG	3:F3:199:SER:O	2.26	0.50
1:G1:615:ILE:HD11	1:G1:666:PRO:HG2	1.93	0.50
3:G3:140:GLU:C	3:G3:142:ASP:H	2.20	0.50
1:C1:649:ILE:HD13	1:C1:734:ILE:HG12	1.94	0.50
1:B1:322:ILE:HG12	1:B1:355:VAL:HG22	1.94	0.50
1:M1:129:TRP:CZ2	1:M1:133:MET:HE3	2.47	0.49
1:M1:165:LYS:HD3	1:M1:236:ILE:HG21	1.92	0.49
1:D1:322:ILE:HG12	1:D1:355:VAL:HG22	1.94	0.49
3:D3:41:SER:OG	3:D3:199:SER:O	2.25	0.49
1:B1:615:ILE:HD11	1:B1:666:PRO:HG2	1.93	0.49
1:P1:162:LEU:HD12	1:P1:217:PRO:HG2	1.93	0.49
1:O1:162:LEU:HD12	1:O1:217:PRO:HG2	1.93	0.49
1:N1:649:ILE:HD13	1:N1:734:ILE:HG12	1.94	0.49
1:A1:657:ALA:HB3	1:A1:670:ASP:HB3	1.94	0.49
1:H1:175:ALA:HB3	1:H1:235:ARG:HH21	1.76	0.49
1:E1:475:ARG:HA	1:D1:584:GLY:HA3	1.94	0.49
1:E1:657:ALA:HB3	1:E1:670:ASP:HB3	1.94	0.49
1:P1:172:ALA:HA	1:P1:235:ARG:NH2	2.27	0.49
1:A1:284:THR:HB	1:A1:292:ALA:HB3	1.92	0.49
1:H1:206:LYS:HA	1:H1:218:ASP:O	2.13	0.49
1:A1:339:GLN:O	1:A1:340:TYR:C	2.56	0.49
3:A3:75:VAL:HG21	3:A3:197:ILE:HD11	1.95	0.49
1:I1:615:ILE:HD11	1:I1:666:PRO:HG2	1.94	0.49
1:F1:172:ALA:HA	1:F1:235:ARG:NH2	2.28	0.49
3:E3:140:GLU:C	3:E3:142:ASP:H	2.20	0.49
1:A1:615:ILE:HD11	1:A1:666:PRO:HG2	1.93	0.49
1:G1:145:VAL:HG12	1:G1:145:VAL:O	2.13	0.49
1:D1:231:GLU:O	1:D1:234:ILE:HG22	2.12	0.49
1:O1:165:LYS:H	1:O1:236:ILE:HD12	1.77	0.49
1:M1:657:ALA:HB3	1:M1:670:ASP:HB3	1.93	0.49
1:A1:649:ILE:HD13	1:A1:734:ILE:HG12	1.94	0.49
3:D3:75:VAL:HG21	3:D3:197:ILE:HD11	1.95	0.49
3:D3:140:GLU:C	3:D3:142:ASP:H	2.20	0.49
1:P1:175:ALA:HB3	1:P1:235:ARG:HH21	1.78	0.49
1:P1:202:ARG:HH21	1:P1:206:LYS:HE3	1.78	0.49
3:L3:77:PHE:HE2	3:L3:194:VAL:HG11	1.77	0.49
1:H1:657:ALA:HB3	1:H1:670:ASP:HB3	1.94	0.49
1:G1:172:ALA:HA	1:G1:235:ARG:NH2	2.27	0.49
3:N3:140:GLU:C	3:N3:142:ASP:H	2.20	0.49
1:L1:129:TRP:CZ2	1:L1:133:MET:HE3	2.48	0.49
1:H1:649:ILE:HD13	1:H1:734:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E1:235:ARG:HB2	1:E1:235:ARG:NH1	2.28	0.49
1:Q1:657:ALA:HB3	1:Q1:670:ASP:HB3	1.94	0.49
1:E1:590:ALA:HB3	1:D1:650:ARG:HH12	1.78	0.49
1:D1:175:ALA:HB3	1:D1:235:ARG:HH21	1.77	0.49
1:Q1:207:PHE:HB2	1:Q1:218:ASP:HB2	1.94	0.49
3:O3:99:ARG:NE	3:O3:104:GLU:OE1	2.41	0.49
1:M1:690:MET:HB2	1:M1:734:ILE:HD13	1.95	0.49
3:F3:140:GLU:C	3:F3:142:ASP:H	2.20	0.49
3:G3:41:SER:OG	3:G3:199:SER:O	2.26	0.49
1:E1:129:TRP:O	1:E1:133:MET:HG2	2.13	0.49
1:D1:145:VAL:HG12	1:D1:145:VAL:O	2.13	0.49
1:C1:615:ILE:HD11	1:C1:666:PRO:HG2	1.94	0.49
1:Q1:75:ASN:OD1	1:B1:152:ARG:NH2	2.42	0.48
1:I1:657:ALA:HB3	1:I1:670:ASP:HB3	1.94	0.48
1:H1:322:ILE:HG12	1:H1:355:VAL:HG22	1.95	0.48
1:H1:615:ILE:HD11	1:H1:666:PRO:HG2	1.95	0.48
1:G1:286:TYR:CE2	1:G1:292:ALA:HB2	2.48	0.48
1:G1:322:ILE:HG12	1:G1:355:VAL:HG22	1.95	0.48
1:P1:177:GLU:HG2	1:P1:202:ARG:HD3	1.93	0.48
1:L1:143:VAL:HB	1:L1:150:VAL:HG13	1.95	0.48
1:C1:61:LEU:C	1:C1:63:SER:H	2.21	0.48
1:O1:143:VAL:HB	1:O1:150:VAL:HG13	1.95	0.48
1:N1:103:THR:OG1	1:N1:107:ARG:NH2	2.45	0.48
1:M1:223:ARG:O	1:M1:227:GLY:HA3	2.13	0.48
1:L1:325:VAL:HG21	1:L1:332:ILE:HG21	1.95	0.48
1:I1:590:ALA:HB3	1:H1:650:ARG:HH12	1.78	0.48
1:H1:172:ALA:HA	1:H1:235:ARG:NH2	2.29	0.48
3:H3:140:GLU:C	3:H3:142:ASP:H	2.19	0.48
1:B1:175:ALA:HB3	1:B1:235:ARG:HH21	1.77	0.48
1:O1:286:TYR:O	1:O1:289:GLY:N	2.39	0.48
1:D1:325:VAL:HG11	1:D1:329:ALA:HB2	1.95	0.48
1:C1:172:ALA:HA	1:C1:235:ARG:NH2	2.28	0.48
1:C1:284:THR:HB	1:C1:292:ALA:HB3	1.95	0.48
1:P1:145:VAL:HG12	1:P1:145:VAL:O	2.14	0.48
1:P1:235:ARG:NH1	1:P1:235:ARG:HB2	2.28	0.48
1:O1:145:VAL:HG12	1:O1:145:VAL:O	2.14	0.48
1:N1:175:ALA:HB3	1:N1:235:ARG:HH21	1.79	0.48
3:N3:194:VAL:HG12	3:N3:194:VAL:O	2.13	0.48
1:L1:152:ARG:NH2	1:A1:75:ASN:OD1	2.38	0.48
1:F1:143:VAL:HB	1:F1:150:VAL:HG13	1.96	0.48
1:F1:145:VAL:HG12	1:F1:145:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F1:657:ALA:HB3	1:F1:670:ASP:HB3	1.96	0.48
1:D1:61:LEU:C	1:D1:63:SER:H	2.21	0.48
3:C3:140:GLU:C	3:C3:142:ASP:H	2.20	0.48
3:B3:75:VAL:HG21	3:B3:197:ILE:HD11	1.96	0.48
1:O1:590:ALA:HB3	1:N1:650:ARG:HH12	1.78	0.48
3:O3:41:SER:OG	3:O3:199:SER:O	2.26	0.48
1:N1:235:ARG:HB2	1:N1:235:ARG:NH1	2.28	0.48
1:L1:274:LEU:HD23	1:L1:283:VAL:HG11	1.96	0.48
1:I1:169:ALA:O	1:I1:210:PRO:HB3	2.14	0.48
3:D3:98:ASP:H	3:D3:106:ALA:HB2	1.79	0.48
1:C1:261:TYR:OH	1:C1:311:ASP:OD2	2.25	0.48
1:A1:325:VAL:HG11	1:A1:329:ALA:HB2	1.96	0.48
1:C1:235:ARG:NH1	1:C1:235:ARG:HB2	2.28	0.48
3:C3:41:SER:OG	3:C3:199:SER:O	2.26	0.48
1:B1:61:LEU:C	1:B1:63:SER:H	2.22	0.48
1:Q1:649:ILE:HD13	1:Q1:734:ILE:HG12	1.95	0.48
1:P1:207:PHE:HB2	1:P1:218:ASP:HB2	1.95	0.48
3:N3:75:VAL:HG21	3:N3:197:ILE:HD11	1.96	0.48
1:I1:61:LEU:C	1:I1:63:SER:H	2.22	0.48
1:I1:325:VAL:HG11	1:I1:329:ALA:HB2	1.96	0.48
1:H1:235:ARG:NH1	1:H1:235:ARG:HB2	2.29	0.48
1:F1:322:ILE:HG12	1:F1:355:VAL:HG22	1.95	0.48
1:E1:690:MET:HB2	1:E1:734:ILE:HD13	1.95	0.48
1:D1:235:ARG:NH1	1:D1:235:ARG:HB2	2.29	0.48
3:N3:99:ARG:NE	3:N3:104:GLU:OE1	2.41	0.48
1:L1:388:VAL:HG22	1:L1:480:ILE:HG12	1.95	0.48
1:I1:649:ILE:HD13	1:I1:734:ILE:HG12	1.96	0.48
1:E1:615:ILE:HD11	1:E1:666:PRO:HG2	1.96	0.48
1:N1:615:ILE:HD11	1:N1:666:PRO:HG2	1.95	0.48
1:M1:150:VAL:HG23	1:L1:71:GLU:O	2.14	0.48
1:F1:61:LEU:C	1:F1:63:SER:H	2.22	0.48
1:F1:175:ALA:HB3	1:F1:235:ARG:HH21	1.79	0.48
1:B1:235:ARG:HB2	1:B1:235:ARG:NH1	2.29	0.48
1:O1:61:LEU:C	1:O1:63:SER:H	2.21	0.47
1:O1:322:ILE:HG12	1:O1:355:VAL:HG22	1.96	0.47
3:L3:140:GLU:C	3:L3:142:ASP:H	2.20	0.47
1:H1:61:LEU:C	1:H1:63:SER:H	2.22	0.47
1:H1:143:VAL:HB	1:H1:150:VAL:HG13	1.96	0.47
1:G1:61:LEU:C	1:G1:63:SER:H	2.22	0.47
1:B1:172:ALA:HA	1:B1:235:ARG:NH2	2.29	0.47
1:Q1:590:ALA:HB3	1:P1:650:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q1:615:ILE:HD11	1:Q1:666:PRO:HG2	1.95	0.47
1:O1:103:THR:O	1:O1:106:GLY:N	2.45	0.47
1:N1:61:LEU:C	1:N1:63:SER:H	2.21	0.47
1:N1:657:ALA:HB3	1:N1:670:ASP:HB3	1.95	0.47
1:L1:103:THR:O	1:L1:106:GLY:N	2.46	0.47
1:A1:103:THR:O	1:A1:106:GLY:N	2.45	0.47
1:B1:143:VAL:HB	1:B1:150:VAL:HG13	1.96	0.47
1:N1:145:VAL:HG12	1:N1:145:VAL:O	2.15	0.47
1:N1:169:ALA:O	1:N1:210:PRO:HB3	2.14	0.47
1:M1:648:ARG:NH1	1:M1:677:GLN:OE1	2.47	0.47
1:L1:231:GLU:O	1:L1:234:ILE:HG22	2.14	0.47
1:L1:286:TYR:O	1:L1:289:GLY:N	2.41	0.47
1:G1:143:VAL:HB	1:G1:150:VAL:HG13	1.97	0.47
1:G1:471:ILE:HB	1:G1:480:ILE:HB	1.97	0.47
1:E1:172:ALA:HA	1:E1:235:ARG:NH2	2.30	0.47
1:O1:519:LEU:HB3	1:O1:567:THR:HB	1.95	0.47
1:N1:172:ALA:HA	1:N1:235:ARG:NH2	2.28	0.47
3:A3:98:ASP:H	3:A3:106:ALA:HB2	1.79	0.47
1:H1:222:LYS:HA	1:H1:222:LYS:HD3	1.61	0.47
1:H1:284:THR:HB	1:H1:292:ALA:HB3	1.95	0.47
1:E1:61:LEU:C	1:E1:63:SER:H	2.21	0.47
1:E1:649:ILE:HD13	1:E1:734:ILE:HG12	1.95	0.47
1:C1:270:VAL:HG13	1:C1:307:LEU:HD11	1.95	0.47
1:B1:145:VAL:HG12	1:B1:145:VAL:O	2.14	0.47
1:B1:657:ALA:HB3	1:B1:670:ASP:HB3	1.95	0.47
1:Q1:222:LYS:HA	1:Q1:222:LYS:HD3	1.51	0.47
1:O1:38:ASP:OD2	1:O1:140:TYR:OH	2.20	0.47
3:M3:194:VAL:HG12	3:M3:194:VAL:O	2.14	0.47
1:L1:322:ILE:HG12	1:L1:355:VAL:HG22	1.97	0.47
1:H1:152:ARG:NH2	1:G1:75:ASN:OD1	2.38	0.47
1:E1:145:VAL:O	1:E1:145:VAL:HG12	2.14	0.47
1:C1:38:ASP:OD2	1:C1:140:TYR:OH	2.18	0.47
1:C1:306:LEU:HD22	1:B1:286:TYR:CD2	2.48	0.47
1:Q1:145:VAL:HG12	1:Q1:145:VAL:O	2.15	0.47
1:N1:661:THR:C	1:N1:663:ASP:H	2.23	0.47
1:A1:61:LEU:C	1:A1:63:SER:H	2.22	0.47
1:I1:103:THR:O	1:I1:106:GLY:N	2.46	0.47
1:C1:302:ARG:HH12	1:B1:286:TYR:HE2	1.62	0.47
1:Q1:61:LEU:C	1:Q1:63:SER:H	2.22	0.47
1:O1:306:LEU:HD22	1:N1:286:TYR:CD2	2.50	0.47
1:N1:274:LEU:HD23	1:N1:283:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N3:98:ASP:H	3:N3:106:ALA:HB2	1.79	0.47
1:M1:284:THR:HB	1:M1:292:ALA:HB3	1.97	0.47
1:L1:615:ILE:HD11	1:L1:666:PRO:HG2	1.96	0.47
1:F1:235:ARG:NH1	1:F1:235:ARG:HB2	2.28	0.47
1:F1:519:LEU:HB3	1:F1:567:THR:HB	1.95	0.47
3:F3:98:ASP:H	3:F3:106:ALA:HB2	1.80	0.47
1:D1:206:LYS:HD2	1:D1:223:ARG:HG2	1.96	0.47
1:C1:145:VAL:HG12	1:C1:145:VAL:O	2.15	0.47
1:I1:145:VAL:HG12	1:I1:145:VAL:O	2.14	0.47
3:E3:98:ASP:H	3:E3:106:ALA:HB2	1.80	0.47
1:D1:143:VAL:HB	1:D1:150:VAL:HG13	1.96	0.47
1:Q1:143:VAL:HB	1:Q1:150:VAL:HG13	1.97	0.47
1:N1:202:ARG:HH21	1:N1:206:LYS:HE3	1.80	0.47
1:M1:61:LEU:C	1:M1:63:SER:H	2.22	0.47
1:M1:206:LYS:HA	1:M1:218:ASP:O	2.15	0.47
1:A1:231:GLU:O	1:A1:234:ILE:HG22	2.15	0.47
1:A1:286:TYR:O	1:A1:289:GLY:N	2.39	0.47
1:H1:590:ALA:HB3	1:G1:650:ARG:HH12	1.80	0.47
1:F1:690:MET:HB2	1:F1:734:ILE:HD13	1.97	0.47
1:Q1:648:ARG:NH2	1:B1:586:ARG:O	2.48	0.47
1:N1:143:VAL:HB	1:N1:150:VAL:HG13	1.95	0.47
1:M1:38:ASP:OD2	1:M1:140:TYR:OH	2.17	0.47
1:M1:590:ALA:HB3	1:L1:650:ARG:HH12	1.80	0.47
1:M1:615:ILE:HD11	1:M1:666:PRO:HG2	1.96	0.47
1:G1:286:TYR:O	1:G1:289:GLY:N	2.42	0.47
1:C1:590:ALA:HB3	1:B1:650:ARG:HH12	1.79	0.47
3:C3:114:ASN:OD1	3:C3:115:ALA:N	2.48	0.47
1:P1:61:LEU:C	1:P1:63:SER:H	2.22	0.46
3:P3:116:LYS:HE3	3:O3:38:ASP:OD1	2.15	0.46
1:L1:690:MET:HB2	1:L1:734:ILE:HD13	1.96	0.46
1:I1:286:TYR:O	1:I1:289:GLY:N	2.38	0.46
3:G3:98:ASP:H	3:G3:106:ALA:HB2	1.81	0.46
1:D1:261:TYR:OH	1:D1:311:ASP:OD2	2.30	0.46
1:C1:177:GLU:HA	1:C1:202:ARG:HD3	1.96	0.46
3:O3:75:VAL:HG21	3:O3:197:ILE:HD11	1.97	0.46
1:N1:157:PRO:HB3	1:M1:226:ILE:HA	1.97	0.46
1:I1:157:PRO:HB3	1:H1:226:ILE:HA	1.97	0.46
1:I1:222:LYS:HA	1:I1:222:LYS:HD3	1.64	0.46
1:H1:274:LEU:HD23	1:H1:283:VAL:HG11	1.96	0.46
1:E1:231:GLU:O	1:E1:234:ILE:HG22	2.14	0.46
1:D1:206:LYS:HE3	1:D1:206:LYS:HB3	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:143:VAL:HB	1:C1:150:VAL:HG13	1.97	0.46
1:Q1:284:THR:HB	1:Q1:292:ALA:HB3	1.97	0.46
1:Q1:661:THR:C	1:Q1:663:ASP:H	2.24	0.46
1:N1:340:TYR:OH	1:N1:365:THR:HG22	2.16	0.46
1:A1:580:THR:O	1:I1:678:SER:OG	2.21	0.46
3:A3:175:VAL:HG12	3:A3:198:VAL:HG22	1.97	0.46
1:I1:274:LEU:HD23	1:I1:283:VAL:HG11	1.96	0.46
3:H3:98:ASP:H	3:H3:106:ALA:HB2	1.80	0.46
1:C1:231:GLU:O	1:C1:234:ILE:HG22	2.15	0.46
1:F1:231:GLU:O	1:F1:234:ILE:HG22	2.14	0.46
1:E1:471:ILE:HB	1:E1:480:ILE:HB	1.97	0.46
1:D1:284:THR:HB	1:D1:292:ALA:HB3	1.96	0.46
1:M1:202:ARG:HH21	1:M1:206:LYS:HE3	1.81	0.46
1:L1:284:THR:HB	1:L1:292:ALA:HB3	1.97	0.46
1:D1:129:TRP:O	1:D1:133:MET:HG2	2.16	0.46
3:B3:98:ASP:H	3:B3:106:ALA:HB2	1.80	0.46
1:Q1:322:ILE:HG12	1:Q1:355:VAL:HG22	1.98	0.46
3:P3:114:ASN:OD1	3:P3:116:LYS:HG3	2.15	0.46
3:L3:98:ASP:H	3:L3:106:ALA:HB2	1.80	0.46
1:A1:274:LEU:HD23	1:A1:283:VAL:HG11	1.97	0.46
1:H1:145:VAL:HG12	1:H1:145:VAL:O	2.15	0.46
3:H3:41:SER:OG	3:H3:199:SER:O	2.29	0.46
1:F1:61:LEU:HD11	1:G1:132:LEU:HD23	1.98	0.46
1:E1:143:VAL:HB	1:E1:150:VAL:HG13	1.97	0.46
1:D1:222:LYS:HB2	1:D1:222:LYS:HE2	1.78	0.46
1:F1:302:ARG:NH2	1:E1:286:TYR:OH	2.44	0.46
1:Q1:226:ILE:HA	1:B1:157:PRO:HB3	1.98	0.46
1:N1:231:GLU:O	1:N1:234:ILE:HG22	2.15	0.46
1:N1:690:MET:HB2	1:N1:734:ILE:HD13	1.97	0.46
1:M1:274:LEU:HD23	1:M1:283:VAL:HG11	1.98	0.46
1:I1:231:GLU:O	1:I1:234:ILE:HG22	2.15	0.46
1:F1:471:ILE:HB	1:F1:480:ILE:HB	1.98	0.46
1:Q1:650:ARG:HH12	1:B1:590:ALA:HB3	1.81	0.46
1:P1:388:VAL:HG22	1:P1:480:ILE:HG12	1.98	0.46
1:P1:590:ALA:HB3	1:O1:650:ARG:HH12	1.81	0.46
1:L1:177:GLU:HG2	1:L1:202:ARG:HD3	1.98	0.46
1:I1:261:TYR:OH	1:I1:311:ASP:OD2	2.29	0.46
1:I1:661:THR:C	1:I1:663:ASP:H	2.24	0.46
1:I1:700:THR:HG22	1:I1:700:THR:O	2.14	0.46
1:H1:325:VAL:HG21	1:H1:332:ILE:HG21	1.98	0.46
1:F1:202:ARG:HH21	1:F1:206:LYS:HE3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:103:THR:O	1:D1:106:GLY:N	2.48	0.46
3:D3:31:ASN:HB3	3:D3:82:ARG:HB2	1.98	0.46
3:C3:98:ASP:H	3:C3:106:ALA:HB2	1.81	0.46
1:B1:231:GLU:O	1:B1:234:ILE:HG22	2.16	0.46
1:N1:590:ALA:HB3	1:M1:650:ARG:HH12	1.81	0.46
1:M1:661:THR:C	1:M1:663:ASP:H	2.24	0.46
1:H1:202:ARG:NH2	1:H1:206:LYS:HE3	2.31	0.46
1:G1:690:MET:HB2	1:G1:734:ILE:HD13	1.98	0.46
1:I1:143:VAL:HB	1:I1:150:VAL:HG13	1.96	0.45
1:F1:661:THR:C	1:F1:663:ASP:H	2.24	0.45
1:D1:690:MET:HB2	1:D1:734:ILE:HD13	1.98	0.45
1:Q1:231:GLU:O	1:Q1:234:ILE:HG22	2.16	0.45
1:O1:157:PRO:HB3	1:N1:226:ILE:HA	1.99	0.45
1:N1:628:TYR:HA	1:N1:654:ASN:OD1	2.16	0.45
3:N3:175:VAL:HG12	3:N3:198:VAL:HG22	1.98	0.45
1:M1:143:VAL:HB	1:M1:150:VAL:HG13	1.97	0.45
1:L1:61:LEU:C	1:L1:63:SER:H	2.23	0.45
3:I3:31:ASN:HB3	3:I3:82:ARG:HB2	1.98	0.45
1:H1:325:VAL:HG11	1:H1:329:ALA:HB2	1.98	0.45
1:E1:661:THR:C	1:E1:663:ASP:H	2.23	0.45
1:C1:103:THR:OG1	1:C1:107:ARG:NH2	2.48	0.45
1:F1:302:ARG:NH1	1:E1:286:TYR:OH	2.47	0.45
1:P1:261:TYR:OH	1:P1:311:ASP:OD2	2.28	0.45
3:P3:98:ASP:H	3:P3:106:ALA:HB2	1.80	0.45
1:O1:274:LEU:HD23	1:O1:283:VAL:HG11	1.98	0.45
1:F1:649:ILE:HD13	1:F1:734:ILE:HG12	1.97	0.45
3:B3:92:GLY:HA2	3:B3:117:MET:HG3	1.99	0.45
3:B3:128:GLU:OE1	3:B3:128:GLU:N	2.48	0.45
1:O1:129:TRP:O	1:O1:133:MET:HG2	2.17	0.45
3:L3:175:VAL:HG12	3:L3:198:VAL:HG22	1.98	0.45
1:A1:661:THR:C	1:A1:663:ASP:H	2.25	0.45
3:I3:128:GLU:OE1	3:I3:128:GLU:N	2.48	0.45
3:I3:175:VAL:HG12	3:I3:198:VAL:HG22	1.97	0.45
1:H1:231:GLU:O	1:H1:234:ILE:HG22	2.16	0.45
1:F1:274:LEU:HD23	1:F1:283:VAL:HG11	1.97	0.45
3:F3:128:GLU:OE1	3:F3:128:GLU:N	2.48	0.45
1:C1:169:ALA:O	1:C1:210:PRO:HB3	2.16	0.45
1:B1:649:ILE:HD13	1:B1:734:ILE:HG12	1.98	0.45
1:P1:132:LEU:HD23	1:O1:61:LEU:HD11	1.98	0.45
1:P1:274:LEU:HD23	1:P1:283:VAL:HG11	1.98	0.45
3:M3:98:ASP:H	3:M3:106:ALA:HB2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:38:ASP:OD2	1:A1:140:TYR:OH	2.19	0.45
1:F1:226:ILE:HA	1:G1:157:PRO:HB3	1.99	0.45
1:G1:628:TYR:HA	1:G1:654:ASN:OD1	2.17	0.45
3:E3:114:ASN:OD1	3:E3:116:LYS:HG3	2.17	0.45
1:D1:325:VAL:HG21	1:D1:332:ILE:HG21	1.98	0.45
1:D1:590:ALA:HB3	1:C1:650:ARG:HH12	1.82	0.45
1:C1:274:LEU:HD23	1:C1:283:VAL:HG11	1.98	0.45
1:B1:661:THR:C	1:B1:663:ASP:H	2.24	0.45
1:O1:325:VAL:HG21	1:O1:332:ILE:HG21	1.97	0.45
1:L1:62:ALA:HA	1:L1:72:VAL:HG21	1.99	0.45
1:A1:143:VAL:HB	1:A1:150:VAL:HG13	1.98	0.45
1:A1:590:ALA:HB3	1:I1:650:ARG:HH12	1.82	0.45
1:G1:661:THR:C	1:G1:663:ASP:H	2.25	0.45
1:P1:206:LYS:HA	1:P1:218:ASP:O	2.16	0.45
1:O1:231:GLU:O	1:O1:234:ILE:HG22	2.17	0.45
1:O1:661:THR:C	1:O1:663:ASP:H	2.24	0.45
1:A1:306:LEU:HD13	1:I1:286:TYR:HD2	1.81	0.45
3:A3:31:ASN:HB3	3:A3:82:ARG:HB2	1.98	0.45
3:B3:175:VAL:HG12	3:B3:198:VAL:HG22	1.99	0.45
3:O3:98:ASP:H	3:O3:106:ALA:HB2	1.81	0.45
3:N3:114:ASN:OD1	3:N3:115:ALA:N	2.50	0.45
3:M3:175:VAL:HG12	3:M3:198:VAL:HG22	1.99	0.45
1:A1:566:GLU:OE1	1:I1:706:PRO:HA	2.17	0.45
1:I1:325:VAL:HG21	1:I1:332:ILE:HG21	1.98	0.45
3:I3:98:ASP:H	3:I3:106:ALA:HB2	1.81	0.45
1:H1:103:THR:O	1:H1:106:GLY:N	2.48	0.45
3:H3:75:VAL:HG21	3:H3:197:ILE:HD11	1.99	0.45
1:F1:590:ALA:HB3	1:E1:650:ARG:HH12	1.82	0.45
3:E3:31:ASN:HB3	3:E3:82:ARG:HB2	1.99	0.45
1:C1:661:THR:C	1:C1:663:ASP:H	2.25	0.45
1:B1:169:ALA:O	1:B1:210:PRO:HB3	2.17	0.45
3:Q3:75:VAL:HG21	3:Q3:197:ILE:HD11	2.00	0.44
1:N1:207:PHE:HB2	1:N1:218:ASP:CB	2.47	0.44
1:L1:386:GLN:NE2	1:A1:493:GLU:OE2	2.49	0.44
2:F2:86:ARG:HH21	1:G1:578:ASN:HD22	1.65	0.44
1:G1:231:GLU:O	1:G1:234:ILE:HG22	2.16	0.44
1:G1:274:LEU:HD23	1:G1:283:VAL:HG11	1.98	0.44
1:D1:388:VAL:HG22	1:D1:480:ILE:HG12	1.99	0.44
1:P1:231:GLU:O	1:P1:234:ILE:HG22	2.17	0.44
1:P1:284:THR:HB	1:P1:292:ALA:HB3	1.99	0.44
1:D1:132:LEU:HD23	1:C1:61:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:222:LYS:HA	1:C1:222:LYS:HD3	1.60	0.44
1:Q1:519:LEU:HB3	1:Q1:567:THR:HB	1.99	0.44
1:O1:637:PRO:HB3	1:O1:647:LEU:HD13	1.99	0.44
1:L1:590:ALA:HB3	1:A1:650:ARG:HH12	1.82	0.44
1:I1:164:LEU:HD12	1:I1:169:ALA:HB2	1.99	0.44
1:F1:650:ARG:HH12	1:G1:590:ALA:HB3	1.83	0.44
1:G1:307:LEU:HA	1:G1:310:VAL:HG22	2.00	0.44
1:E1:169:ALA:O	1:E1:210:PRO:HB3	2.17	0.44
1:E1:690:MET:HB2	1:E1:734:ILE:CD1	2.48	0.44
3:L3:75:VAL:HG21	3:L3:197:ILE:HD11	2.00	0.44
1:A1:325:VAL:HG21	1:A1:332:ILE:HG21	1.98	0.44
1:H1:214:LYS:HZ2	1:G1:237:ARG:HH22	1.64	0.44
3:F3:31:ASN:HB3	3:F3:82:ARG:HB2	2.00	0.44
1:E1:274:LEU:HD23	1:E1:283:VAL:HG11	1.98	0.44
1:D1:661:THR:C	1:D1:663:ASP:H	2.25	0.44
1:P1:661:THR:C	1:P1:663:ASP:H	2.26	0.44
1:M1:231:GLU:O	1:M1:234:ILE:HG22	2.17	0.44
1:A1:157:PRO:HB3	1:I1:226:ILE:HA	2.00	0.44
1:A1:202:ARG:HH21	1:A1:206:LYS:HE3	1.83	0.44
3:F3:175:VAL:HG12	3:F3:198:VAL:HG22	1.99	0.44
1:D1:649:ILE:HD13	1:D1:734:ILE:HG12	1.98	0.44
1:B1:103:THR:O	1:B1:106:GLY:N	2.48	0.44
1:Q1:164:LEU:HD12	1:Q1:169:ALA:HB2	2.00	0.44
1:Q1:340:TYR:OH	1:Q1:365:THR:HG22	2.18	0.44
3:Q3:98:ASP:H	3:Q3:106:ALA:HB2	1.82	0.44
1:O1:690:MET:HB2	1:O1:734:ILE:HD13	1.99	0.44
3:M3:128:GLU:OE1	3:M3:128:GLU:N	2.48	0.44
1:L1:169:ALA:O	1:L1:210:PRO:HB3	2.18	0.44
1:H1:157:PRO:HB3	1:G1:226:ILE:HA	2.00	0.44
3:E3:116:LYS:HE3	3:D3:38:ASP:OD2	2.18	0.44
1:Q1:471:ILE:HB	1:Q1:480:ILE:HB	1.99	0.44
1:P1:224:LEU:O	1:P1:229:ASN:HB2	2.18	0.44
3:P3:175:VAL:HG12	3:P3:198:VAL:HG22	1.99	0.44
1:M1:700:THR:HG22	1:M1:700:THR:O	2.16	0.44
1:A1:322:ILE:HG12	1:A1:355:VAL:HG22	1.99	0.44
1:I1:206:LYS:HA	1:I1:218:ASP:O	2.18	0.44
2:D2:84:GLN:HG2	2:D2:122:GLU:HG3	2.00	0.44
1:C1:690:MET:HB2	1:C1:734:ILE:HD13	1.99	0.44
1:Q1:103:THR:OG1	1:Q1:107:ARG:NH2	2.51	0.44
1:P1:302:ARG:HH12	1:O1:286:TYR:HE2	1.65	0.44
1:O1:471:ILE:HB	1:O1:480:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:169:ALA:O	1:M1:210:PRO:HB3	2.18	0.44
1:L1:520:GLN:NE2	1:L1:566:GLU:HG3	2.33	0.44
1:G1:103:THR:O	1:G1:106:GLY:N	2.48	0.44
1:G1:180:PHE:CZ	1:G1:227:GLY:HA2	2.53	0.44
1:E1:103:THR:O	1:E1:106:GLY:N	2.48	0.44
2:E2:84:GLN:HG2	2:E2:122:GLU:HG3	2.00	0.44
3:E3:175:VAL:HG12	3:E3:198:VAL:HG22	1.99	0.44
1:Q1:274:LEU:HD23	1:Q1:283:VAL:HG11	1.99	0.44
1:L1:661:THR:C	1:L1:663:ASP:H	2.25	0.44
3:L3:114:ASN:OD1	3:L3:115:ALA:N	2.51	0.44
1:D1:115:PRO:HA	1:C1:84:ILE:O	2.17	0.44
2:C2:84:GLN:HG2	2:C2:122:GLU:HG3	2.00	0.44
1:B1:274:LEU:HD23	1:B1:283:VAL:HG11	1.99	0.44
1:P1:103:THR:O	1:P1:106:GLY:N	2.50	0.43
1:O1:388:VAL:HG22	1:O1:480:ILE:HG12	2.00	0.43
3:M3:77:PHE:HE2	3:M3:194:VAL:HG11	1.83	0.43
1:F1:157:PRO:HB3	1:E1:226:ILE:HA	2.00	0.43
1:F1:585:GLN:OE1	1:E1:679:THR:HB	2.18	0.43
1:E1:157:PRO:HB3	1:D1:226:ILE:HA	2.00	0.43
1:C1:103:THR:O	1:C1:106:GLY:N	2.49	0.43
1:B1:632:LEU:HD23	1:B1:651:GLY:HA2	2.00	0.43
1:A1:466:GLN:HB3	1:A1:467:GLN:H	1.56	0.43
3:A3:114:ASN:OD1	3:A3:115:ALA:N	2.51	0.43
2:F2:84:GLN:HG2	2:F2:122:GLU:HG3	2.00	0.43
3:E3:128:GLU:OE1	3:E3:128:GLU:N	2.49	0.43
1:C1:157:PRO:HB3	1:B1:226:ILE:HA	2.00	0.43
3:O3:175:VAL:HG12	3:O3:198:VAL:HG22	1.99	0.43
1:A1:115:PRO:HA	1:I1:84:ILE:O	2.18	0.43
1:A1:164:LEU:HD12	1:A1:169:ALA:HB2	2.01	0.43
1:A1:690:MET:HB2	1:A1:734:ILE:HD13	2.01	0.43
1:H1:661:THR:C	1:H1:663:ASP:H	2.25	0.43
1:D1:274:LEU:HD23	1:D1:283:VAL:HG11	1.99	0.43
3:D3:114:ASN:OD1	3:D3:115:ALA:N	2.51	0.43
3:D3:128:GLU:OE1	3:D3:128:GLU:N	2.49	0.43
3:B3:114:ASN:OD1	3:B3:115:ALA:N	2.51	0.43
1:Q1:628:TYR:HA	1:Q1:654:ASN:OD1	2.18	0.43
1:O1:177:GLU:HA	1:O1:202:ARG:HD3	2.01	0.43
1:N1:150:VAL:HG23	1:M1:71:GLU:O	2.18	0.43
1:L1:340:TYR:OH	1:L1:365:THR:HG22	2.19	0.43
3:L3:31:ASN:HB3	3:L3:82:ARG:HB2	1.99	0.43
1:A1:388:VAL:HG22	1:A1:480:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I1:132:LEU:HD23	1:H1:61:LEU:HD11	2.00	0.43
1:H1:632:LEU:HD23	1:H1:651:GLY:HA2	2.00	0.43
1:D1:524:LEU:HD12	1:D1:561:THR:O	2.18	0.43
1:C1:211:ASN:O	1:C1:213:ILE:HD12	2.18	0.43
1:C1:471:ILE:HB	1:C1:480:ILE:HB	1.98	0.43
1:N1:224:LEU:O	1:N1:229:ASN:HB2	2.18	0.43
1:M1:164:LEU:HD12	1:M1:169:ALA:HB2	2.01	0.43
3:H3:175:VAL:HG12	3:H3:198:VAL:HG22	1.99	0.43
1:F1:75:ASN:HD22	1:F1:222:LYS:NZ	2.17	0.43
2:E2:66:PRO:HB2	2:E2:147:SER:HB3	2.01	0.43
1:D1:324:THR:O	1:D1:324:THR:OG1	2.36	0.43
1:B1:270:VAL:HG13	1:B1:307:LEU:HD11	2.00	0.43
1:Q1:169:ALA:O	1:Q1:210:PRO:HB3	2.18	0.43
2:M2:66:PRO:HB2	2:M2:147:SER:HB3	2.01	0.43
1:A1:524:LEU:HD12	1:A1:561:THR:O	2.19	0.43
1:I1:632:LEU:HD23	1:I1:651:GLY:HA2	2.00	0.43
1:E1:132:LEU:HD23	1:D1:61:LEU:HD11	2.01	0.43
3:E3:114:ASN:OD1	3:E3:115:ALA:N	2.52	0.43
1:D1:224:LEU:O	1:D1:229:ASN:HB2	2.18	0.43
3:C3:128:GLU:OE1	3:C3:128:GLU:N	2.50	0.43
3:C3:175:VAL:HG12	3:C3:198:VAL:HG22	2.00	0.43
3:Q3:175:VAL:HG12	3:Q3:198:VAL:HG22	2.00	0.43
1:P1:164:LEU:HD12	1:P1:169:ALA:HB2	2.01	0.43
2:P2:66:PRO:HB2	2:P2:147:SER:HB3	2.01	0.43
1:O1:164:LEU:HD12	1:O1:169:ALA:HB2	2.01	0.43
2:N2:66:PRO:HB2	2:N2:147:SER:HB3	2.01	0.43
1:M1:632:LEU:HD23	1:M1:651:GLY:HA2	2.00	0.43
1:A1:152:ARG:NH2	1:I1:75:ASN:OD1	2.42	0.43
1:F1:329:ALA:HA	1:F1:332:ILE:HG22	2.01	0.43
3:G3:175:VAL:HG12	3:G3:198:VAL:HG22	2.00	0.43
1:D1:157:PRO:HB3	1:C1:226:ILE:HA	2.00	0.43
1:B1:224:LEU:O	1:B1:229:ASN:HB2	2.19	0.43
1:L1:632:LEU:HD23	1:L1:651:GLY:HA2	2.01	0.43
3:I3:114:ASN:OD1	3:I3:115:ALA:N	2.52	0.43
1:H1:132:LEU:HD23	1:G1:61:LEU:HD11	2.01	0.43
2:G2:84:GLN:HG2	2:G2:122:GLU:HG3	2.00	0.43
2:D2:66:PRO:HB2	2:D2:147:SER:HB3	2.01	0.43
1:C1:132:LEU:HD23	1:B1:61:LEU:HD11	2.00	0.43
2:B2:66:PRO:HB2	2:B2:147:SER:HB3	2.01	0.43
2:B2:84:GLN:HG2	2:B2:122:GLU:HG3	2.00	0.43
1:Q1:84:ILE:O	1:B1:115:PRO:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q1:157:PRO:HB3	1:P1:226:ILE:HA	2.01	0.43
1:Q1:209:LEU:HB2	1:Q1:216:ILE:HB	2.00	0.43
1:N1:164:LEU:HD12	1:N1:169:ALA:HB2	2.01	0.43
1:M1:129:TRP:CE2	1:M1:133:MET:HE3	2.53	0.43
1:L1:132:LEU:HD23	1:A1:61:LEU:HD11	2.00	0.43
1:L1:524:LEU:HD12	1:L1:561:THR:O	2.19	0.43
2:A2:66:PRO:HB2	2:A2:147:SER:HB3	2.01	0.43
2:H2:66:PRO:HB2	2:H2:147:SER:HB3	2.01	0.43
2:F2:66:PRO:HB2	2:F2:147:SER:HB3	2.01	0.43
1:C1:43:SER:HA	1:C1:126:ASN:HB2	2.01	0.43
1:C1:115:PRO:HA	1:B1:84:ILE:O	2.18	0.43
2:C2:66:PRO:HB2	2:C2:147:SER:HB3	2.01	0.43
1:B1:164:LEU:HD12	1:B1:169:ALA:HB2	2.01	0.43
2:O2:66:PRO:HB2	2:O2:147:SER:HB3	2.01	0.43
1:N1:115:PRO:HA	1:M1:84:ILE:O	2.19	0.43
3:N3:31:ASN:HB3	3:N3:82:ARG:HB2	2.00	0.43
2:L2:66:PRO:HB2	2:L2:147:SER:HB3	2.01	0.43
1:A1:213:ILE:HD13	1:I1:237:ARG:NH1	2.34	0.43
2:I2:66:PRO:HB2	2:I2:147:SER:HB3	2.01	0.43
1:F1:132:LEU:HD23	1:E1:61:LEU:HD11	2.01	0.43
1:G1:164:LEU:HD12	1:G1:169:ALA:HB2	2.00	0.43
3:D3:175:VAL:HG12	3:D3:198:VAL:HG22	2.00	0.43
1:C1:632:LEU:HD23	1:C1:651:GLY:HA2	2.01	0.43
2:Q2:66:PRO:HB2	2:Q2:147:SER:HB3	2.01	0.42
3:O3:116:LYS:HE3	3:N3:38:ASP:OD1	2.19	0.42
1:M1:286:TYR:HE2	1:M1:292:ALA:CB	2.30	0.42
3:F3:116:LYS:HB2	3:F3:116:LYS:HE2	1.82	0.42
2:G2:66:PRO:HB2	2:G2:147:SER:HB3	2.01	0.42
1:Q1:132:LEU:HD23	1:P1:61:LEU:HD11	2.00	0.42
1:P1:270:VAL:HG13	1:P1:307:LEU:HD21	2.01	0.42
3:O3:184:SER:OG	3:O3:188:VAL:HG22	2.19	0.42
1:I1:38:ASP:OD2	1:I1:140:TYR:OH	2.17	0.42
1:E1:103:THR:OG1	1:E1:107:ARG:NH2	2.52	0.42
1:E1:224:LEU:O	1:E1:229:ASN:HB2	2.18	0.42
1:D1:302:ARG:NH1	1:C1:286:TYR:OH	2.52	0.42
1:C1:224:LEU:O	1:C1:229:ASN:HB2	2.19	0.42
1:C1:357:ASN:ND2	1:B1:339:GLN:NE2	2.62	0.42
3:C3:31:ASN:HB3	3:C3:82:ARG:HB2	2.01	0.42
1:Q1:72:VAL:HG13	1:B1:153:ILE:HD12	2.01	0.42
1:Q1:129:TRP:CZ2	1:Q1:133:MET:HE3	2.54	0.42
1:Q1:325:VAL:HG11	1:Q1:329:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q3:31:ASN:HB3	3:Q3:82:ARG:HB2	2.01	0.42
2:N2:84:GLN:HG2	2:N2:122:GLU:HG3	2.00	0.42
3:N3:184:SER:OG	3:N3:188:VAL:HG22	2.19	0.42
1:L1:580:THR:O	1:A1:678:SER:OG	2.23	0.42
1:A1:129:TRP:CE2	1:A1:133:MET:HE3	2.55	0.42
1:A1:132:LEU:HD23	1:I1:61:LEU:HD11	2.01	0.42
1:A1:180:PHE:CZ	1:A1:227:GLY:HA2	2.54	0.42
1:A1:264:ARG:HD2	1:A1:312:ARG:HA	2.02	0.42
1:I1:224:LEU:O	1:I1:229:ASN:HB2	2.19	0.42
1:H1:224:LEU:O	1:H1:229:ASN:HB2	2.19	0.42
1:G1:325:VAL:HG21	1:G1:332:ILE:HG21	2.01	0.42
1:C1:282:ILE:HD13	1:C1:282:ILE:HA	1.87	0.42
1:C1:697:THR:OG1	1:C1:726:THR:HB	2.17	0.42
1:Q1:129:TRP:HB3	1:Q1:130:PRO:HD3	2.02	0.42
3:Q3:128:GLU:OE1	3:Q3:128:GLU:N	2.50	0.42
1:N1:206:LYS:HA	1:N1:218:ASP:O	2.20	0.42
1:M1:157:PRO:HB3	1:L1:226:ILE:HA	2.01	0.42
1:L1:157:PRO:HB3	1:A1:226:ILE:HA	2.01	0.42
1:L1:304:ILE:HD13	1:L1:304:ILE:HA	1.93	0.42
1:H1:711:LEU:HD23	1:H1:711:LEU:HA	1.91	0.42
1:E1:264:ARG:HD2	1:E1:312:ARG:HA	2.01	0.42
1:D1:169:ALA:O	1:D1:210:PRO:HB3	2.19	0.42
1:B1:690:MET:HB2	1:B1:734:ILE:HD13	2.02	0.42
2:Q2:84:GLN:HG2	2:Q2:122:GLU:HG3	2.00	0.42
1:N1:207:PHE:HB2	1:N1:218:ASP:CG	2.44	0.42
1:N1:471:ILE:HB	1:N1:480:ILE:HB	2.00	0.42
1:M1:103:THR:OG1	1:M1:107:ARG:NH2	2.53	0.42
1:L1:224:LEU:O	1:L1:229:ASN:HB2	2.20	0.42
1:A1:222:LYS:HB2	1:A1:222:LYS:HE2	1.89	0.42
2:H2:84:GLN:HG2	2:H2:122:GLU:HG3	2.00	0.42
1:F1:325:VAL:HG11	1:F1:329:ALA:HB2	2.01	0.42
1:G1:690:MET:HB2	1:G1:734:ILE:CD1	2.50	0.42
1:E1:270:VAL:HG13	1:E1:307:LEU:HD11	2.00	0.42
1:C1:264:ARG:HD2	1:C1:312:ARG:HA	2.01	0.42
1:B1:370:LEU:HD23	1:B1:370:LEU:HA	1.81	0.42
3:O3:31:ASN:HB3	3:O3:82:ARG:HB2	2.01	0.42
1:N1:520:GLN:NE2	1:N1:566:GLU:HG3	2.34	0.42
2:M2:84:GLN:HG2	2:M2:122:GLU:HG3	2.00	0.42
2:L2:84:GLN:HG2	2:L2:122:GLU:HG3	2.00	0.42
1:A1:129:TRP:HB3	1:A1:130:PRO:HD3	2.02	0.42
3:I3:116:LYS:HB2	3:I3:116:LYS:HE2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F1:115:PRO:HA	1:E1:84:ILE:O	2.19	0.42
1:G1:524:LEU:HD12	1:G1:561:THR:O	2.18	0.42
1:G1:711:LEU:HD23	1:G1:711:LEU:HA	1.89	0.42
1:C1:164:LEU:HD12	1:C1:169:ALA:HB2	2.01	0.42
1:B1:324:THR:O	1:B1:324:THR:OG1	2.38	0.42
1:P1:157:PRO:HB3	1:O1:226:ILE:HA	2.02	0.42
1:O1:222:LYS:HE2	1:O1:222:LYS:HB2	1.79	0.42
2:O2:84:GLN:HG2	2:O2:122:GLU:HG3	2.00	0.42
1:N1:466:GLN:HB3	1:N1:467:GLN:H	1.57	0.42
2:A2:84:GLN:HG2	2:A2:122:GLU:HG3	2.00	0.42
1:E1:524:LEU:HD12	1:E1:561:THR:O	2.19	0.42
1:D1:164:LEU:HD12	1:D1:169:ALA:HB2	2.01	0.42
3:B3:31:ASN:HB3	3:B3:82:ARG:HB2	2.01	0.42
1:O1:224:LEU:O	1:O1:229:ASN:HB2	2.20	0.42
1:N1:132:LEU:HD23	1:M1:61:LEU:HD11	2.01	0.42
1:N1:264:ARG:HD2	1:N1:312:ARG:HA	2.02	0.42
1:L1:164:LEU:HD12	1:L1:169:ALA:HB2	2.02	0.42
1:I1:115:PRO:HA	1:H1:84:ILE:O	2.20	0.42
1:H1:340:TYR:OH	1:H1:365:THR:HG22	2.19	0.42
1:F1:164:LEU:HD12	1:F1:169:ALA:HB2	2.01	0.42
3:G3:31:ASN:HB3	3:G3:82:ARG:HB2	2.02	0.42
1:E1:370:LEU:HD23	1:E1:370:LEU:HA	1.79	0.42
1:C1:524:LEU:HD12	1:C1:561:THR:O	2.20	0.42
3:B3:184:SER:OG	3:B3:188:VAL:HG22	2.19	0.42
1:Q1:150:VAL:HG23	1:P1:71:GLU:O	2.20	0.42
3:P3:128:GLU:OE1	3:P3:128:GLU:N	2.49	0.42
1:O1:524:LEU:HD12	1:O1:561:THR:O	2.20	0.42
1:M1:145:VAL:HG12	1:M1:145:VAL:O	2.19	0.42
3:L3:184:SER:OG	3:L3:188:VAL:HG22	2.20	0.42
1:I1:340:TYR:OH	1:I1:365:THR:HG22	2.19	0.42
1:I1:388:VAL:HG22	1:I1:480:ILE:HG12	2.01	0.42
1:H1:164:LEU:HD12	1:H1:169:ALA:HB2	2.02	0.42
1:G1:697:THR:OG1	1:G1:726:THR:HB	2.20	0.42
1:C1:150:VAL:HG23	1:B1:71:GLU:O	2.20	0.42
1:Q1:71:GLU:O	1:B1:150:VAL:HG23	2.19	0.42
1:Q1:235:ARG:HB2	1:Q1:235:ARG:NH1	2.35	0.42
1:Q1:524:LEU:HD12	1:Q1:561:THR:O	2.19	0.42
3:Q3:184:SER:OG	3:Q3:188:VAL:HG22	2.20	0.42
1:P1:286:TYR:O	1:P1:289:GLY:N	2.41	0.42
1:N1:524:LEU:HD12	1:N1:561:THR:O	2.20	0.42
1:N1:632:LEU:HD23	1:N1:651:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:36:TYR:HB3	1:M1:130:PRO:HB2	2.02	0.42
1:M1:524:LEU:HD12	1:M1:561:THR:O	2.20	0.42
1:L1:133:MET:SD	1:L1:138:LEU:HB2	2.60	0.42
1:A1:264:ARG:HB3	1:A1:311:ASP:OD2	2.20	0.42
1:H1:680:ILE:HD11	1:H1:734:ILE:HG21	2.02	0.42
1:E1:164:LEU:HD12	1:E1:169:ALA:HB2	2.01	0.42
1:D1:466:GLN:HB3	1:D1:467:GLN:H	1.57	0.42
1:O1:264:ARG:HD2	1:O1:312:ARG:HA	2.02	0.41
1:L1:264:ARG:HD2	1:L1:312:ARG:HA	2.02	0.41
1:A1:224:LEU:O	1:A1:229:ASN:HB2	2.20	0.41
2:I2:84:GLN:HG2	2:I2:122:GLU:HG3	2.00	0.41
3:F3:117:MET:HE2	3:F3:117:MET:HB3	1.88	0.41
1:G1:284:THR:HB	1:G1:292:ALA:HB3	2.01	0.41
1:G1:466:GLN:HB3	1:G1:467:GLN:H	1.56	0.41
3:E3:75:VAL:HG21	3:E3:197:ILE:HD11	2.02	0.41
1:D1:270:VAL:HG13	1:D1:307:LEU:HD11	2.00	0.41
1:Q1:329:ALA:HA	1:Q1:332:ILE:HG22	2.01	0.41
1:P1:38:ASP:HB3	1:P1:41:LEU:HD12	2.02	0.41
1:P1:325:VAL:HG21	1:P1:332:ILE:HG21	2.02	0.41
2:P2:84:GLN:HG2	2:P2:122:GLU:HG3	2.00	0.41
1:M1:223:ARG:HA	1:M1:223:ARG:HD3	1.91	0.41
1:M1:471:ILE:HB	1:M1:480:ILE:HB	2.02	0.41
1:F1:304:ILE:HD13	1:F1:304:ILE:HA	1.93	0.41
3:G3:75:VAL:HG21	3:G3:197:ILE:HD11	2.02	0.41
1:D1:153:ILE:HD12	1:C1:72:VAL:HG13	2.01	0.41
1:D1:206:LYS:HA	1:D1:218:ASP:O	2.19	0.41
1:Q1:652:GLN:HB2	1:Q1:675:GLU:HG3	2.03	0.41
1:O1:554:LEU:HD23	1:O1:554:LEU:HA	1.92	0.41
1:M1:115:PRO:HA	1:L1:84:ILE:O	2.19	0.41
1:M1:129:TRP:HB3	1:M1:130:PRO:HD3	2.03	0.41
3:L3:128:GLU:OE1	3:L3:128:GLU:N	2.48	0.41
1:A1:697:THR:OG1	1:A1:726:THR:HB	2.20	0.41
1:I1:711:LEU:HD23	1:I1:711:LEU:HA	1.90	0.41
1:H1:169:ALA:O	1:H1:210:PRO:HB3	2.20	0.41
1:F1:103:THR:O	1:F1:106:GLY:N	2.50	0.41
1:F1:680:ILE:HD11	1:F1:734:ILE:HG21	2.02	0.41
3:F3:184:SER:OG	3:F3:188:VAL:HG22	2.19	0.41
1:E1:150:VAL:HG23	1:D1:71:GLU:O	2.20	0.41
3:P3:75:VAL:HG11	3:P3:197:ILE:HD11	2.02	0.41
3:N3:117:MET:HE2	3:N3:117:MET:HB3	1.91	0.41
1:M1:224:LEU:O	1:M1:229:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:169:ALA:O	1:A1:210:PRO:HB3	2.21	0.41
3:A3:184:SER:OG	3:A3:188:VAL:HG22	2.20	0.41
1:I1:561:THR:HG23	1:H1:546:THR:HG22	2.02	0.41
3:I3:117:MET:HE1	3:I3:180:PHE:CD2	2.54	0.41
1:H1:264:ARG:HD2	1:H1:312:ARG:HA	2.03	0.41
3:H3:114:ASN:OD1	3:H3:115:ALA:N	2.53	0.41
1:F1:224:LEU:O	1:F1:229:ASN:HB2	2.20	0.41
1:E1:129:TRP:HB3	1:E1:130:PRO:HD3	2.02	0.41
1:C1:346:THR:HA	1:C1:347:PRO:HD3	1.91	0.41
1:P1:632:LEU:HD23	1:P1:651:GLY:HA2	2.02	0.41
1:M1:304:ILE:HD13	1:M1:304:ILE:HA	1.93	0.41
3:L3:117:MET:HE2	3:L3:117:MET:HB3	1.90	0.41
1:H1:466:GLN:HB3	1:H1:467:GLN:H	1.56	0.41
3:H3:128:GLU:OE1	3:H3:128:GLU:N	2.50	0.41
1:F1:306:LEU:HD11	1:E1:289:GLY:HA3	2.03	0.41
1:B1:388:VAL:HG22	1:B1:480:ILE:HG12	2.02	0.41
1:O1:115:PRO:HA	1:N1:84:ILE:O	2.21	0.41
1:N1:219:SER:HB2	1:N1:223:ARG:HB2	2.03	0.41
1:N1:222:LYS:HA	1:N1:222:LYS:HD3	1.67	0.41
1:Q1:224:LEU:O	1:Q1:229:ASN:HB2	2.20	0.41
1:Q1:286:TYR:CD2	1:B1:306:LEU:HD22	2.55	0.41
1:N1:711:LEU:HD23	1:N1:711:LEU:HA	1.89	0.41
1:L1:36:TYR:HB3	1:L1:130:PRO:HB2	2.03	0.41
1:L1:637:PRO:HB3	1:L1:647:LEU:HD13	2.03	0.41
1:I1:324:THR:O	1:I1:324:THR:OG1	2.36	0.41
1:I1:471:ILE:HB	1:I1:480:ILE:HB	2.02	0.41
3:I3:184:SER:OG	3:I3:188:VAL:HG22	2.20	0.41
1:G1:224:LEU:O	1:G1:229:ASN:HB2	2.20	0.41
1:C1:325:VAL:HG21	1:C1:332:ILE:HG21	2.01	0.41
1:B1:524:LEU:HD12	1:B1:561:THR:O	2.20	0.41
1:P1:264:ARG:HB3	1:P1:311:ASP:OD2	2.21	0.41
1:P1:520:GLN:NE2	1:P1:566:GLU:HG3	2.35	0.41
1:O1:132:LEU:HD23	1:N1:61:LEU:HD11	2.02	0.41
1:N1:576:ASP:O	1:M1:693:LEU:HA	2.20	0.41
1:I1:211:ASN:HD22	1:H1:237:ARG:HH12	1.69	0.41
1:H1:524:LEU:HD12	1:H1:561:THR:O	2.20	0.41
1:G1:264:ARG:HD2	1:G1:312:ARG:HA	2.03	0.41
1:C1:173:LEU:HD22	1:C1:210:PRO:HG3	2.03	0.41
3:P3:114:ASN:OD1	3:P3:115:ALA:N	2.54	0.41
3:O3:114:ASN:OD1	3:O3:115:ALA:N	2.54	0.41
1:M1:264:ARG:HB3	1:M1:311:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M3:130:LEU:HD12	3:M3:130:LEU:HA	1.90	0.41
1:L1:145:VAL:HG12	1:L1:145:VAL:O	2.19	0.41
1:A1:206:LYS:HA	1:A1:218:ASP:O	2.21	0.41
1:A1:585:GLN:OE1	1:I1:679:THR:HB	2.21	0.41
1:I1:129:TRP:CZ2	1:I1:133:MET:HE2	2.55	0.41
1:I1:165:LYS:HE2	1:I1:236:ILE:HG21	2.03	0.41
1:H1:177:GLU:HA	1:H1:202:ARG:HD3	2.02	0.41
1:F1:264:ARG:HD2	1:F1:312:ARG:HA	2.03	0.41
1:F1:274:LEU:HD12	1:F1:274:LEU:HA	1.87	0.41
1:G1:222:LYS:HA	1:G1:222:LYS:HD3	1.83	0.41
1:G1:519:LEU:HB3	1:G1:567:THR:HB	2.03	0.41
1:G1:632:LEU:HD23	1:G1:651:GLY:HA2	2.01	0.41
3:G3:128:GLU:OE1	3:G3:128:GLU:N	2.49	0.41
1:E1:177:GLU:HG2	1:E1:202:ARG:HD3	2.02	0.41
1:E1:632:LEU:HD23	1:E1:651:GLY:HA2	2.01	0.41
1:C1:370:LEU:HD23	1:C1:370:LEU:HA	1.82	0.41
1:C1:466:GLN:HB3	1:C1:467:GLN:H	1.58	0.41
3:B3:145:ILE:HG13	3:B3:145:ILE:O	2.21	0.41
1:Q1:61:LEU:HD11	1:B1:132:LEU:HD23	2.02	0.41
1:Q1:554:LEU:HD23	1:Q1:554:LEU:HA	1.90	0.41
1:Q1:632:LEU:HD23	1:Q1:651:GLY:HA2	2.03	0.41
1:O1:129:TRP:HB3	1:O1:130:PRO:HD3	2.03	0.41
1:O1:169:ALA:O	1:O1:210:PRO:HB3	2.21	0.41
1:N1:302:ARG:CZ	1:N1:302:ARG:HB3	2.50	0.41
1:N1:580:THR:O	1:M1:678:SER:OG	2.25	0.41
1:N1:680:ILE:HD11	1:N1:734:ILE:HG21	2.03	0.41
2:N2:101:ASP:HA	2:M2:63:THR:HG21	2.03	0.41
1:M1:43:SER:HA	1:M1:126:ASN:HB2	2.02	0.41
1:M1:264:ARG:HD2	1:M1:312:ARG:HA	2.03	0.41
1:I1:133:MET:HE1	1:I1:153:ILE:HD13	2.02	0.41
1:F1:268:GLU:HA	1:F1:271:LEU:HB3	2.03	0.41
1:E1:268:GLU:HA	1:E1:271:LEU:HB3	2.03	0.41
1:E1:329:ALA:HA	1:E1:332:ILE:HG22	2.03	0.41
3:C3:76:THR:HG23	3:C3:76:THR:O	2.21	0.41
1:P1:36:TYR:HB3	1:P1:130:PRO:HB2	2.03	0.40
1:P1:524:LEU:HD12	1:P1:561:THR:O	2.21	0.40
1:P1:690:MET:HB2	1:P1:734:ILE:HD13	2.03	0.40
1:N1:207:PHE:HB2	1:N1:218:ASP:OD2	2.20	0.40
1:M1:132:LEU:HD23	1:L1:61:LEU:HD11	2.02	0.40
1:M1:274:LEU:HD12	1:M1:274:LEU:HA	1.86	0.40
1:M1:388:VAL:HG22	1:M1:480:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:564:ALA:HB1	1:I1:706:PRO:HG2	2.03	0.40
1:I1:524:LEU:HD12	1:I1:561:THR:O	2.21	0.40
1:F1:169:ALA:O	1:F1:210:PRO:HB3	2.20	0.40
1:G1:209:LEU:HB2	1:G1:216:ILE:HB	2.03	0.40
3:G3:130:LEU:HD12	3:G3:130:LEU:HA	1.91	0.40
1:D1:264:ARG:HD2	1:D1:312:ARG:HA	2.03	0.40
1:C1:206:LYS:HA	1:C1:218:ASP:O	2.19	0.40
1:B1:346:THR:HA	1:B1:347:PRO:HD3	1.92	0.40
1:Q1:115:PRO:HA	1:P1:84:ILE:O	2.21	0.40
1:Q1:211:ASN:HD22	1:P1:237:ARG:HH12	1.68	0.40
1:P1:264:ARG:HD2	1:P1:312:ARG:HA	2.03	0.40
3:P3:184:SER:OG	3:P3:188:VAL:HG22	2.21	0.40
1:O1:152:ARG:HH21	1:N1:75:ASN:CG	2.30	0.40
3:M3:184:SER:OG	3:M3:188:VAL:HG22	2.21	0.40
1:A1:471:ILE:HB	1:A1:480:ILE:HB	2.02	0.40
1:A1:554:LEU:HD23	1:A1:554:LEU:HA	1.92	0.40
1:I1:680:ILE:HD11	1:I1:734:ILE:HG21	2.04	0.40
2:H2:127:VAL:HA	2:H2:128:PRO:HD3	1.94	0.40
1:F1:75:ASN:CG	1:G1:152:ARG:HH21	2.29	0.40
1:G1:36:TYR:HB3	1:G1:130:PRO:HB2	2.02	0.40
1:E1:282:ILE:HA	1:E1:282:ILE:HD13	1.86	0.40
1:E1:340:TYR:OH	1:E1:365:THR:HG22	2.22	0.40
1:C1:274:LEU:HD12	1:C1:274:LEU:HA	1.88	0.40
3:C3:184:SER:OG	3:C3:188:VAL:HG22	2.20	0.40
1:B1:336:LEU:HD23	1:B1:336:LEU:HA	1.88	0.40
1:B1:471:ILE:HB	1:B1:480:ILE:HB	2.02	0.40
1:P1:471:ILE:HB	1:P1:480:ILE:HB	2.02	0.40
1:M1:680:ILE:HD11	1:M1:734:ILE:HG21	2.03	0.40
1:L1:206:LYS:HB3	1:L1:206:LYS:HE3	1.53	0.40
1:A1:150:VAL:HG23	1:I1:71:GLU:O	2.20	0.40
1:G1:38:ASP:HB3	1:G1:41:LEU:HD12	2.03	0.40
1:G1:329:ALA:HA	1:G1:332:ILE:HG22	2.04	0.40
3:E3:76:THR:HG23	3:E3:76:THR:O	2.21	0.40
1:D1:632:LEU:HD23	1:D1:651:GLY:HA2	2.03	0.40
1:P1:169:ALA:O	1:P1:210:PRO:HB3	2.21	0.40
1:P1:290:GLY:O	1:P1:291:LEU:HD23	2.21	0.40
1:O1:36:TYR:HB3	1:O1:130:PRO:HB2	2.04	0.40
1:O1:632:LEU:HD23	1:O1:651:GLY:HA2	2.02	0.40
3:M3:31:ASN:HB3	3:M3:82:ARG:HB2	2.03	0.40
1:A1:632:LEU:HD23	1:A1:651:GLY:HA2	2.03	0.40
1:I1:282:ILE:HA	1:I1:282:ILE:HD13	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H1:49:ASN:OD1	1:H1:50:VAL:N	2.54	0.40
1:H1:165:LYS:H	1:H1:236:ILE:HD12	1.87	0.40
1:F1:38:ASP:OD2	1:F1:140:TYR:OH	2.18	0.40
1:E1:637:PRO:HB3	1:E1:647:LEU:HD13	2.03	0.40
3:C3:75:VAL:HG21	3:C3:197:ILE:HD11	2.03	0.40
1:B1:325:VAL:HG11	1:B1:329:ALA:HB2	2.03	0.40
2:Q2:127:VAL:HA	2:Q2:128:PRO:HD3	1.94	0.40
3:P3:94:ARG:CG	3:P3:113:GLU:HG2	2.52	0.40
1:A1:711:LEU:HD23	1:A1:711:LEU:HA	1.89	0.40
1:F1:679:THR:HB	1:G1:585:GLN:OE1	2.22	0.40
1:E1:165:LYS:H	1:E1:236:ILE:HD12	1.85	0.40
1:E1:325:VAL:HG11	1:E1:329:ALA:HB2	2.02	0.40
1:E1:711:LEU:HD23	1:E1:711:LEU:HA	1.88	0.40
1:D1:637:PRO:HB3	1:D1:647:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	599/740 (81%)	538 (90%)	60 (10%)	1 (0%)	43	54
1	B1	599/740 (81%)	540 (90%)	59 (10%)	0	100	100
1	C1	599/740 (81%)	538 (90%)	61 (10%)	0	100	100
1	D1	599/740 (81%)	543 (91%)	56 (9%)	0	100	100
1	E1	599/740 (81%)	541 (90%)	58 (10%)	0	100	100
1	F1	599/740 (81%)	539 (90%)	60 (10%)	0	100	100
1	G1	599/740 (81%)	539 (90%)	60 (10%)	0	100	100
1	H1	599/740 (81%)	537 (90%)	62 (10%)	0	100	100
1	I1	599/740 (81%)	540 (90%)	59 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L1	599/740 (81%)	536 (90%)	62 (10%)	1 (0%)	43	54
1	M1	599/740 (81%)	539 (90%)	60 (10%)	0	100	100
1	N1	599/740 (81%)	541 (90%)	58 (10%)	0	100	100
1	O1	599/740 (81%)	538 (90%)	61 (10%)	0	100	100
1	P1	599/740 (81%)	536 (90%)	63 (10%)	0	100	100
1	Q1	599/740 (81%)	543 (91%)	56 (9%)	0	100	100
2	A2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	B2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	C2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	D2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	E2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	F2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	G2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	H2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	I2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	L2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	M2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	N2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	O2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	P2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
2	Q2	93/155 (60%)	90 (97%)	3 (3%)	0	100	100
3	A3	136/208 (65%)	122 (90%)	13 (10%)	1 (1%)	18	25
3	B3	136/208 (65%)	119 (88%)	16 (12%)	1 (1%)	18	25
3	C3	136/208 (65%)	123 (90%)	12 (9%)	1 (1%)	18	25
3	D3	136/208 (65%)	122 (90%)	13 (10%)	1 (1%)	18	25
3	E3	136/208 (65%)	122 (90%)	13 (10%)	1 (1%)	18	25
3	F3	136/208 (65%)	122 (90%)	13 (10%)	1 (1%)	18	25
3	G3	136/208 (65%)	121 (89%)	14 (10%)	1 (1%)	18	25
3	H3	136/208 (65%)	121 (89%)	14 (10%)	1 (1%)	18	25
3	I3	136/208 (65%)	122 (90%)	13 (10%)	1 (1%)	18	25
3	L3	136/208 (65%)	122 (90%)	13 (10%)	1 (1%)	18	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M3	136/208 (65%)	121 (89%)	14 (10%)	1 (1%)	18	25
3	N3	136/208 (65%)	122 (90%)	13 (10%)	1 (1%)	18	25
3	O3	136/208 (65%)	120 (88%)	15 (11%)	1 (1%)	18	25
3	P3	136/208 (65%)	123 (90%)	12 (9%)	1 (1%)	18	25
3	Q3	136/208 (65%)	123 (90%)	12 (9%)	1 (1%)	18	25
All	All	12420/16545 (75%)	11263 (91%)	1140 (9%)	17 (0%)	49	60

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	339	GLN
1	L1	72	VAL
3	L3	49	ILE
3	H3	49	ILE
3	F3	49	ILE
3	Q3	49	ILE
3	P3	49	ILE
3	O3	49	ILE
3	N3	49	ILE
3	M3	49	ILE
3	A3	49	ILE
3	I3	49	ILE
3	G3	49	ILE
3	E3	49	ILE
3	D3	49	ILE
3	C3	49	ILE
3	B3	49	ILE

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	A1	497/607 (82%)	496 (100%)	1 (0%)	87	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	496/607 (82%)	496 (100%)	0	100	100
1	C1	497/607 (82%)	497 (100%)	0	100	100
1	D1	497/607 (82%)	497 (100%)	0	100	100
1	E1	497/607 (82%)	497 (100%)	0	100	100
1	F1	497/607 (82%)	497 (100%)	0	100	100
1	G1	497/607 (82%)	497 (100%)	0	100	100
1	H1	497/607 (82%)	497 (100%)	0	100	100
1	I1	497/607 (82%)	497 (100%)	0	100	100
1	L1	497/607 (82%)	497 (100%)	0	100	100
1	M1	497/607 (82%)	497 (100%)	0	100	100
1	N1	497/607 (82%)	497 (100%)	0	100	100
1	O1	497/607 (82%)	497 (100%)	0	100	100
1	P1	497/607 (82%)	497 (100%)	0	100	100
1	Q1	497/607 (82%)	497 (100%)	0	100	100
2	A2	71/118 (60%)	71 (100%)	0	100	100
2	B2	71/118 (60%)	71 (100%)	0	100	100
2	C2	71/118 (60%)	71 (100%)	0	100	100
2	D2	71/118 (60%)	71 (100%)	0	100	100
2	E2	71/118 (60%)	71 (100%)	0	100	100
2	F2	71/118 (60%)	71 (100%)	0	100	100
2	G2	71/118 (60%)	71 (100%)	0	100	100
2	H2	71/118 (60%)	71 (100%)	0	100	100
2	I2	71/118 (60%)	71 (100%)	0	100	100
2	L2	71/118 (60%)	71 (100%)	0	100	100
2	M2	71/118 (60%)	71 (100%)	0	100	100
2	N2	71/118 (60%)	71 (100%)	0	100	100
2	O2	71/118 (60%)	71 (100%)	0	100	100
2	P2	71/118 (60%)	71 (100%)	0	100	100
2	Q2	71/118 (60%)	71 (100%)	0	100	100
3	A3	106/164 (65%)	106 (100%)	0	100	100
3	B3	106/164 (65%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C3	106/164 (65%)	106 (100%)	0	100	100
3	D3	106/164 (65%)	106 (100%)	0	100	100
3	E3	106/164 (65%)	106 (100%)	0	100	100
3	F3	106/164 (65%)	106 (100%)	0	100	100
3	G3	106/164 (65%)	106 (100%)	0	100	100
3	H3	105/164 (64%)	105 (100%)	0	100	100
3	I3	106/164 (65%)	106 (100%)	0	100	100
3	L3	106/164 (65%)	106 (100%)	0	100	100
3	M3	106/164 (65%)	106 (100%)	0	100	100
3	N3	106/164 (65%)	106 (100%)	0	100	100
3	O3	106/164 (65%)	106 (100%)	0	100	100
3	P3	106/164 (65%)	106 (100%)	0	100	100
3	Q3	106/164 (65%)	106 (100%)	0	100	100
All	All	10108/13335 (76%)	10107 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	211	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q1	149	ASN
1	Q1	211	ASN
1	Q1	301	ASN
1	Q1	309	GLN
1	Q1	320	GLN
1	Q1	578	ASN
1	Q1	631	ASN
1	Q1	652	GLN
1	Q1	673	ASN
3	Q3	137	GLN
3	Q3	152	GLN
3	Q3	187	ASN
1	P1	122	ASN

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Mol	Chain	Res	Type
1	P1	149	ASN
1	P1	301	ASN
1	P1	320	GLN
1	P1	520	GLN
1	P1	578	ASN
1	P1	701	ASN
3	P3	152	GLN
3	P3	187	ASN
1	O1	149	ASN
1	O1	301	ASN
1	O1	309	GLN
1	O1	515	ASN
1	O1	578	ASN
3	O3	31	ASN
3	O3	152	GLN
3	O3	187	ASN
1	N1	149	ASN
1	N1	301	ASN
1	N1	309	GLN
1	N1	520	GLN
1	N1	578	ASN
1	N1	631	ASN
1	N1	652	GLN
3	N3	152	GLN
1	M1	149	ASN
1	M1	301	ASN
1	M1	309	GLN
1	M1	578	ASN
1	M1	701	ASN
3	M3	31	ASN
3	M3	152	GLN
3	M3	187	ASN
1	L1	149	ASN
1	L1	301	ASN
1	L1	309	GLN
1	L1	515	ASN
1	L1	520	GLN
1	L1	631	ASN
3	L3	137	GLN
3	L3	152	GLN
3	L3	187	ASN
1	A1	149	ASN

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Mol	Chain	Res	Type
1	A1	301	ASN
3	A3	31	ASN
3	A3	152	GLN
3	A3	187	ASN
1	I1	149	ASN
1	I1	211	ASN
1	I1	301	ASN
1	I1	309	GLN
1	I1	320	GLN
3	I3	152	GLN
3	I3	187	ASN
1	H1	122	ASN
1	H1	149	ASN
1	H1	301	ASN
1	H1	309	GLN
1	H1	320	GLN
1	H1	515	ASN
1	H1	578	ASN
3	H3	152	GLN
3	H3	187	ASN
1	F1	149	ASN
1	F1	301	ASN
1	F1	309	GLN
1	F1	320	GLN
1	F1	568	GLN
3	F3	31	ASN
3	F3	152	GLN
3	F3	187	ASN
1	G1	149	ASN
1	G1	515	ASN
3	G3	187	ASN
1	E1	149	ASN
1	E1	301	ASN
1	E1	631	ASN
1	E1	701	ASN
3	E3	152	GLN
3	E3	187	ASN
1	D1	122	ASN
1	D1	149	ASN
1	D1	301	ASN
1	D1	309	GLN
1	D1	578	ASN

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Mol	Chain	Res	Type
3	D3	152	GLN
3	D3	187	ASN
1	C1	149	ASN
1	C1	301	ASN
1	C1	515	ASN
3	C3	31	ASN
3	C3	137	GLN
3	C3	152	GLN
3	C3	187	ASN
1	B1	149	ASN
1	B1	301	ASN
1	B1	309	GLN
1	B1	339	GLN
1	B1	578	ASN
1	B1	701	ASN
3	B3	31	ASN
3	B3	152	GLN
3	B3	187	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

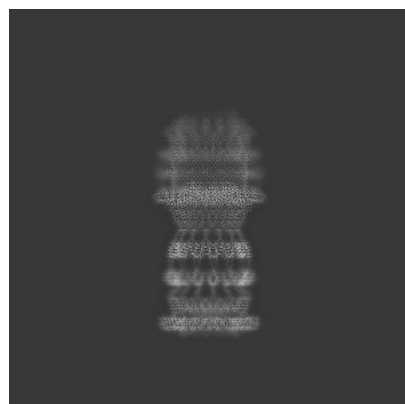
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16770. These allow visual inspection of the internal detail of the map and identification of artifacts.

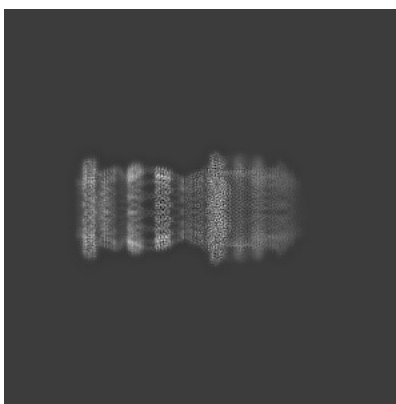
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

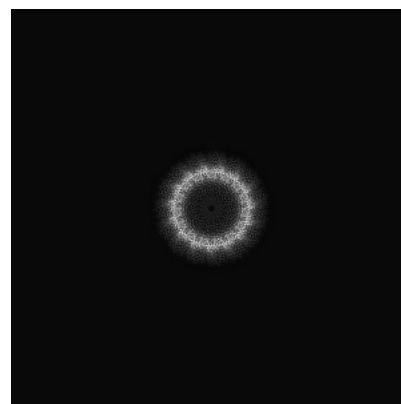
6.1.1 Primary map



X

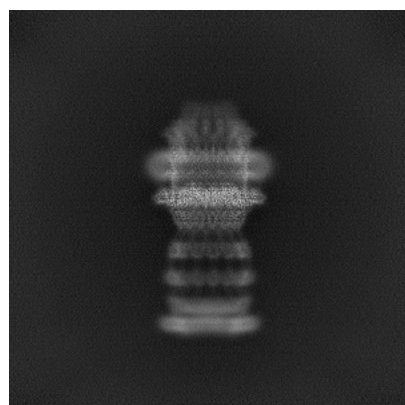


Y

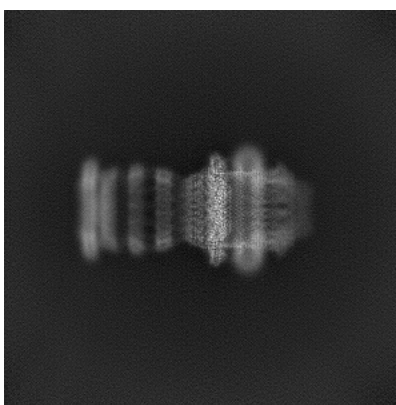


Z

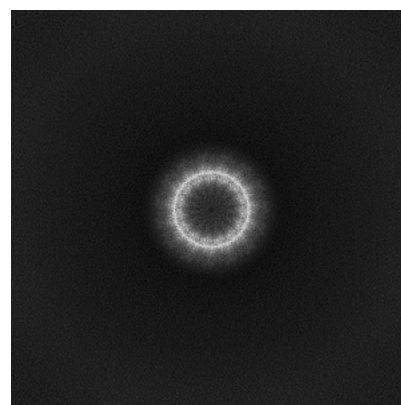
6.1.2 Raw map



X



Y



Z

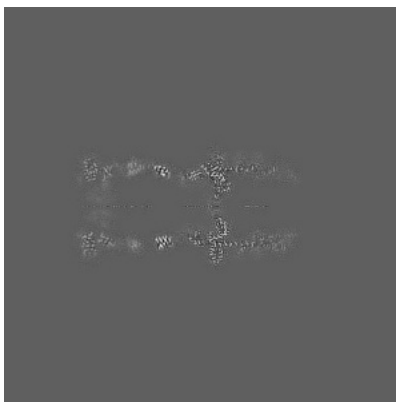
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

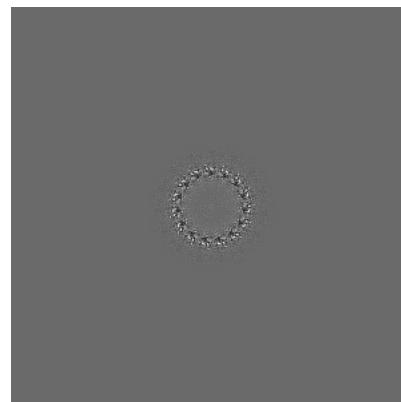
6.2.1 Primary map



X Index: 250

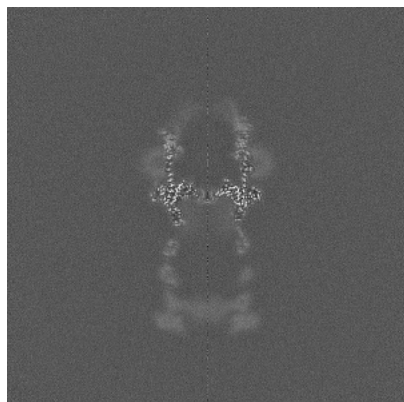


Y Index: 250

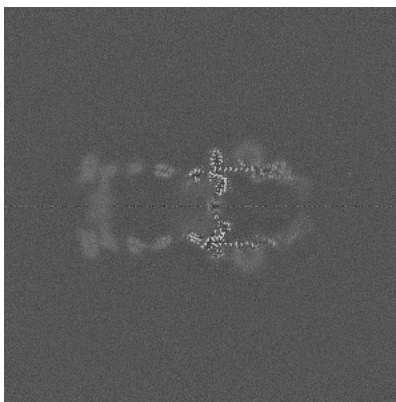


Z Index: 250

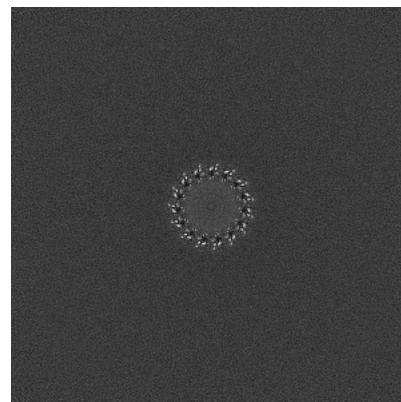
6.2.2 Raw map



X Index: 250



Y Index: 250

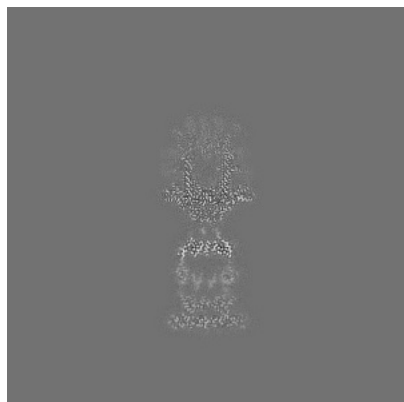


Z Index: 250

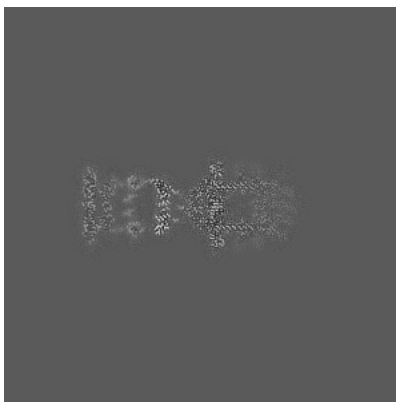
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

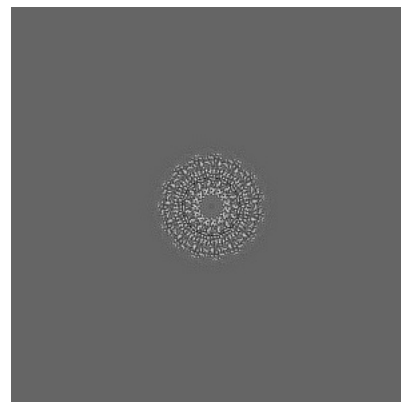
6.3.1 Primary map



X Index: 210

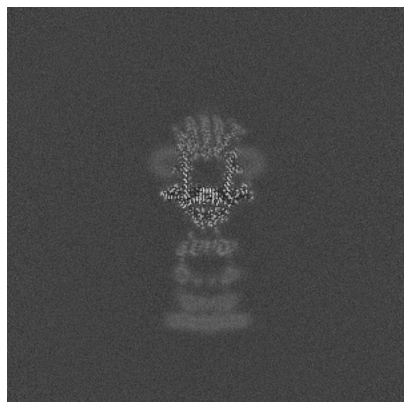


Y Index: 289

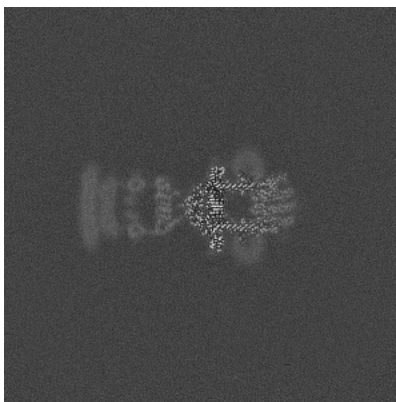


Z Index: 271

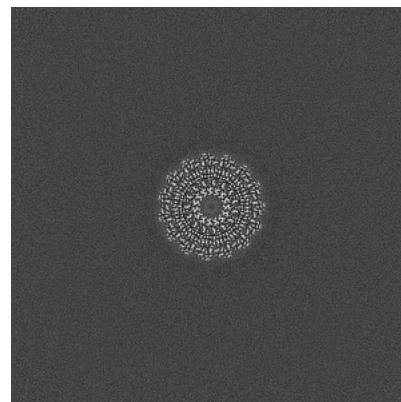
6.3.2 Raw map



X Index: 288



Y Index: 289

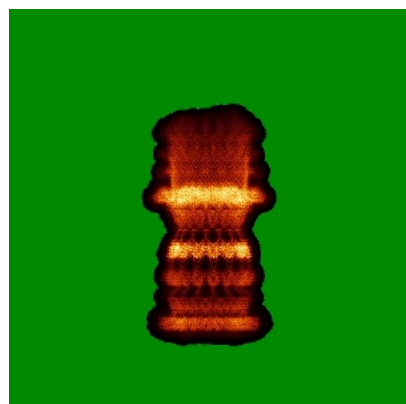


Z Index: 271

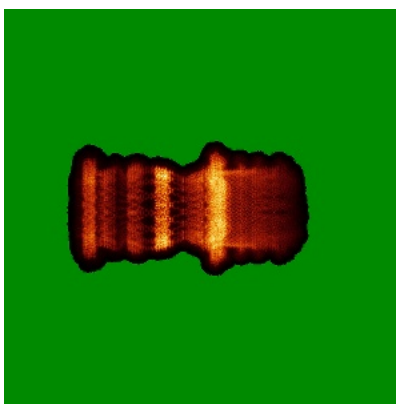
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

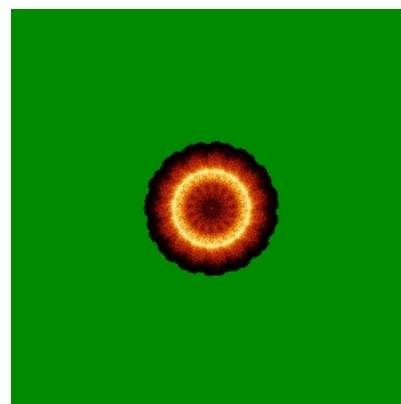
6.4.1 Primary map



X

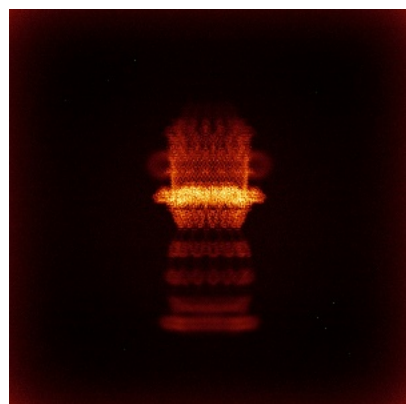


Y

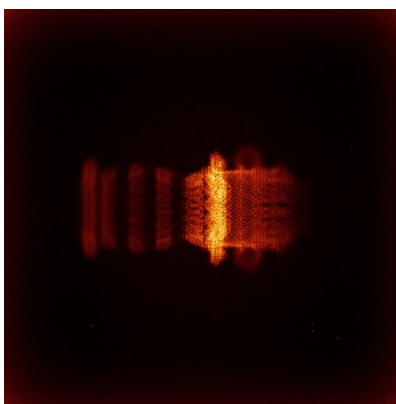


Z

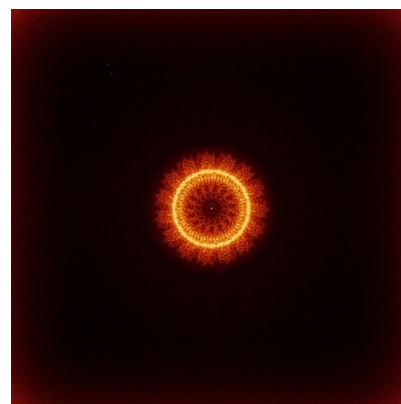
6.4.2 Raw map



X



Y

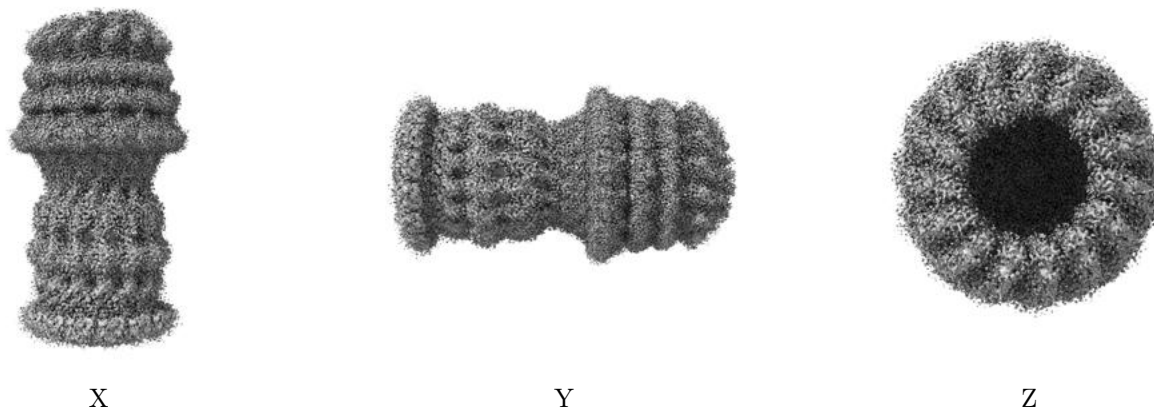


Z

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.

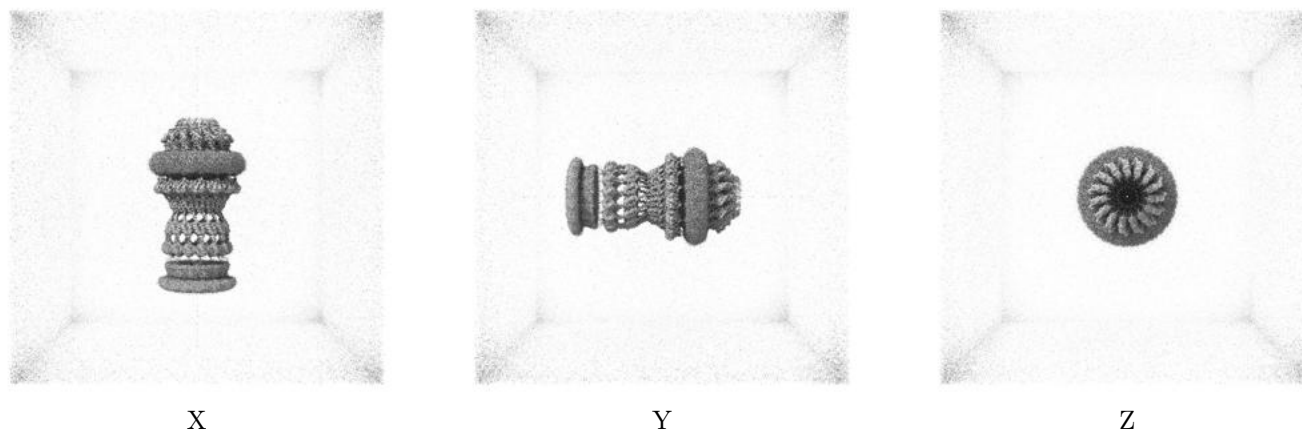
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

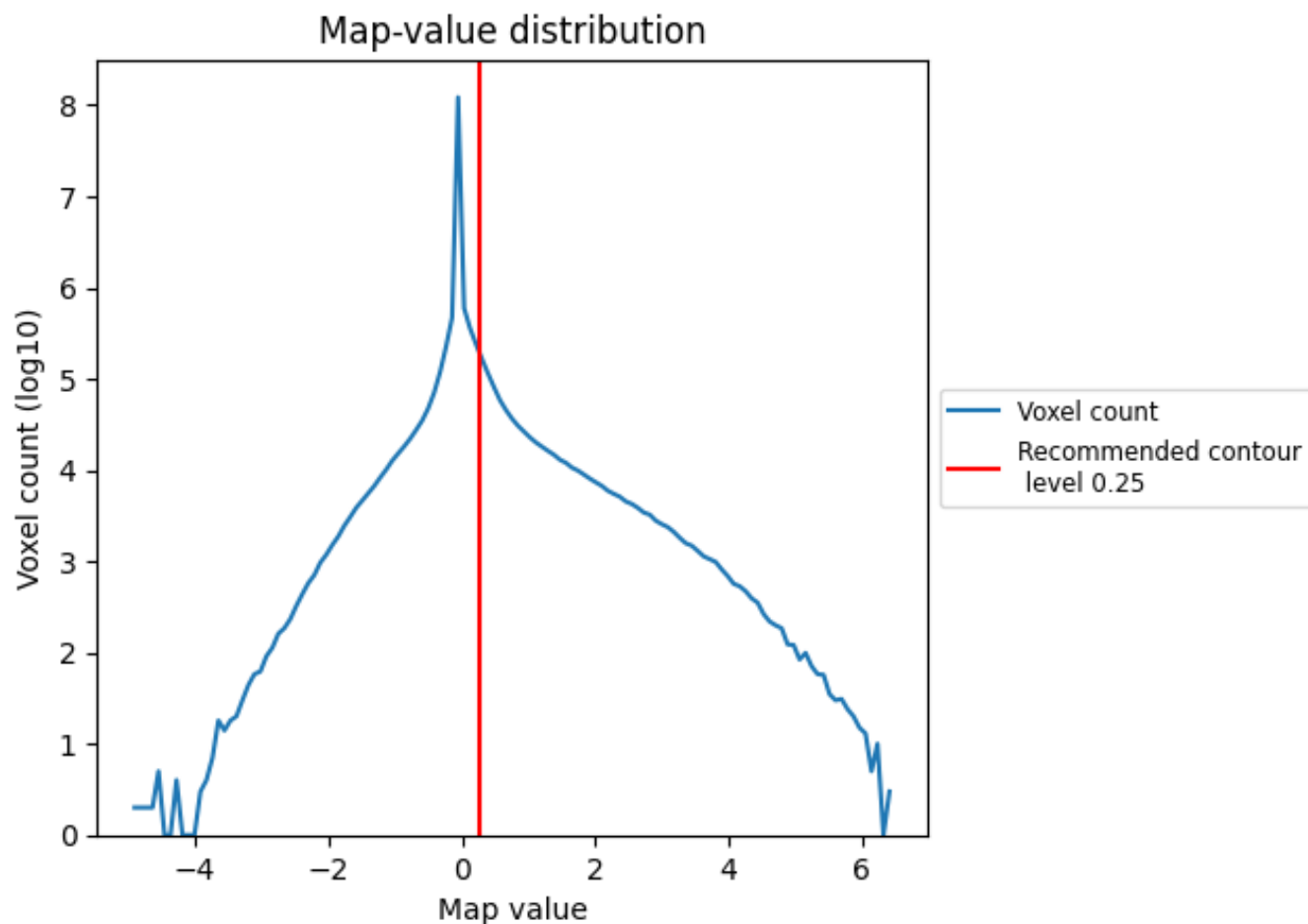
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

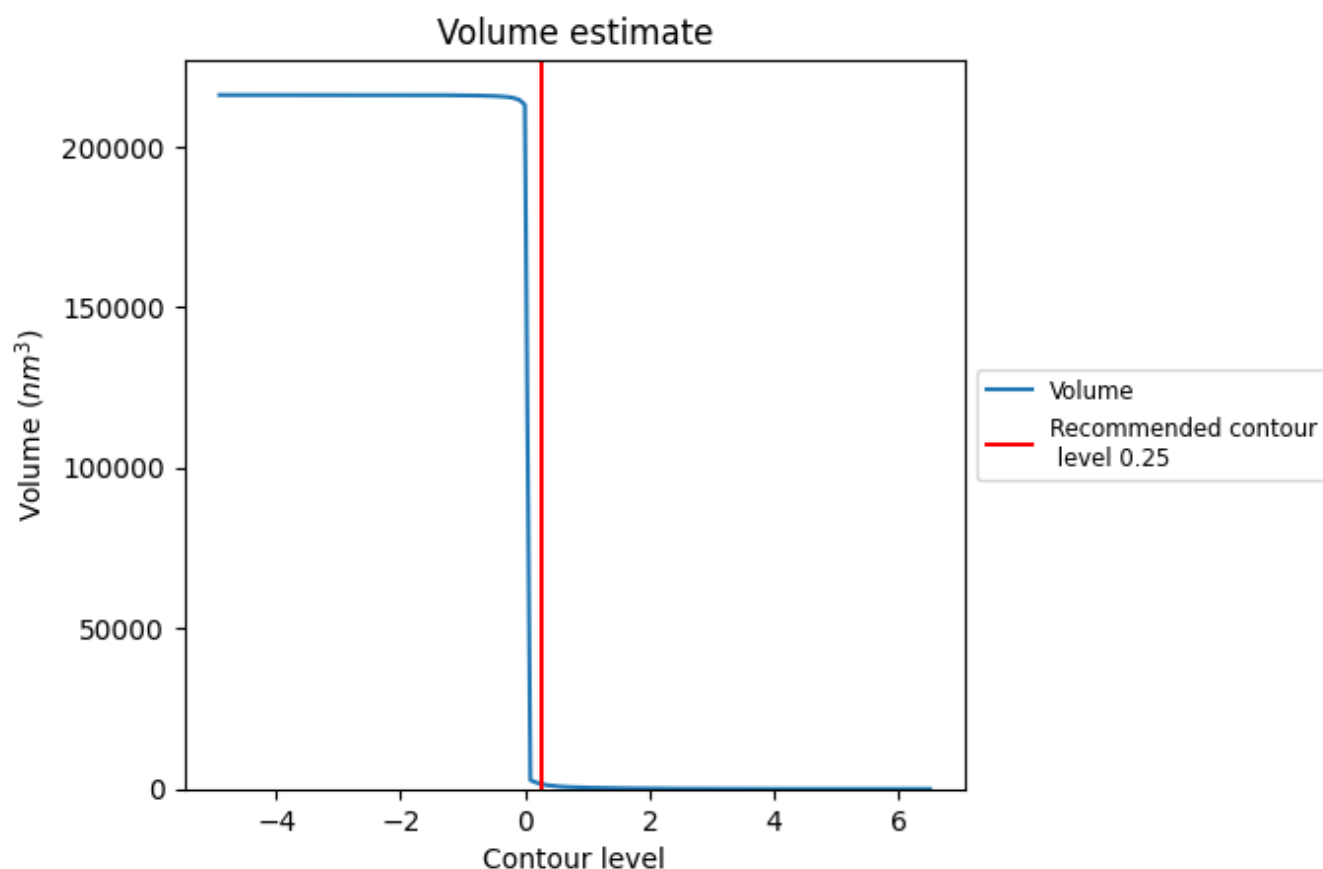
This section contains the results of statistical analysis of the map.

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.

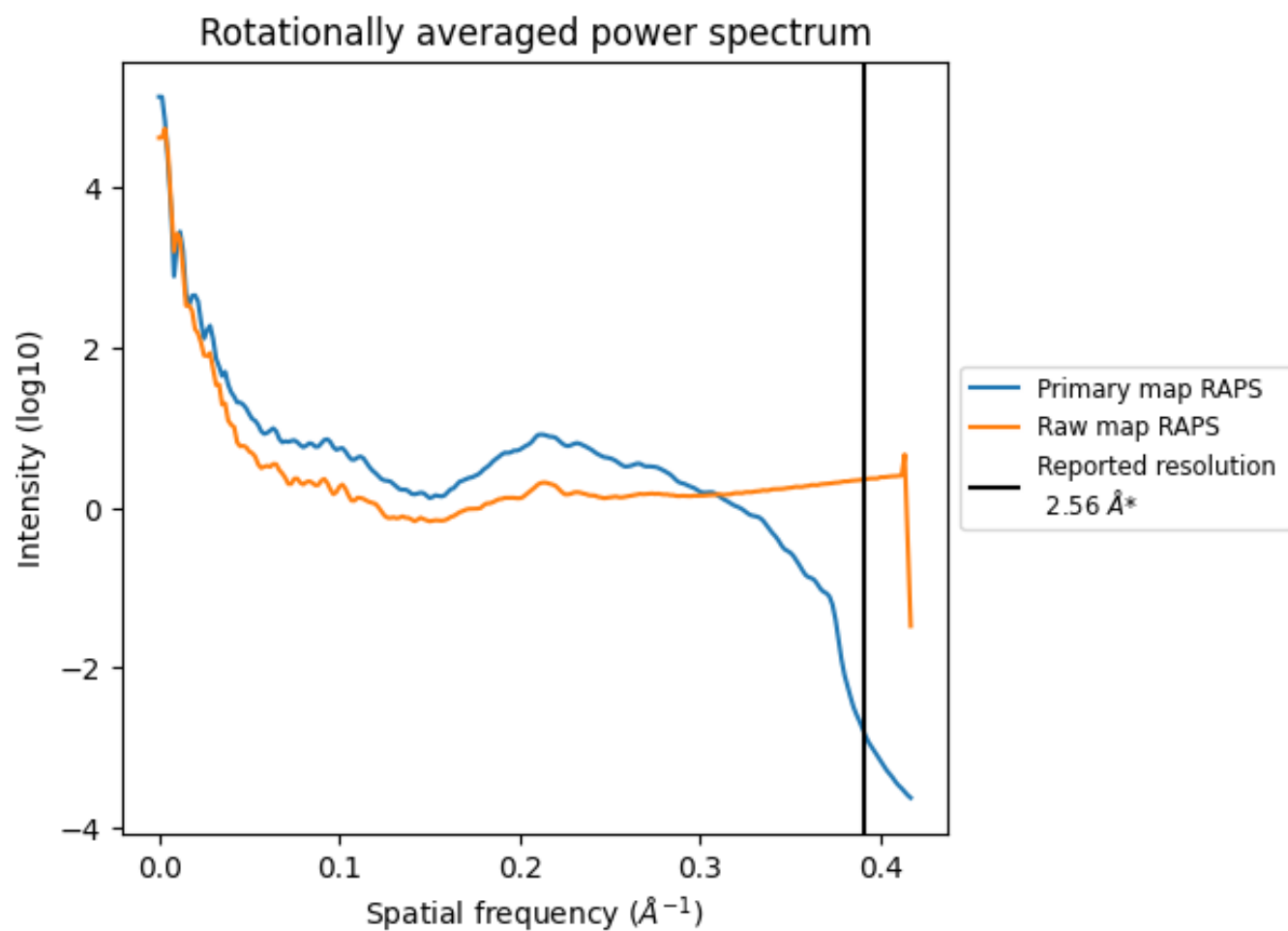
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1595 nm³; this corresponds to an approximate mass of 1441 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 ⓘ

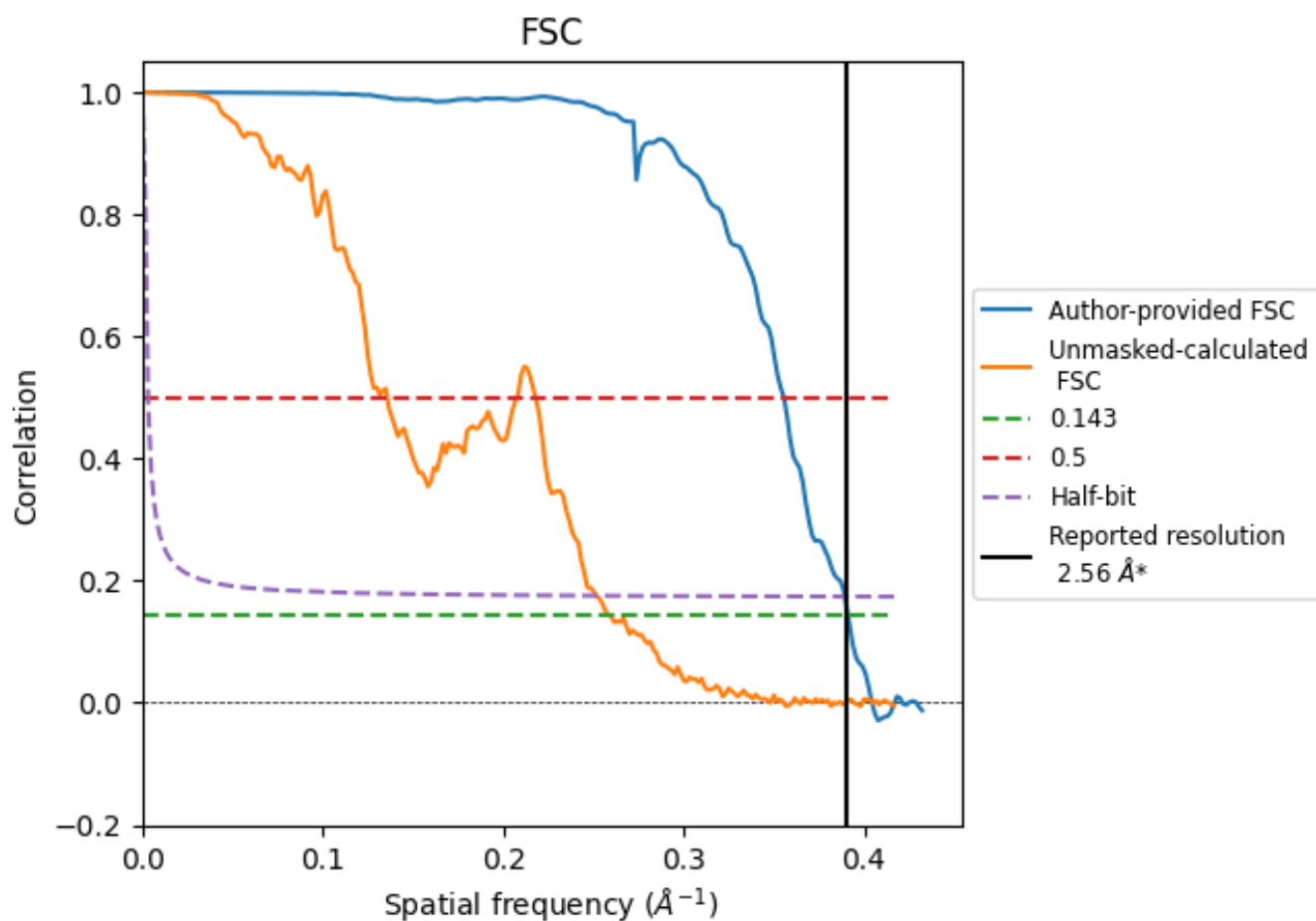


*Reported resolution corresponds to spatial frequency of 0.391 Å⁻¹

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 0.391 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

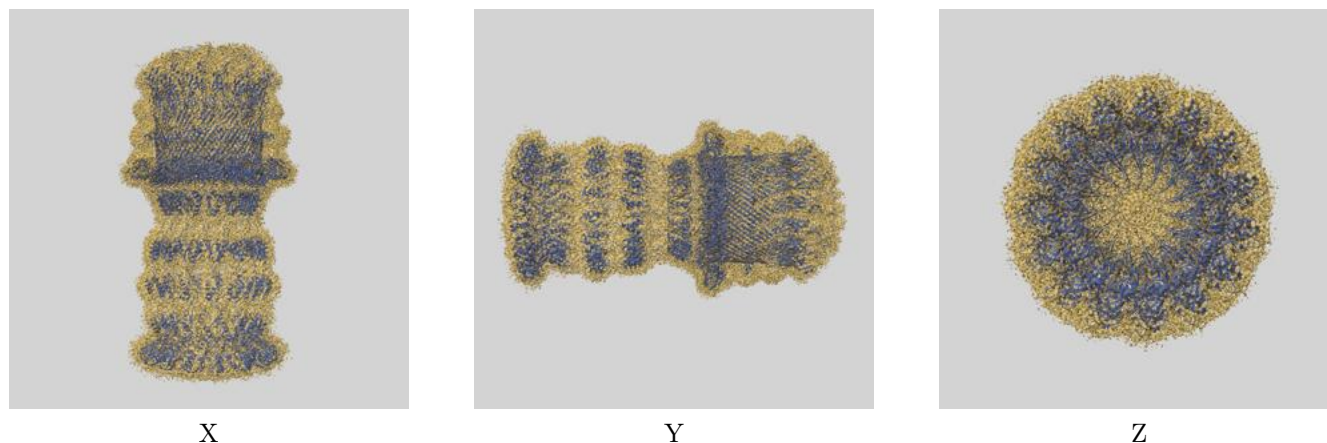
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.56	2.81	2.57
Unmasked-calculated*	3.86	7.36	3.98

*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 3.86 differs from the reported value 2.56 by more than 10 %

9 Map-model fit [i](#)

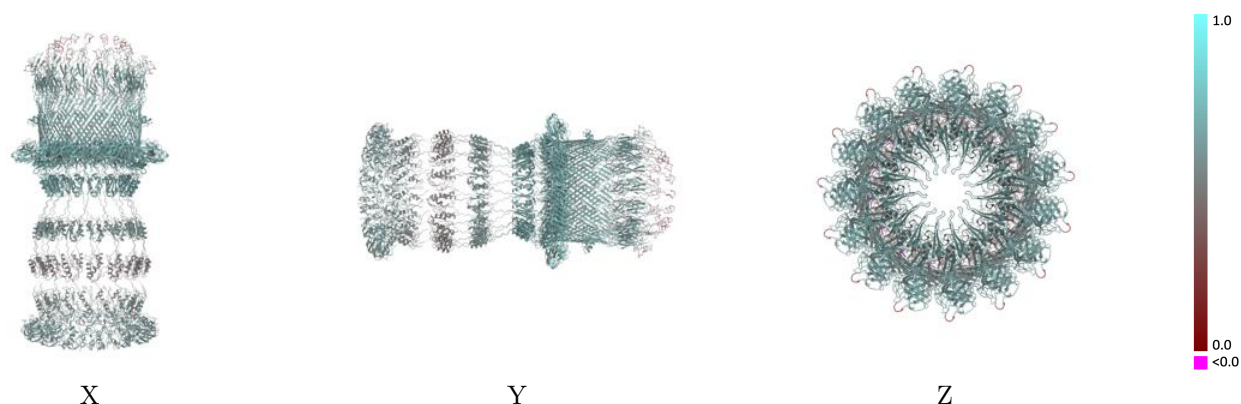
This section contains information regarding the fit between EMDB map EMD-16770 and PDB model 8CO1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



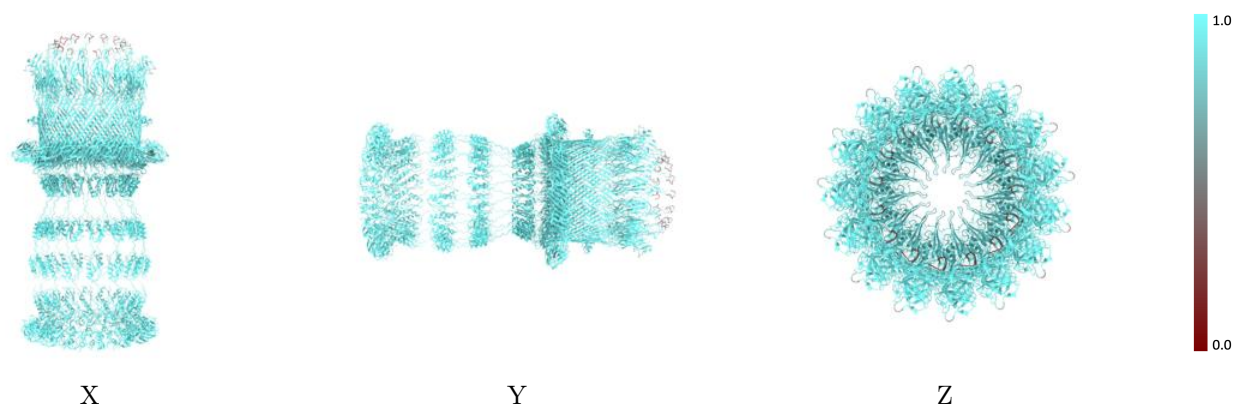
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



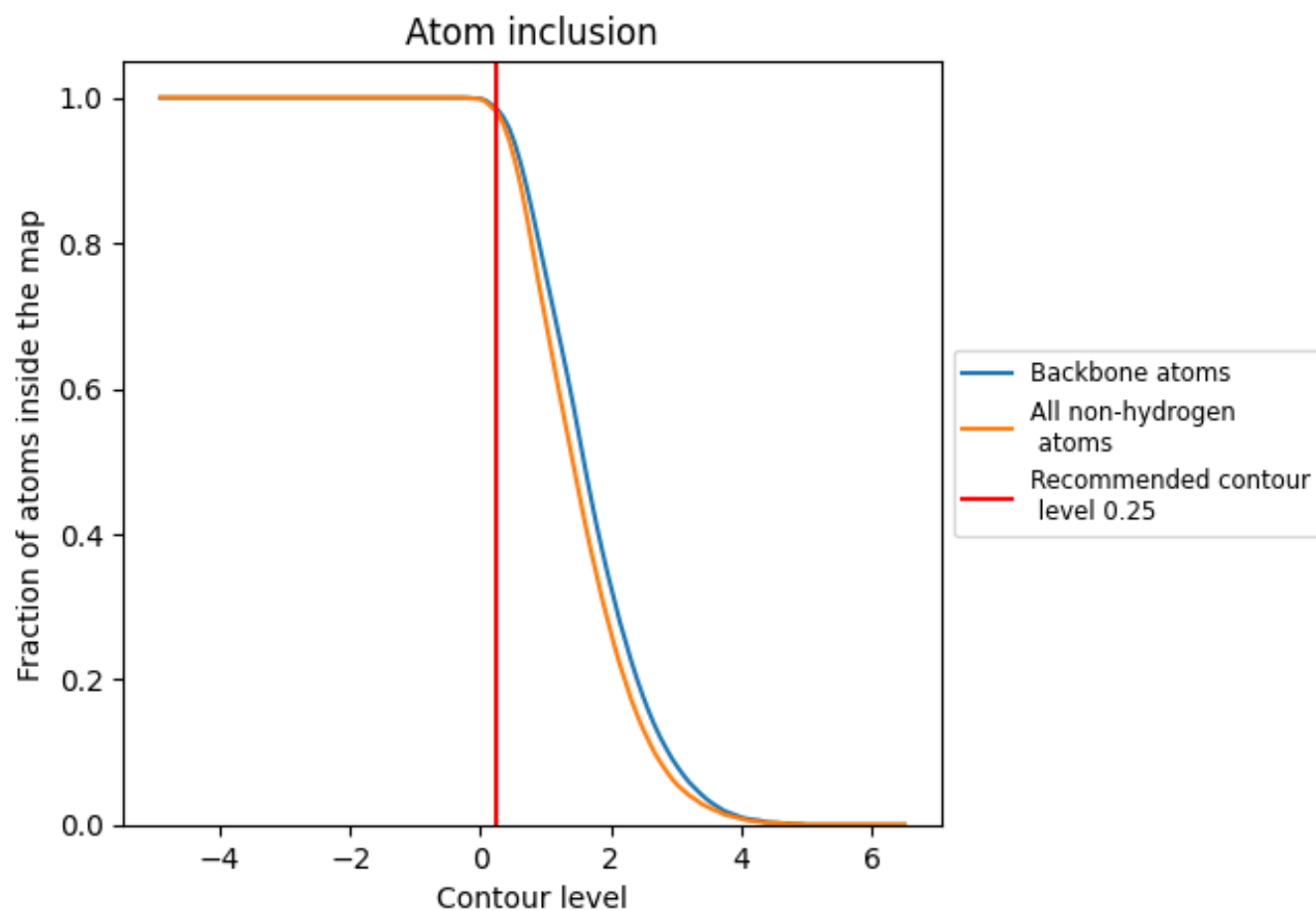
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9800	 0.5740
A1	 0.9890	 0.5760
A2	 0.9990	 0.6350
A3	 0.9280	 0.5290
B1	 0.9890	 0.5750
B2	 1.0000	 0.6360
B3	 0.9320	 0.5280
C1	 0.9870	 0.5780
C2	 1.0000	 0.6380
C3	 0.9350	 0.5320
D1	 0.9890	 0.5760
D2	 1.0000	 0.6340
D3	 0.9320	 0.5200
E1	 0.9870	 0.5750
E2	 0.9990	 0.6360
E3	 0.9400	 0.5280
F1	 0.9870	 0.5760
F2	 1.0000	 0.6360
F3	 0.9280	 0.5210
G1	 0.9890	 0.5760
G2	 0.9990	 0.6400
G3	 0.9320	 0.5240
H1	 0.9880	 0.5760
H2	 1.0000	 0.6370
H3	 0.9330	 0.5220
I1	 0.9900	 0.5760
I2	 0.9990	 0.6370
I3	 0.9330	 0.5250
L1	 0.9910	 0.5770
L2	 0.9990	 0.6390
L3	 0.9240	 0.5230
M1	 0.9890	 0.5750
M2	 1.0000	 0.6370
M3	 0.9250	 0.5250
N1	 0.9890	 0.5770



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Chain	Atom inclusion	Q-score
N2	 1.0000	 0.6350
N3	 0.9230	 0.5250
O1	 0.9890	 0.5770
O2	 1.0000	 0.6340
O3	 0.9180	 0.5260
P1	 0.9880	 0.5770
P2	 1.0000	 0.6360
P3	 0.9310	 0.5280
Q1	 0.9900	 0.5770
Q2	 1.0000	 0.6370
Q3	 0.9350	 0.5280