



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:54 AM UTC

PDB ID : 6QL5 / pdb_00006ql5
EMDB ID : EMD-4577
Title : Structure of fatty acid synthase complex with bound gamma subunit from *Saccharomyces cerevisiae* at 2.8 angstrom
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.
Deposited on : 2019-01-31
Resolution : 2.80 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:

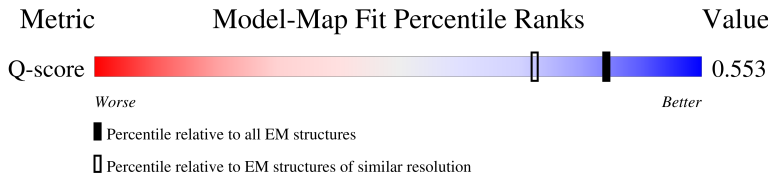
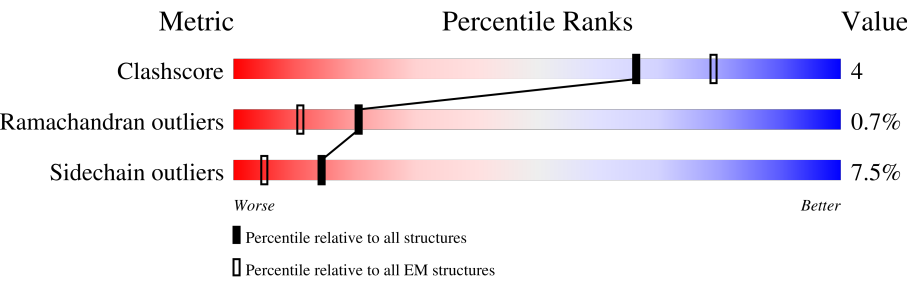
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A	1887	77% 13% • 7%
1	B	1887	77% 13% • 7%
1	C	1887	77% 13% • 7%
1	D	1887	77% 13% • 7%

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Mol	Chain	Length	Quality of chain
1	E	1887	 5% 77% 14% 7%
1	F	1887	 78% 13% 7%
2	G	2040	 85% 13%
2	H	2040	 85% 13%
2	I	2040	 85% 13%
2	J	2040	 85% 13%
2	K	2040	 85% 13%
2	L	2040	 85% 13%
3	M	148	 61% 11% 24%
3	N	148	 61% 11% 24%
3	O	148	 61% 11% 24%
3	P	148	 61% 11% 24%
3	Q	148	 61% 11% 24%
3	R	148	 61% 11% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 183444 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	B	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	C	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	D	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	E	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	F	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	H	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	I	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	J	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	K	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	L	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		

- Molecule 3 is a protein called Translation machinery-associated protein 17.

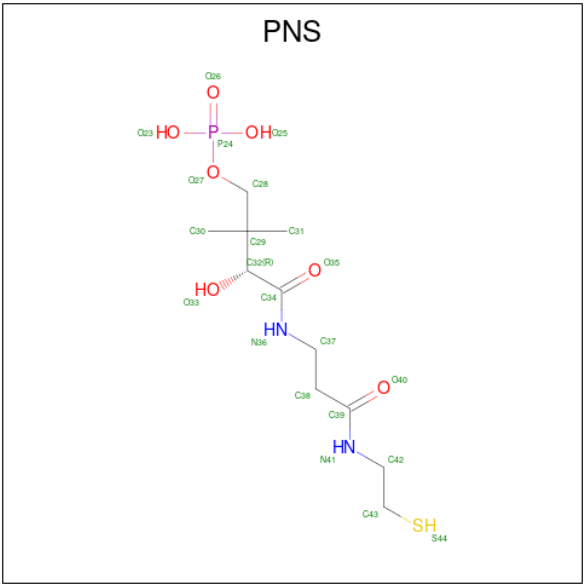
Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	O	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	P	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	Q	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	R	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).

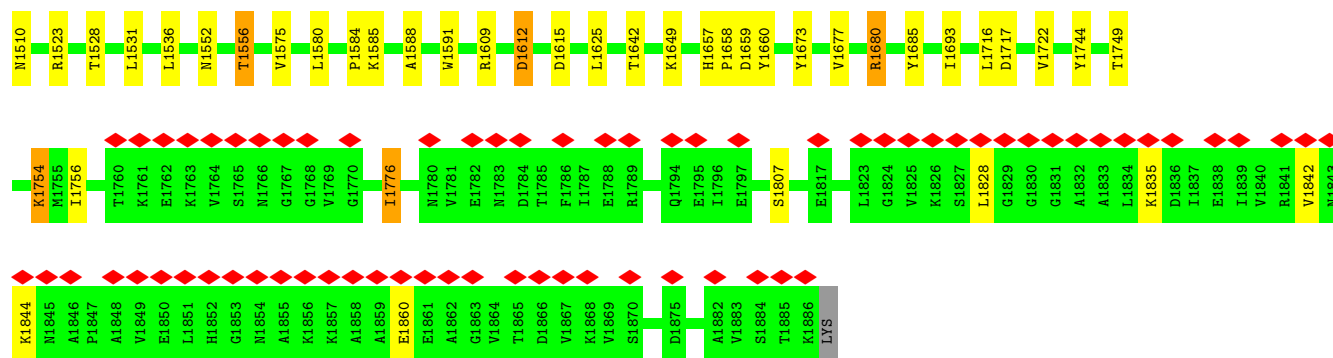


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	B	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	C	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	D	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	E	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	F	1	Total	C	N	O	P	S
			21	11	2	6	1	1

-
- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5) attached to a ribitol chain. The ribitol chain is a five-carbon chain with hydroxyl groups at C2, C3, and C4. The C1 of the ribitol chain is attached to the N10 of the isoalloxazine ring. The C5 of the ribitol chain is attached to a phosphate group (O1P, O2P, O3P, O4P, O5P). The ribitol chain is shown in a chair conformation with the hydroxyl groups at C2, C3, and C4 in the endo position. The phosphate group is shown as a series of oxygen atoms (O1P, O2P, O3P, O4P, O5P) connected by phosphorus atoms (P). The ribitol chain is labeled with C1, C2, C3, C4, and C5. The isoalloxazine ring system is labeled with N1, N5, C2, C4A, C5A, C6, C7, C8, C9, C10, and C10A. The ribitol chain is also labeled with C1, C2, C3, C4, and C5. The phosphate group is labeled with O1P, O2P, O3P, O4P, and O5P.

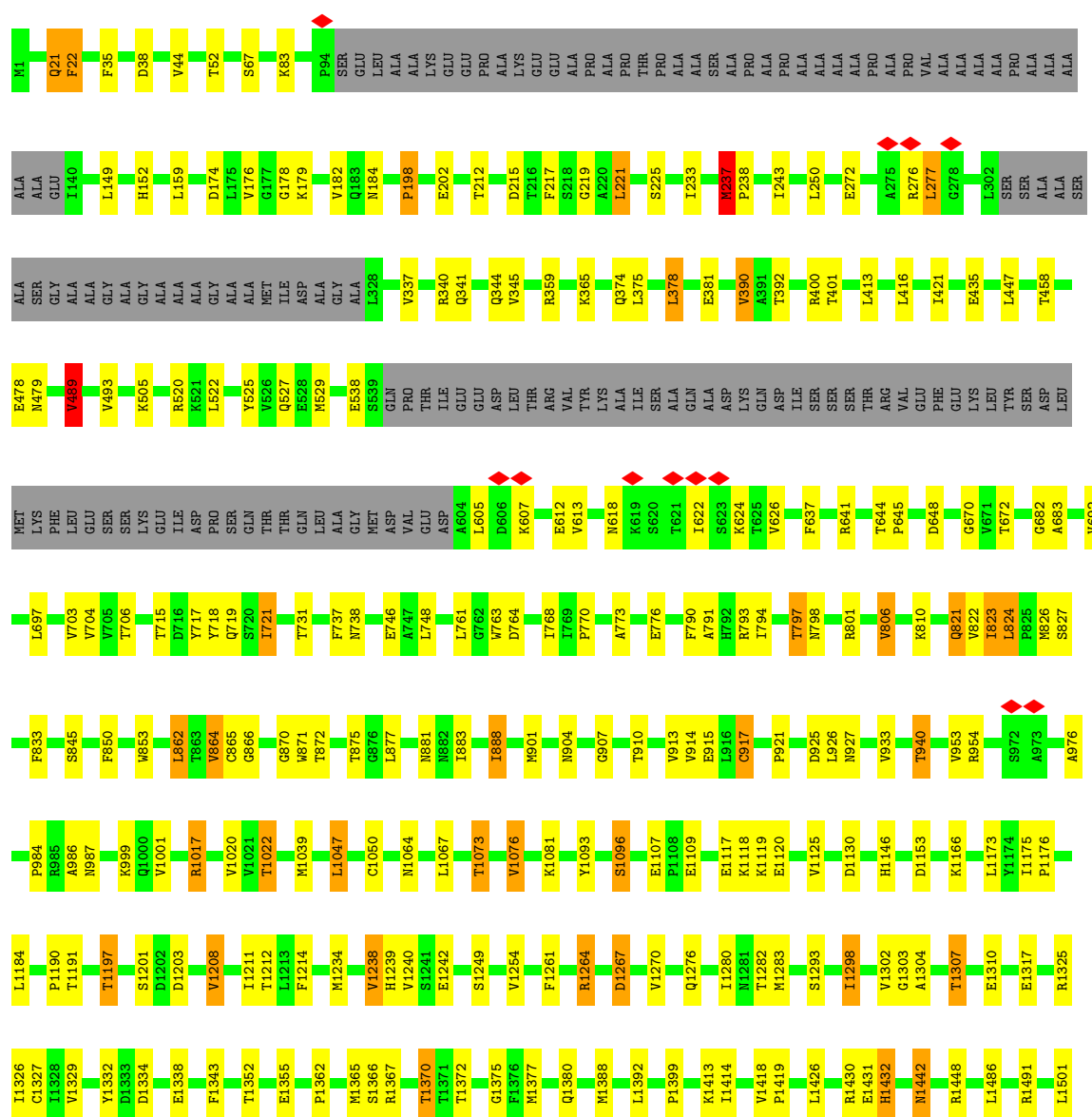
Mol	Chain	Residues	Atoms					AltConf
5	G	1	Total 31	C 17	N 4	O 9	P 1	0
5	H	1	Total 31	C 17	N 4	O 9	P 1	0
5	I	1	Total 31	C 17	N 4	O 9	P 1	0
5	J	1	Total 31	C 17	N 4	O 9	P 1	0
5	K	1	Total 31	C 17	N 4	O 9	P 1	0
5	L	1	Total 31	C 17	N 4	O 9	P 1	0

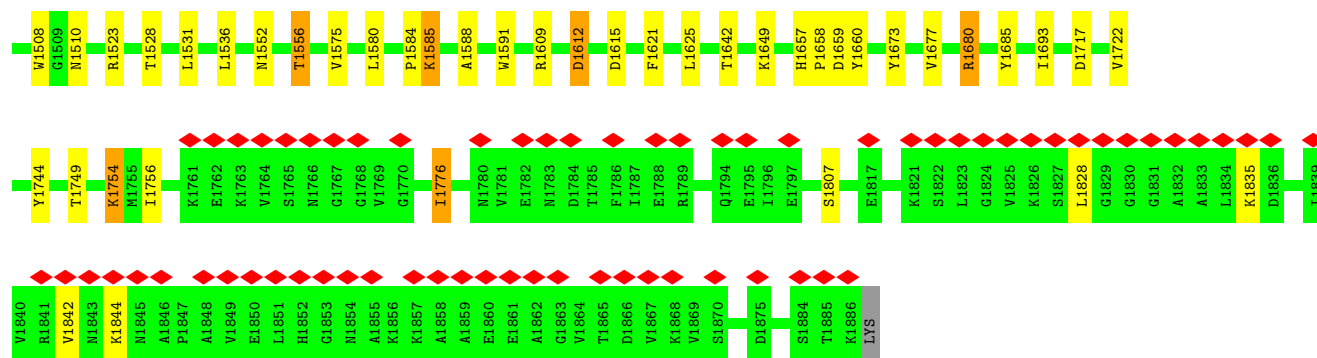




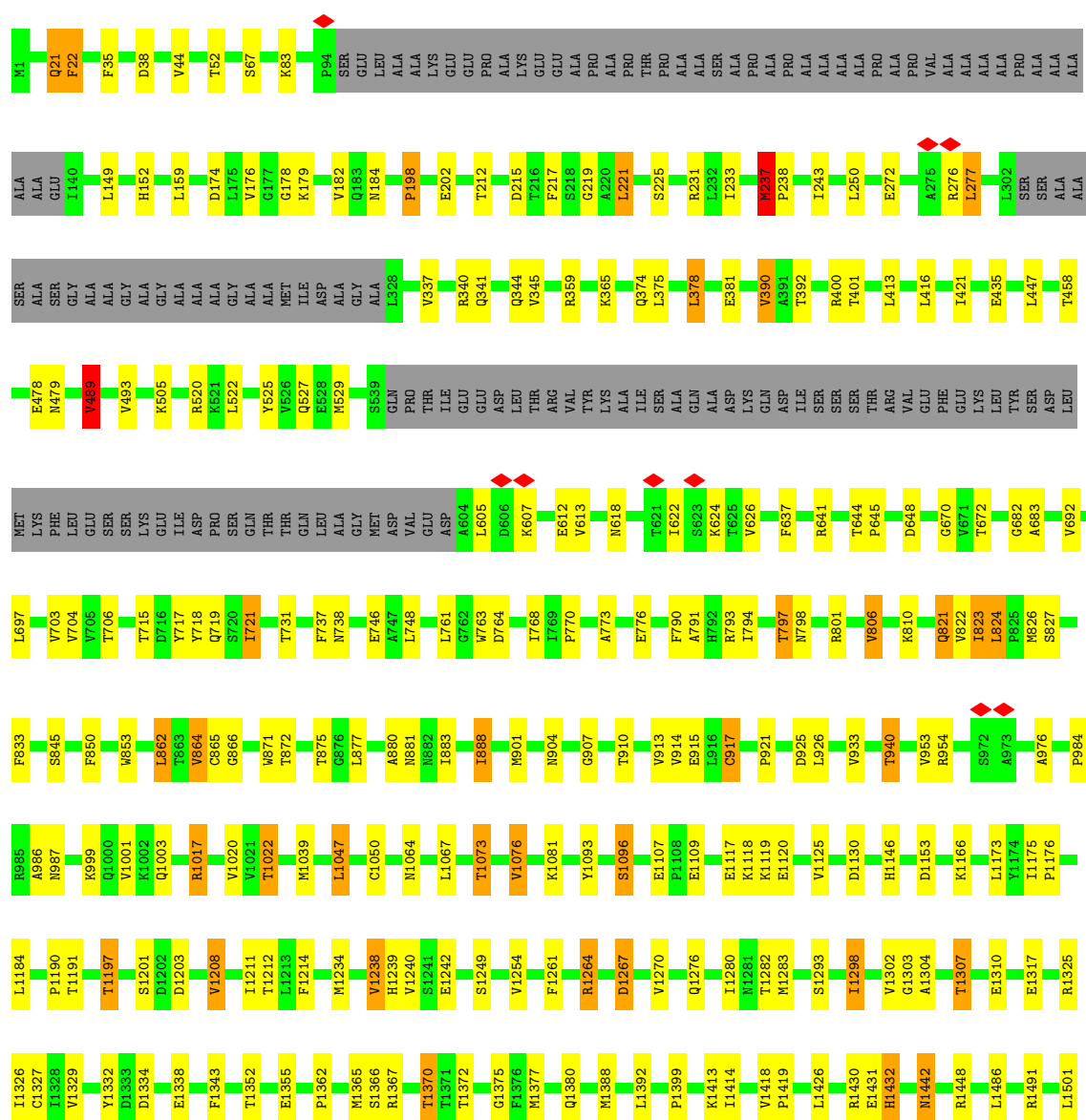
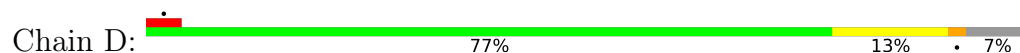
• Molecule 1: Fatty acid synthase subunit alpha

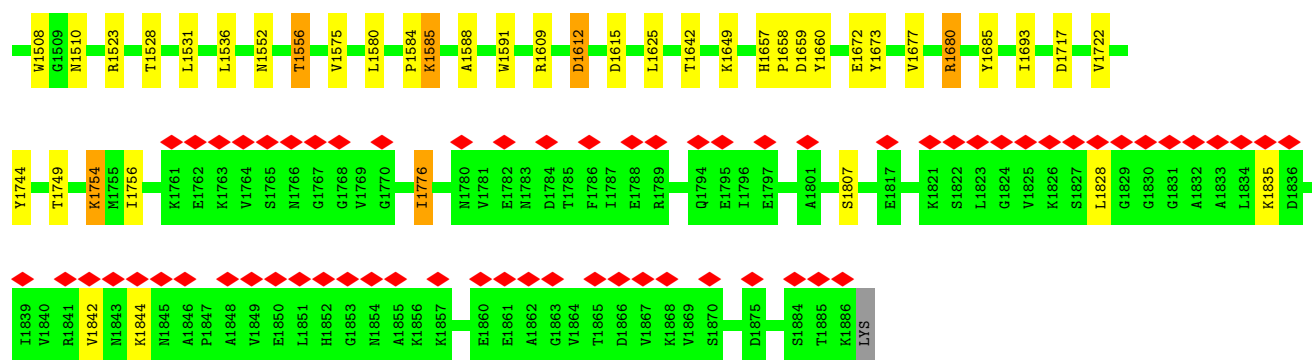
Chain C: 77% 13% 7%



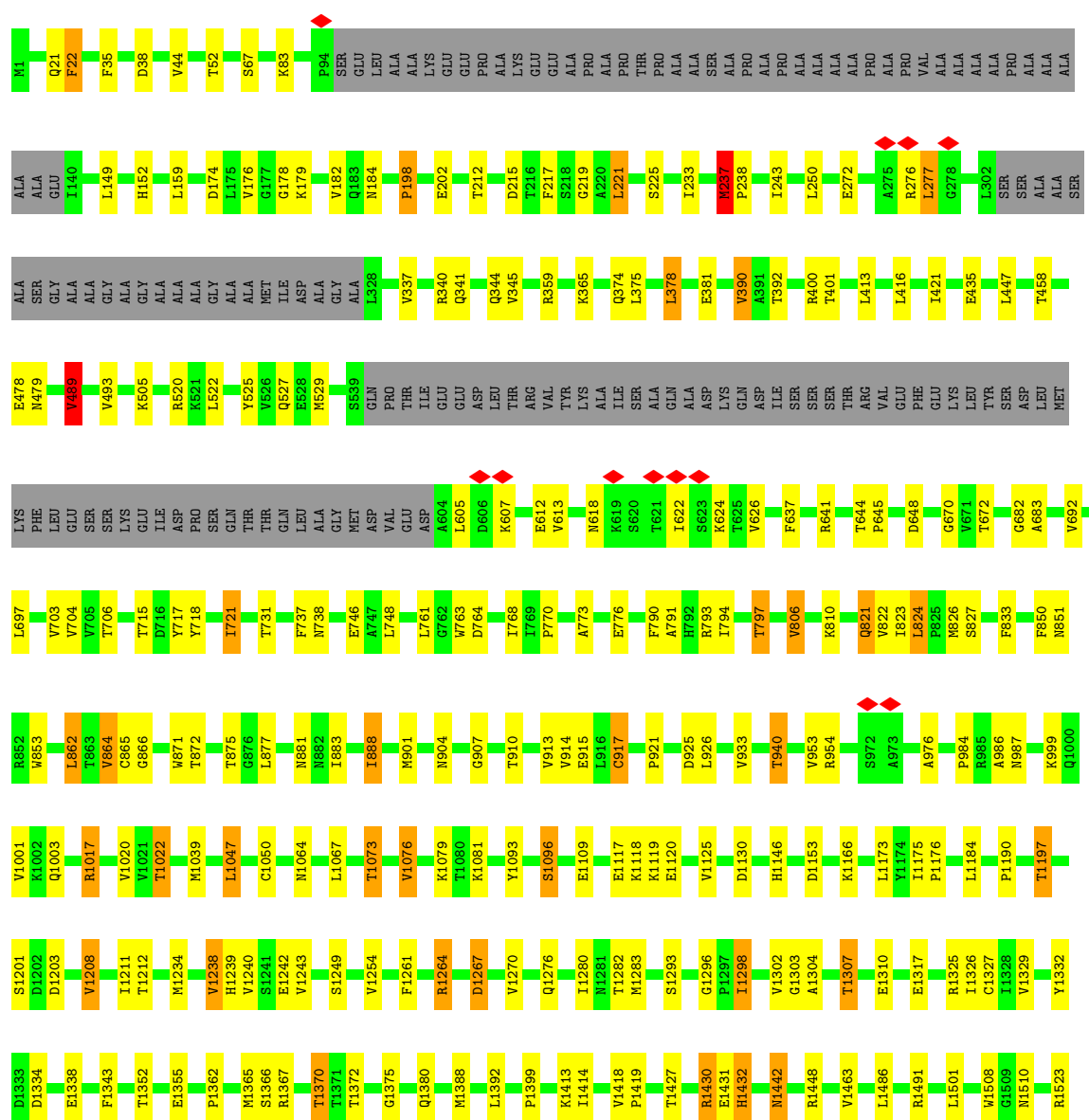


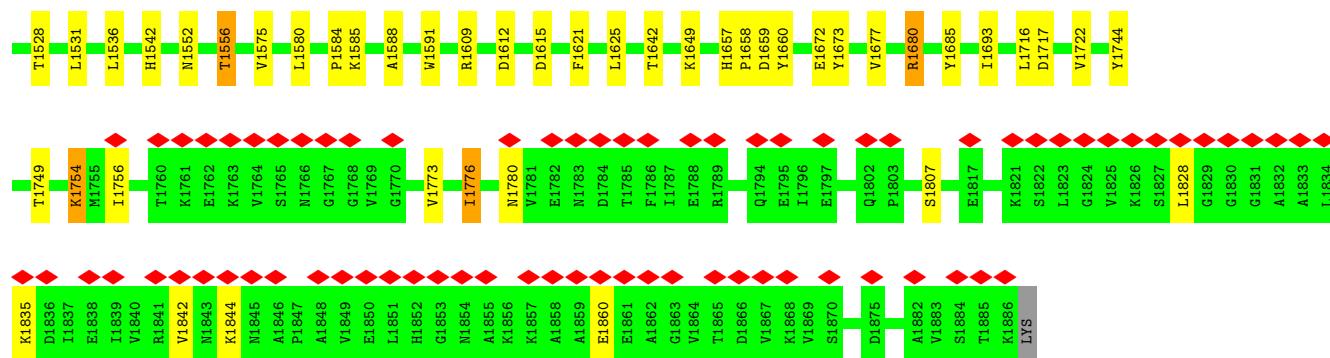
• Molecule 1: Fatty acid synthase subunit alpha



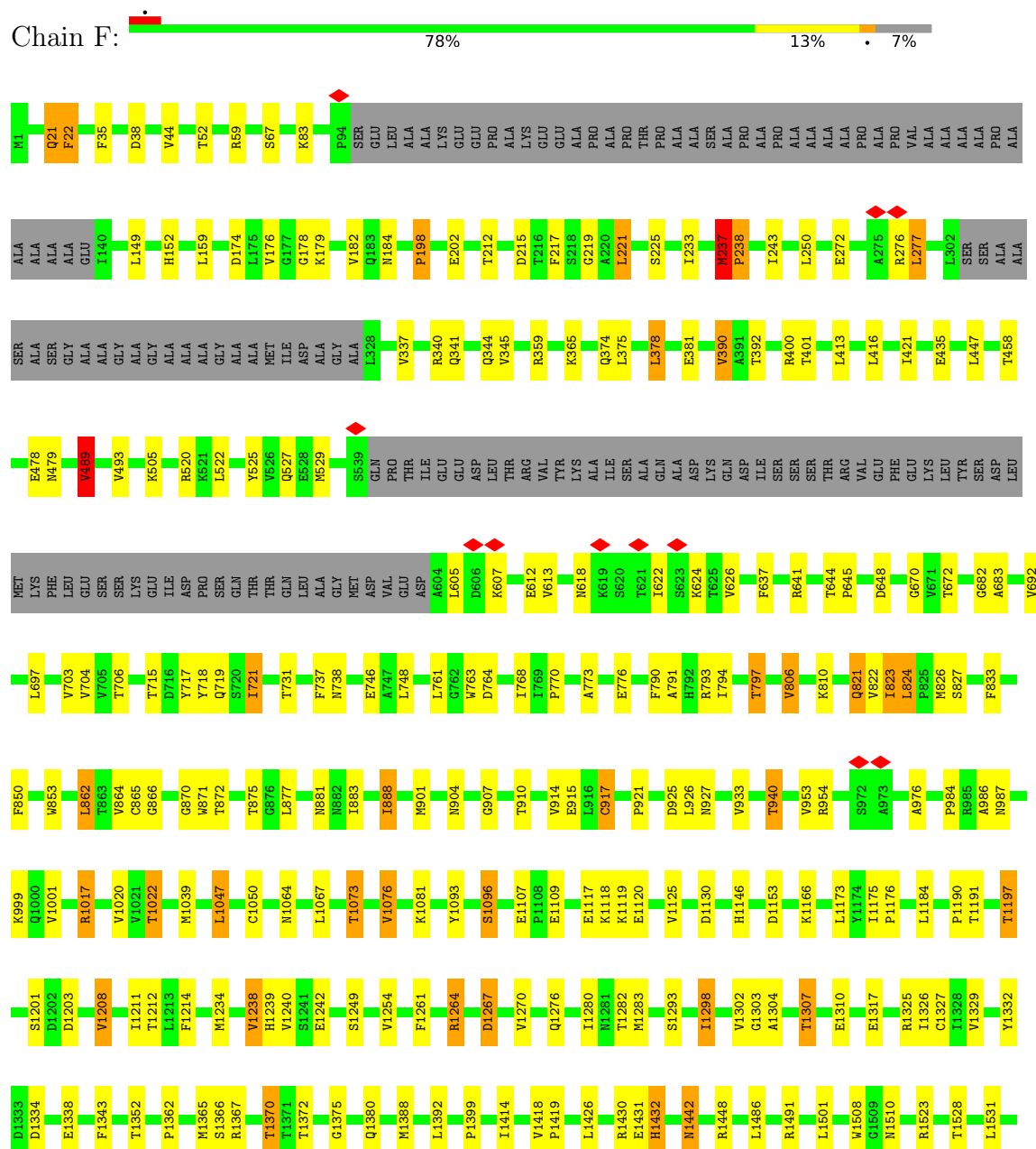


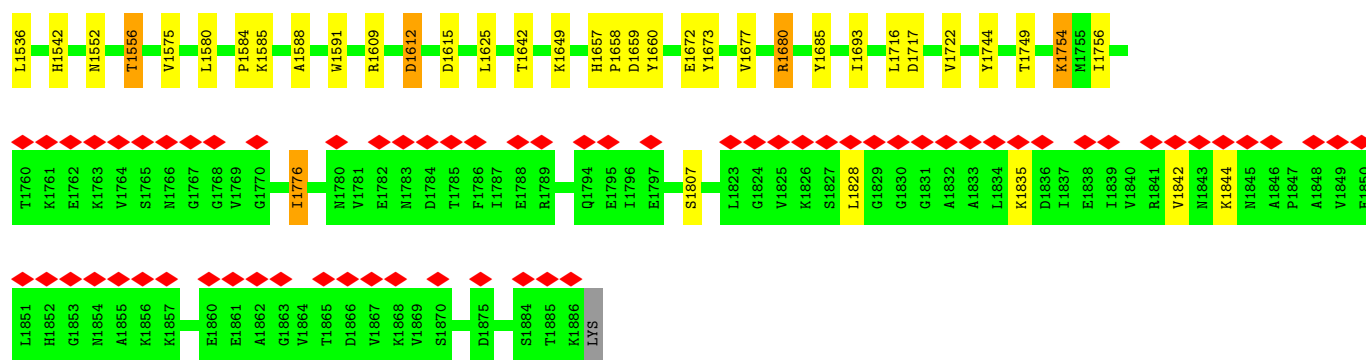
● Molecule 1: Fatty acid synthase subunit alpha





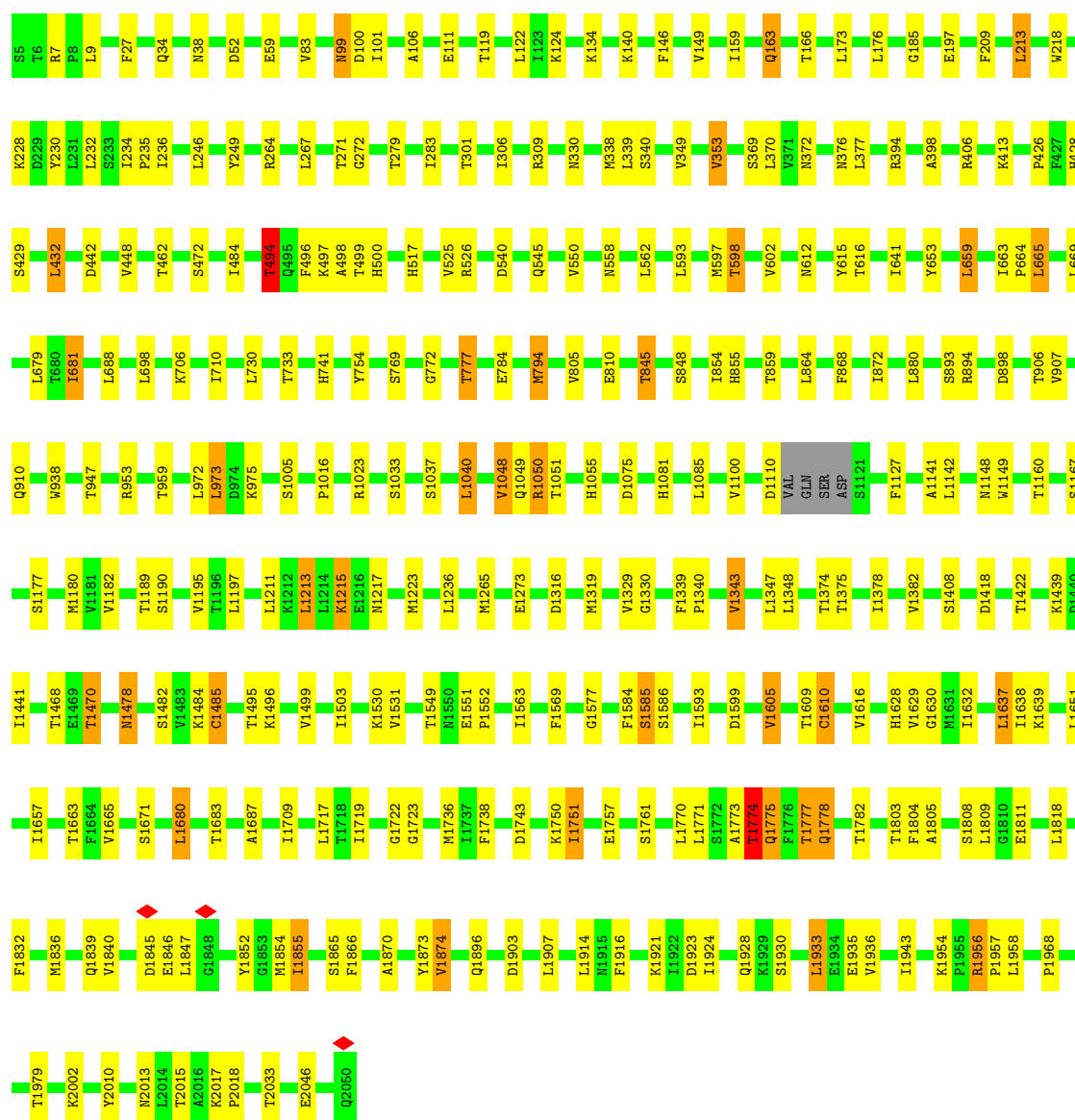
- Molecule 1: Fatty acid synthase subunit alpha





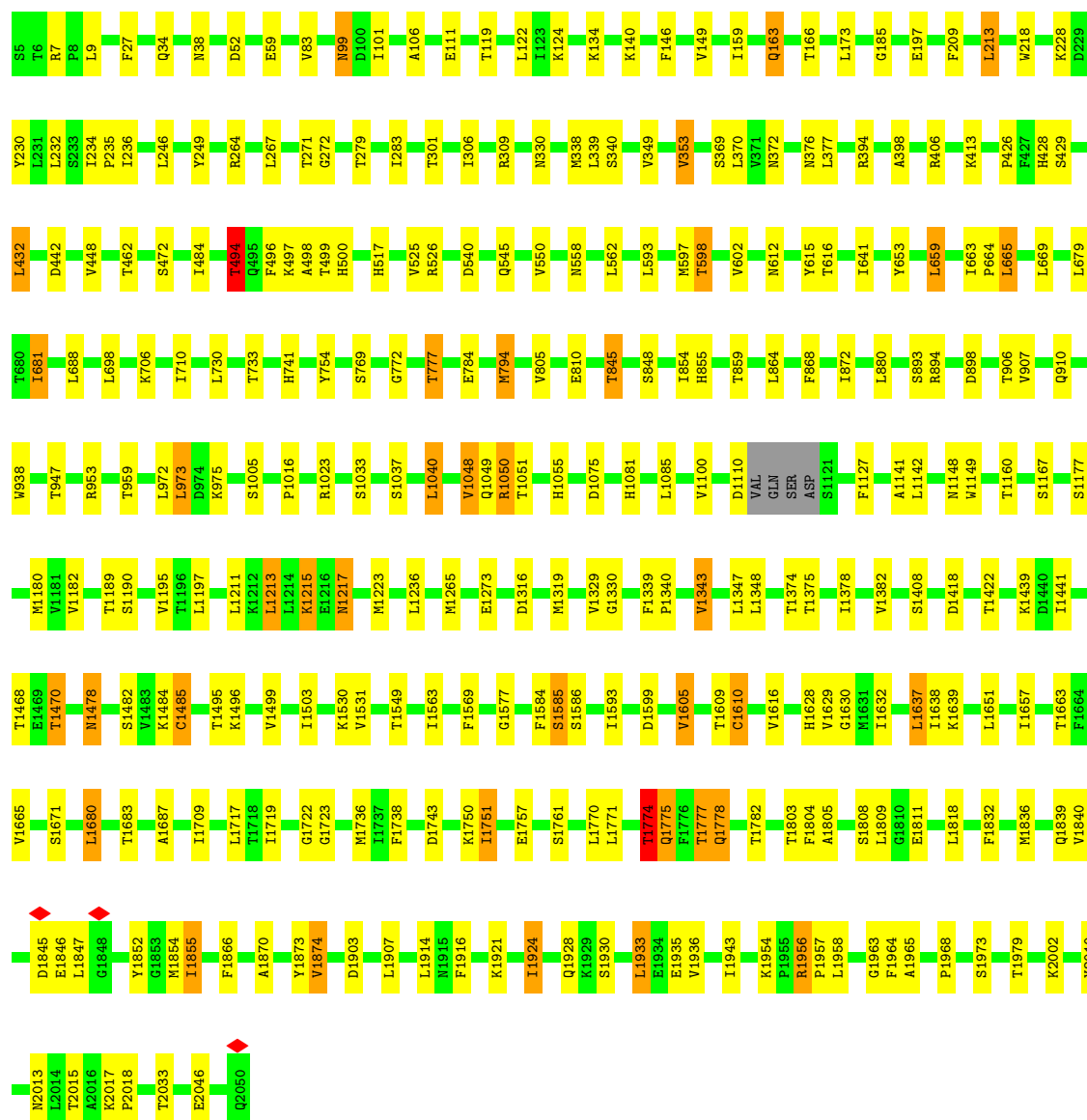
• Molecule 2: Fatty acid synthase subunit beta

Chain G: 85% 13%



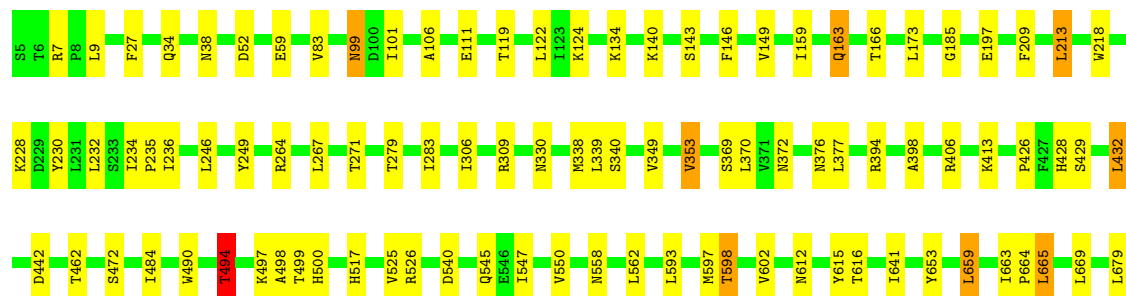
• Molecule 2: Fatty acid synthase subunit beta

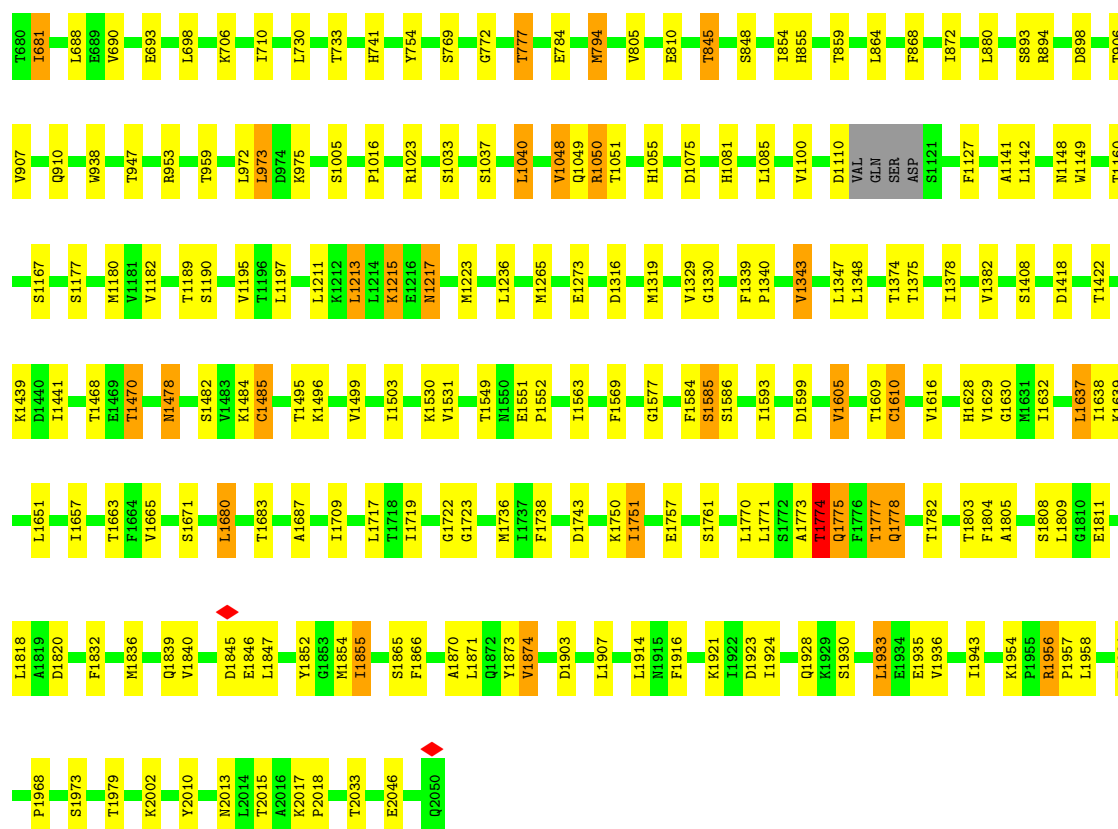
Chain H:  85% 13% .



• Molecule 2: Fatty acid synthase subunit beta

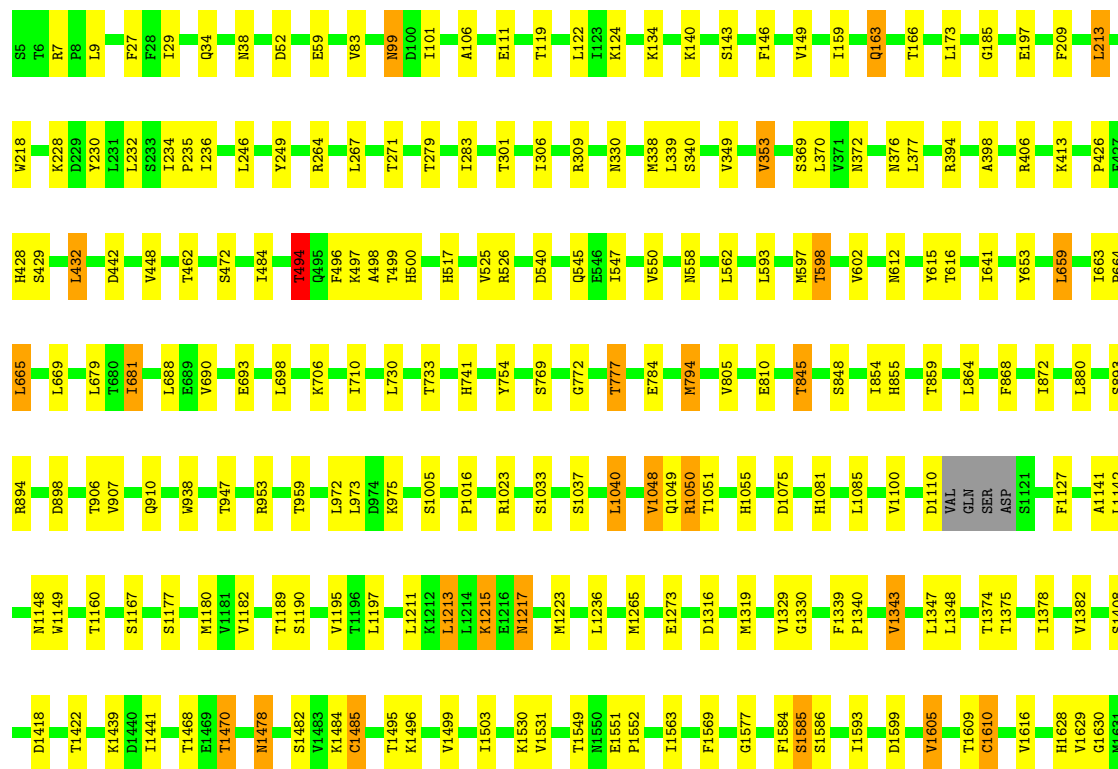
Chain I:  85% 13% .

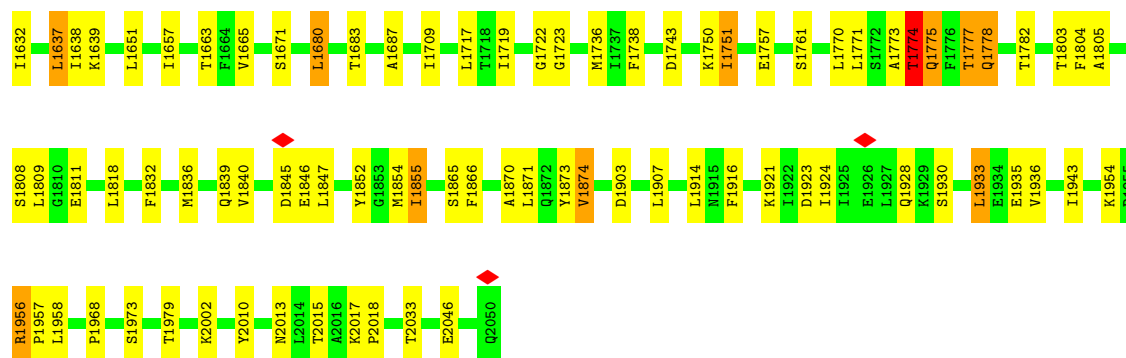




• Molecule 2: Fatty acid synthase subunit beta

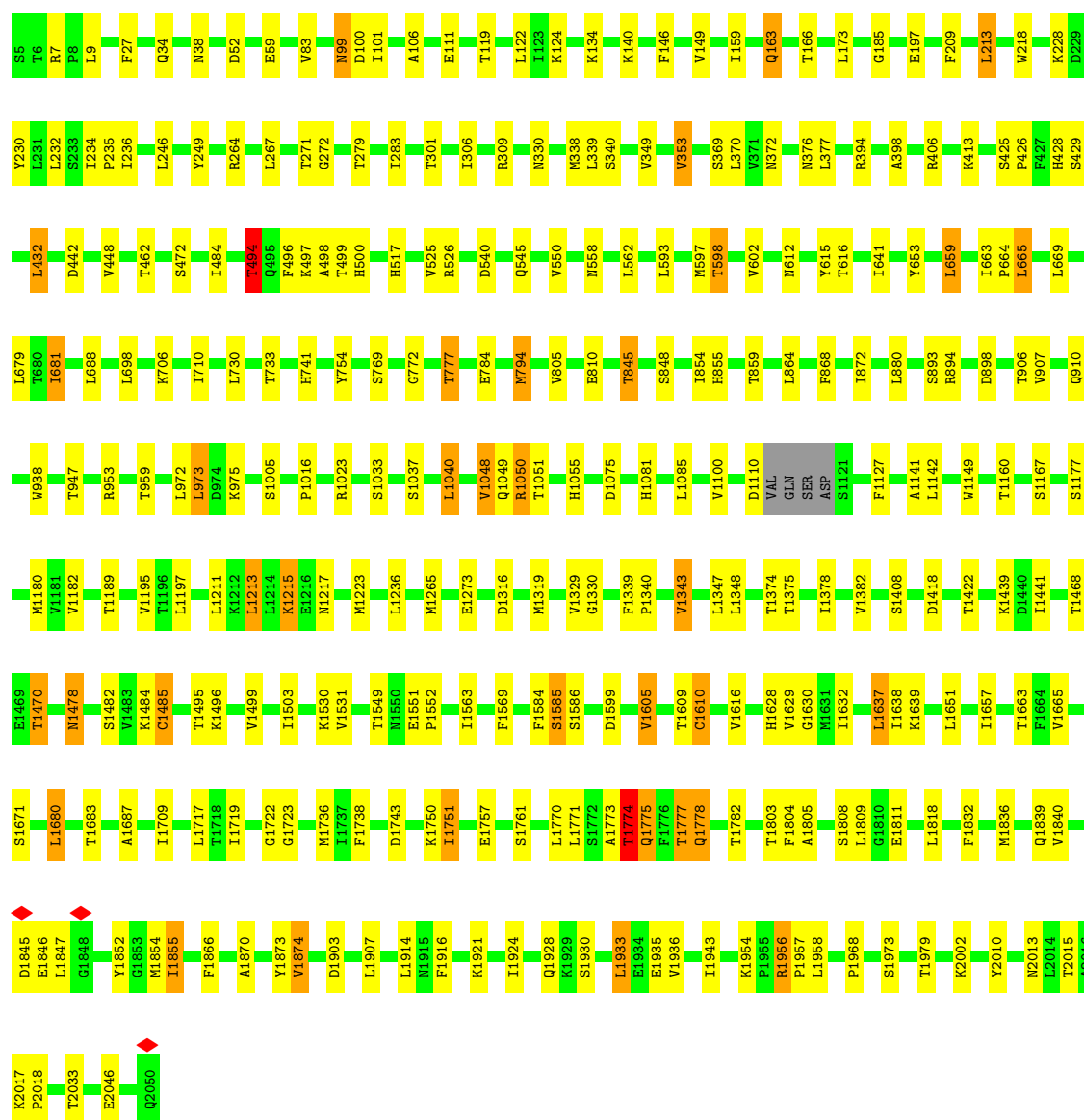
Chain J: 85% 13% .





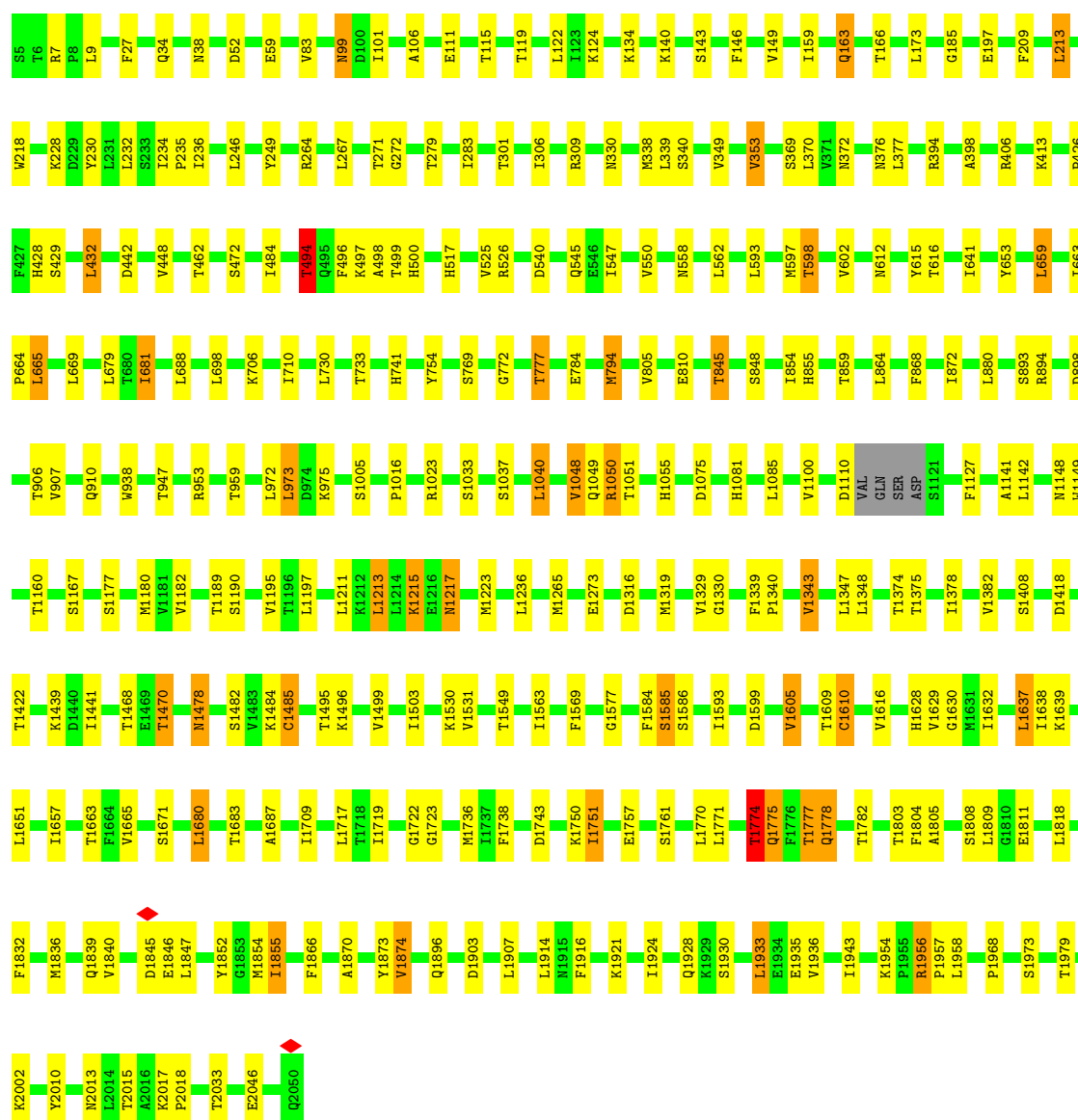
• Molecule 2: Fatty acid synthase subunit beta

Chain K: 85% 13% .



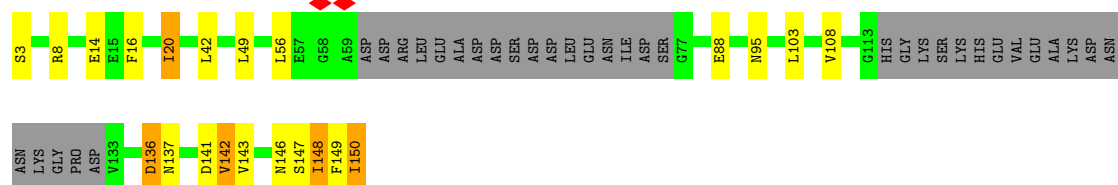
• Molecule 2: Fatty acid synthase subunit beta

Chain L:  85% 13% .



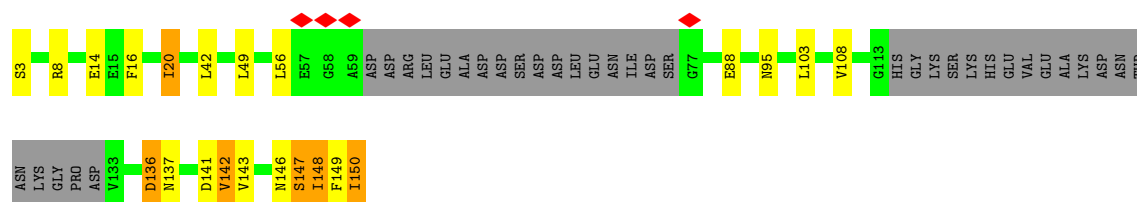
• Molecule 3: Translation machinery-associated protein 17

Chain M:  61% 11% 24% .

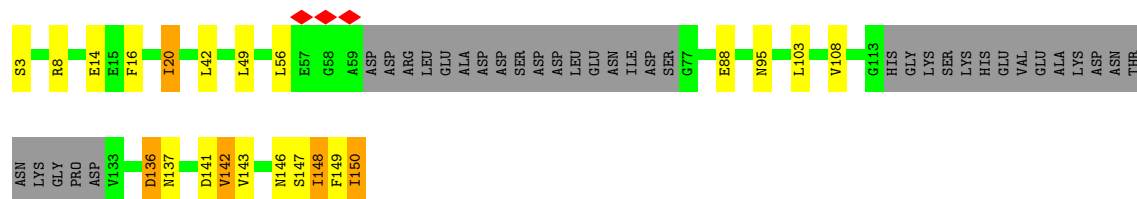


• Molecule 3: Translation machinery-associated protein 17

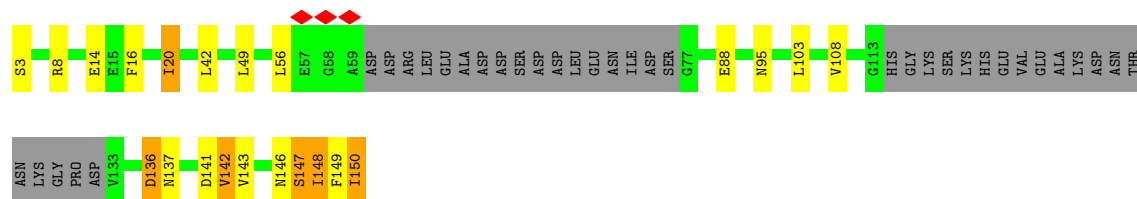
Chain N:  61% 11% 24% .



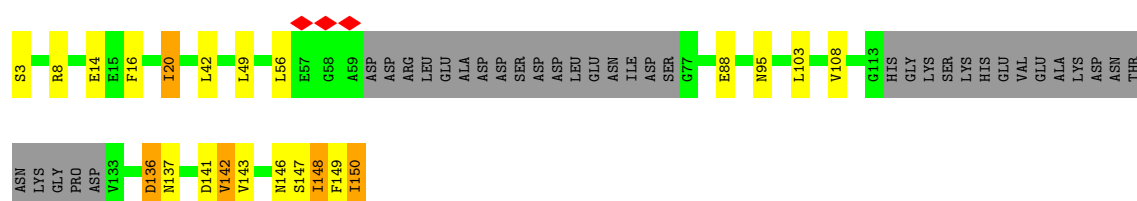
• Molecule 3: Translation machinery-associated protein 17



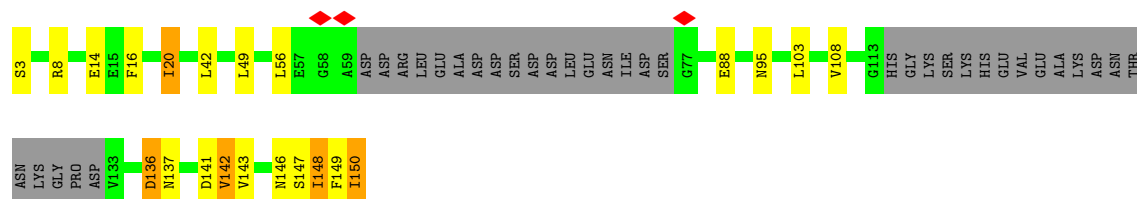
• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	110597	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	132000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.142	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PNS

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	A	1.13	6/13878 (0.0%)	1.59	50/18755 (0.3%)
1	B	1.13	4/13878 (0.0%)	1.59	51/18755 (0.3%)
1	C	1.13	4/13878 (0.0%)	1.59	47/18755 (0.3%)
1	D	1.13	4/13878 (0.0%)	1.59	49/18755 (0.3%)
1	E	1.13	5/13878 (0.0%)	1.59	54/18755 (0.3%)
1	F	1.13	5/13878 (0.0%)	1.59	45/18755 (0.2%)
2	G	1.03	1/16383 (0.0%)	1.50	16/22229 (0.1%)
2	H	1.03	1/16383 (0.0%)	1.49	17/22229 (0.1%)
2	I	1.03	1/16383 (0.0%)	1.50	16/22229 (0.1%)
2	J	1.03	1/16383 (0.0%)	1.50	18/22229 (0.1%)
2	K	1.03	1/16383 (0.0%)	1.50	15/22229 (0.1%)
2	L	1.03	1/16383 (0.0%)	1.50	16/22229 (0.1%)
3	M	1.10	0/885	1.73	0/1189
3	N	1.11	0/885	1.72	0/1189
3	O	1.10	0/885	1.73	0/1189
3	P	1.10	0/885	1.73	0/1189
3	Q	1.11	0/885	1.73	0/1189
3	R	1.10	0/885	1.73	0/1189
All	All	1.08	34/186876 (0.0%)	1.55	394/253038 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	G	0	6
2	H	0	6
2	I	0	6
2	J	0	6
2	K	0	6
2	L	0	6
All	All	0	42

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1399	PRO	C-O	-6.00	1.16	1.23
1	F	1399	PRO	C-O	-5.97	1.16	1.23
1	C	1399	PRO	C-O	-5.93	1.16	1.23
1	E	1399	PRO	C-O	-5.90	1.16	1.23
1	D	1399	PRO	C-O	-5.90	1.16	1.23
1	A	1399	PRO	C-O	-5.87	1.16	1.23
2	H	1273	GLU	N-CA	5.35	1.49	1.46
1	B	1615	ASP	C-O	-5.32	1.17	1.23
2	K	1273	GLU	N-CA	5.31	1.49	1.46
1	E	1615	ASP	C-O	-5.27	1.17	1.23
1	F	1615	ASP	C-O	-5.26	1.17	1.23
1	D	1615	ASP	C-O	-5.25	1.17	1.23
1	C	1615	ASP	C-O	-5.24	1.17	1.23
2	J	1273	GLU	N-CA	5.23	1.49	1.46
2	I	1273	GLU	N-CA	5.23	1.49	1.46
1	A	1615	ASP	C-O	-5.21	1.17	1.23
2	G	1273	GLU	N-CA	5.19	1.49	1.46
1	E	862	LEU	C-O	-5.12	1.17	1.23
1	D	791	ALA	C-O	-5.11	1.18	1.24
1	F	791	ALA	C-O	-5.10	1.18	1.24
1	F	862	LEU	C-O	-5.10	1.17	1.23
1	A	791	ALA	C-O	-5.10	1.18	1.24
1	E	791	ALA	C-O	-5.10	1.18	1.24
1	B	862	LEU	C-O	-5.08	1.17	1.23
1	F	1542	HIS	CE1-NE2	5.07	1.37	1.32
1	C	862	LEU	C-O	-5.06	1.17	1.23
2	L	1273	GLU	N-CA	5.06	1.49	1.46
1	D	862	LEU	C-O	-5.05	1.17	1.23
1	B	791	ALA	C-O	-5.05	1.18	1.24
1	C	791	ALA	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	862	LEU	C-O	-5.03	1.17	1.23
1	E	1542	HIS	CE1-NE2	5.01	1.37	1.32
1	A	1542	HIS	CE1-NE2	5.01	1.37	1.32
1	A	166	ILE	N-CA	5.00	1.50	1.46

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	494	THR	CB-CA-C	7.95	121.66	111.40
2	G	494	THR	CB-CA-C	7.95	121.65	111.40
2	K	494	THR	CB-CA-C	7.92	121.62	111.40
2	I	494	THR	CB-CA-C	7.91	121.61	111.40
2	J	494	THR	CB-CA-C	7.89	121.58	111.40
2	H	494	THR	CB-CA-C	7.85	121.53	111.40
1	B	1176	PRO	CB-CA-C	-7.10	102.14	111.23
1	E	1176	PRO	CB-CA-C	-7.07	102.18	111.23
1	F	1176	PRO	CB-CA-C	-7.04	102.22	111.23
1	C	1176	PRO	CB-CA-C	-7.04	102.22	111.23
1	D	1176	PRO	CB-CA-C	-7.01	102.26	111.23
1	A	1176	PRO	CB-CA-C	-6.98	102.29	111.23
2	H	432	LEU	CA-C-N	6.58	124.39	120.24
2	H	432	LEU	C-N-CA	6.58	124.39	120.24
2	K	432	LEU	CA-C-N	6.56	124.38	120.24
2	K	432	LEU	C-N-CA	6.56	124.38	120.24
2	I	432	LEU	CA-C-N	6.55	124.36	120.24
2	I	432	LEU	C-N-CA	6.55	124.36	120.24
1	E	1612	ASP	CA-CB-CG	6.50	119.10	112.60
1	F	1612	ASP	CA-CB-CG	6.50	119.09	112.60
2	J	432	LEU	CA-C-N	6.49	124.33	120.24
2	J	432	LEU	C-N-CA	6.49	124.33	120.24
2	L	432	LEU	CA-C-N	6.49	124.33	120.24
2	L	432	LEU	C-N-CA	6.49	124.33	120.24
1	B	1612	ASP	CA-CB-CG	6.47	119.07	112.60
1	D	1612	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	1612	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	1612	ASP	CA-CB-CG	6.43	119.03	112.60
1	C	1197	THR	CA-CB-OG1	6.43	119.25	109.60
1	B	1197	THR	CA-CB-OG1	6.33	119.09	109.60
1	A	1197	THR	CA-CB-OG1	6.33	119.09	109.60
1	E	1197	THR	CA-CB-OG1	6.32	119.08	109.60
2	G	432	LEU	CA-C-N	6.30	124.21	120.24
2	G	432	LEU	C-N-CA	6.30	124.21	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1197	THR	CA-CB-OG1	6.26	119.00	109.60
1	F	1197	THR	CA-CB-OG1	6.22	118.93	109.60
2	H	1215	LYS	CA-C-N	6.12	128.77	120.38
2	H	1215	LYS	C-N-CA	6.12	128.77	120.38
1	A	976	ALA	CA-C-N	6.04	128.97	120.28
1	A	976	ALA	C-N-CA	6.04	128.97	120.28
1	B	770	PRO	N-CA-CB	-6.02	98.33	102.73
2	J	1215	LYS	CA-C-N	6.02	128.62	120.38
2	J	1215	LYS	C-N-CA	6.02	128.62	120.38
1	D	976	ALA	CA-C-N	6.01	128.94	120.28
1	D	976	ALA	C-N-CA	6.01	128.94	120.28
1	D	770	PRO	N-CA-CB	-6.01	98.34	102.73
1	A	1264	ARG	CG-CD-NE	-6.01	98.78	112.00
1	E	1264	ARG	CG-CD-NE	-6.01	98.79	112.00
1	D	1264	ARG	CG-CD-NE	-6.00	98.79	112.00
1	F	1264	ARG	CG-CD-NE	-6.00	98.79	112.00
1	C	1264	ARG	CG-CD-NE	-5.99	98.81	112.00
1	B	1264	ARG	CG-CD-NE	-5.97	98.86	112.00
1	F	770	PRO	N-CA-CB	-5.97	98.37	102.73
1	C	770	PRO	N-CA-CB	-5.96	98.38	102.73
1	A	770	PRO	N-CA-CB	-5.95	98.39	102.73
2	K	1215	LYS	CA-C-N	5.93	128.50	120.38
2	K	1215	LYS	C-N-CA	5.93	128.50	120.38
1	E	746	GLU	CA-C-N	5.92	128.13	120.44
1	E	746	GLU	C-N-CA	5.92	128.13	120.44
1	C	746	GLU	CA-C-N	5.91	128.12	120.44
1	C	746	GLU	C-N-CA	5.91	128.12	120.44
1	D	746	GLU	CA-C-N	5.91	128.12	120.44
1	D	746	GLU	C-N-CA	5.91	128.12	120.44
1	E	770	PRO	N-CA-CB	-5.89	98.43	102.73
2	I	1215	LYS	CA-C-N	5.88	128.43	120.38
2	I	1215	LYS	C-N-CA	5.88	128.43	120.38
2	G	1215	LYS	CA-C-N	5.87	128.42	120.38
2	G	1215	LYS	C-N-CA	5.87	128.42	120.38
2	L	1215	LYS	CA-C-N	5.87	128.42	120.38
2	L	1215	LYS	C-N-CA	5.87	128.42	120.38
1	B	976	ALA	CA-C-N	5.76	128.57	120.28
1	B	976	ALA	C-N-CA	5.76	128.57	120.28
2	L	1722	GLY	CA-C-O	-5.75	116.12	121.18
1	A	1588	ALA	CA-C-N	5.74	126.32	120.00
1	A	1588	ALA	C-N-CA	5.74	126.32	120.00
1	F	976	ALA	CA-C-N	5.73	128.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	976	ALA	C-N-CA	5.73	128.53	120.28
2	K	1722	GLY	CA-C-O	-5.72	116.15	121.18
2	G	1722	GLY	CA-C-O	-5.71	116.15	121.18
1	E	1588	ALA	CA-C-N	5.70	126.27	120.00
1	E	1588	ALA	C-N-CA	5.70	126.27	120.00
1	D	1588	ALA	CA-C-N	5.70	126.27	120.00
1	D	1588	ALA	C-N-CA	5.70	126.27	120.00
2	H	1722	GLY	CA-C-O	-5.70	116.17	121.18
1	B	1588	ALA	CA-C-N	5.69	126.26	120.00
1	B	1588	ALA	C-N-CA	5.69	126.26	120.00
1	F	1588	ALA	CA-C-N	5.69	126.26	120.00
1	F	1588	ALA	C-N-CA	5.69	126.26	120.00
1	F	746	GLU	CA-C-N	5.68	128.17	120.44
1	F	746	GLU	C-N-CA	5.68	128.17	120.44
2	I	1722	GLY	CA-C-O	-5.68	116.18	121.18
1	C	1588	ALA	CA-C-N	5.67	126.24	120.00
1	C	1588	ALA	C-N-CA	5.67	126.24	120.00
1	C	1375	GLY	CA-C-O	-5.67	118.37	122.45
1	C	976	ALA	CA-C-N	5.66	128.43	120.28
1	C	976	ALA	C-N-CA	5.66	128.43	120.28
2	J	1722	GLY	CA-C-O	-5.66	116.20	121.18
1	B	746	GLU	CA-C-N	5.64	128.11	120.44
1	B	746	GLU	C-N-CA	5.64	128.11	120.44
1	C	1612	ASP	N-CA-C	-5.64	104.35	111.11
2	H	1723	GLY	CA-C-O	-5.62	117.39	122.57
1	E	976	ALA	CA-C-N	5.62	128.37	120.28
1	E	976	ALA	C-N-CA	5.62	128.37	120.28
1	F	1612	ASP	N-CA-C	-5.61	104.37	111.11
1	A	746	GLU	CA-C-N	5.60	128.05	120.44
1	A	746	GLU	C-N-CA	5.60	128.05	120.44
1	D	1612	ASP	N-CA-C	-5.58	104.42	111.11
1	F	1343	PHE	CA-C-N	5.58	126.13	120.00
1	F	1343	PHE	C-N-CA	5.58	126.13	120.00
1	E	1375	GLY	CA-C-O	-5.56	118.31	122.37
2	J	1723	GLY	CA-C-O	-5.55	117.46	122.57
2	L	1723	GLY	CA-C-O	-5.55	117.46	122.57
1	E	1343	PHE	CA-C-N	5.54	126.10	120.00
1	E	1343	PHE	C-N-CA	5.54	126.10	120.00
1	A	1375	GLY	CA-C-O	-5.53	118.34	122.37
1	A	1612	ASP	N-CA-C	-5.53	104.48	111.11
1	B	1375	GLY	CA-C-O	-5.53	118.34	122.37
1	D	1343	PHE	CA-C-N	5.52	126.08	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1343	PHE	C-N-CA	5.52	126.08	120.00
1	B	1343	PHE	CA-C-N	5.52	126.07	120.00
1	B	1343	PHE	C-N-CA	5.52	126.07	120.00
1	C	1343	PHE	CA-C-N	5.52	126.07	120.00
1	C	1343	PHE	C-N-CA	5.52	126.07	120.00
1	A	1343	PHE	CA-C-N	5.51	126.06	120.00
1	A	1343	PHE	C-N-CA	5.51	126.06	120.00
1	F	1120	GLU	CB-CG-CD	5.50	121.94	112.60
1	F	1375	GLY	CA-C-O	-5.50	118.36	122.37
1	D	1375	GLY	CA-C-O	-5.49	118.36	122.37
2	I	1723	GLY	CA-C-O	-5.48	117.53	122.57
2	K	1723	GLY	CA-C-O	-5.48	117.53	122.57
1	A	1680	ARG	CG-CD-NE	-5.47	99.95	112.00
1	D	1680	ARG	CG-CD-NE	-5.47	99.96	112.00
2	G	1723	GLY	CA-C-O	-5.47	117.54	122.57
1	C	1680	ARG	CG-CD-NE	-5.46	100.00	112.00
1	B	1120	GLU	CB-CG-CD	5.45	121.86	112.60
1	E	1680	ARG	CG-CD-NE	-5.44	100.03	112.00
1	F	692	VAL	N-CA-C	-5.44	105.31	110.42
1	C	1190	PRO	CA-C-O	-5.44	115.41	121.23
1	B	1835	LYS	CA-C-N	5.44	127.51	120.44
1	B	1835	LYS	C-N-CA	5.44	127.51	120.44
1	F	1835	LYS	CA-C-N	5.43	127.50	120.44
1	F	1835	LYS	C-N-CA	5.43	127.50	120.44
1	F	1680	ARG	CG-CD-NE	-5.43	100.06	112.00
1	A	1190	PRO	CA-C-O	-5.42	115.43	121.23
1	E	1612	ASP	N-CA-C	-5.42	104.40	111.02
1	B	250	LEU	CA-C-N	5.42	128.09	120.28
1	B	250	LEU	C-N-CA	5.42	128.09	120.28
1	B	1612	ASP	N-CA-C	-5.42	104.41	111.02
1	B	1190	PRO	CA-C-O	-5.42	115.44	121.23
1	E	692	VAL	N-CA-C	-5.42	105.33	110.42
1	B	915	GLU	CA-C-O	-5.41	115.14	120.82
1	E	1776	ILE	CA-C-N	5.41	127.53	120.28
1	E	1776	ILE	C-N-CA	5.41	127.53	120.28
1	A	915	GLU	CA-C-O	-5.41	115.14	120.82
1	A	692	VAL	N-CA-C	-5.41	105.34	110.42
1	A	1835	LYS	CA-C-N	5.40	127.47	120.44
1	A	1835	LYS	C-N-CA	5.40	127.47	120.44
1	C	1835	LYS	CA-C-N	5.40	127.47	120.44
1	C	1835	LYS	C-N-CA	5.40	127.47	120.44
1	E	1835	LYS	CA-C-N	5.39	127.45	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1835	LYS	C-N-CA	5.39	127.45	120.44
1	B	1680	ARG	CG-CD-NE	-5.39	100.15	112.00
1	A	1120	GLU	CB-CG-CD	5.38	121.75	112.60
1	D	1835	LYS	CA-C-N	5.38	127.44	120.44
1	D	1835	LYS	C-N-CA	5.38	127.44	120.44
1	A	1776	ILE	CA-C-N	5.37	127.48	120.28
1	A	1776	ILE	C-N-CA	5.37	127.48	120.28
1	E	1190	PRO	CA-C-O	-5.37	115.48	121.23
1	B	1119	LYS	CA-C-O	-5.37	114.83	120.58
1	D	692	VAL	N-CA-C	-5.36	105.38	110.42
1	A	250	LEU	CA-C-N	5.36	128.00	120.28
1	A	250	LEU	C-N-CA	5.36	128.00	120.28
1	B	692	VAL	N-CA-C	-5.36	105.38	110.42
1	F	1190	PRO	CA-C-O	-5.36	115.50	121.23
2	G	1329	VAL	CA-C-N	5.36	125.78	119.94
2	G	1329	VAL	C-N-CA	5.36	125.78	119.94
1	D	250	LEU	CA-C-N	5.35	127.99	120.28
1	D	250	LEU	C-N-CA	5.35	127.99	120.28
1	F	915	GLU	CA-C-O	-5.35	115.20	120.82
1	D	915	GLU	CA-C-O	-5.35	115.20	120.82
1	C	915	GLU	CA-C-O	-5.35	115.20	120.82
1	D	1120	GLU	CB-CG-CD	5.35	121.69	112.60
1	E	250	LEU	CA-C-N	5.35	127.98	120.28
1	E	250	LEU	C-N-CA	5.35	127.98	120.28
1	D	1190	PRO	CA-C-O	-5.34	115.51	121.23
1	D	1776	ILE	CA-C-N	5.34	127.44	120.28
1	D	1776	ILE	C-N-CA	5.34	127.44	120.28
1	E	915	GLU	CA-C-O	-5.34	115.21	120.82
1	C	1120	GLU	CB-CG-CD	5.33	121.67	112.60
1	F	1119	LYS	CA-C-O	-5.33	114.88	120.58
1	C	692	VAL	N-CA-C	-5.32	105.42	110.42
2	J	1329	VAL	CA-C-N	5.32	125.74	119.94
2	J	1329	VAL	C-N-CA	5.32	125.74	119.94
1	F	250	LEU	CA-C-N	5.32	127.94	120.28
1	F	250	LEU	C-N-CA	5.32	127.94	120.28
1	B	489	VAL	N-CA-CB	-5.31	102.97	111.58
2	G	1418	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	489	VAL	N-CA-CB	-5.31	102.98	111.58
1	C	1119	LYS	CA-C-O	-5.31	114.90	120.58
1	D	1119	LYS	CA-C-O	-5.31	114.90	120.58
1	C	250	LEU	CA-C-N	5.30	127.92	120.28
1	C	250	LEU	C-N-CA	5.30	127.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1120	GLU	CB-CG-CD	5.30	121.61	112.60
1	C	1776	ILE	CA-C-N	5.29	127.37	120.28
1	C	1776	ILE	C-N-CA	5.29	127.37	120.28
1	F	489	VAL	N-CA-CB	-5.29	103.01	111.58
1	D	697	LEU	N-CA-C	-5.28	105.69	111.82
2	L	1329	VAL	CA-C-N	5.28	125.70	119.94
2	L	1329	VAL	C-N-CA	5.28	125.70	119.94
1	E	1621	PHE	CA-C-N	5.28	127.61	120.38
1	E	1621	PHE	C-N-CA	5.28	127.61	120.38
1	C	1621	PHE	CA-C-N	5.27	127.60	120.38
1	C	1621	PHE	C-N-CA	5.27	127.60	120.38
1	E	489	VAL	N-CA-CB	-5.26	103.06	111.58
1	A	1119	LYS	CA-C-O	-5.26	114.95	120.58
1	B	697	LEU	N-CA-C	-5.26	105.72	111.82
2	H	1329	VAL	CA-C-N	5.26	125.67	119.94
2	H	1329	VAL	C-N-CA	5.26	125.67	119.94
1	D	489	VAL	N-CA-CB	-5.25	103.08	111.58
2	K	1329	VAL	CA-C-N	5.25	125.66	119.94
2	K	1329	VAL	C-N-CA	5.25	125.66	119.94
1	C	152	HIS	CA-C-N	5.24	127.27	120.56
1	C	152	HIS	C-N-CA	5.24	127.27	120.56
1	F	152	HIS	CA-C-N	5.24	127.27	120.56
1	F	152	HIS	C-N-CA	5.24	127.27	120.56
1	F	697	LEU	N-CA-C	-5.24	105.74	111.82
1	A	697	LEU	N-CA-C	-5.24	105.75	111.82
1	E	22	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	489	VAL	N-CA-CB	-5.23	103.11	111.58
1	F	1776	ILE	CA-C-N	5.23	127.28	120.28
1	F	1776	ILE	C-N-CA	5.23	127.28	120.28
1	C	697	LEU	N-CA-C	-5.22	105.76	111.82
1	E	1119	LYS	CA-C-O	-5.22	114.99	120.58
1	B	152	HIS	CA-C-N	5.21	127.23	120.56
1	B	152	HIS	C-N-CA	5.21	127.23	120.56
1	D	152	HIS	CA-C-N	5.21	127.23	120.56
1	D	152	HIS	C-N-CA	5.21	127.23	120.56
1	E	697	LEU	N-CA-C	-5.21	105.78	111.82
1	C	22	PHE	CA-CB-CG	5.20	119.00	113.80
1	E	152	HIS	CA-C-N	5.20	127.22	120.56
1	E	152	HIS	C-N-CA	5.20	127.22	120.56
2	K	1418	ASP	CA-CB-CG	5.20	117.80	112.60
2	I	83	VAL	CA-C-N	5.20	127.19	120.44
2	I	83	VAL	C-N-CA	5.20	127.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1418	ASP	CA-CB-CG	5.20	117.80	112.60
2	K	1719	ILE	CA-C-O	-5.19	114.93	121.11
1	A	152	HIS	CA-C-N	5.19	127.20	120.56
1	A	152	HIS	C-N-CA	5.19	127.20	120.56
1	C	738	ASN	CA-C-O	-5.19	114.79	120.70
2	L	83	VAL	CA-C-N	5.18	127.18	120.44
2	L	83	VAL	C-N-CA	5.18	127.18	120.44
1	B	22	PHE	CA-CB-CG	5.18	118.98	113.80
2	H	1719	ILE	CA-C-O	-5.18	114.94	121.11
2	I	1329	VAL	CA-C-N	5.18	125.58	119.94
2	I	1329	VAL	C-N-CA	5.18	125.58	119.94
2	I	1378	ILE	CB-CA-C	5.18	117.88	111.15
1	B	1776	ILE	CA-C-N	5.17	127.22	120.28
1	B	1776	ILE	C-N-CA	5.17	127.22	120.28
1	D	22	PHE	CA-CB-CG	5.17	118.97	113.80
1	E	35	PHE	CA-CB-CG	5.17	118.97	113.80
1	D	738	ASN	CA-C-O	-5.17	114.80	120.70
1	A	22	PHE	CA-CB-CG	5.16	118.96	113.80
2	G	1719	ILE	CA-C-O	-5.16	114.97	121.11
2	K	1378	ILE	CB-CA-C	5.16	117.85	111.15
2	J	1719	ILE	CA-C-O	-5.15	114.98	121.11
1	E	738	ASN	CA-C-O	-5.15	114.83	120.70
1	F	1693	ILE	CA-C-O	-5.15	114.69	120.25
1	A	738	ASN	CA-C-O	-5.15	114.83	120.70
2	L	1719	ILE	CA-C-O	-5.15	114.98	121.11
1	A	35	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	525	TYR	CA-C-O	-5.14	115.10	120.55
2	G	83	VAL	CA-C-N	5.14	127.13	120.44
2	G	83	VAL	C-N-CA	5.14	127.13	120.44
2	H	83	VAL	CA-C-N	5.14	127.13	120.44
2	H	83	VAL	C-N-CA	5.14	127.13	120.44
1	B	703	VAL	CA-C-O	-5.14	114.91	120.36
1	C	35	PHE	CA-CB-CG	5.14	118.94	113.80
2	J	83	VAL	CA-C-N	5.14	127.13	120.44
2	J	83	VAL	C-N-CA	5.14	127.13	120.44
2	L	1418	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	703	VAL	CA-C-O	-5.14	114.91	120.36
2	K	83	VAL	CA-C-N	5.14	127.12	120.44
2	K	83	VAL	C-N-CA	5.14	127.12	120.44
1	E	703	VAL	CA-C-O	-5.14	114.92	120.36
1	F	22	PHE	CA-CB-CG	5.14	118.94	113.80
1	D	35	PHE	CA-CB-CG	5.13	118.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	525	TYR	CA-C-O	-5.13	115.11	120.55
1	F	703	VAL	CA-C-O	-5.13	114.92	120.36
1	E	1693	ILE	CA-C-O	-5.13	114.71	120.25
1	F	738	ASN	CA-C-O	-5.12	114.86	120.70
2	L	1378	ILE	CB-CA-C	5.12	117.81	111.15
1	D	703	VAL	CA-C-O	-5.12	114.94	120.36
2	I	1839	GLN	N-CA-C	-5.12	107.59	113.88
2	J	1378	ILE	CB-CA-C	5.12	117.80	111.15
1	B	35	PHE	CA-CB-CG	5.11	118.91	113.80
1	F	35	PHE	CA-CB-CG	5.11	118.91	113.80
1	D	1093	TYR	CA-C-O	-5.11	113.10	118.77
1	F	174	ASP	CA-CB-CG	5.11	117.71	112.60
2	G	1378	ILE	CB-CA-C	5.11	117.79	111.15
1	D	1693	ILE	CA-C-O	-5.10	114.75	120.25
2	I	1418	ASP	CA-CB-CG	5.09	117.69	112.60
2	I	1719	ILE	CA-C-O	-5.09	115.05	121.11
2	J	1577	GLY	CA-C-O	-5.09	116.95	122.05
2	H	1378	ILE	CB-CA-C	5.09	117.77	111.15
1	B	1693	ILE	CA-C-O	-5.09	114.75	120.25
2	K	1839	GLN	N-CA-C	-5.09	107.62	113.88
1	C	1093	TYR	CA-C-O	-5.09	113.12	118.77
1	A	1693	ILE	CA-C-O	-5.08	114.76	120.25
1	B	738	ASN	CA-C-O	-5.08	114.91	120.70
1	C	174	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	174	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	525	TYR	CA-C-O	-5.08	115.16	120.55
2	H	1839	GLN	N-CA-C	-5.08	107.63	113.88
2	L	1577	GLY	CA-C-O	-5.08	116.97	122.05
2	H	1418	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	1017	ARG	CB-CA-C	5.07	121.41	110.41
1	F	1093	TYR	CA-C-O	-5.06	113.15	118.77
1	A	174	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	1096	SER	CA-C-N	5.06	127.13	120.60
1	C	1096	SER	C-N-CA	5.06	127.13	120.60
1	A	703	VAL	CA-C-O	-5.06	115.00	120.36
2	G	1577	GLY	CA-C-O	-5.06	116.99	122.05
1	B	1214	PHE	CA-C-O	-5.06	115.17	120.63
1	D	525	TYR	CA-C-O	-5.06	115.19	120.55
1	B	174	ASP	CA-CB-CG	5.06	117.66	112.60
1	F	1096	SER	CA-C-N	5.05	127.12	120.60
1	F	1096	SER	C-N-CA	5.05	127.12	120.60
1	F	1017	ARG	CB-CA-C	5.05	121.37	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	525	TYR	CA-C-O	-5.05	115.20	120.55
1	C	1214	PHE	CA-C-O	-5.05	115.17	120.63
1	A	1096	SER	CA-C-N	5.05	127.11	120.60
1	A	1096	SER	C-N-CA	5.05	127.11	120.60
1	C	1017	ARG	CB-CA-C	5.05	121.36	110.41
1	C	1693	ILE	CA-C-O	-5.05	114.80	120.25
1	E	1093	TYR	CA-C-O	-5.05	113.17	118.77
1	A	1017	ARG	CB-CA-C	5.05	121.36	110.41
1	B	1093	TYR	CA-C-O	-5.05	113.17	118.77
1	F	1672	GLU	CA-C-N	5.05	127.80	120.79
1	F	1672	GLU	C-N-CA	5.05	127.80	120.79
1	A	1003	GLN	CA-C-N	5.04	126.92	120.56
1	A	1003	GLN	C-N-CA	5.04	126.92	120.56
1	E	1003	GLN	CA-C-N	5.04	126.92	120.56
1	E	1003	GLN	C-N-CA	5.04	126.92	120.56
1	E	1017	ARG	CB-CA-C	5.04	121.36	110.41
2	L	1839	GLN	N-CA-C	-5.04	107.67	113.88
1	D	1672	GLU	CA-C-N	5.04	127.80	120.79
1	D	1672	GLU	C-N-CA	5.04	127.80	120.79
1	E	1413	LYS	CA-C-N	5.04	127.34	120.63
1	E	1413	LYS	C-N-CA	5.04	127.34	120.63
1	B	525	TYR	CA-C-O	-5.04	115.21	120.55
1	E	1780	ASN	CA-C-N	5.04	127.01	120.56
1	E	1780	ASN	C-N-CA	5.04	127.01	120.56
1	F	1214	PHE	CA-C-O	-5.04	115.19	120.63
2	J	29	ILE	CA-C-N	5.04	127.03	120.28
2	J	29	ILE	C-N-CA	5.04	127.03	120.28
2	J	1839	GLN	N-CA-C	-5.03	107.69	113.88
1	A	1413	LYS	CA-C-N	5.03	127.32	120.63
1	A	1413	LYS	C-N-CA	5.03	127.32	120.63
1	A	1672	GLU	CA-C-N	5.03	127.78	120.79
1	A	1672	GLU	C-N-CA	5.03	127.78	120.79
1	B	1096	SER	CA-C-N	5.03	127.08	120.60
1	B	1096	SER	C-N-CA	5.03	127.08	120.60
1	B	1860	GLU	CA-C-N	5.03	127.43	120.29
1	B	1860	GLU	C-N-CA	5.03	127.43	120.29
1	D	1017	ARG	CB-CA-C	5.03	121.32	110.41
1	E	1096	SER	CA-C-N	5.03	127.08	120.60
1	E	1096	SER	C-N-CA	5.03	127.08	120.60
2	G	1839	GLN	N-CA-C	-5.03	107.70	113.88
1	B	262	ASP	CA-C-N	5.03	125.66	120.03
1	B	262	ASP	C-N-CA	5.03	125.66	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1413	LYS	CA-C-N	5.02	127.31	120.63
1	B	1413	LYS	C-N-CA	5.02	127.31	120.63
1	D	1096	SER	CA-C-N	5.02	127.08	120.60
1	D	1096	SER	C-N-CA	5.02	127.08	120.60
1	E	174	ASP	CA-CB-CG	5.02	117.62	112.60
1	E	1860	GLU	CA-C-N	5.02	127.42	120.29
1	E	1860	GLU	C-N-CA	5.02	127.42	120.29
1	A	1860	GLU	CA-C-N	5.02	127.42	120.29
1	A	1860	GLU	C-N-CA	5.02	127.42	120.29
1	E	1672	GLU	CA-C-N	5.02	127.76	120.79
1	E	1672	GLU	C-N-CA	5.02	127.76	120.79
1	C	1413	LYS	CA-C-N	5.01	127.30	120.63
1	C	1413	LYS	C-N-CA	5.01	127.30	120.63
2	I	1577	GLY	CA-C-O	-5.01	117.04	122.05
1	B	1003	GLN	CA-C-N	5.01	126.88	120.56
1	B	1003	GLN	C-N-CA	5.01	126.88	120.56
1	D	1413	LYS	CA-C-N	5.01	127.29	120.63
1	D	1413	LYS	C-N-CA	5.01	127.29	120.63
2	H	1924	ILE	CA-C-O	-5.01	116.06	121.27
1	D	1003	GLN	CA-C-N	5.01	126.87	120.56
1	D	1003	GLN	C-N-CA	5.01	126.87	120.56
1	A	1093	TYR	CA-C-O	-5.01	113.21	118.77
1	D	1214	PHE	CA-C-O	-5.00	115.22	120.63
2	H	1577	GLY	CA-C-O	-5.00	117.05	122.05

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	MET	Peptide
1	B	237	MET	Peptide
1	C	237	MET	Peptide
1	D	237	MET	Peptide
1	E	237	MET	Peptide
1	F	237	MET	Peptide
2	G	1050	ARG	Peptide
2	G	1223	MET	Peptide
2	G	1605	VAL	Peptide
2	G	1750	LYS	Peptide
2	G	2046	GLU	Peptide
2	G	975	LYS	Peptide
2	H	1050	ARG	Peptide

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Mol	Chain	Res	Type	Group
2	H	1223	MET	Peptide
2	H	1605	VAL	Peptide
2	H	1750	LYS	Peptide
2	H	2046	GLU	Peptide
2	H	975	LYS	Peptide
2	I	1050	ARG	Peptide
2	I	1223	MET	Peptide
2	I	1605	VAL	Peptide
2	I	1750	LYS	Peptide
2	I	2046	GLU	Peptide
2	I	975	LYS	Peptide
2	J	1050	ARG	Peptide
2	J	1223	MET	Peptide
2	J	1605	VAL	Peptide
2	J	1750	LYS	Peptide
2	J	2046	GLU	Peptide
2	J	975	LYS	Peptide
2	K	1050	ARG	Peptide
2	K	1223	MET	Peptide
2	K	1605	VAL	Peptide
2	K	1750	LYS	Peptide
2	K	2046	GLU	Peptide
2	K	975	LYS	Peptide
2	L	1050	ARG	Peptide
2	L	1223	MET	Peptide
2	L	1605	VAL	Peptide
2	L	1750	LYS	Peptide
2	L	2046	GLU	Peptide
2	L	975	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13625	0	13615	123	0
1	B	13625	0	13615	127	0
1	C	13625	0	13615	130	0
1	D	13625	0	13615	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	13625	0	13615	123	0
1	F	13625	0	13615	125	0
2	G	16018	0	15993	124	0
2	H	16018	0	15993	119	0
2	I	16018	0	15993	120	0
2	J	16018	0	15993	120	0
2	K	16018	0	15993	118	0
2	L	16018	0	15993	120	0
3	M	879	0	871	19	0
3	N	879	0	871	20	0
3	O	879	0	871	19	0
3	P	879	0	871	19	0
3	Q	879	0	871	18	0
3	R	879	0	871	20	0
4	A	21	0	21	3	0
4	B	21	0	21	4	0
4	C	21	0	21	3	0
4	D	21	0	21	3	0
4	E	21	0	21	3	0
4	F	21	0	21	3	0
5	G	31	0	19	2	0
5	H	31	0	19	2	0
5	I	31	0	19	2	0
5	J	31	0	19	2	0
5	K	31	0	19	2	0
5	L	31	0	19	2	0
All	All	183444	0	183114	1446	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 4.

All (1446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1811:GLU:OE2	2:H:2010:TYR:OH	1.80	1.00
2:L:1811:GLU:OE2	2:L:2010:TYR:OH	1.80	1.00
2:K:1811:GLU:OE2	2:K:2010:TYR:OH	1.80	0.99
2:G:1811:GLU:OE2	2:G:2010:TYR:OH	1.80	0.99
2:I:1811:GLU:OE2	2:I:2010:TYR:OH	1.80	0.99
2:J:1811:GLU:OE2	2:J:2010:TYR:OH	1.80	0.98
2:H:894:ARG:NH1	2:H:898:ASP:OD2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:894:ARG:NH1	2:L:898:ASP:OD2	2.15	0.80
2:I:894:ARG:NH1	2:I:898:ASP:OD2	2.15	0.80
2:J:894:ARG:NH1	2:J:898:ASP:OD2	2.15	0.80
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.15	0.79
2:K:894:ARG:NH1	2:K:898:ASP:OD2	2.15	0.79
2:I:1775:GLN:HG2	2:I:1836:MET:HE2	1.66	0.78
2:J:1775:GLN:HG2	2:J:1836:MET:HE2	1.66	0.77
2:G:1775:GLN:HG2	2:G:1836:MET:HE2	1.66	0.77
2:K:1775:GLN:HG2	2:K:1836:MET:HE2	1.67	0.77
2:H:1775:GLN:HG2	2:H:1836:MET:HE2	1.67	0.74
2:L:1775:GLN:HG2	2:L:1836:MET:HE2	1.66	0.74
1:C:871:TRP:HA	3:O:146:ASN:ND2	2.04	0.73
1:D:871:TRP:HA	3:P:146:ASN:ND2	2.05	0.72
1:E:871:TRP:HA	3:Q:146:ASN:ND2	2.06	0.71
1:F:871:TRP:HA	3:R:146:ASN:ND2	2.05	0.70
1:C:1552:ASN:O	1:C:1556:THR:HG22	1.91	0.70
1:D:1552:ASN:O	1:D:1556:THR:HG22	1.91	0.70
1:B:1552:ASN:O	1:B:1556:THR:HG22	1.91	0.70
1:F:1552:ASN:O	1:F:1556:THR:HG22	1.91	0.70
1:A:871:TRP:HA	3:M:146:ASN:ND2	2.07	0.70
1:C:872:THR:H	3:O:146:ASN:HD21	1.40	0.69
1:A:1552:ASN:O	1:A:1556:THR:HG22	1.91	0.69
1:B:871:TRP:HA	3:N:146:ASN:ND2	2.07	0.69
1:E:1552:ASN:O	1:E:1556:THR:HG22	1.91	0.69
1:B:793:ARG:HA	1:B:797:THR:HG23	1.76	0.68
1:F:793:ARG:HA	1:F:797:THR:HG23	1.76	0.68
1:A:793:ARG:HA	1:A:797:THR:HG23	1.76	0.68
1:E:793:ARG:HA	1:E:797:THR:HG23	1.76	0.68
1:C:793:ARG:HA	1:C:797:THR:HG23	1.76	0.68
1:D:793:ARG:HA	1:D:797:THR:HG23	1.76	0.68
2:I:406:ARG:HG2	3:O:88:GLU:HG2	1.76	0.67
2:L:406:ARG:HG2	3:R:88:GLU:HG2	1.76	0.67
2:J:406:ARG:HG2	3:P:88:GLU:HG2	1.77	0.67
2:J:1775:GLN:CG	2:J:1836:MET:HE2	2.25	0.67
2:L:612:ASN:HD21	2:L:641:ILE:HA	1.60	0.67
2:I:1775:GLN:CG	2:I:1836:MET:HE2	2.25	0.66
2:G:1775:GLN:CG	2:G:1836:MET:HE2	2.25	0.66
2:H:612:ASN:HD21	2:H:641:ILE:HA	1.61	0.66
2:K:1775:GLN:CG	2:K:1836:MET:HE2	2.26	0.66
1:C:400:ARG:NH1	1:C:715:THR:HG21	2.11	0.66
1:D:400:ARG:NH1	1:D:715:THR:HG21	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.60	0.66
2:K:612:ASN:HD21	2:K:641:ILE:HA	1.60	0.66
1:A:717:TYR:CZ	1:A:721:ILE:HD11	2.31	0.66
1:E:400:ARG:NH1	1:E:715:THR:HG21	2.11	0.66
1:E:717:TYR:CZ	1:E:721:ILE:HD11	2.31	0.66
1:A:400:ARG:NH1	1:A:715:THR:HG21	2.11	0.66
1:E:872:THR:H	3:Q:146:ASN:HD21	1.42	0.66
1:F:872:THR:H	3:R:146:ASN:HD21	1.41	0.66
1:B:400:ARG:NH1	1:B:715:THR:HG21	2.11	0.66
2:H:1775:GLN:CG	2:H:1836:MET:HE2	2.25	0.65
1:C:717:TYR:CZ	1:C:721:ILE:HD11	2.31	0.65
1:D:717:TYR:CZ	1:D:721:ILE:HD11	2.31	0.65
1:F:400:ARG:NH1	1:F:715:THR:HG21	2.11	0.65
2:J:612:ASN:HD21	2:J:641:ILE:HA	1.60	0.65
1:B:717:TYR:CZ	1:B:721:ILE:HD11	2.31	0.65
2:G:1924:ILE:O	2:G:1928:GLN:HB2	1.97	0.65
2:H:406:ARG:HG2	3:N:88:GLU:HG2	1.76	0.65
2:L:1775:GLN:CG	2:L:1836:MET:HE2	2.25	0.65
1:F:717:TYR:CZ	1:F:721:ILE:HD11	2.31	0.65
2:G:406:ARG:HG2	3:M:88:GLU:HG2	1.77	0.65
2:K:1924:ILE:O	2:K:1928:GLN:HB2	1.97	0.65
2:I:612:ASN:HD21	2:I:641:ILE:HA	1.60	0.65
2:I:1924:ILE:O	2:I:1928:GLN:HB2	1.97	0.65
2:J:1924:ILE:O	2:J:1928:GLN:HB2	1.97	0.65
2:K:406:ARG:HG2	3:Q:88:GLU:HG2	1.78	0.65
1:D:872:THR:H	3:P:146:ASN:HD21	1.45	0.65
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.79	0.65
2:K:848:SER:HB3	2:K:854:ILE:HD11	1.79	0.64
1:B:1491:ARG:NH1	1:B:1744:TYR:O	2.31	0.64
2:L:848:SER:HB3	2:L:854:ILE:HD11	1.79	0.64
1:C:1491:ARG:NH1	1:C:1744:TYR:O	2.31	0.64
1:D:1491:ARG:NH1	1:D:1744:TYR:O	2.31	0.64
1:F:1491:ARG:NH1	1:F:1744:TYR:O	2.31	0.64
2:H:848:SER:HB3	2:H:854:ILE:HD11	1.79	0.64
2:J:848:SER:HB3	2:J:854:ILE:HD11	1.79	0.64
2:I:848:SER:HB3	2:I:854:ILE:HD11	1.79	0.64
1:B:872:THR:H	3:N:146:ASN:HD21	1.44	0.64
4:D:1901:PNS:H382	2:L:372:ASN:HD21	1.63	0.64
1:E:1491:ARG:NH1	1:E:1744:TYR:O	2.30	0.64
1:F:1448:ARG:HD2	1:F:1508:TRP:O	1.98	0.63
2:L:1924:ILE:O	2:L:1928:GLN:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:ARG:HD2	1:A:1508:TRP:O	1.98	0.63
1:B:1448:ARG:HD2	1:B:1508:TRP:O	1.98	0.63
2:H:1924:ILE:O	2:H:1928:GLN:HB2	1.97	0.63
1:A:1491:ARG:NH1	1:A:1744:TYR:O	2.31	0.63
1:D:1448:ARG:HD2	1:D:1508:TRP:O	1.98	0.63
1:C:1448:ARG:HD2	1:C:1508:TRP:O	1.98	0.63
1:E:1448:ARG:HD2	1:E:1508:TRP:O	1.98	0.63
1:A:872:THR:H	3:M:146:ASN:HD21	1.45	0.62
4:C:1901:PNS:H421	2:H:163:GLN:O	1.99	0.62
1:B:1125:VAL:HG11	1:B:1175:ILE:HD12	1.81	0.62
1:F:1125:VAL:HG11	1:F:1175:ILE:HD12	1.81	0.62
4:B:1901:PNS:H382	2:G:372:ASN:HD21	1.64	0.62
1:D:1064:ASN:ND2	1:D:1073:THR:OG1	2.33	0.62
4:A:1901:PNS:H382	2:I:372:ASN:HD21	1.65	0.61
1:B:1064:ASN:ND2	1:B:1073:THR:OG1	2.33	0.61
1:C:1064:ASN:ND2	1:C:1073:THR:OG1	2.33	0.61
1:F:1064:ASN:ND2	1:F:1073:THR:OG1	2.33	0.61
1:A:1064:ASN:ND2	1:A:1073:THR:OG1	2.33	0.61
1:C:1414:ILE:HG12	1:F:1293:SER:HB2	1.83	0.61
1:E:1064:ASN:ND2	1:E:1073:THR:OG1	2.33	0.61
1:E:1125:VAL:HG11	1:E:1175:ILE:HD12	1.81	0.61
2:I:1771:LEU:O	2:I:1777:THR:OG1	2.19	0.61
1:B:1017:ARG:HG2	1:B:1510:ASN:HD22	1.66	0.61
2:J:1771:LEU:O	2:J:1777:THR:OG1	2.19	0.61
1:A:1125:VAL:HG11	1:A:1175:ILE:HD12	1.81	0.61
4:A:1901:PNS:O23	4:A:1901:PNS:H312	2.00	0.61
1:C:1125:VAL:HG11	1:C:1175:ILE:HD12	1.81	0.61
1:F:1017:ARG:HG2	1:F:1510:ASN:HD22	1.66	0.61
2:I:1180:MET:HE3	2:I:1197:LEU:HD11	1.83	0.61
1:F:1352:THR:HG23	1:F:1365:MET:HE1	1.83	0.61
2:K:1180:MET:HE3	2:K:1197:LEU:HD11	1.83	0.61
1:D:1125:VAL:HG11	1:D:1175:ILE:HD12	1.81	0.61
1:F:237:MET:HB2	1:F:277:LEU:HD12	1.82	0.61
2:L:1632:ILE:HG22	2:L:1637:LEU:HD23	1.83	0.61
1:B:237:MET:HB2	1:B:277:LEU:HD12	1.82	0.60
1:B:1234:MET:HE3	1:B:1326:ILE:HG21	1.83	0.60
1:B:1352:THR:HG23	1:B:1365:MET:HE1	1.83	0.60
4:B:1901:PNS:H312	4:B:1901:PNS:O23	2.01	0.60
4:F:1901:PNS:H312	4:F:1901:PNS:O26	2.00	0.60
2:J:1180:MET:HE3	2:J:1197:LEU:HD11	1.83	0.60
4:D:1901:PNS:H312	4:D:1901:PNS:O26	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1180:MET:HE3	2:G:1197:LEU:HD11	1.83	0.60
2:H:1632:ILE:HG22	2:H:1637:LEU:HD23	1.83	0.60
2:G:1771:LEU:O	2:G:1777:THR:OG1	2.19	0.60
1:F:1234:MET:HE3	1:F:1326:ILE:HG21	1.84	0.60
2:K:1771:LEU:O	2:K:1777:THR:OG1	2.19	0.60
1:A:1017:ARG:HG2	1:A:1510:ASN:HD22	1.66	0.60
1:C:1017:ARG:HG2	1:C:1510:ASN:HD22	1.66	0.60
1:D:1017:ARG:HG2	1:D:1510:ASN:HD22	1.66	0.60
2:K:101:ILE:HD11	2:K:122:LEU:CD2	2.32	0.60
1:A:1352:THR:HG23	1:A:1365:MET:HE1	1.83	0.60
1:C:940:THR:HG21	3:O:150:ILE:C	2.26	0.60
4:E:1901:PNS:H312	4:E:1901:PNS:O26	2.00	0.60
4:A:1901:PNS:H421	2:I:163:GLN:O	2.01	0.60
4:C:1901:PNS:O23	4:C:1901:PNS:H312	2.00	0.60
1:C:237:MET:HB2	1:C:277:LEU:HD12	1.82	0.60
1:E:1017:ARG:HG2	1:E:1510:ASN:HD22	1.66	0.60
1:E:1352:THR:HG23	1:E:1365:MET:HE1	1.83	0.60
1:B:1293:SER:HB2	1:D:1414:ILE:HG12	1.84	0.60
1:C:1208:VAL:HG13	1:C:1212:THR:HB	1.84	0.60
1:E:1234:MET:HE3	1:E:1326:ILE:HG21	1.83	0.60
1:A:1234:MET:HE3	1:A:1326:ILE:HG21	1.84	0.60
1:A:1293:SER:HB2	1:E:1414:ILE:HG12	1.83	0.60
1:D:1208:VAL:HG13	1:D:1212:THR:HB	1.84	0.60
2:G:101:ILE:HD11	2:G:122:LEU:CD2	2.32	0.60
2:H:1771:LEU:O	2:H:1777:THR:OG1	2.19	0.59
2:I:1632:ILE:HG22	2:I:1637:LEU:HD23	1.83	0.59
2:J:1632:ILE:HG22	2:J:1637:LEU:HD23	1.83	0.59
1:A:1208:VAL:HG13	1:A:1212:THR:HB	1.84	0.59
1:D:1234:MET:HE3	1:D:1326:ILE:HG21	1.84	0.59
1:E:1208:VAL:HG13	1:E:1212:THR:HB	1.84	0.59
4:F:1901:PNS:H382	2:K:372:ASN:HD21	1.67	0.59
2:L:1771:LEU:O	2:L:1777:THR:OG1	2.19	0.59
1:C:1352:THR:HG23	1:C:1365:MET:HE1	1.83	0.59
1:D:1352:THR:HG23	1:D:1365:MET:HE1	1.83	0.59
2:K:1632:ILE:HG22	2:K:1637:LEU:HD23	1.83	0.59
1:A:1022:THR:HG21	1:A:1388:MET:HE3	1.84	0.59
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.36	0.59
1:C:1234:MET:HE3	1:C:1326:ILE:HG21	1.84	0.59
1:F:1039:MET:O	1:F:1609:ARG:NH2	2.36	0.59
2:G:1632:ILE:HG22	2:G:1637:LEU:HD23	1.83	0.59
2:L:101:ILE:HD11	2:L:122:LEU:CD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MET:HB2	1:A:277:LEU:HD12	1.82	0.59
1:D:237:MET:HB2	1:D:277:LEU:HD12	1.82	0.59
1:E:1022:THR:HG21	1:E:1388:MET:HE3	1.84	0.59
1:F:1208:VAL:HG13	1:F:1212:THR:HB	1.84	0.59
2:I:101:ILE:HD11	2:I:122:LEU:CD2	2.32	0.59
1:B:1208:VAL:HG13	1:B:1212:THR:HB	1.84	0.59
1:D:940:THR:HG21	3:P:150:ILE:C	2.27	0.59
2:H:101:ILE:HD11	2:H:122:LEU:CD2	2.32	0.59
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.35	0.59
1:C:1293:SER:HB2	1:F:1414:ILE:HG12	1.83	0.59
4:D:1901:PNS:H421	2:L:163:GLN:O	2.03	0.59
4:E:1901:PNS:H421	2:J:163:GLN:O	2.02	0.59
1:F:940:THR:HG21	3:R:150:ILE:C	2.28	0.59
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.36	0.59
1:B:1276:GLN:O	1:B:1282:THR:HG21	2.03	0.59
1:D:1039:MET:O	1:D:1609:ARG:NH2	2.36	0.59
1:E:237:MET:HB2	1:E:277:LEU:HD12	1.82	0.59
4:E:1901:PNS:H382	2:J:372:ASN:HD21	1.68	0.59
1:F:1276:GLN:O	1:F:1282:THR:HG21	2.03	0.59
2:J:101:ILE:HD11	2:J:122:LEU:CD2	2.32	0.59
1:B:1414:ILE:HG12	1:D:1293:SER:HB2	1.84	0.59
4:F:1901:PNS:H421	2:K:163:GLN:O	2.02	0.59
1:B:940:THR:HG21	3:N:150:ILE:C	2.28	0.58
1:B:1022:THR:HG21	1:B:1388:MET:HE3	1.84	0.58
1:D:1276:GLN:O	1:D:1282:THR:HG21	2.03	0.58
1:E:1039:MET:O	1:E:1609:ARG:NH2	2.36	0.58
1:F:1022:THR:HG21	1:F:1388:MET:HE3	1.85	0.58
2:L:1180:MET:HE3	2:L:1197:LEU:HD11	1.83	0.58
1:C:1276:GLN:O	1:C:1282:THR:HG21	2.03	0.58
1:A:1276:GLN:O	1:A:1282:THR:HG21	2.03	0.58
1:D:1022:THR:HG21	1:D:1388:MET:HE3	1.84	0.58
2:H:1180:MET:HE3	2:H:1197:LEU:HD11	1.83	0.58
1:A:1414:ILE:HG12	1:E:1293:SER:HB2	1.84	0.58
1:C:1022:THR:HG21	1:C:1388:MET:HE3	1.85	0.58
1:E:1276:GLN:O	1:E:1282:THR:HG21	2.03	0.58
1:A:940:THR:HG21	3:M:150:ILE:C	2.29	0.58
1:E:940:THR:HG21	3:Q:150:ILE:C	2.29	0.58
1:D:221:LEU:O	1:D:225:SER:OG	2.22	0.57
1:C:221:LEU:O	1:C:225:SER:OG	2.23	0.57
3:M:16:PHE:CE2	3:M:20:ILE:HD12	2.40	0.57
1:F:1238:VAL:HG22	1:F:1325:ARG:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:16:PHE:CE2	3:Q:20:ILE:HD12	2.40	0.57
3:P:16:PHE:CE2	3:P:20:ILE:HD12	2.40	0.57
1:B:1238:VAL:HG22	1:B:1325:ARG:HD3	1.87	0.57
1:A:833:PHE:CZ	3:M:150:ILE:HG13	2.40	0.57
4:B:1901:PNS:H421	2:G:163:GLN:O	2.03	0.57
2:L:1680:LEU:HD13	2:L:1687:ALA:HB2	1.86	0.57
2:H:1680:LEU:HD13	2:H:1687:ALA:HB2	1.86	0.57
3:O:16:PHE:CE2	3:O:20:ILE:HD12	2.40	0.57
2:G:1680:LEU:HD13	2:G:1687:ALA:HB2	1.86	0.56
3:N:16:PHE:CE2	3:N:20:ILE:HD12	2.40	0.56
3:R:16:PHE:CE2	3:R:20:ILE:HD12	2.40	0.56
1:B:221:LEU:O	1:B:225:SER:OG	2.23	0.56
4:C:1901:PNS:H382	2:H:372:ASN:HD21	1.69	0.56
1:D:833:PHE:CZ	3:P:150:ILE:HG13	2.40	0.56
2:H:218:TRP:HH2	2:H:236:ILE:HD11	1.71	0.56
2:K:1680:LEU:HD13	2:K:1687:ALA:HB2	1.86	0.56
2:L:845:THR:HG22	2:L:855:HIS:CD2	2.40	0.56
1:F:221:LEU:O	1:F:225:SER:OG	2.22	0.56
2:I:1680:LEU:HD13	2:I:1687:ALA:HB2	1.86	0.56
2:H:845:THR:HG22	2:H:855:HIS:CD2	2.41	0.56
2:J:845:THR:HG22	2:J:855:HIS:CD2	2.41	0.56
2:G:845:THR:HG22	2:G:855:HIS:CD2	2.40	0.56
2:I:845:THR:HG22	2:I:855:HIS:CD2	2.41	0.56
2:J:1680:LEU:HD13	2:J:1687:ALA:HB2	1.86	0.56
2:L:1343:VAL:O	2:L:1343:VAL:HG22	2.06	0.56
1:A:1238:VAL:HG22	1:A:1325:ARG:HD3	1.87	0.56
2:K:845:THR:HG22	2:K:855:HIS:CD2	2.41	0.56
2:H:1343:VAL:HG22	2:H:1343:VAL:O	2.06	0.56
2:I:1343:VAL:HG22	2:I:1343:VAL:O	2.06	0.56
2:I:1775:GLN:HG2	2:I:1836:MET:CE	2.36	0.56
2:H:1610:CYS:SG	2:H:1651:LEU:HD22	2.46	0.56
2:J:1775:GLN:HG2	2:J:1836:MET:CE	2.36	0.56
1:E:1238:VAL:HG22	1:E:1325:ARG:HD3	1.87	0.55
2:I:1610:CYS:SG	2:I:1651:LEU:HD22	2.46	0.55
2:J:1343:VAL:O	2:J:1343:VAL:HG22	2.06	0.55
2:J:1610:CYS:SG	2:J:1651:LEU:HD22	2.46	0.55
2:K:1343:VAL:HG22	2:K:1343:VAL:O	2.06	0.55
1:A:768:ILE:HD11	1:A:806:VAL:HG11	1.88	0.55
1:B:833:PHE:CZ	3:N:150:ILE:HG13	2.42	0.55
1:E:768:ILE:HD11	1:E:806:VAL:HG11	1.88	0.55
2:H:1866:PHE:CE1	2:H:1870:ALA:HB1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1610:CYS:SG	2:L:1651:LEU:HD22	2.46	0.55
2:G:1343:VAL:O	2:G:1343:VAL:HG22	2.06	0.55
2:K:218:TRP:HH2	2:K:236:ILE:HD11	1.71	0.55
1:E:833:PHE:CZ	3:Q:150:ILE:HG13	2.42	0.55
1:F:768:ILE:HD11	1:F:806:VAL:HG11	1.88	0.55
2:L:1866:PHE:CE1	2:L:1870:ALA:HB1	2.42	0.55
1:C:1238:VAL:HG22	1:C:1325:ARG:HD3	1.87	0.55
1:D:877:LEU:HD12	1:D:883:ILE:CG2	2.37	0.55
2:H:597:MET:HA	5:H:2101:FMN:N5	2.22	0.55
2:H:106:ALA:HB2	2:H:545:GLN:HG2	1.89	0.55
2:L:218:TRP:HH2	2:L:236:ILE:HD11	1.72	0.55
2:L:1775:GLN:HG2	2:L:1836:MET:CE	2.36	0.55
1:B:768:ILE:HD11	1:B:806:VAL:HG11	1.88	0.55
1:D:1238:VAL:HG22	1:D:1325:ARG:HD3	1.87	0.55
1:C:877:LEU:HD12	1:C:883:ILE:CG2	2.37	0.55
2:J:615:TYR:OH	2:J:1075:ASP:OD1	2.17	0.55
1:D:768:ILE:HD11	1:D:806:VAL:HG11	1.88	0.54
2:H:1775:GLN:HG2	2:H:1836:MET:CE	2.36	0.54
2:I:1709:ILE:HD11	2:I:1717:LEU:HD22	1.89	0.54
2:J:1709:ILE:HD11	2:J:1717:LEU:HD22	1.89	0.54
2:L:1808:SER:H	2:L:2013:ASN:HD21	1.54	0.54
2:G:1709:ILE:HD11	2:G:1717:LEU:HD22	1.89	0.54
2:G:1866:PHE:CE1	2:G:1870:ALA:HB1	2.42	0.54
2:I:106:ALA:HB2	2:I:545:GLN:HG2	1.88	0.54
2:K:1866:PHE:CE1	2:K:1870:ALA:HB1	2.42	0.54
1:C:768:ILE:HD11	1:C:806:VAL:HG11	1.88	0.54
2:G:1610:CYS:SG	2:G:1651:LEU:HD22	2.46	0.54
2:I:615:TYR:OH	2:I:1075:ASP:OD1	2.17	0.54
2:K:106:ALA:HB2	2:K:545:GLN:HG2	1.89	0.54
2:K:1610:CYS:SG	2:K:1651:LEU:HD22	2.46	0.54
2:K:1709:ILE:HD11	2:K:1717:LEU:HD22	1.89	0.54
3:N:137:ASN:HB3	3:N:141:ASP:HA	1.89	0.54
1:F:833:PHE:CZ	3:R:150:ILE:HG13	2.42	0.54
2:H:1808:SER:H	2:H:2013:ASN:HD21	1.54	0.54
1:B:1153:ASP:OD2	1:C:359:ARG:NH1	2.41	0.54
1:F:877:LEU:HD12	1:F:883:ILE:CG2	2.37	0.54
2:L:106:ALA:HB2	2:L:545:GLN:HG2	1.89	0.54
1:A:221:LEU:O	1:A:225:SER:OG	2.23	0.54
1:B:877:LEU:HD12	1:B:883:ILE:CG2	2.37	0.54
2:J:1866:PHE:CE1	2:J:1870:ALA:HB1	2.42	0.54
3:R:137:ASN:HB3	3:R:141:ASP:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:NH1	1:C:1153:ASP:OD2	2.40	0.54
2:G:1808:SER:H	2:G:2013:ASN:HD21	1.53	0.54
2:J:1808:SER:H	2:J:2013:ASN:HD21	1.54	0.54
3:P:137:ASN:HB3	3:P:141:ASP:HA	1.89	0.54
2:I:1866:PHE:CE1	2:I:1870:ALA:HB1	2.42	0.54
3:M:137:ASN:HB3	3:M:141:ASP:HA	1.89	0.54
1:D:359:ARG:NH1	1:F:1153:ASP:OD2	2.41	0.54
1:E:221:LEU:O	1:E:225:SER:OG	2.22	0.54
2:H:432:LEU:HB3	2:H:484:ILE:HG23	1.89	0.54
2:J:432:LEU:HB3	2:J:484:ILE:HG23	1.90	0.54
2:L:1709:ILE:HD11	2:L:1717:LEU:HD22	1.89	0.54
1:C:833:PHE:CZ	3:O:150:ILE:HG13	2.42	0.54
2:G:1177:SER:O	2:G:1180:MET:HG2	2.08	0.54
2:J:106:ALA:HB2	2:J:545:GLN:HG2	1.89	0.54
2:K:1177:SER:O	2:K:1180:MET:HG2	2.08	0.54
3:O:137:ASN:HB3	3:O:141:ASP:HA	1.90	0.54
2:I:218:TRP:HH2	2:I:236:ILE:HD11	1.71	0.53
2:I:1177:SER:O	2:I:1180:MET:HG2	2.08	0.53
2:K:1775:GLN:HG2	2:K:1836:MET:CE	2.36	0.53
1:A:877:LEU:HD12	1:A:883:ILE:CG2	2.37	0.53
2:H:1709:ILE:HD11	2:H:1717:LEU:HD22	1.90	0.53
2:K:498:ALA:O	2:K:525:VAL:HG22	2.09	0.53
3:Q:137:ASN:HB3	3:Q:141:ASP:HA	1.89	0.53
1:E:237:MET:HE3	1:E:276:ARG:HA	1.91	0.53
2:G:218:TRP:HH2	2:G:236:ILE:HD11	1.73	0.53
2:G:1775:GLN:HG2	2:G:1836:MET:CE	2.36	0.53
2:J:1177:SER:O	2:J:1180:MET:HG2	2.08	0.53
2:K:1808:SER:H	2:K:2013:ASN:HD21	1.54	0.53
1:D:1153:ASP:OD2	1:E:359:ARG:NH1	2.41	0.53
2:J:597:MET:HA	5:J:2101:FMN:N5	2.24	0.53
2:L:526:ARG:HH11	2:L:558:ASN:HD21	1.56	0.53
1:A:237:MET:HE3	1:A:276:ARG:HA	1.91	0.53
2:H:526:ARG:HH11	2:H:558:ASN:HD21	1.57	0.53
2:I:1808:SER:H	2:I:2013:ASN:HD21	1.54	0.53
2:J:218:TRP:HH2	2:J:236:ILE:HD11	1.71	0.53
2:L:432:LEU:HB3	2:L:484:ILE:HG23	1.91	0.53
2:L:597:MET:HA	5:L:2101:FMN:N5	2.24	0.53
3:N:20:ILE:HD11	3:N:103:LEU:CD2	2.39	0.53
1:E:877:LEU:HD12	1:E:883:ILE:CG2	2.37	0.53
2:G:106:ALA:HB2	2:G:545:GLN:HG2	1.90	0.53
2:G:498:ALA:O	2:G:525:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:597:MET:HA	5:K:2101:FMN:N5	2.22	0.53
1:F:237:MET:HE3	1:F:276:ARG:HA	1.91	0.53
2:H:1177:SER:O	2:H:1180:MET:HG2	2.08	0.53
2:I:597:MET:HA	5:I:2101:FMN:N5	2.24	0.53
2:K:526:ARG:HH11	2:K:558:ASN:HD21	1.56	0.53
3:R:20:ILE:HD11	3:R:103:LEU:CD2	2.39	0.53
1:E:1153:ASP:OD2	1:F:359:ARG:NH1	2.41	0.53
2:I:143:SER:OG	2:I:547:ILE:O	2.23	0.53
2:J:146:PHE:HA	2:J:149:VAL:HG12	1.91	0.53
1:B:237:MET:HE3	1:B:276:ARG:HA	1.91	0.52
2:I:146:PHE:HA	2:I:149:VAL:HG12	1.91	0.52
2:I:432:LEU:HB3	2:I:484:ILE:HG23	1.91	0.52
2:L:1177:SER:O	2:L:1180:MET:HG2	2.08	0.52
1:A:159:LEU:HD21	1:A:176:VAL:CG1	2.39	0.52
1:B:381:GLU:HG3	1:E:390:VAL:HG13	1.92	0.52
2:L:1774:THR:O	2:L:1778:GLN:HB2	2.09	0.52
3:P:20:ILE:HD11	3:P:103:LEU:CD2	2.39	0.52
2:G:526:ARG:HH11	2:G:558:ASN:HD21	1.57	0.52
1:A:1153:ASP:OD2	1:B:359:ARG:NH1	2.42	0.52
1:C:237:MET:HE3	1:C:276:ARG:HA	1.91	0.52
2:G:146:PHE:HA	2:G:149:VAL:HG12	1.91	0.52
2:H:1774:THR:O	2:H:1778:GLN:HB2	2.09	0.52
2:K:1774:THR:O	2:K:1778:GLN:HB2	2.09	0.52
1:D:871:TRP:CZ3	1:D:888:ILE:HD13	2.45	0.52
2:I:498:ALA:O	2:I:525:VAL:HG22	2.09	0.52
2:G:1774:THR:O	2:G:1778:GLN:HB2	2.09	0.52
2:H:498:ALA:O	2:H:525:VAL:HG22	2.09	0.52
2:I:526:ARG:HH11	2:I:558:ASN:HD21	1.56	0.52
2:K:146:PHE:HA	2:K:149:VAL:HG12	1.91	0.52
2:L:146:PHE:HA	2:L:149:VAL:HG12	1.91	0.52
1:C:871:TRP:CZ3	1:C:888:ILE:HD13	2.45	0.52
2:H:146:PHE:HA	2:H:149:VAL:HG12	1.91	0.52
2:J:498:ALA:O	2:J:525:VAL:HG22	2.09	0.52
2:J:1774:THR:O	2:J:1778:GLN:HB2	2.09	0.52
3:M:20:ILE:HD11	3:M:103:LEU:CD2	2.39	0.52
1:A:390:VAL:HG13	1:F:381:GLU:HG3	1.92	0.52
2:G:432:LEU:HB3	2:G:484:ILE:HG23	1.90	0.52
2:G:1956:ARG:NE	2:G:1956:ARG:O	2.43	0.52
2:H:309:ARG:NH1	2:H:442:ASP:OD2	2.43	0.52
2:L:309:ARG:NH1	2:L:442:ASP:OD2	2.43	0.52
3:O:20:ILE:HD11	3:O:103:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD21	1:D:176:VAL:CG1	2.40	0.52
1:D:237:MET:HE3	1:D:276:ARG:HA	1.91	0.52
1:E:871:TRP:CZ3	1:E:888:ILE:HD13	2.45	0.52
1:F:1531:LEU:HD21	1:F:1660:TYR:CZ	2.45	0.52
2:J:526:ARG:HH11	2:J:558:ASN:HD21	1.57	0.52
2:K:432:LEU:HB3	2:K:484:ILE:HG23	1.90	0.52
2:K:1956:ARG:O	2:K:1956:ARG:NE	2.43	0.52
2:L:498:ALA:O	2:L:525:VAL:HG22	2.09	0.52
3:Q:20:ILE:HD11	3:Q:103:LEU:CD2	2.39	0.52
1:A:871:TRP:CZ3	1:A:888:ILE:HD13	2.45	0.51
1:B:1531:LEU:HD21	1:B:1660:TYR:CZ	2.45	0.51
1:F:773:ALA:HB3	3:R:142:VAL:HG23	1.92	0.51
2:I:898:ASP:O	2:I:1050:ARG:HA	2.11	0.51
2:I:1040:LEU:HD21	2:I:1048:VAL:HG13	1.92	0.51
2:I:1774:THR:O	2:I:1778:GLN:HB2	2.09	0.51
2:J:330:ASN:HD22	2:J:394:ARG:CZ	2.24	0.51
2:I:330:ASN:HD22	2:I:394:ARG:CZ	2.24	0.51
2:J:898:ASP:O	2:J:1050:ARG:HA	2.11	0.51
2:H:1663:THR:HA	2:H:1803:THR:O	2.11	0.51
2:J:1040:LEU:HD21	2:J:1048:VAL:HG13	1.92	0.51
2:K:1040:LEU:HD21	2:K:1048:VAL:HG13	1.92	0.51
2:L:1663:THR:HA	2:L:1803:THR:O	2.11	0.51
1:C:159:LEU:HD21	1:C:176:VAL:CG1	2.40	0.51
1:C:773:ALA:HB3	3:O:142:VAL:HG23	1.92	0.51
1:C:1657:HIS:HD2	1:C:1659:ASP:H	1.58	0.51
1:D:1657:HIS:HD2	1:D:1659:ASP:H	1.58	0.51
2:I:706:LYS:NZ	5:I:2101:FMN:O2'	2.44	0.51
2:L:1339:PHE:N	2:L:1340:PRO:CD	2.74	0.51
1:E:159:LEU:HD21	1:E:176:VAL:CG1	2.40	0.51
1:B:871:TRP:CZ3	1:B:888:ILE:HD13	2.45	0.51
1:B:1744:TYR:HB2	1:D:1432:HIS:CE1	2.46	0.51
1:C:1531:LEU:HD21	1:C:1660:TYR:CZ	2.45	0.51
1:E:773:ALA:HB3	3:Q:142:VAL:HG23	1.92	0.51
2:H:1339:PHE:N	2:H:1340:PRO:CD	2.74	0.51
2:L:898:ASP:O	2:L:1050:ARG:HA	2.11	0.51
1:C:821:GLN:HE22	1:C:914:VAL:HG22	1.75	0.51
2:G:330:ASN:HD22	2:G:394:ARG:CZ	2.23	0.51
2:G:1663:THR:HA	2:G:1803:THR:O	2.11	0.51
2:H:898:ASP:O	2:H:1050:ARG:HA	2.11	0.51
2:K:330:ASN:HD22	2:K:394:ARG:CZ	2.24	0.51
2:K:1663:THR:HA	2:K:1803:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.45	0.51
1:D:1531:LEU:HD21	1:D:1660:TYR:CZ	2.45	0.51
1:F:159:LEU:HD21	1:F:176:VAL:CG1	2.40	0.51
2:G:1040:LEU:HD21	2:G:1048:VAL:HG13	1.93	0.51
2:L:234:ILE:N	2:L:235:PRO:CD	2.74	0.51
1:B:159:LEU:HD21	1:B:176:VAL:CG1	2.41	0.51
1:D:865:CYS:HB2	1:D:917:CYS:SG	2.51	0.51
1:E:1531:LEU:HD21	1:E:1660:TYR:CZ	2.45	0.51
1:F:865:CYS:HB2	1:F:917:CYS:SG	2.51	0.51
2:G:597:MET:HA	5:G:2101:FMN:N5	2.25	0.51
2:H:1040:LEU:HD21	2:H:1048:VAL:HG13	1.92	0.51
2:J:1956:ARG:O	2:J:1956:ARG:NE	2.43	0.51
2:K:898:ASP:O	2:K:1050:ARG:HA	2.11	0.51
2:L:1040:LEU:HD21	2:L:1048:VAL:HG13	1.92	0.51
1:A:381:GLU:HG3	1:F:390:VAL:HG13	1.92	0.51
1:C:865:CYS:HB2	1:C:917:CYS:SG	2.51	0.51
1:D:821:GLN:HE22	1:D:914:VAL:HG22	1.76	0.51
1:F:871:TRP:CZ3	1:F:888:ILE:HD13	2.45	0.51
2:G:898:ASP:O	2:G:1050:ARG:HA	2.11	0.51
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.74	0.51
2:H:234:ILE:N	2:H:235:PRO:CD	2.74	0.51
2:I:1956:ARG:NE	2:I:1956:ARG:O	2.43	0.51
1:B:682:GLY:HA2	3:N:136:ASP:HA	1.93	0.50
1:B:865:CYS:HB2	1:B:917:CYS:SG	2.51	0.50
1:B:1109:GLU:CD	1:B:1109:GLU:H	2.20	0.50
1:F:904:ASN:HB3	1:F:926:LEU:HD13	1.93	0.50
1:F:1109:GLU:H	1:F:1109:GLU:CD	2.20	0.50
2:K:1339:PHE:N	2:K:1340:PRO:CD	2.74	0.50
1:B:1657:HIS:HD2	1:B:1659:ASP:H	1.58	0.50
1:D:529:MET:HE3	1:D:637:PHE:HB2	1.94	0.50
1:E:821:GLN:HE22	1:E:914:VAL:HG22	1.75	0.50
1:F:682:GLY:HA2	3:R:136:ASP:HA	1.93	0.50
1:F:1657:HIS:HD2	1:F:1659:ASP:H	1.58	0.50
2:K:1665:VAL:HA	2:K:1805:ALA:O	2.11	0.50
2:L:615:TYR:OH	2:L:1075:ASP:OD1	2.17	0.50
1:B:390:VAL:HG13	1:E:381:GLU:HG3	1.93	0.50
1:B:904:ASN:HB3	1:B:926:LEU:HD13	1.93	0.50
1:C:505:LYS:O	1:C:954:ARG:HG2	2.12	0.50
1:C:529:MET:HE3	1:C:637:PHE:HB2	1.94	0.50
1:D:682:GLY:HA2	3:P:136:ASP:HA	1.94	0.50
1:D:1238:VAL:HG13	1:D:1242:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:ASN:ND2	1:E:613:VAL:O	2.45	0.50
2:I:1751:ILE:HG23	2:I:1840:VAL:HG21	1.93	0.50
2:J:1339:PHE:N	2:J:1340:PRO:CD	2.74	0.50
2:K:517:HIS:CE1	2:K:540:ASP:HB3	2.46	0.50
1:A:821:GLN:HE22	1:A:914:VAL:HG22	1.76	0.50
1:B:529:MET:HE3	1:B:637:PHE:HB2	1.93	0.50
1:C:682:GLY:HA2	3:O:136:ASP:HA	1.93	0.50
1:E:682:GLY:HA2	3:Q:136:ASP:HA	1.93	0.50
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.11	0.50
2:H:615:TYR:OH	2:H:1075:ASP:OD1	2.17	0.50
2:I:234:ILE:N	2:I:235:PRO:CD	2.74	0.50
2:J:234:ILE:N	2:J:235:PRO:CD	2.74	0.50
2:J:1663:THR:HA	2:J:1803:THR:O	2.11	0.50
1:A:479:ASN:ND2	1:A:613:VAL:O	2.45	0.50
1:C:1238:VAL:HG13	1:C:1242:GLU:HB2	1.94	0.50
1:D:505:LYS:O	1:D:954:ARG:HG2	2.12	0.50
1:F:529:MET:HE3	1:F:637:PHE:HB2	1.94	0.50
2:I:1339:PHE:N	2:I:1340:PRO:CD	2.74	0.50
2:I:1663:THR:HA	2:I:1803:THR:O	2.11	0.50
2:J:706:LYS:NZ	5:J:2101:FMN:O2'	2.45	0.50
2:L:1751:ILE:HG23	2:L:1840:VAL:HG21	1.94	0.50
1:A:682:GLY:HA2	3:M:136:ASP:HA	1.93	0.50
1:B:1238:VAL:HG13	1:B:1242:GLU:HB2	1.94	0.50
1:F:505:LYS:O	1:F:954:ARG:HG2	2.12	0.50
1:F:1238:VAL:HG13	1:F:1242:GLU:HB2	1.93	0.50
2:H:330:ASN:HD22	2:H:394:ARG:CZ	2.24	0.50
2:L:330:ASN:HD22	2:L:394:ARG:CZ	2.24	0.50
2:L:706:LYS:NZ	5:L:2101:FMN:O2'	2.45	0.50
1:C:381:GLU:HG3	1:D:390:VAL:HG13	1.92	0.50
1:C:390:VAL:HG13	1:D:381:GLU:HG3	1.92	0.50
2:G:234:ILE:N	2:G:235:PRO:CD	2.74	0.50
2:I:1665:VAL:HA	2:I:1805:ALA:O	2.11	0.50
2:J:1665:VAL:HA	2:J:1805:ALA:O	2.11	0.50
2:K:234:ILE:N	2:K:235:PRO:CD	2.74	0.50
2:K:706:LYS:NZ	5:K:2101:FMN:O2'	2.45	0.50
2:K:1751:ILE:HG23	2:K:1840:VAL:HG21	1.94	0.50
1:E:865:CYS:HB2	1:E:917:CYS:SG	2.51	0.50
2:I:99:ASN:HD21	2:I:550:VAL:H	1.60	0.50
2:I:517:HIS:CE1	2:I:540:ASP:HB3	2.46	0.50
1:A:529:MET:HE3	1:A:637:PHE:HB2	1.94	0.50
1:B:505:LYS:O	1:B:954:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1239:HIS:CE1	1:D:1717:ASP:O	2.65	0.50
1:E:529:MET:HE3	1:E:637:PHE:HB2	1.94	0.50
1:E:1657:HIS:HD2	1:E:1659:ASP:H	1.58	0.50
2:H:517:HIS:CE1	2:H:540:ASP:HB3	2.47	0.50
2:H:706:LYS:NZ	5:H:2101:FMN:O2'	2.45	0.50
2:J:99:ASN:HD21	2:J:550:VAL:H	1.60	0.50
1:A:865:CYS:HB2	1:A:917:CYS:SG	2.51	0.49
1:A:904:ASN:HB3	1:A:926:LEU:HD13	1.93	0.49
1:B:773:ALA:HB3	3:N:142:VAL:HG23	1.94	0.49
1:C:1239:HIS:CE1	1:C:1717:ASP:O	2.65	0.49
1:E:505:LYS:O	1:E:954:ARG:HG2	2.12	0.49
1:A:505:LYS:O	1:A:954:ARG:HG2	2.12	0.49
1:A:1109:GLU:H	1:A:1109:GLU:CD	2.20	0.49
1:A:1657:HIS:HD2	1:A:1659:ASP:H	1.58	0.49
1:A:1744:TYR:HB2	1:E:1432:HIS:CE1	2.47	0.49
1:B:821:GLN:HE22	1:B:914:VAL:HG22	1.76	0.49
1:B:1280:ILE:HD12	1:D:1280:ILE:HD12	1.94	0.49
1:C:1280:ILE:HD12	1:F:1280:ILE:HD12	1.94	0.49
1:E:904:ASN:HB3	1:E:926:LEU:HD13	1.93	0.49
1:E:1238:VAL:HG13	1:E:1242:GLU:HB2	1.93	0.49
2:H:1665:VAL:HA	2:H:1805:ALA:O	2.11	0.49
2:K:309:ARG:NH1	2:K:442:ASP:OD2	2.43	0.49
2:K:1638:ILE:HG13	2:K:1657:ILE:HD12	1.94	0.49
2:L:1665:VAL:HA	2:L:1805:ALA:O	2.11	0.49
1:C:479:ASN:ND2	1:C:613:VAL:O	2.45	0.49
1:D:479:ASN:ND2	1:D:613:VAL:O	2.45	0.49
1:E:1109:GLU:CD	1:E:1109:GLU:H	2.20	0.49
1:F:821:GLN:HE22	1:F:914:VAL:HG22	1.76	0.49
2:G:1638:ILE:HG13	2:G:1657:ILE:HD12	1.94	0.49
2:H:1470:THR:HA	2:H:1484:LYS:O	2.12	0.49
2:L:517:HIS:CE1	2:L:540:ASP:HB3	2.47	0.49
1:A:375:LEU:HD21	1:F:374:GLN:OE1	2.12	0.49
1:A:378:LEU:HD23	1:F:378:LEU:HD23	1.95	0.49
1:A:1238:VAL:HG13	1:A:1242:GLU:HB2	1.93	0.49
1:A:1432:HIS:CE1	1:E:1744:TYR:HB2	2.47	0.49
1:B:375:LEU:HD21	1:E:374:GLN:OE1	2.13	0.49
1:E:1239:HIS:CE1	1:E:1717:ASP:O	2.65	0.49
1:F:479:ASN:ND2	1:F:613:VAL:O	2.45	0.49
1:F:704:VAL:HG23	1:F:763:TRP:CZ3	2.48	0.49
2:G:99:ASN:HD21	2:G:550:VAL:H	1.60	0.49
2:G:330:ASN:ND2	2:G:394:ARG:CZ	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1751:ILE:HG23	2:G:1840:VAL:HG21	1.95	0.49
2:J:1470:THR:HA	2:J:1484:LYS:O	2.12	0.49
2:K:330:ASN:ND2	2:K:394:ARG:CZ	2.76	0.49
2:L:330:ASN:ND2	2:L:394:ARG:CZ	2.76	0.49
1:A:1239:HIS:CE1	1:A:1717:ASP:O	2.65	0.49
1:C:704:VAL:HG23	1:C:763:TRP:CZ3	2.47	0.49
1:C:1109:GLU:CD	1:C:1109:GLU:H	2.20	0.49
1:D:1109:GLU:H	1:D:1109:GLU:CD	2.20	0.49
2:H:101:ILE:HD11	2:H:122:LEU:HD23	1.93	0.49
2:H:330:ASN:ND2	2:H:394:ARG:CZ	2.76	0.49
2:J:517:HIS:CE1	2:J:540:ASP:HB3	2.47	0.49
2:K:99:ASN:HD21	2:K:550:VAL:H	1.60	0.49
2:K:101:ILE:HD11	2:K:122:LEU:HD23	1.93	0.49
2:L:159:ILE:HA	2:L:271:THR:O	2.13	0.49
2:L:1470:THR:HA	2:L:1484:LYS:O	2.13	0.49
1:A:1280:ILE:HD12	1:E:1280:ILE:HD12	1.94	0.49
1:B:378:LEU:HD23	1:E:378:LEU:HD23	1.95	0.49
1:B:479:ASN:ND2	1:B:613:VAL:O	2.45	0.49
1:B:704:VAL:HG23	1:B:763:TRP:CZ3	2.48	0.49
1:C:871:TRP:HA	3:O:146:ASN:HD22	1.78	0.49
1:D:704:VAL:HG23	1:D:763:TRP:CZ3	2.48	0.49
1:E:704:VAL:HG23	1:E:763:TRP:CZ3	2.47	0.49
1:F:850:PHE:HZ	1:F:866:GLY:HA3	1.78	0.49
2:G:159:ILE:HA	2:G:271:THR:O	2.13	0.49
2:I:330:ASN:ND2	2:I:394:ARG:CZ	2.76	0.49
2:K:615:TYR:OH	2:K:1075:ASP:OD1	2.17	0.49
2:L:1638:ILE:HG13	2:L:1657:ILE:HD12	1.94	0.49
1:B:850:PHE:HZ	1:B:866:GLY:HA3	1.78	0.49
2:G:309:ARG:NH1	2:G:442:ASP:OD2	2.43	0.49
2:G:1470:THR:HA	2:G:1484:LYS:O	2.13	0.49
2:H:159:ILE:HA	2:H:271:THR:O	2.13	0.49
2:H:1956:ARG:O	2:H:1956:ARG:NE	2.43	0.49
2:I:309:ARG:NH1	2:I:442:ASP:OD2	2.43	0.49
2:I:1470:THR:HA	2:I:1484:LYS:O	2.13	0.49
2:J:330:ASN:ND2	2:J:394:ARG:CZ	2.76	0.49
2:K:159:ILE:HA	2:K:271:THR:O	2.13	0.49
2:K:1585:SER:HB3	2:K:1651:LEU:HD11	1.95	0.49
2:L:1956:ARG:NE	2:L:1956:ARG:O	2.43	0.49
1:A:374:GLN:OE1	1:F:375:LEU:HD21	2.13	0.49
1:C:821:GLN:NE2	1:C:914:VAL:HG22	2.28	0.49
1:C:833:PHE:CE2	3:O:150:ILE:HG13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:821:GLN:NE2	1:D:914:VAL:HG22	2.28	0.49
2:G:517:HIS:CE1	2:G:540:ASP:HB3	2.48	0.49
2:J:309:ARG:NH1	2:J:442:ASP:OD2	2.43	0.49
2:K:1470:THR:HA	2:K:1484:LYS:O	2.13	0.49
1:A:704:VAL:HG23	1:A:763:TRP:CZ3	2.48	0.49
1:C:904:ASN:HB3	1:C:926:LEU:HD13	1.93	0.49
1:D:904:ASN:HB3	1:D:926:LEU:HD13	1.93	0.49
2:G:1585:SER:HB3	2:G:1651:LEU:HD11	1.95	0.49
1:B:529:MET:HE3	1:B:637:PHE:CB	2.43	0.49
2:I:101:ILE:HD11	2:I:122:LEU:HD23	1.93	0.49
3:P:146:ASN:HA	3:P:150:ILE:HG12	1.95	0.49
1:B:641:ARG:NH2	1:B:925:ASP:OD2	2.46	0.48
1:E:605:LEU:HG	1:E:612:GLU:HG3	1.95	0.48
1:E:641:ARG:NH2	1:E:925:ASP:OD2	2.46	0.48
1:E:850:PHE:HZ	1:E:866:GLY:HA3	1.77	0.48
1:F:529:MET:HE3	1:F:637:PHE:CB	2.43	0.48
1:F:821:GLN:NE2	1:F:914:VAL:HG22	2.28	0.48
1:F:833:PHE:CE2	3:R:150:ILE:HG13	2.48	0.48
1:F:1239:HIS:CE1	1:F:1717:ASP:O	2.65	0.48
2:H:1751:ILE:HG23	2:H:1840:VAL:HG21	1.95	0.48
2:J:101:ILE:HD11	2:J:122:LEU:HD23	1.93	0.48
1:A:529:MET:HE3	1:A:637:PHE:CB	2.43	0.48
1:B:821:GLN:NE2	1:B:914:VAL:HG22	2.28	0.48
1:B:1239:HIS:CE1	1:B:1717:ASP:O	2.65	0.48
1:C:850:PHE:HZ	1:C:866:GLY:HA3	1.78	0.48
1:D:850:PHE:HZ	1:D:866:GLY:HA3	1.78	0.48
1:F:641:ARG:NH2	1:F:925:ASP:OD2	2.46	0.48
2:H:1638:ILE:HG13	2:H:1657:ILE:HD12	1.95	0.48
1:A:641:ARG:NH2	1:A:925:ASP:OD2	2.46	0.48
2:J:1751:ILE:HG23	2:J:1840:VAL:HG21	1.95	0.48
2:L:101:ILE:HD11	2:L:122:LEU:HD23	1.94	0.48
1:B:374:GLN:OE1	1:E:375:LEU:HD21	2.13	0.48
1:E:529:MET:HE3	1:E:637:PHE:CB	2.43	0.48
2:I:59:GLU:HA	2:I:122:LEU:HD12	1.96	0.48
1:A:773:ALA:HB3	3:M:142:VAL:HG23	1.95	0.48
1:C:374:GLN:OE1	1:D:375:LEU:HD21	2.13	0.48
1:C:605:LEU:HG	1:C:612:GLU:HG3	1.95	0.48
1:D:529:MET:HE3	1:D:637:PHE:CB	2.43	0.48
2:G:101:ILE:HD11	2:G:122:LEU:HD23	1.94	0.48
1:A:821:GLN:NE2	1:A:914:VAL:HG22	2.28	0.48
1:A:850:PHE:HZ	1:A:866:GLY:HA3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1432:HIS:CE1	1:D:1744:TYR:HB2	2.49	0.48
1:C:378:LEU:HD23	1:D:378:LEU:HD23	1.95	0.48
1:E:833:PHE:CE2	3:Q:150:ILE:HG13	2.48	0.48
2:I:1638:ILE:HG13	2:I:1657:ILE:HD12	1.94	0.48
3:N:146:ASN:HA	3:N:150:ILE:HG12	1.95	0.48
1:A:605:LEU:HG	1:A:612:GLU:HG3	1.96	0.48
1:C:529:MET:HE3	1:C:637:PHE:CB	2.43	0.48
1:C:641:ARG:NH2	1:C:925:ASP:OD2	2.46	0.48
1:D:641:ARG:NH2	1:D:925:ASP:OD2	2.46	0.48
1:D:773:ALA:HB3	3:P:142:VAL:HG23	1.95	0.48
1:E:489:VAL:HG13	1:E:670:GLY:HA3	1.96	0.48
2:I:1127:PHE:CE1	2:I:1141:ALA:HB1	2.49	0.48
2:L:99:ASN:HD21	2:L:550:VAL:H	1.60	0.48
2:L:1808:SER:H	2:L:2013:ASN:ND2	2.12	0.48
1:E:1584:PRO:HG3	1:E:1591:TRP:CE3	2.49	0.48
2:G:370:LEU:HD21	2:G:428:HIS:CD2	2.49	0.48
2:J:1127:PHE:CE1	2:J:1141:ALA:HB1	2.49	0.48
1:A:489:VAL:HG13	1:A:670:GLY:HA3	1.96	0.48
1:B:489:VAL:HG13	1:B:670:GLY:HA3	1.96	0.48
1:C:1261:PHE:CD1	1:F:1338:GLU:HG2	2.49	0.48
1:E:821:GLN:NE2	1:E:914:VAL:HG22	2.28	0.48
1:F:605:LEU:HG	1:F:612:GLU:HG3	1.96	0.48
2:G:1496:LYS:HD3	2:G:2002:LYS:HG2	1.96	0.48
2:H:99:ASN:HD21	2:H:550:VAL:H	1.60	0.48
2:H:1808:SER:H	2:H:2013:ASN:ND2	2.12	0.48
2:I:159:ILE:HA	2:I:271:THR:O	2.13	0.48
2:I:1478:ASN:OD1	2:I:1478:ASN:N	2.47	0.48
2:J:59:GLU:HA	2:J:122:LEU:HD12	1.96	0.48
2:J:1638:ILE:HG13	2:J:1657:ILE:HD12	1.94	0.48
3:O:146:ASN:HA	3:O:150:ILE:HG12	1.96	0.48
3:R:146:ASN:HA	3:R:150:ILE:HG12	1.96	0.48
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.49	0.48
1:B:605:LEU:HG	1:B:612:GLU:HG3	1.96	0.48
1:F:489:VAL:HG13	1:F:670:GLY:HA3	1.96	0.48
1:F:1584:PRO:HG3	1:F:1591:TRP:CE3	2.49	0.48
2:G:706:LYS:NZ	5:G:2101:FMN:O2'	2.47	0.48
2:H:1855:ILE:HG22	2:H:1968:PRO:HA	1.96	0.48
2:J:1478:ASN:OD1	2:J:1478:ASN:N	2.47	0.48
1:C:489:VAL:HG13	1:C:670:GLY:HA3	1.96	0.47
1:D:605:LEU:HG	1:D:612:GLU:HG3	1.96	0.47
1:D:833:PHE:CE2	3:P:150:ILE:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:159:ILE:HA	2:J:271:THR:O	2.13	0.47
1:B:1584:PRO:HG3	1:B:1591:TRP:CE3	2.49	0.47
1:C:375:LEU:HD21	1:D:374:GLN:OE1	2.14	0.47
2:G:1808:SER:H	2:G:2013:ASN:ND2	2.12	0.47
2:G:1855:ILE:HG22	2:G:1968:PRO:HA	1.96	0.47
2:H:1585:SER:HB3	2:H:1651:LEU:HD11	1.95	0.47
2:I:1585:SER:HB3	2:I:1651:LEU:HD11	1.95	0.47
2:J:1808:SER:H	2:J:2013:ASN:ND2	2.12	0.47
2:K:370:LEU:HD21	2:K:428:HIS:CD2	2.49	0.47
2:K:663:ILE:HB	2:K:664:PRO:HD3	1.96	0.47
2:L:1585:SER:HB3	2:L:1651:LEU:HD11	1.95	0.47
1:A:1338:GLU:HG2	1:E:1261:PHE:CD1	2.49	0.47
1:B:1261:PHE:CD1	1:D:1338:GLU:HG2	2.49	0.47
1:C:1338:GLU:HG2	1:F:1261:PHE:CD1	2.49	0.47
1:C:1657:HIS:CD2	1:C:1658:PRO:HD2	2.50	0.47
2:H:1478:ASN:OD1	2:H:1478:ASN:N	2.47	0.47
2:J:370:LEU:HD21	2:J:428:HIS:CD2	2.49	0.47
2:K:1855:ILE:HG22	2:K:1968:PRO:HA	1.97	0.47
3:M:146:ASN:HA	3:M:150:ILE:HG12	1.95	0.47
1:A:1201:SER:OG	1:A:1203:ASP:OD1	2.29	0.47
1:A:1261:PHE:CD1	1:E:1338:GLU:HG2	2.49	0.47
1:B:1338:GLU:HG2	1:D:1261:PHE:CD1	2.50	0.47
1:D:1107:GLU:OE1	1:D:1191:THR:OG1	2.29	0.47
2:H:1736:MET:HE1	2:H:1832:PHE:CD2	2.49	0.47
2:I:1808:SER:H	2:I:2013:ASN:ND2	2.12	0.47
2:J:1585:SER:HB3	2:J:1651:LEU:HD11	1.95	0.47
2:K:1808:SER:H	2:K:2013:ASN:ND2	2.12	0.47
1:D:1584:PRO:HG3	1:D:1591:TRP:CE3	2.49	0.47
1:D:1657:HIS:CD2	1:D:1658:PRO:HD2	2.50	0.47
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.97	0.47
2:G:1736:MET:HE1	2:G:1832:PHE:CD2	2.49	0.47
2:H:598:THR:O	2:H:602:VAL:HB	2.15	0.47
2:K:1736:MET:HE1	2:K:1832:PHE:CD2	2.49	0.47
2:L:1478:ASN:OD1	2:L:1478:ASN:N	2.47	0.47
1:C:1584:PRO:HG3	1:C:1591:TRP:CE3	2.49	0.47
1:D:489:VAL:HG13	1:D:670:GLY:HA3	1.96	0.47
1:E:1201:SER:OG	1:E:1203:ASP:OD1	2.29	0.47
2:L:1736:MET:HE1	2:L:1832:PHE:CD2	2.50	0.47
1:C:1107:GLU:OE1	1:C:1191:THR:OG1	2.29	0.47
2:G:1757:GLU:OE1	2:G:1757:GLU:N	2.38	0.47
2:H:370:LEU:HD21	2:H:428:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:ILE:HD11	2:I:122:LEU:HD21	1.96	0.47
2:I:370:LEU:HD21	2:I:428:HIS:CD2	2.50	0.47
2:I:598:THR:O	2:I:602:VAL:HB	2.15	0.47
2:J:598:THR:O	2:J:602:VAL:HB	2.15	0.47
2:L:370:LEU:HD21	2:L:428:HIS:CD2	2.49	0.47
2:L:598:THR:O	2:L:602:VAL:HB	2.15	0.47
2:L:1496:LYS:HD3	2:L:2002:LYS:HG2	1.97	0.47
1:A:764:ASP:OD1	1:A:810:LYS:NZ	2.48	0.47
1:A:833:PHE:CE2	3:M:150:ILE:HG13	2.49	0.47
1:A:1657:HIS:CD2	1:A:1658:PRO:HD2	2.50	0.47
1:C:706:THR:HB	1:C:737:PHE:HB3	1.97	0.47
1:D:706:THR:HB	1:D:737:PHE:HB3	1.97	0.47
2:G:1478:ASN:OD1	2:G:1478:ASN:N	2.47	0.47
2:K:598:THR:O	2:K:602:VAL:HB	2.15	0.47
2:K:1757:GLU:OE1	2:K:1757:GLU:N	2.38	0.47
2:L:1855:ILE:HG22	2:L:1968:PRO:HA	1.97	0.47
1:E:764:ASP:OD1	1:E:810:LYS:NZ	2.48	0.47
1:F:1657:HIS:CD2	1:F:1658:PRO:HD2	2.50	0.47
2:H:1738:PHE:CZ	2:H:1840:VAL:HG12	2.50	0.47
2:J:1736:MET:HE1	2:J:1832:PHE:CD2	2.49	0.47
2:J:1855:ILE:HG22	2:J:1968:PRO:HA	1.96	0.47
2:K:1478:ASN:OD1	2:K:1478:ASN:N	2.47	0.47
1:B:1657:HIS:CD2	1:B:1658:PRO:HD2	2.50	0.47
1:D:1017:ARG:HG2	1:D:1510:ASN:ND2	2.31	0.47
1:E:1657:HIS:CD2	1:E:1658:PRO:HD2	2.50	0.47
2:G:598:THR:O	2:G:602:VAL:HB	2.15	0.47
2:G:1127:PHE:CE1	2:G:1141:ALA:HB1	2.49	0.47
3:Q:146:ASN:HA	3:Q:150:ILE:HG12	1.96	0.47
1:B:198:PRO:HG3	1:B:212:THR:HG21	1.96	0.46
1:C:1017:ARG:HG2	1:C:1510:ASN:ND2	2.31	0.46
2:I:1736:MET:HE1	2:I:1832:PHE:CD2	2.49	0.46
2:I:1804:PHE:CZ	2:I:2010:TYR:HB2	2.51	0.46
2:J:1804:PHE:CZ	2:J:2010:TYR:HB2	2.50	0.46
2:L:59:GLU:HA	2:L:122:LEU:HD12	1.96	0.46
1:C:1432:HIS:CE1	1:F:1744:TYR:HB2	2.50	0.46
2:J:101:ILE:HD11	2:J:122:LEU:HD21	1.97	0.46
2:K:101:ILE:HD11	2:K:122:LEU:HD21	1.96	0.46
1:B:833:PHE:CE2	3:N:150:ILE:HG13	2.51	0.46
1:C:987:ASN:ND2	1:C:1685:TYR:OH	2.49	0.46
1:D:987:ASN:ND2	1:D:1685:TYR:OH	2.49	0.46
1:E:198:PRO:HG3	1:E:212:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1127:PHE:CE1	2:H:1141:ALA:HB1	2.49	0.46
2:J:1142:LEU:HD22	2:J:1182:VAL:HG11	1.97	0.46
2:J:1265:MET:HE1	2:J:1569:PHE:CZ	2.51	0.46
2:J:1738:PHE:CZ	2:J:1840:VAL:HG12	2.50	0.46
2:K:59:GLU:HA	2:K:122:LEU:HD12	1.96	0.46
2:K:1127:PHE:CE1	2:K:1141:ALA:HB1	2.49	0.46
2:L:1127:PHE:CE1	2:L:1141:ALA:HB1	2.49	0.46
1:A:198:PRO:HG3	1:A:212:THR:HG21	1.97	0.46
1:A:706:THR:HB	1:A:737:PHE:HB3	1.97	0.46
1:E:706:THR:HB	1:E:737:PHE:HB3	1.97	0.46
2:G:101:ILE:HD11	2:G:122:LEU:HD21	1.96	0.46
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.50	0.46
2:H:59:GLU:HA	2:H:122:LEU:HD12	1.96	0.46
2:K:1804:PHE:CZ	2:K:2010:TYR:HB2	2.50	0.46
1:C:1310:GLU:OE1	1:C:1649:LYS:CE	2.64	0.46
2:G:615:TYR:OH	2:G:1075:ASP:OD1	2.17	0.46
1:A:1334:ASP:OD1	1:A:1380:GLN:NE2	2.49	0.46
1:B:764:ASP:OD1	1:B:810:LYS:NZ	2.48	0.46
1:D:1310:GLU:OE1	1:D:1649:LYS:CE	2.64	0.46
1:E:1334:ASP:OD1	1:E:1380:GLN:NE2	2.49	0.46
1:F:764:ASP:OD1	1:F:810:LYS:NZ	2.48	0.46
2:I:1855:ILE:HG22	2:I:1968:PRO:HA	1.97	0.46
1:B:881:ASN:ND2	3:N:146:ASN:O	2.48	0.46
1:D:881:ASN:ND2	3:P:146:ASN:O	2.48	0.46
1:F:1334:ASP:OD1	1:F:1380:GLN:NE2	2.49	0.46
2:G:1142:LEU:HD22	2:G:1182:VAL:HG11	1.97	0.46
2:H:663:ILE:HB	2:H:664:PRO:HD3	1.96	0.46
2:H:1804:PHE:CZ	2:H:2010:TYR:HB2	2.50	0.46
2:L:101:ILE:HD11	2:L:122:LEU:HD21	1.96	0.46
2:L:868:PHE:CD1	2:L:872:ILE:HD12	2.51	0.46
1:B:1334:ASP:OD1	1:B:1380:GLN:NE2	2.49	0.46
1:C:1334:ASP:OD1	1:C:1380:GLN:NE2	2.49	0.46
1:D:1201:SER:OG	1:D:1203:ASP:OD1	2.29	0.46
1:D:1334:ASP:OD1	1:D:1380:GLN:NE2	2.49	0.46
1:F:198:PRO:HG3	1:F:212:THR:HG21	1.97	0.46
1:F:871:TRP:CZ3	3:R:150:ILE:HG21	2.51	0.46
2:H:868:PHE:CD1	2:H:872:ILE:HD12	2.51	0.46
2:I:868:PHE:CD1	2:I:872:ILE:HD12	2.51	0.46
2:L:663:ILE:HB	2:L:664:PRO:HD3	1.96	0.46
1:A:1249:SER:HB3	1:A:1280:ILE:HG23	1.98	0.46
1:C:764:ASP:OD1	1:C:810:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:ASP:OD1	1:D:810:LYS:NZ	2.48	0.46
1:E:1249:SER:HB3	1:E:1280:ILE:HG23	1.98	0.46
1:F:706:THR:HB	1:F:737:PHE:HB3	1.97	0.46
2:G:1265:MET:HE1	2:G:1569:PHE:CZ	2.51	0.46
2:H:101:ILE:HD11	2:H:122:LEU:HD21	1.97	0.46
2:I:1142:LEU:HD22	2:I:1182:VAL:HG11	1.98	0.46
2:K:1496:LYS:HD3	2:K:2002:LYS:HG2	1.98	0.46
2:L:1738:PHE:CZ	2:L:1840:VAL:HG12	2.51	0.46
1:B:21:GLN:HE21	1:B:21:GLN:HB3	1.64	0.46
1:B:706:THR:HB	1:B:737:PHE:HB3	1.97	0.46
1:C:871:TRP:CZ3	3:O:150:ILE:HG21	2.51	0.46
1:C:1201:SER:OG	1:C:1203:ASP:OD1	2.29	0.46
2:K:868:PHE:CD1	2:K:872:ILE:HD12	2.51	0.46
1:A:1310:GLU:OE1	1:A:1649:LYS:CE	2.64	0.45
1:C:1744:TYR:HB2	1:F:1432:HIS:CE1	2.51	0.45
1:E:1304:ALA:O	1:E:1307:THR:HG23	2.17	0.45
2:G:868:PHE:CD1	2:G:872:ILE:HD12	2.51	0.45
2:G:1738:PHE:CZ	2:G:1840:VAL:HG12	2.51	0.45
2:I:663:ILE:HB	2:I:664:PRO:HD3	1.96	0.45
2:J:754:TYR:CD1	2:J:794:MET:HG2	2.51	0.45
2:L:1804:PHE:CZ	2:L:2010:TYR:HB2	2.51	0.45
1:A:881:ASN:ND2	3:M:146:ASN:O	2.49	0.45
1:A:1107:GLU:OE1	1:A:1191:THR:OG1	2.29	0.45
1:F:233:ILE:HG13	1:F:243:ILE:HD13	1.99	0.45
2:H:754:TYR:CD1	2:H:794:MET:HG2	2.52	0.45
2:H:1149:TRP:CE2	2:H:1213:LEU:HD23	2.52	0.45
2:L:754:TYR:CD1	2:L:794:MET:HG2	2.52	0.45
2:L:1265:MET:HE1	2:L:1569:PHE:CZ	2.51	0.45
1:A:233:ILE:HG13	1:A:243:ILE:HD13	1.99	0.45
1:A:1304:ALA:O	1:A:1307:THR:HG23	2.17	0.45
1:E:1310:GLU:OE1	1:E:1649:LYS:CE	2.64	0.45
1:F:1017:ARG:HG2	1:F:1510:ASN:ND2	2.30	0.45
2:G:59:GLU:HA	2:G:122:LEU:HD12	1.97	0.45
2:H:230:TYR:CE2	2:H:236:ILE:HD13	2.52	0.45
2:I:1265:MET:HE1	2:I:1569:PHE:CZ	2.52	0.45
2:J:868:PHE:CD1	2:J:872:ILE:HD12	2.51	0.45
2:J:1496:LYS:HD3	2:J:2002:LYS:HG2	1.98	0.45
2:L:249:TYR:CE2	2:L:283:ILE:HD12	2.52	0.45
2:L:1142:LEU:HD22	2:L:1182:VAL:HG11	1.97	0.45
1:B:1310:GLU:OE1	1:B:1649:LYS:CE	2.64	0.45
1:C:233:ILE:HG13	1:C:243:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:845:SER:HG	1:D:845:SER:HG	1.36	0.45
1:F:1107:GLU:OE1	1:F:1191:THR:OG1	2.29	0.45
2:H:249:TYR:CE2	2:H:283:ILE:HD12	2.52	0.45
2:H:1037:SER:HA	2:H:1051:THR:HG21	1.98	0.45
2:I:754:TYR:CD1	2:I:794:MET:HG2	2.52	0.45
2:J:1037:SER:HA	2:J:1051:THR:HG21	1.98	0.45
2:J:1330:GLY:HA2	2:J:1374:THR:HG21	1.99	0.45
2:K:9:LEU:HD21	2:K:34:GLN:HG3	1.98	0.45
2:K:1142:LEU:HD22	2:K:1182:VAL:HG11	1.97	0.45
2:L:1149:TRP:CE2	2:L:1213:LEU:HD23	2.52	0.45
1:B:1017:ARG:HG2	1:B:1510:ASN:ND2	2.30	0.45
1:E:233:ILE:HG13	1:E:243:ILE:HD13	1.99	0.45
1:F:21:GLN:HE21	1:F:21:GLN:HB3	1.64	0.45
1:F:1310:GLU:OE1	1:F:1649:LYS:CE	2.64	0.45
2:G:754:TYR:CD1	2:G:794:MET:HG2	2.51	0.45
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.99	0.45
2:H:1142:LEU:HD22	2:H:1182:VAL:HG11	1.97	0.45
2:H:1265:MET:HE1	2:H:1569:PHE:CZ	2.51	0.45
2:I:1081:HIS:O	2:I:1085:LEU:HB2	2.17	0.45
2:J:663:ILE:HB	2:J:664:PRO:HD3	1.97	0.45
2:J:1081:HIS:O	2:J:1085:LEU:HB2	2.17	0.45
2:L:398:ALA:HB2	2:L:413:LYS:HB2	1.99	0.45
2:L:1854:MET:HA	2:L:1907:LEU:HD21	1.98	0.45
1:A:1264:ARG:NH1	1:A:1270:VAL:HB	2.32	0.45
1:B:233:ILE:HG13	1:B:243:ILE:HD13	1.99	0.45
1:B:1304:ALA:O	1:B:1307:THR:HG23	2.17	0.45
1:D:1304:ALA:O	1:D:1307:THR:HG23	2.17	0.45
1:F:1304:ALA:O	1:F:1307:THR:HG23	2.17	0.45
1:F:1584:PRO:HG3	1:F:1591:TRP:CZ3	2.52	0.45
2:G:499:THR:OG1	2:G:500:HIS:HD2	2.00	0.45
2:I:1037:SER:HA	2:I:1051:THR:HG21	1.98	0.45
2:I:1330:GLY:HA2	2:I:1374:THR:HG21	1.99	0.45
2:I:1738:PHE:CZ	2:I:1840:VAL:HG12	2.51	0.45
1:B:1249:SER:HB3	1:B:1280:ILE:HG23	1.98	0.45
1:B:1584:PRO:HG3	1:B:1591:TRP:CZ3	2.52	0.45
1:C:198:PRO:HG3	1:C:212:THR:HG21	1.97	0.45
1:D:198:PRO:HG3	1:D:212:THR:HG21	1.97	0.45
1:E:1264:ARG:NH1	1:E:1270:VAL:HB	2.32	0.45
2:G:249:TYR:CE2	2:G:283:ILE:HD12	2.52	0.45
2:H:1081:HIS:O	2:H:1085:LEU:HB2	2.17	0.45
2:I:9:LEU:HD21	2:I:34:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:230:TYR:CE2	2:J:236:ILE:HD13	2.52	0.45
2:K:499:THR:OG1	2:K:500:HIS:HD2	2.00	0.45
2:K:754:TYR:CD1	2:K:794:MET:HG2	2.52	0.45
2:L:499:THR:OG1	2:L:500:HIS:HD2	2.00	0.45
1:C:340:ARG:HH12	1:C:344:GLN:HE21	1.65	0.45
1:C:1304:ALA:O	1:C:1307:THR:HG23	2.17	0.45
1:E:400:ARG:HH11	1:E:715:THR:HG21	1.80	0.45
1:F:1249:SER:HB3	1:F:1280:ILE:HG23	1.98	0.45
2:G:1149:TRP:CE2	2:G:1213:LEU:HD23	2.52	0.45
2:G:1933:LEU:HD13	2:G:1933:LEU:N	2.32	0.45
2:H:2017:LYS:O	2:H:2018:PRO:C	2.59	0.45
2:I:1496:LYS:HD3	2:I:2002:LYS:HG2	1.98	0.45
2:J:249:TYR:CE2	2:J:283:ILE:HD12	2.52	0.45
2:K:1738:PHE:CZ	2:K:1840:VAL:HG12	2.51	0.45
2:L:1081:HIS:O	2:L:1085:LEU:HB2	2.17	0.45
2:L:2017:LYS:O	2:L:2018:PRO:C	2.59	0.45
1:A:871:TRP:CZ3	3:M:150:ILE:HG21	2.52	0.45
1:C:1264:ARG:NH1	1:C:1270:VAL:HB	2.32	0.45
1:E:871:TRP:CZ3	3:Q:150:ILE:HG21	2.52	0.45
1:E:1304:ALA:O	1:E:1307:THR:CG2	2.65	0.45
2:J:1757:GLU:OE1	2:J:1757:GLU:N	2.38	0.45
2:K:249:TYR:CE2	2:K:283:ILE:HD12	2.52	0.45
2:K:1037:SER:HA	2:K:1051:THR:HG21	1.98	0.45
2:K:1265:MET:HE1	2:K:1569:PHE:CZ	2.51	0.45
2:L:1037:SER:HA	2:L:1051:THR:HG21	1.98	0.45
3:N:42:LEU:HD23	3:N:42:LEU:HA	1.89	0.45
3:R:42:LEU:HD23	3:R:42:LEU:HA	1.89	0.45
1:A:400:ARG:HH11	1:A:715:THR:HG21	1.80	0.45
1:A:1304:ALA:O	1:A:1307:THR:CG2	2.65	0.45
1:B:871:TRP:CZ3	3:N:150:ILE:HG21	2.52	0.45
1:D:1264:ARG:NH1	1:D:1270:VAL:HB	2.32	0.45
1:F:987:ASN:ND2	1:F:1685:TYR:OH	2.49	0.45
1:F:1304:ALA:O	1:F:1307:THR:CG2	2.65	0.45
2:G:679:LEU:HD21	2:G:681:ILE:HD11	1.99	0.45
2:G:1037:SER:HA	2:G:1051:THR:HG21	1.98	0.45
2:H:7:ARG:HD3	2:H:27:PHE:CD1	2.53	0.45
2:H:499:THR:OG1	2:H:500:HIS:HD2	2.00	0.45
2:H:1496:LYS:HD3	2:H:2002:LYS:HG2	1.99	0.45
2:J:9:LEU:HD21	2:J:34:GLN:HG3	1.99	0.45
2:J:1149:TRP:CE2	2:J:1213:LEU:HD23	2.52	0.45
2:K:1330:GLY:HA2	2:K:1374:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:741:HIS:CD2	2:L:855:HIS:ND1	2.85	0.45
1:A:1418:VAL:N	1:A:1419:PRO:HD2	2.32	0.44
1:B:987:ASN:ND2	1:B:1685:TYR:OH	2.49	0.44
1:B:1264:ARG:NH1	1:B:1270:VAL:HB	2.32	0.44
1:B:1304:ALA:O	1:B:1307:THR:CG2	2.66	0.44
1:D:233:ILE:HG13	1:D:243:ILE:HD13	1.99	0.44
1:D:340:ARG:HH12	1:D:344:GLN:HE21	1.65	0.44
1:E:987:ASN:ND2	1:E:1685:TYR:OH	2.49	0.44
1:E:1584:PRO:HG3	1:E:1591:TRP:CZ3	2.52	0.44
1:F:1264:ARG:NH1	1:F:1270:VAL:HB	2.32	0.44
2:H:9:LEU:HD21	2:H:34:GLN:HG3	1.99	0.44
2:I:741:HIS:CD2	2:I:855:HIS:ND1	2.85	0.44
2:I:1854:MET:HA	2:I:1907:LEU:HD21	1.98	0.44
2:K:679:LEU:HD21	2:K:681:ILE:HD11	1.99	0.44
2:K:1081:HIS:O	2:K:1085:LEU:HB2	2.17	0.44
2:K:1933:LEU:N	2:K:1933:LEU:HD13	2.33	0.44
1:A:984:PRO:HB3	2:G:959:THR:HG23	1.99	0.44
1:A:987:ASN:ND2	1:A:1685:TYR:OH	2.48	0.44
1:C:1418:VAL:N	1:C:1419:PRO:HD2	2.32	0.44
1:E:1418:VAL:N	1:E:1419:PRO:HD2	2.32	0.44
2:G:398:ALA:HB2	2:G:413:LYS:HB2	1.98	0.44
2:G:741:HIS:CD2	2:G:855:HIS:ND1	2.85	0.44
2:I:398:ALA:HB2	2:I:413:LYS:HB2	1.99	0.44
2:J:741:HIS:CD2	2:J:855:HIS:ND1	2.85	0.44
2:K:741:HIS:CD2	2:K:855:HIS:ND1	2.85	0.44
1:B:159:LEU:CD2	1:B:176:VAL:CG1	2.96	0.44
1:D:1418:VAL:N	1:D:1419:PRO:HD2	2.32	0.44
2:G:1081:HIS:O	2:G:1085:LEU:HB2	2.17	0.44
2:H:741:HIS:CD2	2:H:855:HIS:ND1	2.85	0.44
2:I:249:TYR:CE2	2:I:283:ILE:HD12	2.52	0.44
2:J:1873:TYR:O	2:J:1874:VAL:C	2.60	0.44
2:K:1149:TRP:CE2	2:K:1213:LEU:HD23	2.52	0.44
2:L:7:ARG:HD3	2:L:27:PHE:CD1	2.53	0.44
3:N:20:ILE:HD11	3:N:103:LEU:HD23	2.00	0.44
1:A:1584:PRO:HG3	1:A:1591:TRP:CZ3	2.52	0.44
1:B:1173:LEU:CD2	1:D:1175:ILE:HG12	2.47	0.44
1:C:1175:ILE:HG12	1:F:1173:LEU:CD2	2.48	0.44
1:C:1249:SER:HB3	1:C:1280:ILE:HG23	1.98	0.44
1:D:231:ARG:HH21	2:L:115:THR:HG21	1.83	0.44
1:D:871:TRP:CZ3	3:P:150:ILE:HG21	2.52	0.44
1:F:1418:VAL:N	1:F:1419:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:665:LEU:HD22	2:H:665:LEU:O	2.17	0.44
2:H:1854:MET:HA	2:H:1907:LEU:HD21	1.99	0.44
2:I:1852:TYR:HD1	2:I:1903:ASP:HA	1.82	0.44
2:I:1873:TYR:O	2:I:1874:VAL:C	2.60	0.44
2:K:1854:MET:HA	2:K:1907:LEU:HD21	1.98	0.44
2:K:2017:LYS:O	2:K:2018:PRO:C	2.59	0.44
2:L:230:TYR:CE2	2:L:236:ILE:HD13	2.53	0.44
2:L:665:LEU:O	2:L:665:LEU:HD22	2.17	0.44
2:L:1852:TYR:HD1	2:L:1903:ASP:HA	1.83	0.44
1:B:1146:HIS:HE1	1:D:1117:GLU:O	2.01	0.44
1:B:1418:VAL:N	1:B:1419:PRO:HD2	2.32	0.44
1:D:1249:SER:HB3	1:D:1280:ILE:HG23	1.98	0.44
1:F:159:LEU:CD2	1:F:176:VAL:CG1	2.96	0.44
1:F:984:PRO:HB3	2:L:959:THR:HG23	2.00	0.44
2:G:9:LEU:HD21	2:G:34:GLN:HG3	2.00	0.44
2:J:7:ARG:HD3	2:J:27:PHE:CD1	2.53	0.44
2:J:499:THR:OG1	2:J:500:HIS:HD2	2.00	0.44
2:L:1330:GLY:HA2	2:L:1374:THR:HG21	1.99	0.44
1:A:986:ALA:HB2	1:A:1047:LEU:HD13	2.00	0.44
2:G:2017:LYS:O	2:G:2018:PRO:C	2.59	0.44
2:H:898:ASP:O	2:H:1050:ARG:HG2	2.18	0.44
2:I:1757:GLU:OE1	2:I:1757:GLU:N	2.38	0.44
2:J:398:ALA:HB2	2:J:413:LYS:HB2	1.99	0.44
2:L:9:LEU:HD21	2:L:34:GLN:HG3	1.99	0.44
2:L:679:LEU:HD21	2:L:681:ILE:HD11	1.99	0.44
3:O:141:ASP:OD1	3:O:143:VAL:HG12	2.18	0.44
1:B:1303:GLY:H	1:B:1307:THR:HG22	1.83	0.44
1:C:1117:GLU:O	1:F:1146:HIS:HE1	2.01	0.44
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.99	0.44
2:H:1852:TYR:HD1	2:H:1903:ASP:HA	1.83	0.44
2:I:499:THR:OG1	2:I:500:HIS:HD2	2.00	0.44
2:I:1149:TRP:CE2	2:I:1213:LEU:HD23	2.52	0.44
2:L:898:ASP:O	2:L:1050:ARG:HG2	2.18	0.44
1:C:1173:LEU:CD2	1:F:1175:ILE:HG12	2.48	0.44
1:C:1584:PRO:HG3	1:C:1591:TRP:CZ3	2.52	0.44
1:F:1303:GLY:H	1:F:1307:THR:HG22	1.83	0.44
2:G:230:TYR:CE2	2:G:236:ILE:HD13	2.52	0.44
2:H:679:LEU:HD21	2:H:681:ILE:HD11	1.99	0.44
2:I:7:ARG:HD3	2:I:27:PHE:CD1	2.53	0.44
2:I:230:TYR:CE2	2:I:236:ILE:HD13	2.53	0.44
2:K:1852:TYR:HD1	2:K:1903:ASP:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:141:ASP:OD1	3:R:143:VAL:HG12	2.18	0.44
1:A:1017:ARG:HG2	1:A:1510:ASN:ND2	2.30	0.44
1:C:833:PHE:CZ	3:O:150:ILE:HG23	2.52	0.44
1:C:1585:LYS:HE3	1:C:1585:LYS:HB2	1.81	0.44
1:D:1584:PRO:HG3	1:D:1591:TRP:CZ3	2.52	0.44
1:E:340:ARG:HH12	1:E:344:GLN:HE21	1.65	0.44
1:E:986:ALA:HB2	1:E:1047:LEU:HD13	2.00	0.44
1:F:871:TRP:HA	3:R:146:ASN:HD22	1.79	0.44
1:F:881:ASN:ND2	3:R:146:ASN:O	2.51	0.44
2:G:665:LEU:O	2:G:665:LEU:HD22	2.18	0.44
2:G:1852:TYR:HD1	2:G:1903:ASP:HA	1.83	0.44
2:G:1854:MET:HA	2:G:1907:LEU:HD21	1.99	0.44
2:I:679:LEU:HD21	2:I:681:ILE:HD11	1.99	0.44
2:K:665:LEU:O	2:K:665:LEU:HD22	2.17	0.44
2:K:898:ASP:O	2:K:1050:ARG:HG2	2.17	0.44
2:L:1933:LEU:HD13	2:L:1933:LEU:N	2.32	0.44
1:A:159:LEU:CD2	1:A:176:VAL:CG1	2.95	0.43
1:C:159:LEU:CD2	1:C:176:VAL:CG1	2.95	0.43
1:C:1303:GLY:H	1:C:1307:THR:HG22	1.83	0.43
1:D:1426:LEU:HD23	1:D:1426:LEU:HA	1.90	0.43
1:D:1585:LYS:HE3	1:D:1585:LYS:HB2	1.81	0.43
1:E:1673:TYR:CZ	1:E:1677:VAL:HG21	2.53	0.43
1:F:59:ARG:HD2	2:L:1896:GLN:NE2	2.33	0.43
2:I:2017:LYS:O	2:I:2018:PRO:C	2.59	0.43
2:J:679:LEU:HD21	2:J:681:ILE:HD11	1.99	0.43
2:J:2017:LYS:O	2:J:2018:PRO:C	2.59	0.43
2:K:777:THR:HG23	2:K:1081:HIS:NE2	2.33	0.43
3:N:141:ASP:OD1	3:N:143:VAL:HG12	2.18	0.43
3:P:141:ASP:OD1	3:P:143:VAL:HG12	2.18	0.43
3:R:20:ILE:HD11	3:R:103:LEU:HD23	2.00	0.43
1:A:381:GLU:OE1	1:F:793:ARG:NH2	2.51	0.43
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.65	0.43
1:D:1303:GLY:H	1:D:1307:THR:HG22	1.83	0.43
1:F:1673:TYR:CZ	1:F:1677:VAL:HG21	2.53	0.43
2:G:898:ASP:O	2:G:1050:ARG:HG2	2.18	0.43
2:G:1873:TYR:O	2:G:1874:VAL:C	2.60	0.43
2:H:777:THR:HG23	2:H:1081:HIS:NE2	2.33	0.43
2:I:1584:PHE:CD2	2:I:1584:PHE:C	2.97	0.43
2:J:898:ASP:O	2:J:1050:ARG:HG2	2.18	0.43
2:J:1584:PHE:CD2	2:J:1584:PHE:C	2.97	0.43
2:J:1852:TYR:HD1	2:J:1903:ASP:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1873:TYR:O	2:K:1874:VAL:C	2.60	0.43
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.65	0.43
1:B:986:ALA:HB2	1:B:1047:LEU:HD13	2.00	0.43
1:B:1175:ILE:HG12	1:D:1173:LEU:CD2	2.48	0.43
1:C:793:ARG:NH2	1:D:381:GLU:OE1	2.51	0.43
1:C:984:PRO:HB3	2:I:959:THR:HG23	2.01	0.43
1:C:1304:ALA:O	1:C:1307:THR:CG2	2.66	0.43
1:E:159:LEU:CD2	1:E:176:VAL:CG1	2.95	0.43
1:F:400:ARG:HH11	1:F:715:THR:HG21	1.80	0.43
1:F:986:ALA:HB2	1:F:1047:LEU:HD13	2.00	0.43
2:G:777:THR:HG23	2:G:1081:HIS:NE2	2.33	0.43
2:H:398:ALA:HB2	2:H:413:LYS:HB2	2.00	0.43
2:I:898:ASP:O	2:I:1050:ARG:HG2	2.18	0.43
2:J:665:LEU:HD22	2:J:665:LEU:O	2.17	0.43
2:J:1854:MET:HA	2:J:1907:LEU:HD21	1.99	0.43
2:K:230:TYR:CE2	2:K:236:ILE:HD13	2.52	0.43
3:Q:141:ASP:OD1	3:Q:143:VAL:HG12	2.18	0.43
1:A:1173:LEU:CD2	1:E:1175:ILE:HG12	2.47	0.43
1:B:400:ARG:HH11	1:B:715:THR:HG21	1.80	0.43
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.54	0.43
1:C:1146:HIS:HE1	1:F:1117:GLU:O	2.01	0.43
1:D:159:LEU:CD2	1:D:176:VAL:CG1	2.95	0.43
1:D:984:PRO:HB3	2:J:959:THR:HG23	2.01	0.43
1:D:1304:ALA:O	1:D:1307:THR:CG2	2.66	0.43
2:I:349:VAL:O	2:I:353:VAL:HG13	2.18	0.43
2:I:665:LEU:O	2:I:665:LEU:HD22	2.17	0.43
2:J:209:PHE:CD1	2:J:213:LEU:CD2	3.02	0.43
2:J:349:VAL:O	2:J:353:VAL:HG13	2.18	0.43
2:J:1933:LEU:HD13	2:J:1933:LEU:N	2.32	0.43
2:L:1778:GLN:HG3	2:L:1809:LEU:HD22	2.00	0.43
1:A:683:ALA:O	1:A:718:TYR:OH	2.34	0.43
1:A:1117:GLU:O	1:E:1146:HIS:HE1	2.01	0.43
1:A:1146:HIS:HE1	1:E:1117:GLU:O	2.01	0.43
1:A:1303:GLY:H	1:A:1307:THR:HG22	1.83	0.43
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.54	0.43
1:B:1302:VAL:HG23	1:D:1302:VAL:HG23	2.01	0.43
1:C:381:GLU:OE1	1:D:793:ARG:NH2	2.51	0.43
1:C:1302:VAL:HG23	1:F:1302:VAL:HG23	2.01	0.43
1:E:1017:ARG:HG2	1:E:1510:ASN:ND2	2.31	0.43
1:E:1303:GLY:H	1:E:1307:THR:HG22	1.83	0.43
2:I:777:THR:HG23	2:I:1081:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1778:GLN:HG3	2:I:1809:LEU:HD22	2.00	0.43
2:I:1933:LEU:N	2:I:1933:LEU:HD13	2.33	0.43
2:J:777:THR:HG23	2:J:1081:HIS:NE2	2.33	0.43
2:K:7:ARG:HD3	2:K:27:PHE:CD1	2.53	0.43
2:K:426:PRO:O	2:K:429:SER:OG	2.37	0.43
2:L:1873:TYR:O	2:L:1874:VAL:C	2.60	0.43
1:B:1117:GLU:O	1:D:1146:HIS:HE1	2.01	0.43
1:C:644:THR:HG22	1:C:648:ASP:O	2.19	0.43
1:D:644:THR:HG22	1:D:648:ASP:O	2.19	0.43
1:E:683:ALA:O	1:E:718:TYR:OH	2.34	0.43
1:E:881:ASN:ND2	3:Q:146:ASN:O	2.51	0.43
1:E:984:PRO:HB3	2:K:959:THR:HG23	2.01	0.43
2:H:1933:LEU:HD13	2:H:1933:LEU:N	2.33	0.43
2:I:209:PHE:CD1	2:I:213:LEU:CD2	3.02	0.43
2:J:143:SER:OG	2:J:547:ILE:O	2.23	0.43
2:K:398:ALA:HB2	2:K:413:LYS:HB2	1.99	0.43
1:A:1431:GLU:OE2	1:A:1523:ARG:NH1	2.52	0.43
1:C:400:ARG:HH11	1:C:715:THR:HG21	1.80	0.43
1:F:340:ARG:HH12	1:F:344:GLN:HE21	1.65	0.43
2:G:7:ARG:HD3	2:G:27:PHE:CD1	2.53	0.43
2:G:426:PRO:O	2:G:429:SER:OG	2.37	0.43
2:H:1778:GLN:HG3	2:H:1809:LEU:HD22	2.01	0.43
2:L:777:THR:HG23	2:L:1081:HIS:NE2	2.33	0.43
3:M:20:ILE:HD11	3:M:103:LEU:HD23	2.00	0.43
3:Q:20:ILE:HD11	3:Q:103:LEU:HD23	2.00	0.43
1:B:793:ARG:NH2	1:E:381:GLU:OE1	2.52	0.43
1:C:683:ALA:O	1:C:718:TYR:OH	2.34	0.43
1:C:1776:ILE:HD12	1:C:1807:SER:HA	2.01	0.43
1:D:1431:GLU:OE2	1:D:1523:ARG:NH1	2.52	0.43
1:E:907:GLY:O	1:E:910:THR:HG23	2.19	0.43
1:F:833:PHE:CZ	3:R:150:ILE:HG23	2.54	0.43
2:H:859:THR:HA	2:H:1049:GLN:HE22	1.84	0.43
2:K:349:VAL:O	2:K:353:VAL:HG13	2.18	0.43
2:L:426:PRO:O	2:L:429:SER:OG	2.37	0.43
3:M:141:ASP:OD1	3:M:143:VAL:HG12	2.18	0.43
3:Q:42:LEU:HD23	3:Q:42:LEU:HA	1.89	0.43
1:A:644:THR:HG22	1:A:648:ASP:O	2.19	0.43
1:C:986:ALA:HB2	1:C:1047:LEU:HD13	2.00	0.43
1:C:1673:TYR:CZ	1:C:1677:VAL:HG21	2.54	0.43
1:D:790:PHE:CE2	1:D:794:ILE:HD11	2.54	0.43
1:D:986:ALA:HB2	1:D:1047:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1776:ILE:HD12	1:D:1807:SER:HA	2.01	0.43
1:E:790:PHE:CE2	1:E:794:ILE:HD11	2.54	0.43
2:G:349:VAL:O	2:G:353:VAL:HG13	2.18	0.43
2:H:1468:THR:CG2	2:H:1485:CYS:SG	3.07	0.43
2:H:1873:TYR:O	2:H:1874:VAL:C	2.60	0.43
2:J:1217:ASN:HD22	2:J:1217:ASN:HA	1.66	0.43
2:L:859:THR:HA	2:L:1049:GLN:HE22	1.84	0.43
1:A:790:PHE:CE2	1:A:794:ILE:HD11	2.54	0.43
1:C:790:PHE:CE2	1:C:794:ILE:HD11	2.54	0.43
1:C:1442:ASN:HD22	1:C:1442:ASN:HA	1.69	0.43
1:D:400:ARG:HH11	1:D:715:THR:HG21	1.80	0.43
1:D:683:ALA:O	1:D:718:TYR:OH	2.34	0.43
1:D:1673:TYR:CZ	1:D:1677:VAL:HG21	2.54	0.43
1:E:644:THR:HG22	1:E:648:ASP:O	2.19	0.43
1:E:1431:GLU:OE2	1:E:1523:ARG:NH1	2.52	0.43
1:E:1776:ILE:HD12	1:E:1807:SER:HA	2.00	0.43
1:F:907:GLY:O	1:F:910:THR:HG23	2.19	0.43
1:F:1201:SER:OG	1:F:1203:ASP:OD1	2.29	0.43
2:G:653:TYR:CD1	2:G:659:LEU:HD21	2.54	0.43
2:H:426:PRO:O	2:H:429:SER:OG	2.37	0.43
2:H:1217:ASN:HD22	2:H:1217:ASN:HA	1.66	0.43
2:H:1584:PHE:CD2	2:H:1584:PHE:C	2.97	0.43
2:K:209:PHE:CD1	2:K:213:LEU:CD2	3.02	0.43
2:K:653:TYR:CD1	2:K:659:LEU:HD21	2.54	0.43
1:A:907:GLY:O	1:A:910:THR:HG23	2.19	0.42
1:B:907:GLY:O	1:B:910:THR:HG23	2.19	0.42
1:C:907:GLY:O	1:C:910:THR:HG23	2.19	0.42
1:C:1431:GLU:OE2	1:C:1523:ARG:NH1	2.52	0.42
1:D:1303:GLY:HA2	1:D:1649:LYS:HE2	2.02	0.42
1:E:833:PHE:CZ	3:Q:150:ILE:HG23	2.53	0.42
2:G:973:LEU:HD13	2:G:973:LEU:HA	1.90	0.42
2:G:1584:PHE:CD2	2:G:1584:PHE:C	2.97	0.42
2:K:1584:PHE:CD2	2:K:1584:PHE:C	2.96	0.42
2:L:1217:ASN:HD22	2:L:1217:ASN:HA	1.67	0.42
2:L:1584:PHE:CD2	2:L:1584:PHE:C	2.97	0.42
3:M:42:LEU:HD23	3:M:42:LEU:HA	1.89	0.42
1:A:1302:VAL:HG23	1:E:1302:VAL:HG23	2.01	0.42
1:B:381:GLU:OE1	1:E:793:ARG:NH2	2.51	0.42
1:B:1201:SER:OG	1:B:1203:ASP:OD1	2.29	0.42
1:B:1431:GLU:OE2	1:B:1523:ARG:NH1	2.52	0.42
1:C:1303:GLY:HA2	1:C:1649:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1431:GLU:OE2	1:F:1523:ARG:NH1	2.52	0.42
2:G:301:THR:HG21	2:G:448:VAL:HG21	2.01	0.42
2:H:209:PHE:CD1	2:H:213:LEU:CD2	3.02	0.42
2:H:330:ASN:HD22	2:H:394:ARG:NH1	2.18	0.42
2:H:349:VAL:O	2:H:353:VAL:HG13	2.18	0.42
2:H:1916:PHE:CE2	2:H:1943:ILE:HD12	2.55	0.42
2:I:653:TYR:CD1	2:I:659:LEU:HD21	2.54	0.42
2:J:653:TYR:CD1	2:J:659:LEU:HD21	2.54	0.42
2:L:349:VAL:O	2:L:353:VAL:HG13	2.18	0.42
1:A:793:ARG:NH2	1:F:381:GLU:OE1	2.51	0.42
1:B:984:PRO:HB3	2:H:959:THR:HG23	2.01	0.42
1:C:853:TRP:CE3	1:C:921:PRO:HD3	2.54	0.42
1:C:881:ASN:ND2	3:O:146:ASN:O	2.51	0.42
2:G:271:THR:OG1	2:G:272:GLY:N	2.52	0.42
2:I:426:PRO:O	2:I:429:SER:OG	2.37	0.42
2:I:1217:ASN:HD22	2:I:1217:ASN:HA	1.66	0.42
2:J:426:PRO:O	2:J:429:SER:OG	2.37	0.42
2:J:1468:THR:CG2	2:J:1485:CYS:SG	3.07	0.42
2:L:330:ASN:HD22	2:L:394:ARG:NH1	2.18	0.42
2:L:1468:THR:CG2	2:L:1485:CYS:SG	3.08	0.42
1:B:1776:ILE:HD12	1:B:1807:SER:HA	2.00	0.42
4:B:1901:PNS:H382	2:G:372:ASN:ND2	2.33	0.42
1:C:21:GLN:HE21	1:C:21:GLN:HB3	1.64	0.42
2:G:209:PHE:CD1	2:G:213:LEU:CD2	3.02	0.42
2:G:1468:THR:CG2	2:G:1485:CYS:SG	3.07	0.42
2:J:330:ASN:HD22	2:J:394:ARG:NH1	2.18	0.42
2:J:1778:GLN:HG3	2:J:1809:LEU:HD22	2.01	0.42
2:K:973:LEU:HD13	2:K:973:LEU:HA	1.90	0.42
2:K:1778:GLN:HG3	2:K:1809:LEU:HD22	2.00	0.42
2:L:271:THR:OG1	2:L:272:GLY:N	2.52	0.42
1:A:853:TRP:CE3	1:A:921:PRO:HD3	2.54	0.42
1:A:1175:ILE:HG12	1:E:1173:LEU:CD2	2.48	0.42
1:A:1776:ILE:HD12	1:A:1807:SER:HA	2.01	0.42
1:D:21:GLN:HE21	1:D:21:GLN:HB3	1.64	0.42
1:E:1303:GLY:HA2	1:E:1649:LYS:HE2	2.02	0.42
2:H:271:THR:OG1	2:H:272:GLY:N	2.52	0.42
2:I:330:ASN:HD22	2:I:394:ARG:NH1	2.18	0.42
2:J:754:TYR:CG	2:J:794:MET:HG2	2.55	0.42
2:K:271:THR:OG1	2:K:272:GLY:N	2.52	0.42
2:K:1468:THR:CG2	2:K:1485:CYS:SG	3.08	0.42
2:K:1956:ARG:HB3	2:K:1957:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:GLY:HA2	1:A:1649:LYS:HE2	2.02	0.42
1:B:790:PHE:CE2	1:B:794:ILE:HD11	2.54	0.42
1:D:822:VAL:HG12	1:D:824:LEU:HD13	2.02	0.42
1:D:853:TRP:CE3	1:D:921:PRO:HD3	2.54	0.42
1:D:907:GLY:O	1:D:910:THR:HG23	2.19	0.42
1:E:337:VAL:HG12	1:E:341:GLN:NE2	2.35	0.42
1:E:853:TRP:CE3	1:E:921:PRO:HD3	2.54	0.42
2:G:330:ASN:HD22	2:G:394:ARG:NH1	2.18	0.42
2:H:1956:ARG:HE	2:H:1956:ARG:C	2.27	0.42
2:L:209:PHE:CD1	2:L:213:LEU:CD2	3.02	0.42
3:O:42:LEU:HD23	3:O:42:LEU:HA	1.89	0.42
3:P:42:LEU:HD23	3:P:42:LEU:HA	1.89	0.42
1:A:337:VAL:HG12	1:A:341:GLN:NE2	2.35	0.42
1:C:822:VAL:HG12	1:C:824:LEU:HD13	2.02	0.42
1:D:337:VAL:HG12	1:D:341:GLN:NE2	2.35	0.42
1:F:1776:ILE:HD12	1:F:1807:SER:HA	2.01	0.42
2:G:1956:ARG:HB3	2:G:1957:PRO:HD3	2.02	0.42
3:P:20:ILE:HD11	3:P:103:LEU:HD23	2.00	0.42
1:A:864:VAL:HG22	1:A:921:PRO:HB3	2.02	0.42
1:D:1442:ASN:HD22	1:D:1442:ASN:HA	1.69	0.42
2:J:228:LYS:O	2:J:232:LEU:HD13	2.20	0.42
2:J:1956:ARG:HE	2:J:1956:ARG:C	2.28	0.42
2:K:330:ASN:HD22	2:K:394:ARG:NH1	2.18	0.42
2:K:1956:ARG:HE	2:K:1956:ARG:C	2.28	0.42
2:L:228:LYS:O	2:L:232:LEU:HD13	2.20	0.42
1:D:1298:ILE:HG23	1:D:1298:ILE:O	2.20	0.42
1:F:790:PHE:CE2	1:F:794:ILE:HD11	2.54	0.42
2:G:859:THR:HA	2:G:1049:GLN:HE22	1.84	0.42
2:H:754:TYR:CG	2:H:794:MET:HG2	2.55	0.42
2:I:1468:THR:CG2	2:I:1485:CYS:SG	3.08	0.42
2:J:1916:PHE:CE2	2:J:1943:ILE:HD12	2.55	0.42
2:K:859:THR:HA	2:K:1049:GLN:HE22	1.84	0.42
2:L:653:TYR:CD1	2:L:659:LEU:HD21	2.54	0.42
1:B:644:THR:HG22	1:B:648:ASP:O	2.19	0.42
1:C:1298:ILE:HG23	1:C:1298:ILE:O	2.20	0.42
1:D:1367:ARG:HD2	1:D:1370:THR:HG21	2.02	0.42
1:E:864:VAL:HG22	1:E:921:PRO:HB3	2.02	0.42
1:F:644:THR:HG22	1:F:648:ASP:O	2.19	0.42
2:G:406:ARG:HG2	3:M:88:GLU:CG	2.49	0.42
2:G:1778:GLN:HG3	2:G:1809:LEU:HD22	2.01	0.42
2:G:1956:ARG:HE	2:G:1956:ARG:C	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:228:LYS:O	2:H:232:LEU:HD13	2.20	0.42
2:I:228:LYS:O	2:I:232:LEU:HD13	2.20	0.42
2:I:754:TYR:CG	2:I:794:MET:HG2	2.55	0.42
2:I:1956:ARG:HE	2:I:1956:ARG:C	2.28	0.42
2:L:1593:ILE:HG22	2:L:1657:ILE:HD11	2.02	0.42
1:B:775:PRO:HA	3:N:142:VAL:HG11	2.02	0.41
1:B:1303:GLY:HA2	1:B:1649:LYS:HE2	2.02	0.41
1:B:1426:LEU:HD23	1:B:1426:LEU:HA	1.90	0.41
1:C:1367:ARG:HD2	1:C:1370:THR:HG21	2.02	0.41
1:F:337:VAL:HG12	1:F:341:GLN:NE2	2.35	0.41
1:F:1303:GLY:HA2	1:F:1649:LYS:HE2	2.02	0.41
2:H:653:TYR:CD1	2:H:659:LEU:HD21	2.54	0.41
2:H:938:TRP:CH2	2:H:947:THR:HG21	2.55	0.41
2:H:1757:GLU:OE1	2:H:1757:GLU:N	2.38	0.41
2:I:1956:ARG:HE	2:I:1956:ARG:CA	2.33	0.41
2:J:1871:LEU:HD23	2:J:1871:LEU:HA	1.94	0.41
2:J:1956:ARG:HB3	2:J:1957:PRO:HD3	2.02	0.41
1:B:1716:LEU:HD21	1:D:1426:LEU:HD22	2.02	0.41
1:C:337:VAL:HG12	1:C:341:GLN:NE2	2.35	0.41
1:E:1298:ILE:HG23	1:E:1298:ILE:O	2.20	0.41
2:G:228:LYS:O	2:G:232:LEU:HD13	2.19	0.41
2:I:1916:PHE:CE2	2:I:1943:ILE:HD12	2.56	0.41
2:K:1956:ARG:HE	2:K:1956:ARG:CA	2.33	0.41
2:L:938:TRP:CH2	2:L:947:THR:HG21	2.55	0.41
2:L:1956:ARG:HE	2:L:1956:ARG:C	2.28	0.41
3:O:20:ILE:HD11	3:O:103:LEU:HD23	2.00	0.41
1:A:1298:ILE:O	1:A:1298:ILE:HG23	2.20	0.41
1:B:337:VAL:HG12	1:B:341:GLN:NE2	2.35	0.41
1:B:853:TRP:CE3	1:B:921:PRO:HD3	2.54	0.41
1:B:1118:LYS:HE2	1:D:1146:HIS:O	2.20	0.41
1:F:853:TRP:CE3	1:F:921:PRO:HD3	2.54	0.41
2:G:1632:ILE:CG2	2:G:1637:LEU:HD23	2.50	0.41
2:G:1773:ALA:O	2:G:1775:GLN:N	2.47	0.41
2:H:301:THR:HG21	2:H:448:VAL:HG21	2.01	0.41
2:H:1593:ILE:HG22	2:H:1657:ILE:HD11	2.02	0.41
2:I:1956:ARG:HB3	2:I:1957:PRO:HD3	2.02	0.41
2:J:301:THR:HG21	2:J:448:VAL:HG21	2.01	0.41
2:J:938:TRP:CH2	2:J:947:THR:HG21	2.55	0.41
2:J:1593:ILE:HG22	2:J:1657:ILE:HD11	2.02	0.41
2:J:1956:ARG:HE	2:J:1956:ARG:CA	2.34	0.41
2:K:938:TRP:CH2	2:K:947:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:143:SER:OG	2:L:547:ILE:O	2.23	0.41
1:A:1076:VAL:HG13	1:A:1081:LYS:HA	2.03	0.41
1:A:1754:LYS:HA	1:A:1754:LYS:HE2	2.03	0.41
1:B:871:TRP:HA	3:N:146:ASN:HD22	1.82	0.41
1:E:1427:THR:O	1:E:1430:ARG:HD2	2.21	0.41
2:G:938:TRP:CH2	2:G:947:THR:HG21	2.55	0.41
2:G:1956:ARG:HE	2:G:1956:ARG:CA	2.34	0.41
2:H:1628:HIS:HE1	2:H:1630:GLY:O	2.03	0.41
2:H:1956:ARG:HB3	2:H:1957:PRO:HD3	2.01	0.41
2:I:938:TRP:CH2	2:I:947:THR:HG21	2.55	0.41
2:I:1956:ARG:HE	2:I:1956:ARG:HA	1.86	0.41
2:L:754:TYR:CG	2:L:794:MET:HG2	2.55	0.41
2:L:1757:GLU:OE1	2:L:1757:GLU:N	2.38	0.41
1:A:237:MET:HE3	1:A:277:LEU:H	1.86	0.41
1:A:775:PRO:HA	3:M:142:VAL:HG11	2.01	0.41
1:A:1367:ARG:HD2	1:A:1370:THR:HG21	2.02	0.41
1:A:1427:THR:O	1:A:1430:ARG:HD2	2.21	0.41
1:B:719:GLN:HG3	1:B:1612:ASP:HA	2.03	0.41
1:B:1146:HIS:O	1:D:1118:LYS:HE2	2.21	0.41
1:B:1298:ILE:HG23	1:B:1298:ILE:O	2.20	0.41
1:B:1442:ASN:HD22	1:B:1442:ASN:HA	1.69	0.41
1:D:237:MET:HE3	1:D:277:LEU:H	1.86	0.41
1:E:1367:ARG:HD2	1:E:1370:THR:HG21	2.02	0.41
1:F:1076:VAL:HG13	1:F:1081:LYS:HA	2.03	0.41
1:F:1298:ILE:HG23	1:F:1298:ILE:O	2.20	0.41
1:F:1426:LEU:HD23	1:F:1426:LEU:HA	1.90	0.41
2:G:754:TYR:CG	2:G:794:MET:HG2	2.55	0.41
2:I:1871:LEU:HD23	2:I:1871:LEU:HA	1.94	0.41
2:K:228:LYS:O	2:K:232:LEU:HD13	2.20	0.41
2:K:1632:ILE:CG2	2:K:1637:LEU:HD23	2.50	0.41
2:L:1916:PHE:CE2	2:L:1943:ILE:HD12	2.56	0.41
1:D:719:GLN:HG3	1:D:1612:ASP:HA	2.03	0.41
1:D:880:ALA:HA	3:P:147:SER:HA	2.02	0.41
1:E:822:VAL:HG12	1:E:824:LEU:HD13	2.02	0.41
1:E:1076:VAL:HG13	1:E:1081:LYS:HA	2.03	0.41
1:F:719:GLN:HG3	1:F:1612:ASP:HA	2.03	0.41
1:F:822:VAL:HG12	1:F:824:LEU:HD13	2.02	0.41
2:I:1593:ILE:HG22	2:I:1657:ILE:HD11	2.02	0.41
2:J:1148:ASN:HD22	2:J:1190:SER:HB3	1.86	0.41
2:K:1773:ALA:O	2:K:1775:GLN:N	2.47	0.41
2:L:1628:HIS:HE1	2:L:1630:GLY:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:TYR:CZ	1:A:721:ILE:CD1	3.03	0.41
1:A:822:VAL:HG12	1:A:824:LEU:HD13	2.02	0.41
1:A:1118:LYS:HE2	1:E:1146:HIS:O	2.20	0.41
1:A:1442:ASN:HD22	1:A:1442:ASN:HA	1.69	0.41
1:B:683:ALA:O	1:B:718:TYR:OH	2.34	0.41
1:B:822:VAL:HG12	1:B:824:LEU:HD13	2.02	0.41
1:B:1076:VAL:HG13	1:B:1081:LYS:HA	2.03	0.41
1:C:237:MET:HB2	1:C:277:LEU:CD1	2.50	0.41
1:C:719:GLN:HG3	1:C:1612:ASP:HA	2.03	0.41
1:C:1146:HIS:O	1:F:1118:LYS:HE2	2.21	0.41
1:E:1463:VAL:HB	1:E:1773:VAL:HG21	2.03	0.41
1:E:1754:LYS:HA	1:E:1754:LYS:HE2	2.03	0.41
1:A:1355:GLU:HG3	1:A:1365:MET:HE3	2.03	0.41
1:C:1076:VAL:HG13	1:C:1081:LYS:HA	2.03	0.41
1:C:1118:LYS:HE2	1:F:1146:HIS:O	2.21	0.41
1:D:1076:VAL:HG13	1:D:1081:LYS:HA	2.03	0.41
1:E:717:TYR:CZ	1:E:721:ILE:CD1	3.03	0.41
1:E:1355:GLU:HG3	1:E:1365:MET:HE3	2.03	0.41
2:K:301:THR:HG21	2:K:448:VAL:HG21	2.02	0.41
2:K:754:TYR:CG	2:K:794:MET:HG2	2.55	0.41
2:K:1916:PHE:CE2	2:K:1943:ILE:HD12	2.55	0.41
2:L:1956:ARG:HB3	2:L:1957:PRO:HD3	2.02	0.41
1:A:59:ARG:HD2	2:G:1896:GLN:NE2	2.36	0.41
1:B:880:ALA:HA	3:N:147:SER:HA	2.02	0.41
1:B:1107:GLU:OE1	1:B:1191:THR:OG1	2.29	0.41
1:C:1426:LEU:HD23	1:C:1426:LEU:HA	1.90	0.41
1:D:237:MET:HB2	1:D:277:LEU:CD1	2.51	0.41
1:D:1754:LYS:HE2	1:D:1754:LYS:HA	2.03	0.41
1:E:1442:ASN:HD22	1:E:1442:ASN:HA	1.69	0.41
1:F:683:ALA:O	1:F:718:TYR:OH	2.34	0.41
1:F:1442:ASN:HD22	1:F:1442:ASN:HA	1.69	0.41
2:G:1148:ASN:HD22	2:G:1190:SER:HB3	1.85	0.41
2:G:1484:LYS:HE3	2:G:1484:LYS:HB2	1.91	0.41
2:G:1628:HIS:HE1	2:G:1630:GLY:O	2.04	0.41
2:H:494:THR:HA	2:H:496:PHE:CE1	2.56	0.41
2:H:973:LEU:HD13	2:H:973:LEU:HA	1.90	0.41
2:J:859:THR:HA	2:J:1049:GLN:HE22	1.84	0.41
2:J:1865:SER:HB3	2:J:1923:ASP:OD1	2.21	0.41
2:J:1956:ARG:HE	2:J:1956:ARG:HA	1.86	0.41
2:K:1484:LYS:HE3	2:K:1484:LYS:HB2	1.91	0.41
2:L:494:THR:HA	2:L:496:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:864:LEU:HD11	2:L:868:PHE:CZ	2.56	0.41
1:A:390:VAL:HG13	1:A:390:VAL:O	2.22	0.41
1:C:237:MET:HE3	1:C:277:LEU:H	1.86	0.41
1:C:1754:LYS:HA	1:C:1754:LYS:HE2	2.03	0.41
1:D:864:VAL:HG22	1:D:921:PRO:HB3	2.02	0.41
1:E:237:MET:HE3	1:E:277:LEU:H	1.86	0.41
1:E:390:VAL:HG13	1:E:390:VAL:O	2.22	0.41
1:F:870:GLY:HA3	1:F:927:ASN:HA	2.03	0.41
1:F:1367:ARG:O	1:F:1370:THR:HB	2.21	0.41
2:G:100:ASP:OD1	2:G:101:ILE:N	2.53	0.41
2:H:864:LEU:HD11	2:H:868:PHE:CZ	2.56	0.41
2:H:1484:LYS:HE3	2:H:1484:LYS:HB2	1.90	0.41
2:I:690:VAL:O	2:I:693:GLU:N	2.54	0.41
2:J:1628:HIS:HE1	2:J:1630:GLY:O	2.03	0.41
2:K:1628:HIS:HE1	2:K:1630:GLY:O	2.03	0.41
2:L:973:LEU:HD13	2:L:973:LEU:HA	1.90	0.41
2:L:1148:ASN:HD22	2:L:1190:SER:HB3	1.86	0.41
1:B:870:GLY:HA3	1:B:927:ASN:HA	2.03	0.40
1:B:1367:ARG:O	1:B:1370:THR:HB	2.21	0.40
1:B:1754:LYS:HE2	1:B:1754:LYS:HA	2.03	0.40
1:F:237:MET:HE3	1:F:277:LEU:H	1.86	0.40
1:F:1367:ARG:HD2	1:F:1370:THR:HG21	2.02	0.40
1:F:1754:LYS:HE2	1:F:1754:LYS:HA	2.03	0.40
2:G:494:THR:HA	2:G:496:PHE:CE1	2.56	0.40
2:I:490:TRP:O	2:I:494:THR:HG22	2.21	0.40
2:I:859:THR:HA	2:I:1049:GLN:HE22	1.84	0.40
2:I:1628:HIS:HE1	2:I:1630:GLY:O	2.03	0.40
2:J:1773:ALA:O	2:J:1775:GLN:N	2.47	0.40
1:C:823:ILE:HA	1:C:865:CYS:O	2.21	0.40
1:C:864:VAL:HG22	1:C:921:PRO:HB3	2.02	0.40
1:C:1367:ARG:O	1:C:1370:THR:HB	2.21	0.40
1:D:798:ASN:OD1	1:D:801:ARG:NH1	2.54	0.40
1:D:1355:GLU:HG3	1:D:1365:MET:HE3	2.03	0.40
1:E:851:ASN:HD22	1:E:851:ASN:HA	1.77	0.40
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.56	0.40
2:I:973:LEU:HD13	2:I:973:LEU:HA	1.90	0.40
2:J:690:VAL:O	2:J:693:GLU:N	2.54	0.40
2:K:100:ASP:OD1	2:K:101:ILE:N	2.53	0.40
1:B:1367:ARG:HD2	1:B:1370:THR:HG21	2.02	0.40
1:C:798:ASN:OD1	1:C:801:ARG:NH1	2.54	0.40
1:C:1355:GLU:HG3	1:C:1365:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:823:ILE:HA	1:D:865:CYS:O	2.22	0.40
1:D:1367:ARG:O	1:D:1370:THR:HB	2.21	0.40
2:H:1148:ASN:HD22	2:H:1190:SER:HB3	1.86	0.40
2:H:1632:ILE:CG2	2:H:1637:LEU:HD23	2.50	0.40
2:I:864:LEU:HD11	2:I:868:PHE:CZ	2.56	0.40
2:I:1148:ASN:HD22	2:I:1190:SER:HB3	1.86	0.40
2:I:1773:ALA:O	2:I:1775:GLN:N	2.47	0.40
2:K:494:THR:HA	2:K:496:PHE:CE1	2.56	0.40
2:K:864:LEU:HD11	2:K:868:PHE:CZ	2.57	0.40
1:A:1426:LEU:HD22	1:E:1716:LEU:HD21	2.02	0.40
1:B:237:MET:N	1:B:238:PRO:CD	2.85	0.40
1:B:823:ILE:HA	1:B:865:CYS:O	2.21	0.40
1:C:1426:LEU:HD22	1:F:1716:LEU:HD21	2.03	0.40
1:D:237:MET:CE	1:D:276:ARG:HA	2.51	0.40
2:G:1593:ILE:HG22	2:G:1657:ILE:HD11	2.02	0.40
2:G:1865:SER:HB3	2:G:1923:ASP:OD1	2.21	0.40
2:G:1916:PHE:CE2	2:G:1943:ILE:HD12	2.56	0.40
2:H:1628:HIS:CE1	2:H:1630:GLY:O	2.75	0.40
2:H:1963:GLY:O	2:H:1965:ALA:N	2.55	0.40
2:I:1551:GLU:N	2:I:1552:PRO:HD2	2.36	0.40
2:J:864:LEU:HD11	2:J:868:PHE:CZ	2.56	0.40
2:J:1551:GLU:N	2:J:1552:PRO:HD2	2.36	0.40
2:K:234:ILE:HG21	2:K:425:SER:HB3	2.03	0.40
2:K:1551:GLU:N	2:K:1552:PRO:HD2	2.36	0.40
1:A:823:ILE:HA	1:A:865:CYS:O	2.21	0.40
1:A:1146:HIS:O	1:E:1118:LYS:HE2	2.21	0.40
1:B:237:MET:HE3	1:B:277:LEU:H	1.86	0.40
1:B:864:VAL:HG22	1:B:921:PRO:HB3	2.02	0.40
1:B:1427:THR:O	1:B:1430:ARG:HD2	2.22	0.40
1:C:870:GLY:HA3	1:C:927:ASN:HA	2.03	0.40
1:C:1365:MET:HE2	1:C:1377:MET:HE1	2.03	0.40
1:D:833:PHE:CZ	3:P:150:ILE:HG23	2.57	0.40
1:D:1365:MET:HE2	1:D:1377:MET:HE1	2.03	0.40
1:E:1243:VAL:O	1:E:1296:GLY:HA3	2.22	0.40
1:F:237:MET:N	1:F:238:PRO:CD	2.85	0.40
1:F:823:ILE:HA	1:F:865:CYS:O	2.21	0.40
2:G:176:LEU:C	2:G:176:LEU:HD23	2.47	0.40
2:G:1551:GLU:N	2:G:1552:PRO:HD2	2.36	0.40
2:H:1956:ARG:HE	2:H:1956:ARG:CA	2.34	0.40
2:I:1865:SER:HB3	2:I:1923:ASP:OD1	2.22	0.40
2:J:494:THR:HA	2:J:496:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:301:THR:HG21	2:L:448:VAL:HG21	2.03	0.40
2:L:406:ARG:HG2	3:R:88:GLU:CG	2.50	0.40
2:L:1628:HIS:CE1	2:L:1630:GLY:O	2.75	0.40
2:L:1956:ARG:HE	2:L:1956:ARG:CA	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	B	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	C	1744/1887 (92%)	1612 (92%)	119 (7%)	13 (1%)	18	47
1	D	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	E	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	F	1744/1887 (92%)	1613 (92%)	119 (7%)	12 (1%)	18	47
2	G	2032/2040 (100%)	1843 (91%)	177 (9%)	12 (1%)	21	51
2	H	2032/2040 (100%)	1843 (91%)	176 (9%)	13 (1%)	21	51
2	I	2032/2040 (100%)	1844 (91%)	174 (9%)	14 (1%)	18	47
2	J	2032/2040 (100%)	1842 (91%)	178 (9%)	12 (1%)	21	51
2	K	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	21	51
2	L	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	21	51
3	M	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	N	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	O	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	P	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	R	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
All	All	23292/24450 (95%)	21327 (92%)	1805 (8%)	160 (1%)	20	47

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	ASP
1	B	1130	ASP
1	C	1130	ASP
1	D	1130	ASP
1	E	1130	ASP
1	F	1130	ASP
2	G	1215	LYS
2	G	1845	ASP
2	H	1215	LYS
2	H	1845	ASP
2	I	1215	LYS
2	I	1845	ASP
2	J	1215	LYS
2	J	1845	ASP
2	K	1215	LYS
2	K	1845	ASP
2	L	1215	LYS
2	L	1845	ASP
3	M	149	PHE
3	N	149	PHE
3	O	149	PHE
3	P	149	PHE
3	Q	149	PHE
3	R	149	PHE
1	A	178	GLY
1	A	875	THR
1	B	178	GLY
1	B	875	THR
1	C	178	GLY
1	C	875	THR
1	D	178	GLY
1	D	875	THR
1	E	178	GLY
1	E	875	THR

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Mol	Chain	Res	Type
1	F	178	GLY
1	F	875	THR
2	G	185	GLY
2	G	769	SER
2	G	1874	VAL
2	H	185	GLY
2	H	769	SER
2	H	1874	VAL
2	I	185	GLY
2	I	769	SER
2	I	1874	VAL
2	J	185	GLY
2	J	769	SER
2	J	1874	VAL
2	K	185	GLY
2	K	769	SER
2	K	1874	VAL
2	L	185	GLY
2	L	769	SER
2	L	1874	VAL
3	M	148	ILE
3	N	148	ILE
3	O	148	ILE
3	P	148	ILE
3	Q	148	ILE
3	R	148	ILE
1	A	198	PRO
1	A	238	PRO
1	A	618	ASN
1	B	238	PRO
1	B	618	ASN
1	C	238	PRO
1	C	618	ASN
1	D	198	PRO
1	D	238	PRO
1	D	618	ASN
1	E	238	PRO
1	E	618	ASN
1	F	198	PRO
1	F	238	PRO
1	F	618	ASN
2	G	1316	ASP

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Mol	Chain	Res	Type
2	G	1774	THR
2	H	1316	ASP
2	H	1774	THR
2	H	1846	GLU
2	I	1316	ASP
2	I	1774	THR
2	J	1316	ASP
2	J	1774	THR
2	K	1316	ASP
2	K	1774	THR
2	L	1316	ASP
2	L	1774	THR
1	A	215	ASP
1	A	607	LYS
1	A	917	CYS
1	A	1267	ASP
1	A	1536	LEU
1	B	198	PRO
1	B	215	ASP
1	B	607	LYS
1	B	917	CYS
1	B	1267	ASP
1	B	1536	LEU
1	C	198	PRO
1	C	215	ASP
1	C	917	CYS
1	C	1267	ASP
1	C	1536	LEU
1	D	215	ASP
1	D	607	LYS
1	D	917	CYS
1	D	1267	ASP
1	D	1536	LEU
1	E	198	PRO
1	E	215	ASP
1	E	917	CYS
1	E	1267	ASP
1	E	1536	LEU
1	F	215	ASP
1	F	607	LYS
1	F	917	CYS
1	F	1267	ASP

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Mol	Chain	Res	Type
1	F	1536	LEU
2	G	134	LYS
2	G	1743	ASP
2	G	1846	GLU
2	H	134	LYS
2	H	1743	ASP
2	I	134	LYS
2	I	1743	ASP
2	I	1846	GLU
2	J	134	LYS
2	J	1743	ASP
2	J	1846	GLU
2	K	134	LYS
2	K	1743	ASP
2	K	1846	GLU
2	L	134	LYS
2	L	1743	ASP
2	L	1846	GLU
1	C	607	LYS
1	E	607	LYS
2	G	140	LYS
2	G	772	GLY
2	H	140	LYS
2	H	772	GLY
2	I	140	LYS
2	I	772	GLY
2	J	140	LYS
2	J	772	GLY
2	K	140	LYS
2	K	772	GLY
2	L	140	LYS
2	L	772	GLY
1	C	538	GLU
2	H	1964	PHE
2	I	1820	ASP
2	I	1964	PHE
1	B	219	GLY
1	C	219	GLY
1	D	219	GLY
1	E	219	GLY
1	F	219	GLY
1	A	219	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1476/1566 (94%)	1367 (93%)	109 (7%)	13	37
1	B	1476/1566 (94%)	1365 (92%)	111 (8%)	12	37
1	C	1476/1566 (94%)	1365 (92%)	111 (8%)	12	37
1	D	1476/1566 (94%)	1365 (92%)	111 (8%)	12	37
1	E	1476/1566 (94%)	1364 (92%)	112 (8%)	12	36
1	F	1476/1566 (94%)	1366 (92%)	110 (8%)	12	37
2	G	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	H	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	I	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	J	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	K	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	L	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
3	M	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	N	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	O	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	P	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	Q	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	R	97/129 (75%)	84 (87%)	13 (13%)	4	13
All	All	20088/20844 (96%)	18572 (92%)	1516 (8%)	14	37

All (1516) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	22	PHE
1	A	38	ASP
1	A	44	VAL
1	A	52	THR
1	A	67	SER

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Mol	Chain	Res	Type
1	A	83	LYS
1	A	149	LEU
1	A	179	LYS
1	A	182	VAL
1	A	184	ASN
1	A	202	GLU
1	A	217	PHE
1	A	221	LEU
1	A	237	MET
1	A	272	GLU
1	A	277	LEU
1	A	345	VAL
1	A	365	LYS
1	A	378	LEU
1	A	390	VAL
1	A	392	THR
1	A	401	THR
1	A	413	LEU
1	A	416	LEU
1	A	421	ILE
1	A	435	GLU
1	A	447	LEU
1	A	458	THR
1	A	478	GLU
1	A	489	VAL
1	A	493	VAL
1	A	520	ARG
1	A	522	LEU
1	A	527	GLN
1	A	622	ILE
1	A	624	LYS
1	A	626	VAL
1	A	672	THR
1	A	721	ILE
1	A	731	THR
1	A	748	LEU
1	A	761	LEU
1	A	776	GLU
1	A	797	THR
1	A	806	VAL
1	A	821	GLN
1	A	823	ILE

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Mol	Chain	Res	Type
1	A	824	LEU
1	A	826	MET
1	A	827	SER
1	A	862	LEU
1	A	864	VAL
1	A	888	ILE
1	A	901	MET
1	A	913	VAL
1	A	933	VAL
1	A	940	THR
1	A	953	VAL
1	A	999	LYS
1	A	1001	VAL
1	A	1020	VAL
1	A	1022	THR
1	A	1047	LEU
1	A	1050	CYS
1	A	1067	LEU
1	A	1073	THR
1	A	1076	VAL
1	A	1096	SER
1	A	1166	LYS
1	A	1184	LEU
1	A	1197	THR
1	A	1208	VAL
1	A	1211	ILE
1	A	1238	VAL
1	A	1240	VAL
1	A	1254	VAL
1	A	1267	ASP
1	A	1283	MET
1	A	1298	ILE
1	A	1307	THR
1	A	1317	GLU
1	A	1327	CYS
1	A	1329	VAL
1	A	1332	TYR
1	A	1362	PRO
1	A	1366	SER
1	A	1370	THR
1	A	1372	THR
1	A	1392	LEU

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Mol	Chain	Res	Type
1	A	1430	ARG
1	A	1432	HIS
1	A	1442	ASN
1	A	1486	LEU
1	A	1501	LEU
1	A	1528	THR
1	A	1556	THR
1	A	1575	VAL
1	A	1580	LEU
1	A	1585	LYS
1	A	1625	LEU
1	A	1642	THR
1	A	1722	VAL
1	A	1749	THR
1	A	1754	LYS
1	A	1756	ILE
1	A	1828	LEU
1	A	1842	VAL
1	A	1844	LYS
1	B	21	GLN
1	B	22	PHE
1	B	38	ASP
1	B	44	VAL
1	B	52	THR
1	B	67	SER
1	B	83	LYS
1	B	149	LEU
1	B	179	LYS
1	B	182	VAL
1	B	184	ASN
1	B	202	GLU
1	B	217	PHE
1	B	221	LEU
1	B	237	MET
1	B	272	GLU
1	B	277	LEU
1	B	345	VAL
1	B	365	LYS
1	B	378	LEU
1	B	390	VAL
1	B	392	THR
1	B	401	THR

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Mol	Chain	Res	Type
1	B	413	LEU
1	B	416	LEU
1	B	421	ILE
1	B	435	GLU
1	B	447	LEU
1	B	458	THR
1	B	478	GLU
1	B	489	VAL
1	B	493	VAL
1	B	520	ARG
1	B	522	LEU
1	B	527	GLN
1	B	622	ILE
1	B	624	LYS
1	B	626	VAL
1	B	645	PRO
1	B	672	THR
1	B	721	ILE
1	B	731	THR
1	B	748	LEU
1	B	761	LEU
1	B	776	GLU
1	B	797	THR
1	B	806	VAL
1	B	821	GLN
1	B	823	ILE
1	B	824	LEU
1	B	826	MET
1	B	827	SER
1	B	862	LEU
1	B	864	VAL
1	B	888	ILE
1	B	901	MET
1	B	913	VAL
1	B	933	VAL
1	B	940	THR
1	B	953	VAL
1	B	999	LYS
1	B	1001	VAL
1	B	1020	VAL
1	B	1022	THR
1	B	1047	LEU

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Mol	Chain	Res	Type
1	B	1050	CYS
1	B	1067	LEU
1	B	1073	THR
1	B	1076	VAL
1	B	1096	SER
1	B	1166	LYS
1	B	1184	LEU
1	B	1197	THR
1	B	1208	VAL
1	B	1211	ILE
1	B	1238	VAL
1	B	1240	VAL
1	B	1254	VAL
1	B	1267	ASP
1	B	1283	MET
1	B	1298	ILE
1	B	1307	THR
1	B	1317	GLU
1	B	1327	CYS
1	B	1329	VAL
1	B	1332	TYR
1	B	1362	PRO
1	B	1366	SER
1	B	1370	THR
1	B	1372	THR
1	B	1392	LEU
1	B	1430	ARG
1	B	1432	HIS
1	B	1442	ASN
1	B	1486	LEU
1	B	1501	LEU
1	B	1528	THR
1	B	1556	THR
1	B	1575	VAL
1	B	1580	LEU
1	B	1585	LYS
1	B	1625	LEU
1	B	1642	THR
1	B	1680	ARG
1	B	1722	VAL
1	B	1749	THR
1	B	1754	LYS

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Mol	Chain	Res	Type
1	B	1756	ILE
1	B	1828	LEU
1	B	1842	VAL
1	B	1844	LYS
1	C	21	GLN
1	C	22	PHE
1	C	38	ASP
1	C	44	VAL
1	C	52	THR
1	C	67	SER
1	C	83	LYS
1	C	149	LEU
1	C	179	LYS
1	C	182	VAL
1	C	184	ASN
1	C	202	GLU
1	C	217	PHE
1	C	221	LEU
1	C	237	MET
1	C	272	GLU
1	C	277	LEU
1	C	345	VAL
1	C	365	LYS
1	C	378	LEU
1	C	390	VAL
1	C	392	THR
1	C	401	THR
1	C	413	LEU
1	C	416	LEU
1	C	421	ILE
1	C	435	GLU
1	C	447	LEU
1	C	458	THR
1	C	478	GLU
1	C	489	VAL
1	C	493	VAL
1	C	520	ARG
1	C	522	LEU
1	C	527	GLN
1	C	622	ILE
1	C	624	LYS
1	C	626	VAL

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Mol	Chain	Res	Type
1	C	645	PRO
1	C	672	THR
1	C	721	ILE
1	C	731	THR
1	C	748	LEU
1	C	761	LEU
1	C	776	GLU
1	C	797	THR
1	C	806	VAL
1	C	821	GLN
1	C	823	ILE
1	C	824	LEU
1	C	826	MET
1	C	827	SER
1	C	862	LEU
1	C	864	VAL
1	C	888	ILE
1	C	901	MET
1	C	913	VAL
1	C	933	VAL
1	C	940	THR
1	C	953	VAL
1	C	999	LYS
1	C	1001	VAL
1	C	1020	VAL
1	C	1022	THR
1	C	1047	LEU
1	C	1050	CYS
1	C	1067	LEU
1	C	1073	THR
1	C	1076	VAL
1	C	1096	SER
1	C	1166	LYS
1	C	1184	LEU
1	C	1197	THR
1	C	1208	VAL
1	C	1211	ILE
1	C	1238	VAL
1	C	1240	VAL
1	C	1254	VAL
1	C	1267	ASP
1	C	1283	MET

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Mol	Chain	Res	Type
1	C	1298	ILE
1	C	1307	THR
1	C	1317	GLU
1	C	1327	CYS
1	C	1329	VAL
1	C	1332	TYR
1	C	1362	PRO
1	C	1366	SER
1	C	1370	THR
1	C	1372	THR
1	C	1392	LEU
1	C	1430	ARG
1	C	1432	HIS
1	C	1442	ASN
1	C	1486	LEU
1	C	1501	LEU
1	C	1528	THR
1	C	1556	THR
1	C	1575	VAL
1	C	1580	LEU
1	C	1585	LYS
1	C	1625	LEU
1	C	1642	THR
1	C	1680	ARG
1	C	1722	VAL
1	C	1749	THR
1	C	1754	LYS
1	C	1756	ILE
1	C	1828	LEU
1	C	1842	VAL
1	C	1844	LYS
1	D	21	GLN
1	D	22	PHE
1	D	38	ASP
1	D	44	VAL
1	D	52	THR
1	D	67	SER
1	D	83	LYS
1	D	149	LEU
1	D	179	LYS
1	D	182	VAL
1	D	184	ASN

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Mol	Chain	Res	Type
1	D	202	GLU
1	D	217	PHE
1	D	221	LEU
1	D	237	MET
1	D	272	GLU
1	D	277	LEU
1	D	345	VAL
1	D	365	LYS
1	D	378	LEU
1	D	390	VAL
1	D	392	THR
1	D	401	THR
1	D	413	LEU
1	D	416	LEU
1	D	421	ILE
1	D	435	GLU
1	D	447	LEU
1	D	458	THR
1	D	478	GLU
1	D	489	VAL
1	D	493	VAL
1	D	520	ARG
1	D	522	LEU
1	D	527	GLN
1	D	622	ILE
1	D	624	LYS
1	D	626	VAL
1	D	645	PRO
1	D	672	THR
1	D	721	ILE
1	D	731	THR
1	D	748	LEU
1	D	761	LEU
1	D	776	GLU
1	D	797	THR
1	D	806	VAL
1	D	821	GLN
1	D	823	ILE
1	D	824	LEU
1	D	826	MET
1	D	827	SER
1	D	862	LEU

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Mol	Chain	Res	Type
1	D	864	VAL
1	D	888	ILE
1	D	901	MET
1	D	913	VAL
1	D	933	VAL
1	D	940	THR
1	D	953	VAL
1	D	999	LYS
1	D	1001	VAL
1	D	1020	VAL
1	D	1022	THR
1	D	1047	LEU
1	D	1050	CYS
1	D	1067	LEU
1	D	1073	THR
1	D	1076	VAL
1	D	1096	SER
1	D	1166	LYS
1	D	1184	LEU
1	D	1197	THR
1	D	1208	VAL
1	D	1211	ILE
1	D	1238	VAL
1	D	1240	VAL
1	D	1254	VAL
1	D	1267	ASP
1	D	1283	MET
1	D	1298	ILE
1	D	1307	THR
1	D	1317	GLU
1	D	1327	CYS
1	D	1329	VAL
1	D	1332	TYR
1	D	1362	PRO
1	D	1366	SER
1	D	1370	THR
1	D	1372	THR
1	D	1392	LEU
1	D	1430	ARG
1	D	1432	HIS
1	D	1442	ASN
1	D	1486	LEU

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Mol	Chain	Res	Type
1	D	1501	LEU
1	D	1528	THR
1	D	1556	THR
1	D	1575	VAL
1	D	1580	LEU
1	D	1585	LYS
1	D	1625	LEU
1	D	1642	THR
1	D	1680	ARG
1	D	1722	VAL
1	D	1749	THR
1	D	1754	LYS
1	D	1756	ILE
1	D	1828	LEU
1	D	1842	VAL
1	D	1844	LYS
1	E	21	GLN
1	E	22	PHE
1	E	38	ASP
1	E	44	VAL
1	E	52	THR
1	E	67	SER
1	E	83	LYS
1	E	149	LEU
1	E	179	LYS
1	E	182	VAL
1	E	184	ASN
1	E	202	GLU
1	E	217	PHE
1	E	221	LEU
1	E	237	MET
1	E	272	GLU
1	E	277	LEU
1	E	345	VAL
1	E	365	LYS
1	E	378	LEU
1	E	390	VAL
1	E	392	THR
1	E	401	THR
1	E	413	LEU
1	E	416	LEU
1	E	421	ILE

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Mol	Chain	Res	Type
1	E	435	GLU
1	E	447	LEU
1	E	458	THR
1	E	478	GLU
1	E	489	VAL
1	E	493	VAL
1	E	520	ARG
1	E	522	LEU
1	E	527	GLN
1	E	622	ILE
1	E	624	LYS
1	E	626	VAL
1	E	645	PRO
1	E	672	THR
1	E	721	ILE
1	E	731	THR
1	E	748	LEU
1	E	761	LEU
1	E	776	GLU
1	E	797	THR
1	E	806	VAL
1	E	821	GLN
1	E	823	ILE
1	E	824	LEU
1	E	826	MET
1	E	827	SER
1	E	862	LEU
1	E	864	VAL
1	E	888	ILE
1	E	901	MET
1	E	913	VAL
1	E	933	VAL
1	E	940	THR
1	E	953	VAL
1	E	999	LYS
1	E	1001	VAL
1	E	1020	VAL
1	E	1022	THR
1	E	1047	LEU
1	E	1050	CYS
1	E	1067	LEU
1	E	1073	THR

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Mol	Chain	Res	Type
1	E	1076	VAL
1	E	1079	LYS
1	E	1096	SER
1	E	1166	LYS
1	E	1184	LEU
1	E	1197	THR
1	E	1208	VAL
1	E	1211	ILE
1	E	1238	VAL
1	E	1240	VAL
1	E	1254	VAL
1	E	1267	ASP
1	E	1283	MET
1	E	1298	ILE
1	E	1307	THR
1	E	1317	GLU
1	E	1327	CYS
1	E	1329	VAL
1	E	1332	TYR
1	E	1362	PRO
1	E	1366	SER
1	E	1370	THR
1	E	1372	THR
1	E	1392	LEU
1	E	1430	ARG
1	E	1432	HIS
1	E	1442	ASN
1	E	1486	LEU
1	E	1501	LEU
1	E	1528	THR
1	E	1556	THR
1	E	1575	VAL
1	E	1580	LEU
1	E	1585	LYS
1	E	1625	LEU
1	E	1642	THR
1	E	1680	ARG
1	E	1722	VAL
1	E	1749	THR
1	E	1754	LYS
1	E	1756	ILE
1	E	1828	LEU

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Mol	Chain	Res	Type
1	E	1842	VAL
1	E	1844	LYS
1	F	21	GLN
1	F	22	PHE
1	F	38	ASP
1	F	44	VAL
1	F	52	THR
1	F	67	SER
1	F	83	LYS
1	F	149	LEU
1	F	179	LYS
1	F	182	VAL
1	F	184	ASN
1	F	202	GLU
1	F	217	PHE
1	F	221	LEU
1	F	237	MET
1	F	272	GLU
1	F	277	LEU
1	F	345	VAL
1	F	365	LYS
1	F	378	LEU
1	F	390	VAL
1	F	392	THR
1	F	401	THR
1	F	413	LEU
1	F	416	LEU
1	F	421	ILE
1	F	435	GLU
1	F	447	LEU
1	F	458	THR
1	F	478	GLU
1	F	489	VAL
1	F	493	VAL
1	F	520	ARG
1	F	522	LEU
1	F	527	GLN
1	F	622	ILE
1	F	624	LYS
1	F	626	VAL
1	F	645	PRO
1	F	672	THR

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Mol	Chain	Res	Type
1	F	721	ILE
1	F	731	THR
1	F	748	LEU
1	F	761	LEU
1	F	776	GLU
1	F	797	THR
1	F	806	VAL
1	F	821	GLN
1	F	823	ILE
1	F	824	LEU
1	F	826	MET
1	F	827	SER
1	F	862	LEU
1	F	864	VAL
1	F	888	ILE
1	F	901	MET
1	F	933	VAL
1	F	940	THR
1	F	953	VAL
1	F	999	LYS
1	F	1001	VAL
1	F	1020	VAL
1	F	1022	THR
1	F	1047	LEU
1	F	1050	CYS
1	F	1067	LEU
1	F	1073	THR
1	F	1076	VAL
1	F	1096	SER
1	F	1166	LYS
1	F	1184	LEU
1	F	1197	THR
1	F	1208	VAL
1	F	1211	ILE
1	F	1238	VAL
1	F	1240	VAL
1	F	1254	VAL
1	F	1267	ASP
1	F	1283	MET
1	F	1298	ILE
1	F	1307	THR
1	F	1317	GLU

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Mol	Chain	Res	Type
1	F	1327	CYS
1	F	1329	VAL
1	F	1332	TYR
1	F	1362	PRO
1	F	1366	SER
1	F	1370	THR
1	F	1372	THR
1	F	1392	LEU
1	F	1430	ARG
1	F	1432	HIS
1	F	1442	ASN
1	F	1486	LEU
1	F	1501	LEU
1	F	1528	THR
1	F	1556	THR
1	F	1575	VAL
1	F	1580	LEU
1	F	1585	LYS
1	F	1625	LEU
1	F	1642	THR
1	F	1680	ARG
1	F	1722	VAL
1	F	1749	THR
1	F	1754	LYS
1	F	1756	ILE
1	F	1828	LEU
1	F	1842	VAL
1	F	1844	LYS
2	G	38	ASN
2	G	52	ASP
2	G	99	ASN
2	G	111	GLU
2	G	119	THR
2	G	124	LYS
2	G	163	GLN
2	G	166	THR
2	G	173	LEU
2	G	197	GLU
2	G	213	LEU
2	G	246	LEU
2	G	264	ARG
2	G	267	LEU

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Mol	Chain	Res	Type
2	G	279	THR
2	G	306	ILE
2	G	338	MET
2	G	339	LEU
2	G	340	SER
2	G	353	VAL
2	G	369	SER
2	G	376	ASN
2	G	377	LEU
2	G	462	THR
2	G	472	SER
2	G	494	THR
2	G	497	LYS
2	G	562	LEU
2	G	593	LEU
2	G	598	THR
2	G	616	THR
2	G	659	LEU
2	G	665	LEU
2	G	669	LEU
2	G	681	ILE
2	G	688	LEU
2	G	698	LEU
2	G	710	ILE
2	G	730	LEU
2	G	733	THR
2	G	777	THR
2	G	784	GLU
2	G	794	MET
2	G	805	VAL
2	G	810	GLU
2	G	845	THR
2	G	880	LEU
2	G	893	SER
2	G	906	THR
2	G	907	VAL
2	G	910	GLN
2	G	953	ARG
2	G	972	LEU
2	G	973	LEU
2	G	1005	SER
2	G	1016	PRO

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Mol	Chain	Res	Type
2	G	1023	ARG
2	G	1033	SER
2	G	1040	LEU
2	G	1048	VAL
2	G	1055	HIS
2	G	1100	VAL
2	G	1110	ASP
2	G	1160	THR
2	G	1167	SER
2	G	1189	THR
2	G	1195	VAL
2	G	1211	LEU
2	G	1213	LEU
2	G	1217	ASN
2	G	1236	LEU
2	G	1319	MET
2	G	1343	VAL
2	G	1347	LEU
2	G	1348	LEU
2	G	1375	THR
2	G	1382	VAL
2	G	1408	SER
2	G	1422	THR
2	G	1439	LYS
2	G	1441	ILE
2	G	1470	THR
2	G	1478	ASN
2	G	1482	SER
2	G	1485	CYS
2	G	1495	THR
2	G	1499	VAL
2	G	1503	ILE
2	G	1530	LYS
2	G	1531	VAL
2	G	1549	THR
2	G	1563	ILE
2	G	1585	SER
2	G	1586	SER
2	G	1599	ASP
2	G	1605	VAL
2	G	1609	THR
2	G	1610	CYS

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Mol	Chain	Res	Type
2	G	1616	VAL
2	G	1629	VAL
2	G	1637	LEU
2	G	1639	LYS
2	G	1671	SER
2	G	1680	LEU
2	G	1683	THR
2	G	1751	ILE
2	G	1761	SER
2	G	1770	LEU
2	G	1774	THR
2	G	1775	GLN
2	G	1777	THR
2	G	1778	GLN
2	G	1782	THR
2	G	1818	LEU
2	G	1847	LEU
2	G	1855	ILE
2	G	1914	LEU
2	G	1921	LYS
2	G	1930	SER
2	G	1933	LEU
2	G	1935	GLU
2	G	1936	VAL
2	G	1954	LYS
2	G	1956	ARG
2	G	1958	LEU
2	G	1973	SER
2	G	1979	THR
2	G	2015	THR
2	G	2033	THR
2	H	38	ASN
2	H	52	ASP
2	H	99	ASN
2	H	111	GLU
2	H	119	THR
2	H	124	LYS
2	H	163	GLN
2	H	166	THR
2	H	173	LEU
2	H	197	GLU
2	H	213	LEU

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Mol	Chain	Res	Type
2	H	246	LEU
2	H	264	ARG
2	H	267	LEU
2	H	279	THR
2	H	306	ILE
2	H	338	MET
2	H	339	LEU
2	H	340	SER
2	H	353	VAL
2	H	369	SER
2	H	376	ASN
2	H	377	LEU
2	H	462	THR
2	H	472	SER
2	H	494	THR
2	H	497	LYS
2	H	562	LEU
2	H	593	LEU
2	H	598	THR
2	H	616	THR
2	H	659	LEU
2	H	665	LEU
2	H	669	LEU
2	H	681	ILE
2	H	688	LEU
2	H	698	LEU
2	H	710	ILE
2	H	730	LEU
2	H	733	THR
2	H	777	THR
2	H	784	GLU
2	H	794	MET
2	H	805	VAL
2	H	810	GLU
2	H	845	THR
2	H	880	LEU
2	H	893	SER
2	H	906	THR
2	H	907	VAL
2	H	910	GLN
2	H	953	ARG
2	H	972	LEU

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Mol	Chain	Res	Type
2	H	973	LEU
2	H	1005	SER
2	H	1016	PRO
2	H	1023	ARG
2	H	1033	SER
2	H	1040	LEU
2	H	1048	VAL
2	H	1055	HIS
2	H	1100	VAL
2	H	1110	ASP
2	H	1160	THR
2	H	1167	SER
2	H	1189	THR
2	H	1195	VAL
2	H	1211	LEU
2	H	1213	LEU
2	H	1217	ASN
2	H	1236	LEU
2	H	1319	MET
2	H	1343	VAL
2	H	1347	LEU
2	H	1348	LEU
2	H	1375	THR
2	H	1382	VAL
2	H	1408	SER
2	H	1422	THR
2	H	1439	LYS
2	H	1441	ILE
2	H	1470	THR
2	H	1478	ASN
2	H	1482	SER
2	H	1485	CYS
2	H	1495	THR
2	H	1499	VAL
2	H	1503	ILE
2	H	1530	LYS
2	H	1531	VAL
2	H	1549	THR
2	H	1563	ILE
2	H	1585	SER
2	H	1586	SER
2	H	1599	ASP

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Mol	Chain	Res	Type
2	H	1605	VAL
2	H	1609	THR
2	H	1610	CYS
2	H	1616	VAL
2	H	1629	VAL
2	H	1637	LEU
2	H	1639	LYS
2	H	1671	SER
2	H	1680	LEU
2	H	1683	THR
2	H	1751	ILE
2	H	1761	SER
2	H	1770	LEU
2	H	1774	THR
2	H	1775	GLN
2	H	1777	THR
2	H	1778	GLN
2	H	1782	THR
2	H	1818	LEU
2	H	1847	LEU
2	H	1855	ILE
2	H	1914	LEU
2	H	1921	LYS
2	H	1930	SER
2	H	1933	LEU
2	H	1935	GLU
2	H	1936	VAL
2	H	1954	LYS
2	H	1956	ARG
2	H	1958	LEU
2	H	1973	SER
2	H	1979	THR
2	H	2015	THR
2	H	2033	THR
2	I	38	ASN
2	I	52	ASP
2	I	99	ASN
2	I	111	GLU
2	I	119	THR
2	I	124	LYS
2	I	163	GLN
2	I	166	THR

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Mol	Chain	Res	Type
2	I	173	LEU
2	I	197	GLU
2	I	213	LEU
2	I	246	LEU
2	I	264	ARG
2	I	267	LEU
2	I	279	THR
2	I	306	ILE
2	I	338	MET
2	I	339	LEU
2	I	340	SER
2	I	353	VAL
2	I	369	SER
2	I	376	ASN
2	I	377	LEU
2	I	462	THR
2	I	472	SER
2	I	494	THR
2	I	497	LYS
2	I	562	LEU
2	I	593	LEU
2	I	598	THR
2	I	616	THR
2	I	659	LEU
2	I	665	LEU
2	I	669	LEU
2	I	681	ILE
2	I	688	LEU
2	I	698	LEU
2	I	710	ILE
2	I	730	LEU
2	I	733	THR
2	I	777	THR
2	I	784	GLU
2	I	794	MET
2	I	805	VAL
2	I	810	GLU
2	I	845	THR
2	I	880	LEU
2	I	893	SER
2	I	906	THR
2	I	907	VAL

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Mol	Chain	Res	Type
2	I	910	GLN
2	I	953	ARG
2	I	972	LEU
2	I	973	LEU
2	I	1005	SER
2	I	1016	PRO
2	I	1023	ARG
2	I	1033	SER
2	I	1040	LEU
2	I	1048	VAL
2	I	1055	HIS
2	I	1100	VAL
2	I	1110	ASP
2	I	1160	THR
2	I	1167	SER
2	I	1189	THR
2	I	1195	VAL
2	I	1211	LEU
2	I	1213	LEU
2	I	1217	ASN
2	I	1236	LEU
2	I	1319	MET
2	I	1343	VAL
2	I	1347	LEU
2	I	1348	LEU
2	I	1375	THR
2	I	1382	VAL
2	I	1408	SER
2	I	1422	THR
2	I	1439	LYS
2	I	1441	ILE
2	I	1470	THR
2	I	1478	ASN
2	I	1482	SER
2	I	1485	CYS
2	I	1495	THR
2	I	1499	VAL
2	I	1503	ILE
2	I	1530	LYS
2	I	1531	VAL
2	I	1549	THR
2	I	1563	ILE

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Mol	Chain	Res	Type
2	I	1585	SER
2	I	1586	SER
2	I	1599	ASP
2	I	1605	VAL
2	I	1609	THR
2	I	1610	CYS
2	I	1616	VAL
2	I	1629	VAL
2	I	1637	LEU
2	I	1639	LYS
2	I	1671	SER
2	I	1680	LEU
2	I	1683	THR
2	I	1751	ILE
2	I	1761	SER
2	I	1770	LEU
2	I	1774	THR
2	I	1775	GLN
2	I	1777	THR
2	I	1778	GLN
2	I	1782	THR
2	I	1818	LEU
2	I	1847	LEU
2	I	1855	ILE
2	I	1914	LEU
2	I	1921	LYS
2	I	1930	SER
2	I	1933	LEU
2	I	1935	GLU
2	I	1936	VAL
2	I	1954	LYS
2	I	1956	ARG
2	I	1958	LEU
2	I	1973	SER
2	I	1979	THR
2	I	2015	THR
2	I	2033	THR
2	J	38	ASN
2	J	52	ASP
2	J	99	ASN
2	J	111	GLU
2	J	119	THR

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Mol	Chain	Res	Type
2	J	124	LYS
2	J	163	GLN
2	J	166	THR
2	J	173	LEU
2	J	197	GLU
2	J	213	LEU
2	J	246	LEU
2	J	264	ARG
2	J	267	LEU
2	J	279	THR
2	J	306	ILE
2	J	338	MET
2	J	339	LEU
2	J	340	SER
2	J	353	VAL
2	J	369	SER
2	J	376	ASN
2	J	377	LEU
2	J	462	THR
2	J	472	SER
2	J	494	THR
2	J	497	LYS
2	J	562	LEU
2	J	593	LEU
2	J	598	THR
2	J	616	THR
2	J	659	LEU
2	J	665	LEU
2	J	669	LEU
2	J	681	ILE
2	J	688	LEU
2	J	698	LEU
2	J	710	ILE
2	J	730	LEU
2	J	733	THR
2	J	777	THR
2	J	784	GLU
2	J	794	MET
2	J	805	VAL
2	J	810	GLU
2	J	845	THR
2	J	880	LEU

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Mol	Chain	Res	Type
2	J	893	SER
2	J	906	THR
2	J	907	VAL
2	J	910	GLN
2	J	953	ARG
2	J	972	LEU
2	J	973	LEU
2	J	1005	SER
2	J	1016	PRO
2	J	1023	ARG
2	J	1033	SER
2	J	1040	LEU
2	J	1048	VAL
2	J	1055	HIS
2	J	1100	VAL
2	J	1110	ASP
2	J	1160	THR
2	J	1167	SER
2	J	1189	THR
2	J	1195	VAL
2	J	1211	LEU
2	J	1213	LEU
2	J	1217	ASN
2	J	1236	LEU
2	J	1319	MET
2	J	1343	VAL
2	J	1347	LEU
2	J	1348	LEU
2	J	1375	THR
2	J	1382	VAL
2	J	1408	SER
2	J	1422	THR
2	J	1439	LYS
2	J	1441	ILE
2	J	1470	THR
2	J	1478	ASN
2	J	1482	SER
2	J	1485	CYS
2	J	1495	THR
2	J	1499	VAL
2	J	1503	ILE
2	J	1530	LYS

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Mol	Chain	Res	Type
2	J	1531	VAL
2	J	1549	THR
2	J	1563	ILE
2	J	1585	SER
2	J	1586	SER
2	J	1599	ASP
2	J	1605	VAL
2	J	1609	THR
2	J	1610	CYS
2	J	1616	VAL
2	J	1629	VAL
2	J	1637	LEU
2	J	1639	LYS
2	J	1671	SER
2	J	1680	LEU
2	J	1683	THR
2	J	1751	ILE
2	J	1761	SER
2	J	1770	LEU
2	J	1774	THR
2	J	1775	GLN
2	J	1777	THR
2	J	1778	GLN
2	J	1782	THR
2	J	1818	LEU
2	J	1847	LEU
2	J	1855	ILE
2	J	1914	LEU
2	J	1921	LYS
2	J	1930	SER
2	J	1933	LEU
2	J	1935	GLU
2	J	1936	VAL
2	J	1954	LYS
2	J	1956	ARG
2	J	1958	LEU
2	J	1973	SER
2	J	1979	THR
2	J	2015	THR
2	J	2033	THR
2	K	38	ASN
2	K	52	ASP

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Mol	Chain	Res	Type
2	K	99	ASN
2	K	111	GLU
2	K	119	THR
2	K	124	LYS
2	K	163	GLN
2	K	166	THR
2	K	173	LEU
2	K	197	GLU
2	K	213	LEU
2	K	246	LEU
2	K	264	ARG
2	K	267	LEU
2	K	279	THR
2	K	306	ILE
2	K	338	MET
2	K	339	LEU
2	K	340	SER
2	K	353	VAL
2	K	369	SER
2	K	376	ASN
2	K	377	LEU
2	K	462	THR
2	K	472	SER
2	K	494	THR
2	K	497	LYS
2	K	562	LEU
2	K	593	LEU
2	K	598	THR
2	K	616	THR
2	K	659	LEU
2	K	665	LEU
2	K	669	LEU
2	K	681	ILE
2	K	688	LEU
2	K	698	LEU
2	K	710	ILE
2	K	730	LEU
2	K	733	THR
2	K	777	THR
2	K	784	GLU
2	K	794	MET
2	K	805	VAL

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Mol	Chain	Res	Type
2	K	810	GLU
2	K	845	THR
2	K	880	LEU
2	K	893	SER
2	K	906	THR
2	K	907	VAL
2	K	910	GLN
2	K	953	ARG
2	K	972	LEU
2	K	973	LEU
2	K	1005	SER
2	K	1016	PRO
2	K	1023	ARG
2	K	1033	SER
2	K	1040	LEU
2	K	1048	VAL
2	K	1055	HIS
2	K	1100	VAL
2	K	1110	ASP
2	K	1160	THR
2	K	1167	SER
2	K	1189	THR
2	K	1195	VAL
2	K	1211	LEU
2	K	1213	LEU
2	K	1217	ASN
2	K	1236	LEU
2	K	1319	MET
2	K	1343	VAL
2	K	1347	LEU
2	K	1348	LEU
2	K	1375	THR
2	K	1382	VAL
2	K	1408	SER
2	K	1422	THR
2	K	1439	LYS
2	K	1441	ILE
2	K	1470	THR
2	K	1478	ASN
2	K	1482	SER
2	K	1485	CYS
2	K	1495	THR

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Mol	Chain	Res	Type
2	K	1499	VAL
2	K	1503	ILE
2	K	1530	LYS
2	K	1531	VAL
2	K	1549	THR
2	K	1563	ILE
2	K	1585	SER
2	K	1586	SER
2	K	1599	ASP
2	K	1605	VAL
2	K	1609	THR
2	K	1610	CYS
2	K	1616	VAL
2	K	1629	VAL
2	K	1637	LEU
2	K	1639	LYS
2	K	1671	SER
2	K	1680	LEU
2	K	1683	THR
2	K	1751	ILE
2	K	1761	SER
2	K	1770	LEU
2	K	1774	THR
2	K	1775	GLN
2	K	1777	THR
2	K	1778	GLN
2	K	1782	THR
2	K	1818	LEU
2	K	1847	LEU
2	K	1855	ILE
2	K	1914	LEU
2	K	1921	LYS
2	K	1930	SER
2	K	1933	LEU
2	K	1935	GLU
2	K	1936	VAL
2	K	1954	LYS
2	K	1956	ARG
2	K	1958	LEU
2	K	1973	SER
2	K	1979	THR
2	K	2015	THR

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Mol	Chain	Res	Type
2	K	2033	THR
2	L	38	ASN
2	L	52	ASP
2	L	99	ASN
2	L	111	GLU
2	L	119	THR
2	L	124	LYS
2	L	163	GLN
2	L	166	THR
2	L	173	LEU
2	L	197	GLU
2	L	213	LEU
2	L	246	LEU
2	L	264	ARG
2	L	267	LEU
2	L	279	THR
2	L	306	ILE
2	L	338	MET
2	L	339	LEU
2	L	340	SER
2	L	353	VAL
2	L	369	SER
2	L	376	ASN
2	L	377	LEU
2	L	462	THR
2	L	472	SER
2	L	494	THR
2	L	497	LYS
2	L	562	LEU
2	L	593	LEU
2	L	598	THR
2	L	616	THR
2	L	659	LEU
2	L	665	LEU
2	L	669	LEU
2	L	681	ILE
2	L	688	LEU
2	L	698	LEU
2	L	710	ILE
2	L	730	LEU
2	L	733	THR
2	L	777	THR

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Mol	Chain	Res	Type
2	L	784	GLU
2	L	794	MET
2	L	805	VAL
2	L	810	GLU
2	L	845	THR
2	L	880	LEU
2	L	893	SER
2	L	906	THR
2	L	907	VAL
2	L	910	GLN
2	L	953	ARG
2	L	972	LEU
2	L	973	LEU
2	L	1005	SER
2	L	1016	PRO
2	L	1023	ARG
2	L	1033	SER
2	L	1040	LEU
2	L	1048	VAL
2	L	1055	HIS
2	L	1100	VAL
2	L	1110	ASP
2	L	1160	THR
2	L	1167	SER
2	L	1189	THR
2	L	1195	VAL
2	L	1211	LEU
2	L	1213	LEU
2	L	1217	ASN
2	L	1236	LEU
2	L	1319	MET
2	L	1343	VAL
2	L	1347	LEU
2	L	1348	LEU
2	L	1375	THR
2	L	1382	VAL
2	L	1408	SER
2	L	1422	THR
2	L	1439	LYS
2	L	1441	ILE
2	L	1470	THR
2	L	1478	ASN

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Mol	Chain	Res	Type
2	L	1482	SER
2	L	1485	CYS
2	L	1495	THR
2	L	1499	VAL
2	L	1503	ILE
2	L	1530	LYS
2	L	1531	VAL
2	L	1549	THR
2	L	1563	ILE
2	L	1585	SER
2	L	1586	SER
2	L	1599	ASP
2	L	1605	VAL
2	L	1609	THR
2	L	1610	CYS
2	L	1616	VAL
2	L	1629	VAL
2	L	1637	LEU
2	L	1639	LYS
2	L	1671	SER
2	L	1680	LEU
2	L	1683	THR
2	L	1751	ILE
2	L	1761	SER
2	L	1770	LEU
2	L	1774	THR
2	L	1775	GLN
2	L	1777	THR
2	L	1778	GLN
2	L	1782	THR
2	L	1818	LEU
2	L	1847	LEU
2	L	1855	ILE
2	L	1914	LEU
2	L	1921	LYS
2	L	1930	SER
2	L	1933	LEU
2	L	1935	GLU
2	L	1936	VAL
2	L	1954	LYS
2	L	1956	ARG
2	L	1958	LEU

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Mol	Chain	Res	Type
2	L	1973	SER
2	L	1979	THR
2	L	2015	THR
2	L	2033	THR
3	M	3	SER
3	M	8	ARG
3	M	14	GLU
3	M	20	ILE
3	M	49	LEU
3	M	56	LEU
3	M	95	ASN
3	M	108	VAL
3	M	136	ASP
3	M	142	VAL
3	M	147	SER
3	M	148	ILE
3	M	150	ILE
3	N	3	SER
3	N	8	ARG
3	N	14	GLU
3	N	20	ILE
3	N	49	LEU
3	N	56	LEU
3	N	95	ASN
3	N	108	VAL
3	N	136	ASP
3	N	142	VAL
3	N	147	SER
3	N	148	ILE
3	N	150	ILE
3	O	3	SER
3	O	8	ARG
3	O	14	GLU
3	O	20	ILE
3	O	49	LEU
3	O	56	LEU
3	O	95	ASN
3	O	108	VAL
3	O	136	ASP
3	O	142	VAL
3	O	147	SER
3	O	148	ILE

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Mol	Chain	Res	Type
3	O	150	ILE
3	P	3	SER
3	P	8	ARG
3	P	14	GLU
3	P	20	ILE
3	P	49	LEU
3	P	56	LEU
3	P	95	ASN
3	P	108	VAL
3	P	136	ASP
3	P	142	VAL
3	P	147	SER
3	P	148	ILE
3	P	150	ILE
3	Q	3	SER
3	Q	8	ARG
3	Q	14	GLU
3	Q	20	ILE
3	Q	49	LEU
3	Q	56	LEU
3	Q	95	ASN
3	Q	108	VAL
3	Q	136	ASP
3	Q	142	VAL
3	Q	147	SER
3	Q	148	ILE
3	Q	150	ILE
3	R	3	SER
3	R	8	ARG
3	R	14	GLU
3	R	20	ILE
3	R	49	LEU
3	R	56	LEU
3	R	95	ASN
3	R	108	VAL
3	R	136	ASP
3	R	142	VAL
3	R	147	SER
3	R	148	ILE
3	R	150	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (542) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	40	ASN
1	A	261	GLN
1	A	292	GLN
1	A	335	HIS
1	A	344	GLN
1	A	438	ASN
1	A	454	HIS
1	A	618	ASN
1	A	669	ASN
1	A	719	GLN
1	A	738	ASN
1	A	739	GLN
1	A	743	GLN
1	A	851	ASN
1	A	979	GLN
1	A	987	ASN
1	A	1146	HIS
1	A	1239	HIS
1	A	1245	ASN
1	A	1271	GLN
1	A	1389	GLN
1	A	1442	ASN
1	A	1444	ASN
1	A	1507	GLN
1	A	1510	ASN
1	A	1552	ASN
1	A	1563	HIS
1	A	1610	ASN
1	A	1657	HIS
1	A	1690	ASN
1	A	1780	ASN
1	A	1783	ASN
1	A	1790	ASN
1	B	21	GLN
1	B	40	ASN
1	B	184	ASN
1	B	261	GLN
1	B	292	GLN
1	B	344	GLN
1	B	438	ASN
1	B	454	HIS
1	B	618	ASN

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Mol	Chain	Res	Type
1	B	669	ASN
1	B	719	GLN
1	B	738	ASN
1	B	739	GLN
1	B	743	GLN
1	B	851	ASN
1	B	979	GLN
1	B	987	ASN
1	B	1146	HIS
1	B	1239	HIS
1	B	1245	ASN
1	B	1271	GLN
1	B	1389	GLN
1	B	1432	HIS
1	B	1442	ASN
1	B	1444	ASN
1	B	1507	GLN
1	B	1510	ASN
1	B	1552	ASN
1	B	1563	HIS
1	B	1577	GLN
1	B	1610	ASN
1	B	1657	HIS
1	B	1690	ASN
1	B	1780	ASN
1	B	1783	ASN
1	B	1790	ASN
1	C	21	GLN
1	C	40	ASN
1	C	261	GLN
1	C	292	GLN
1	C	335	HIS
1	C	344	GLN
1	C	438	ASN
1	C	454	HIS
1	C	618	ASN
1	C	669	ASN
1	C	719	GLN
1	C	738	ASN
1	C	739	GLN
1	C	743	GLN
1	C	851	ASN

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Mol	Chain	Res	Type
1	C	979	GLN
1	C	987	ASN
1	C	1146	HIS
1	C	1239	HIS
1	C	1271	GLN
1	C	1288	ASN
1	C	1389	GLN
1	C	1442	ASN
1	C	1444	ASN
1	C	1507	GLN
1	C	1510	ASN
1	C	1552	ASN
1	C	1563	HIS
1	C	1610	ASN
1	C	1657	HIS
1	C	1690	ASN
1	C	1695	ASN
1	C	1780	ASN
1	C	1783	ASN
1	C	1790	ASN
1	D	21	GLN
1	D	40	ASN
1	D	184	ASN
1	D	261	GLN
1	D	292	GLN
1	D	335	HIS
1	D	344	GLN
1	D	438	ASN
1	D	454	HIS
1	D	618	ASN
1	D	669	ASN
1	D	719	GLN
1	D	738	ASN
1	D	739	GLN
1	D	743	GLN
1	D	851	ASN
1	D	979	GLN
1	D	987	ASN
1	D	1146	HIS
1	D	1239	HIS
1	D	1271	GLN
1	D	1288	ASN

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Mol	Chain	Res	Type
1	D	1389	GLN
1	D	1442	ASN
1	D	1444	ASN
1	D	1507	GLN
1	D	1510	ASN
1	D	1552	ASN
1	D	1563	HIS
1	D	1610	ASN
1	D	1657	HIS
1	D	1690	ASN
1	D	1780	ASN
1	D	1783	ASN
1	D	1790	ASN
1	E	21	GLN
1	E	40	ASN
1	E	261	GLN
1	E	292	GLN
1	E	335	HIS
1	E	344	GLN
1	E	438	ASN
1	E	454	HIS
1	E	618	ASN
1	E	669	ASN
1	E	719	GLN
1	E	738	ASN
1	E	739	GLN
1	E	743	GLN
1	E	851	ASN
1	E	979	GLN
1	E	987	ASN
1	E	1146	HIS
1	E	1239	HIS
1	E	1245	ASN
1	E	1271	GLN
1	E	1389	GLN
1	E	1442	ASN
1	E	1444	ASN
1	E	1507	GLN
1	E	1510	ASN
1	E	1552	ASN
1	E	1563	HIS
1	E	1610	ASN

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Mol	Chain	Res	Type
1	E	1657	HIS
1	E	1690	ASN
1	E	1780	ASN
1	E	1783	ASN
1	E	1790	ASN
1	F	21	GLN
1	F	40	ASN
1	F	184	ASN
1	F	261	GLN
1	F	292	GLN
1	F	344	GLN
1	F	438	ASN
1	F	454	HIS
1	F	618	ASN
1	F	669	ASN
1	F	719	GLN
1	F	738	ASN
1	F	739	GLN
1	F	743	GLN
1	F	851	ASN
1	F	979	GLN
1	F	987	ASN
1	F	1146	HIS
1	F	1239	HIS
1	F	1245	ASN
1	F	1271	GLN
1	F	1389	GLN
1	F	1432	HIS
1	F	1442	ASN
1	F	1444	ASN
1	F	1507	GLN
1	F	1510	ASN
1	F	1552	ASN
1	F	1563	HIS
1	F	1577	GLN
1	F	1610	ASN
1	F	1657	HIS
1	F	1690	ASN
1	F	1780	ASN
1	F	1783	ASN
1	F	1790	ASN
2	G	99	ASN

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Mol	Chain	Res	Type
2	G	165	ASN
2	G	211	GLN
2	G	224	ASN
2	G	248	HIS
2	G	330	ASN
2	G	331	ASN
2	G	384	GLN
2	G	500	HIS
2	G	517	HIS
2	G	558	ASN
2	G	572	ASN
2	G	612	ASN
2	G	718	ASN
2	G	741	HIS
2	G	747	HIS
2	G	900	GLN
2	G	910	GLN
2	G	993	GLN
2	G	1008	GLN
2	G	1049	GLN
2	G	1055	HIS
2	G	1078	HIS
2	G	1148	ASN
2	G	1178	GLN
2	G	1217	ASN
2	G	1220	GLN
2	G	1302	HIS
2	G	1341	ASN
2	G	1383	ASN
2	G	1421	ASN
2	G	1434	HIS
2	G	1451	GLN
2	G	1476	ASN
2	G	1529	GLN
2	G	1595	ASN
2	G	1611	GLN
2	G	1628	HIS
2	G	1659	GLN
2	G	1669	GLN
2	G	1712	ASN
2	G	1716	ASN
2	G	1775	GLN

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Mol	Chain	Res	Type
2	G	1807	HIS
2	G	1890	ASN
2	G	1895	ASN
2	G	1995	ASN
2	G	2013	ASN
2	G	2020	GLN
2	H	18	HIS
2	H	99	ASN
2	H	102	HIS
2	H	165	ASN
2	H	211	GLN
2	H	224	ASN
2	H	248	HIS
2	H	330	ASN
2	H	331	ASN
2	H	384	GLN
2	H	500	HIS
2	H	517	HIS
2	H	558	ASN
2	H	572	ASN
2	H	612	ASN
2	H	650	ASN
2	H	718	ASN
2	H	741	HIS
2	H	747	HIS
2	H	900	GLN
2	H	910	GLN
2	H	993	GLN
2	H	1008	GLN
2	H	1049	GLN
2	H	1055	HIS
2	H	1078	HIS
2	H	1148	ASN
2	H	1178	GLN
2	H	1217	ASN
2	H	1220	GLN
2	H	1302	HIS
2	H	1341	ASN
2	H	1383	ASN
2	H	1421	ASN
2	H	1434	HIS
2	H	1451	GLN

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Mol	Chain	Res	Type
2	H	1476	ASN
2	H	1529	GLN
2	H	1595	ASN
2	H	1611	GLN
2	H	1628	HIS
2	H	1659	GLN
2	H	1669	GLN
2	H	1712	ASN
2	H	1716	ASN
2	H	1775	GLN
2	H	1807	HIS
2	H	1890	ASN
2	H	1895	ASN
2	H	1995	ASN
2	H	2013	ASN
2	H	2020	GLN
2	I	99	ASN
2	I	102	HIS
2	I	181	HIS
2	I	224	ASN
2	I	248	HIS
2	I	330	ASN
2	I	331	ASN
2	I	384	GLN
2	I	500	HIS
2	I	517	HIS
2	I	558	ASN
2	I	572	ASN
2	I	612	ASN
2	I	718	ASN
2	I	741	HIS
2	I	747	HIS
2	I	900	GLN
2	I	910	GLN
2	I	993	GLN
2	I	1008	GLN
2	I	1049	GLN
2	I	1055	HIS
2	I	1078	HIS
2	I	1148	ASN
2	I	1178	GLN
2	I	1217	ASN

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Mol	Chain	Res	Type
2	I	1220	GLN
2	I	1302	HIS
2	I	1341	ASN
2	I	1383	ASN
2	I	1421	ASN
2	I	1434	HIS
2	I	1451	GLN
2	I	1476	ASN
2	I	1529	GLN
2	I	1550	ASN
2	I	1595	ASN
2	I	1611	GLN
2	I	1628	HIS
2	I	1669	GLN
2	I	1712	ASN
2	I	1716	ASN
2	I	1775	GLN
2	I	1807	HIS
2	I	1890	ASN
2	I	1895	ASN
2	I	1995	ASN
2	I	2013	ASN
2	I	2020	GLN
2	J	99	ASN
2	J	102	HIS
2	J	165	ASN
2	J	181	HIS
2	J	224	ASN
2	J	248	HIS
2	J	330	ASN
2	J	331	ASN
2	J	384	GLN
2	J	500	HIS
2	J	517	HIS
2	J	558	ASN
2	J	572	ASN
2	J	612	ASN
2	J	718	ASN
2	J	741	HIS
2	J	747	HIS
2	J	900	GLN
2	J	910	GLN

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Mol	Chain	Res	Type
2	J	993	GLN
2	J	1008	GLN
2	J	1049	GLN
2	J	1055	HIS
2	J	1078	HIS
2	J	1148	ASN
2	J	1178	GLN
2	J	1217	ASN
2	J	1220	GLN
2	J	1302	HIS
2	J	1341	ASN
2	J	1383	ASN
2	J	1421	ASN
2	J	1434	HIS
2	J	1451	GLN
2	J	1476	ASN
2	J	1529	GLN
2	J	1595	ASN
2	J	1611	GLN
2	J	1628	HIS
2	J	1669	GLN
2	J	1712	ASN
2	J	1716	ASN
2	J	1775	GLN
2	J	1807	HIS
2	J	1890	ASN
2	J	1895	ASN
2	J	1995	ASN
2	J	2013	ASN
2	J	2020	GLN
2	K	99	ASN
2	K	102	HIS
2	K	165	ASN
2	K	181	HIS
2	K	211	GLN
2	K	224	ASN
2	K	248	HIS
2	K	330	ASN
2	K	331	ASN
2	K	384	GLN
2	K	500	HIS
2	K	517	HIS

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Mol	Chain	Res	Type
2	K	558	ASN
2	K	572	ASN
2	K	612	ASN
2	K	718	ASN
2	K	741	HIS
2	K	747	HIS
2	K	900	GLN
2	K	910	GLN
2	K	993	GLN
2	K	1008	GLN
2	K	1049	GLN
2	K	1055	HIS
2	K	1078	HIS
2	K	1148	ASN
2	K	1178	GLN
2	K	1217	ASN
2	K	1220	GLN
2	K	1302	HIS
2	K	1341	ASN
2	K	1383	ASN
2	K	1421	ASN
2	K	1434	HIS
2	K	1451	GLN
2	K	1476	ASN
2	K	1529	GLN
2	K	1595	ASN
2	K	1611	GLN
2	K	1628	HIS
2	K	1659	GLN
2	K	1669	GLN
2	K	1712	ASN
2	K	1716	ASN
2	K	1775	GLN
2	K	1807	HIS
2	K	1890	ASN
2	K	1895	ASN
2	K	1995	ASN
2	K	2013	ASN
2	K	2020	GLN
2	L	18	HIS
2	L	99	ASN
2	L	165	ASN

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Mol	Chain	Res	Type
2	L	211	GLN
2	L	224	ASN
2	L	248	HIS
2	L	330	ASN
2	L	331	ASN
2	L	384	GLN
2	L	500	HIS
2	L	517	HIS
2	L	558	ASN
2	L	572	ASN
2	L	612	ASN
2	L	718	ASN
2	L	741	HIS
2	L	747	HIS
2	L	900	GLN
2	L	910	GLN
2	L	993	GLN
2	L	1008	GLN
2	L	1049	GLN
2	L	1055	HIS
2	L	1078	HIS
2	L	1148	ASN
2	L	1178	GLN
2	L	1217	ASN
2	L	1220	GLN
2	L	1302	HIS
2	L	1341	ASN
2	L	1383	ASN
2	L	1421	ASN
2	L	1434	HIS
2	L	1451	GLN
2	L	1476	ASN
2	L	1512	HIS
2	L	1529	GLN
2	L	1595	ASN
2	L	1611	GLN
2	L	1628	HIS
2	L	1659	GLN
2	L	1669	GLN
2	L	1712	ASN
2	L	1716	ASN
2	L	1775	GLN

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Mol	Chain	Res	Type
2	L	1807	HIS
2	L	1890	ASN
2	L	1895	ASN
2	L	1995	ASN
2	L	2013	ASN
2	L	2020	GLN
3	M	40	ASN
3	M	94	ASN
3	M	95	ASN
3	M	97	ASN
3	M	146	ASN
3	N	40	ASN
3	N	94	ASN
3	N	95	ASN
3	N	97	ASN
3	N	146	ASN
3	O	40	ASN
3	O	94	ASN
3	O	95	ASN
3	O	97	ASN
3	O	146	ASN
3	P	40	ASN
3	P	89	ASN
3	P	94	ASN
3	P	95	ASN
3	P	97	ASN
3	P	146	ASN
3	Q	40	ASN
3	Q	94	ASN
3	Q	95	ASN
3	Q	97	ASN
3	Q	146	ASN
3	R	40	ASN
3	R	94	ASN
3	R	95	ASN
3	R	97	ASN
3	R	146	ASN

5.3.3 RNA ⓘ

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FMN	J	2101	-	33,33,33	1.59	8 (24%)	48,50,50	1.82	15 (31%)
4	PNS	D	1901	1	14,20,21	0.87	0	18,26,29	1.50	3 (16%)
4	PNS	F	1901	1	14,20,21	0.87	0	18,26,29	1.50	3 (16%)
5	FMN	G	2101	-	33,33,33	1.56	8 (24%)	48,50,50	1.84	15 (31%)
5	FMN	I	2101	-	33,33,33	1.58	7 (21%)	48,50,50	1.80	15 (31%)
4	PNS	C	1901	1	14,20,21	0.88	0	18,26,29	1.51	3 (16%)
4	PNS	B	1901	1	14,20,21	0.85	0	18,26,29	1.49	2 (11%)
4	PNS	A	1901	1	14,20,21	0.87	0	18,26,29	1.51	3 (16%)
5	FMN	L	2101	-	33,33,33	1.58	8 (24%)	48,50,50	1.82	15 (31%)
4	PNS	E	1901	1	14,20,21	0.88	0	18,26,29	1.50	3 (16%)
5	FMN	H	2101	-	33,33,33	1.57	8 (24%)	48,50,50	1.82	15 (31%)
5	FMN	K	2101	-	33,33,33	1.55	8 (24%)	48,50,50	1.83	15 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FMN	J	2101	-	-	6/18/18/18	0/3/3/3
4	PNS	D	1901	1	-	7/24/26/27	-
4	PNS	F	1901	1	-	6/24/26/27	-
5	FMN	G	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
4	PNS	C	1901	1	-	6/24/26/27	-
4	PNS	B	1901	1	-	7/24/26/27	-
4	PNS	A	1901	1	-	6/24/26/27	-
5	FMN	L	2101	-	-	6/18/18/18	0/3/3/3
4	PNS	E	1901	1	-	6/24/26/27	-
5	FMN	H	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	K	2101	-	-	6/18/18/18	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2101	FMN	C9A-C5A	4.04	1.47	1.41
5	G	2101	FMN	C9A-C5A	4.03	1.47	1.41
5	I	2101	FMN	C9A-C5A	4.01	1.47	1.41
5	H	2101	FMN	C9A-C5A	3.96	1.47	1.41
5	L	2101	FMN	C9A-C5A	3.94	1.47	1.41
5	K	2101	FMN	C9A-C5A	3.92	1.47	1.41
5	L	2101	FMN	C5A-N5	-3.53	1.32	1.39
5	J	2101	FMN	C5A-N5	-3.52	1.33	1.39
5	I	2101	FMN	C5A-N5	-3.51	1.33	1.39
5	H	2101	FMN	C5A-N5	-3.44	1.33	1.39
5	K	2101	FMN	C5A-N5	-3.40	1.33	1.39
5	G	2101	FMN	C5A-N5	-3.38	1.33	1.39
5	I	2101	FMN	C4-N3	-3.12	1.33	1.38
5	J	2101	FMN	C4-N3	-3.11	1.33	1.38
5	L	2101	FMN	C4-N3	-2.98	1.33	1.38
5	K	2101	FMN	C4-N3	-2.97	1.33	1.38
5	G	2101	FMN	C4-N3	-2.97	1.33	1.38
5	H	2101	FMN	C4-N3	-2.96	1.33	1.38
5	L	2101	FMN	C7M-C7	-2.73	1.45	1.51
5	H	2101	FMN	C7M-C7	-2.70	1.45	1.51
5	J	2101	FMN	C7M-C7	-2.65	1.46	1.51
5	K	2101	FMN	C7M-C7	-2.56	1.46	1.51
5	I	2101	FMN	C7M-C7	-2.56	1.46	1.51
5	G	2101	FMN	C7M-C7	-2.52	1.46	1.51
5	I	2101	FMN	C8-C7	2.46	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	2101	FMN	C8-C7	2.42	1.46	1.40
5	J	2101	FMN	C8-C7	2.40	1.46	1.40
5	H	2101	FMN	C8-C7	2.39	1.46	1.40
5	L	2101	FMN	C8-C7	2.39	1.46	1.40
5	G	2101	FMN	C8-C7	2.35	1.46	1.40
5	I	2101	FMN	C2-N3	-2.17	1.34	1.39
5	G	2101	FMN	C6-C5A	-2.15	1.36	1.40
5	J	2101	FMN	C2-N3	-2.15	1.34	1.39
5	I	2101	FMN	C9A-N10	-2.11	1.37	1.41
5	L	2101	FMN	C2-N3	-2.10	1.34	1.39
5	J	2101	FMN	C6-C5A	-2.08	1.36	1.40
5	J	2101	FMN	C9A-N10	-2.05	1.37	1.41
5	H	2101	FMN	C2-N3	-2.05	1.34	1.39
5	L	2101	FMN	C9A-N10	-2.05	1.37	1.41
5	K	2101	FMN	C2-N3	-2.04	1.34	1.39
5	K	2101	FMN	C9A-N10	-2.04	1.37	1.41
5	L	2101	FMN	C6-C5A	-2.04	1.36	1.40
5	G	2101	FMN	C2-N3	-2.04	1.34	1.39
5	H	2101	FMN	C9A-N10	-2.03	1.37	1.41
5	G	2101	FMN	C9A-N10	-2.02	1.37	1.41
5	K	2101	FMN	C6-C7	-2.00	1.36	1.39
5	H	2101	FMN	C6-C5A	-2.00	1.36	1.40

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2101	FMN	O3P-P-O5'	-4.36	95.31	106.67
5	H	2101	FMN	O3P-P-O5'	-4.28	95.51	106.67
5	J	2101	FMN	O3P-P-O5'	-4.22	95.67	106.67
5	L	2101	FMN	O3P-P-O5'	-4.20	95.70	106.67
5	K	2101	FMN	O3P-P-O5'	-4.08	96.03	106.67
5	I	2101	FMN	O3P-P-O5'	-3.93	96.43	106.67
5	K	2101	FMN	C4-C4A-N5	3.78	123.43	118.21
5	I	2101	FMN	C4-C4A-N5	3.72	123.35	118.21
5	H	2101	FMN	C4-C4A-N5	3.62	123.21	118.21
5	L	2101	FMN	C4-C4A-N5	3.58	123.15	118.21
5	K	2101	FMN	O5'-P-O1P	-3.56	96.83	106.44
5	I	2101	FMN	O5'-P-O1P	-3.53	96.89	106.44
5	G	2101	FMN	C4-C4A-N5	3.53	123.09	118.21
5	J	2101	FMN	C4-C4A-N5	3.53	123.08	118.21
5	L	2101	FMN	O5'-P-O1P	-3.37	97.33	106.44
5	J	2101	FMN	O5'-P-O1P	-3.36	97.35	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2101	FMN	O5'-P-O1P	-3.34	97.41	106.44
5	H	2101	FMN	O5'-P-O1P	-3.32	97.47	106.44
4	A	1901	PNS	C37-C38-C39	-3.09	107.24	112.39
4	F	1901	PNS	C37-C38-C39	-3.08	107.27	112.39
4	B	1901	PNS	C37-C38-C39	-3.07	107.28	112.39
4	D	1901	PNS	C37-C38-C39	-3.06	107.29	112.39
4	E	1901	PNS	C37-C38-C39	-3.05	107.31	112.39
4	C	1901	PNS	C37-C38-C39	-3.00	107.39	112.39
5	G	2101	FMN	O2-C2-N1	-2.97	116.86	121.80
5	G	2101	FMN	O2P-P-O5'	2.90	114.22	106.67
5	L	2101	FMN	O2P-P-O5'	2.88	114.18	106.67
5	H	2101	FMN	O2P-P-O5'	2.87	114.15	106.67
5	K	2101	FMN	C4A-C10-N10	2.82	120.53	116.48
5	K	2101	FMN	O2P-P-O5'	2.81	114.00	106.67
5	J	2101	FMN	O2P-P-O5'	2.80	113.97	106.67
5	I	2101	FMN	C4A-C10-N10	2.77	120.44	116.48
5	I	2101	FMN	O2P-P-O5'	2.76	113.87	106.67
5	G	2101	FMN	O4-C4-C4A	-2.76	119.26	126.53
5	G	2101	FMN	O4'-C4'-C5'	-2.75	103.93	109.99
5	J	2101	FMN	C10-N1-C2	2.75	122.80	116.85
5	G	2101	FMN	C4A-C10-N10	2.74	120.41	116.48
5	I	2101	FMN	C10-N1-C2	2.73	122.77	116.85
5	J	2101	FMN	O4'-C4'-C5'	-2.73	103.96	109.99
5	L	2101	FMN	C10-N1-C2	2.71	122.72	116.85
5	H	2101	FMN	C10-N1-C2	2.71	122.71	116.85
5	K	2101	FMN	O2-C2-N1	-2.70	117.32	121.80
5	K	2101	FMN	C10-N1-C2	2.69	122.67	116.85
5	L	2101	FMN	C4A-C10-N10	2.68	120.32	116.48
5	J	2101	FMN	C4A-C10-N10	2.68	120.32	116.48
5	K	2101	FMN	O4'-C4'-C5'	-2.67	104.09	109.99
5	J	2101	FMN	O4-C4-C4A	-2.67	119.48	126.53
5	J	2101	FMN	O4'-C4'-C3'	2.66	115.47	109.25
5	L	2101	FMN	O4'-C4'-C5'	-2.66	104.13	109.99
5	H	2101	FMN	C4A-C10-N10	2.64	120.26	116.48
5	G	2101	FMN	C10-N1-C2	2.63	122.53	116.85
5	H	2101	FMN	O4'-C4'-C5'	-2.62	104.21	109.99
5	H	2101	FMN	O4-C4-C4A	-2.62	119.62	126.53
5	L	2101	FMN	O4-C4-C4A	-2.61	119.65	126.53
5	I	2101	FMN	O4'-C4'-C3'	2.59	115.32	109.25
5	I	2101	FMN	O4'-C4'-C5'	-2.59	104.27	109.99
5	H	2101	FMN	C7M-C7-C6	-2.57	115.05	119.57
5	I	2101	FMN	O4-C4-C4A	-2.56	119.78	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	2101	FMN	O2-C2-N1	-2.53	117.59	121.80
5	L	2101	FMN	C7M-C7-C6	-2.51	115.15	119.57
5	I	2101	FMN	O2-C2-N1	-2.51	117.64	121.80
5	G	2101	FMN	C9A-C5A-N5	2.50	125.11	122.45
5	H	2101	FMN	O4'-C4'-C3'	2.49	115.07	109.25
5	K	2101	FMN	O4-C4-C4A	-2.49	119.97	126.53
5	J	2101	FMN	O2-C2-N1	-2.49	117.67	121.80
5	H	2101	FMN	O2-C2-N1	-2.48	117.68	121.80
5	L	2101	FMN	O4'-C4'-C3'	2.47	115.04	109.25
5	G	2101	FMN	O4'-C4'-C3'	2.47	115.03	109.25
5	K	2101	FMN	C7M-C7-C6	-2.46	115.24	119.57
5	J	2101	FMN	C9A-C5A-N5	2.45	125.06	122.45
5	J	2101	FMN	C4A-C10-N1	-2.45	118.59	124.59
5	I	2101	FMN	C4A-C10-N1	-2.43	118.63	124.59
5	L	2101	FMN	C9A-C5A-N5	2.42	125.02	122.45
5	K	2101	FMN	O4'-C4'-C3'	2.42	114.91	109.25
5	L	2101	FMN	C4A-C10-N1	-2.41	118.69	124.59
5	K	2101	FMN	C4A-C10-N1	-2.41	118.69	124.59
5	J	2101	FMN	C4A-C4-N3	2.39	119.33	113.25
5	H	2101	FMN	C4A-C4-N3	2.38	119.31	113.25
5	I	2101	FMN	C4A-C4-N3	2.37	119.28	113.25
5	H	2101	FMN	C4A-C10-N1	-2.37	118.79	124.59
5	H	2101	FMN	C9A-C5A-N5	2.37	124.97	122.45
5	K	2101	FMN	C9A-C5A-N5	2.36	124.96	122.45
5	I	2101	FMN	C9A-C5A-N5	2.35	124.94	122.45
5	G	2101	FMN	C4A-C10-N1	-2.34	118.85	124.59
5	L	2101	FMN	C4A-C4-N3	2.34	119.20	113.25
5	I	2101	FMN	C7M-C7-C6	-2.33	115.47	119.57
5	G	2101	FMN	C4A-C4-N3	2.32	119.15	113.25
5	K	2101	FMN	C4A-C4-N3	2.32	119.15	113.25
5	I	2101	FMN	C4'-C3'-C2'	-2.29	109.77	113.57
5	J	2101	FMN	C4'-C3'-C2'	-2.28	109.77	113.57
5	J	2101	FMN	C7M-C7-C6	-2.23	115.64	119.57
5	G	2101	FMN	C4'-C3'-C2'	-2.22	109.88	113.57
5	G	2101	FMN	C7M-C7-C6	-2.21	115.68	119.57
5	H	2101	FMN	C4'-C3'-C2'	-2.21	109.90	113.57
4	A	1901	PNS	C43-C42-N41	2.19	117.28	112.31
5	L	2101	FMN	C4'-C3'-C2'	-2.19	109.92	113.57
4	C	1901	PNS	C30-C29-C28	2.19	111.84	108.22
4	B	1901	PNS	C30-C29-C28	2.18	111.82	108.22
4	E	1901	PNS	C30-C29-C28	2.18	111.82	108.22
4	D	1901	PNS	C30-C29-C28	2.17	111.80	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1901	PNS	C30-C29-C28	2.15	111.77	108.22
4	F	1901	PNS	C43-C42-N41	2.14	117.17	112.31
4	C	1901	PNS	C43-C42-N41	2.14	117.15	112.31
5	K	2101	FMN	C4'-C3'-C2'	-2.13	110.03	113.57
4	F	1901	PNS	C30-C29-C28	2.12	111.72	108.22
4	E	1901	PNS	C43-C42-N41	2.05	116.95	112.31
4	D	1901	PNS	C43-C42-N41	2.00	116.85	112.31

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1901	PNS	O27-C28-C29-C32
4	A	1901	PNS	N36-C37-C38-C39
4	A	1901	PNS	N41-C42-C43-S44
4	B	1901	PNS	O27-C28-C29-C32
4	B	1901	PNS	N36-C37-C38-C39
4	B	1901	PNS	N41-C42-C43-S44
4	C	1901	PNS	O27-C28-C29-C32
4	C	1901	PNS	N36-C37-C38-C39
4	C	1901	PNS	N41-C42-C43-S44
4	D	1901	PNS	O27-C28-C29-C31
4	D	1901	PNS	O27-C28-C29-C32
4	D	1901	PNS	N36-C37-C38-C39
4	D	1901	PNS	N41-C42-C43-S44
4	E	1901	PNS	O27-C28-C29-C32
4	E	1901	PNS	N36-C37-C38-C39
4	E	1901	PNS	N41-C42-C43-S44
4	F	1901	PNS	O27-C28-C29-C32
4	F	1901	PNS	N36-C37-C38-C39
4	F	1901	PNS	N41-C42-C43-S44
4	A	1901	PNS	C38-C37-N36-C34
4	B	1901	PNS	C38-C37-N36-C34
4	C	1901	PNS	C38-C37-N36-C34
4	D	1901	PNS	C38-C37-N36-C34
4	E	1901	PNS	C38-C37-N36-C34
4	F	1901	PNS	C38-C37-N36-C34
5	G	2101	FMN	O3'-C3'-C4'-C5'
5	H	2101	FMN	O3'-C3'-C4'-C5'
5	I	2101	FMN	O3'-C3'-C4'-C5'
5	J	2101	FMN	O3'-C3'-C4'-C5'
5	L	2101	FMN	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
5	G	2101	FMN	C2'-C3'-C4'-C5'
5	H	2101	FMN	C2'-C3'-C4'-C5'
5	I	2101	FMN	C2'-C3'-C4'-C5'
5	J	2101	FMN	C2'-C3'-C4'-C5'
5	K	2101	FMN	C2'-C3'-C4'-C5'
5	L	2101	FMN	C2'-C3'-C4'-C5'
5	J	2101	FMN	C2'-C3'-C4'-O4'
5	K	2101	FMN	O3'-C3'-C4'-C5'
5	G	2101	FMN	C2'-C3'-C4'-O4'
5	H	2101	FMN	C2'-C3'-C4'-O4'
5	I	2101	FMN	C2'-C3'-C4'-O4'
5	K	2101	FMN	C2'-C3'-C4'-O4'
5	L	2101	FMN	C2'-C3'-C4'-O4'
5	G	2101	FMN	C3'-C4'-C5'-O5'
5	J	2101	FMN	C3'-C4'-C5'-O5'
5	J	2101	FMN	O3'-C3'-C4'-O4'
5	G	2101	FMN	O3'-C3'-C4'-O4'
5	H	2101	FMN	C3'-C4'-C5'-O5'
5	I	2101	FMN	C3'-C4'-C5'-O5'
5	L	2101	FMN	C3'-C4'-C5'-O5'
5	H	2101	FMN	O3'-C3'-C4'-O4'
5	I	2101	FMN	O3'-C3'-C4'-O4'
5	L	2101	FMN	O3'-C3'-C4'-O4'
4	A	1901	PNS	O27-C28-C29-C30
4	A	1901	PNS	O27-C28-C29-C31
4	B	1901	PNS	O27-C28-C29-C30
4	B	1901	PNS	O27-C28-C29-C31
4	C	1901	PNS	O27-C28-C29-C30
4	C	1901	PNS	O27-C28-C29-C31
4	D	1901	PNS	O27-C28-C29-C30
4	E	1901	PNS	O27-C28-C29-C30
4	E	1901	PNS	O27-C28-C29-C31
4	F	1901	PNS	O27-C28-C29-C30
4	F	1901	PNS	O27-C28-C29-C31
5	K	2101	FMN	O3'-C3'-C4'-O4'
5	K	2101	FMN	C3'-C4'-C5'-O5'
5	G	2101	FMN	C4'-C5'-O5'-P
5	I	2101	FMN	C4'-C5'-O5'-P
5	K	2101	FMN	C4'-C5'-O5'-P
5	H	2101	FMN	C4'-C5'-O5'-P
5	J	2101	FMN	C4'-C5'-O5'-P
5	L	2101	FMN	C4'-C5'-O5'-P

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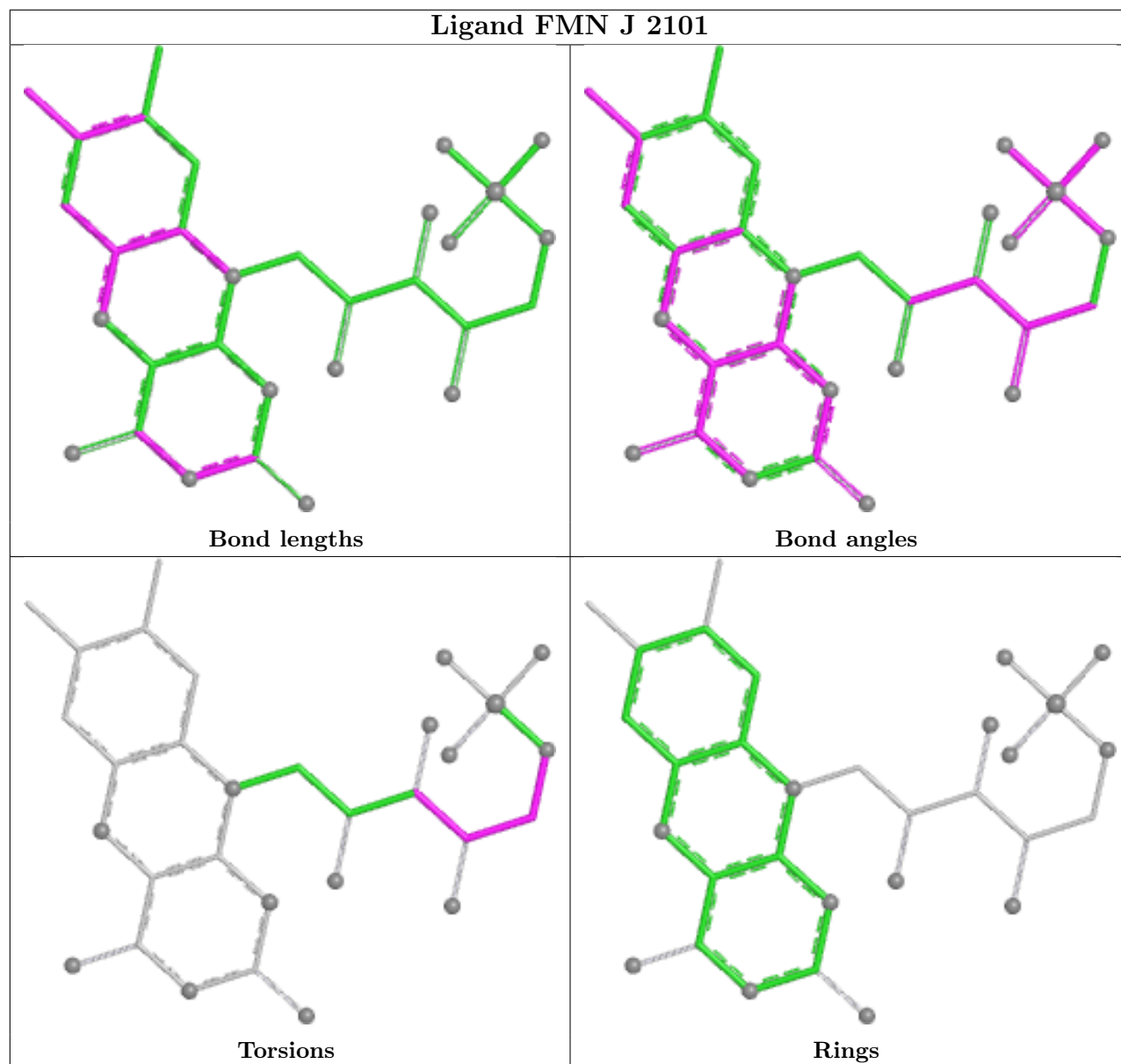
Mol	Chain	Res	Type	Atoms
4	B	1901	PNS	C38-C39-N41-C42
4	D	1901	PNS	C38-C39-N41-C42

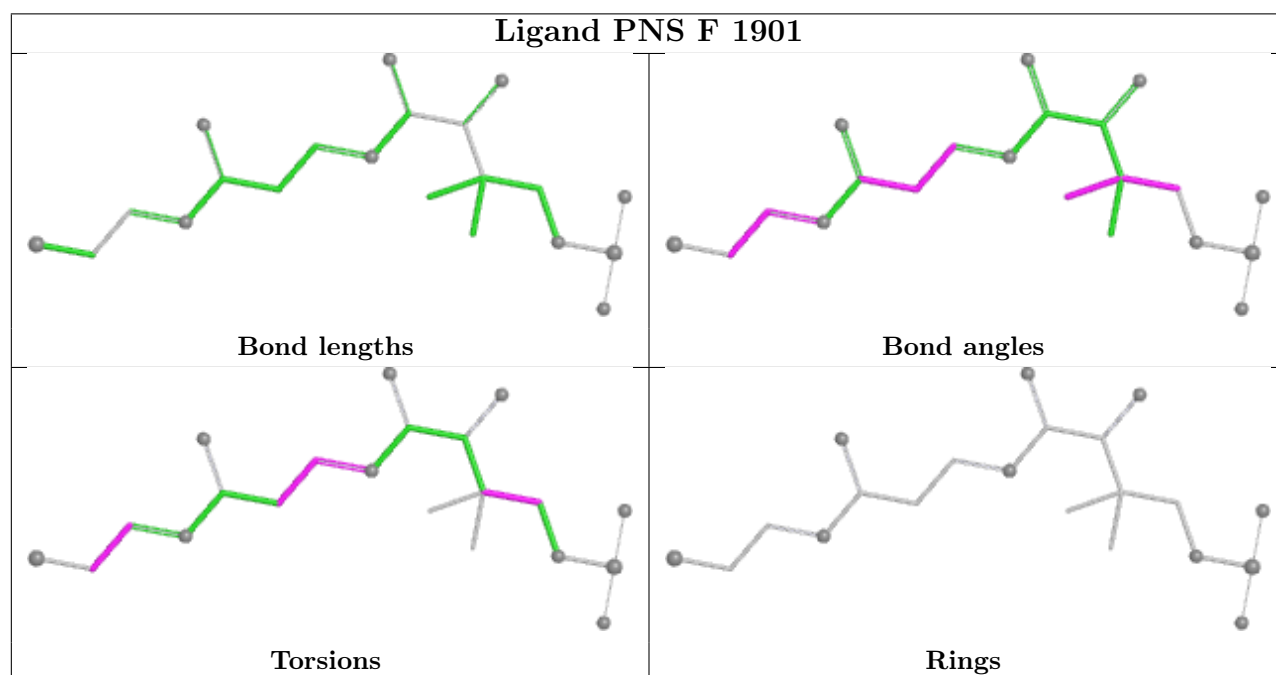
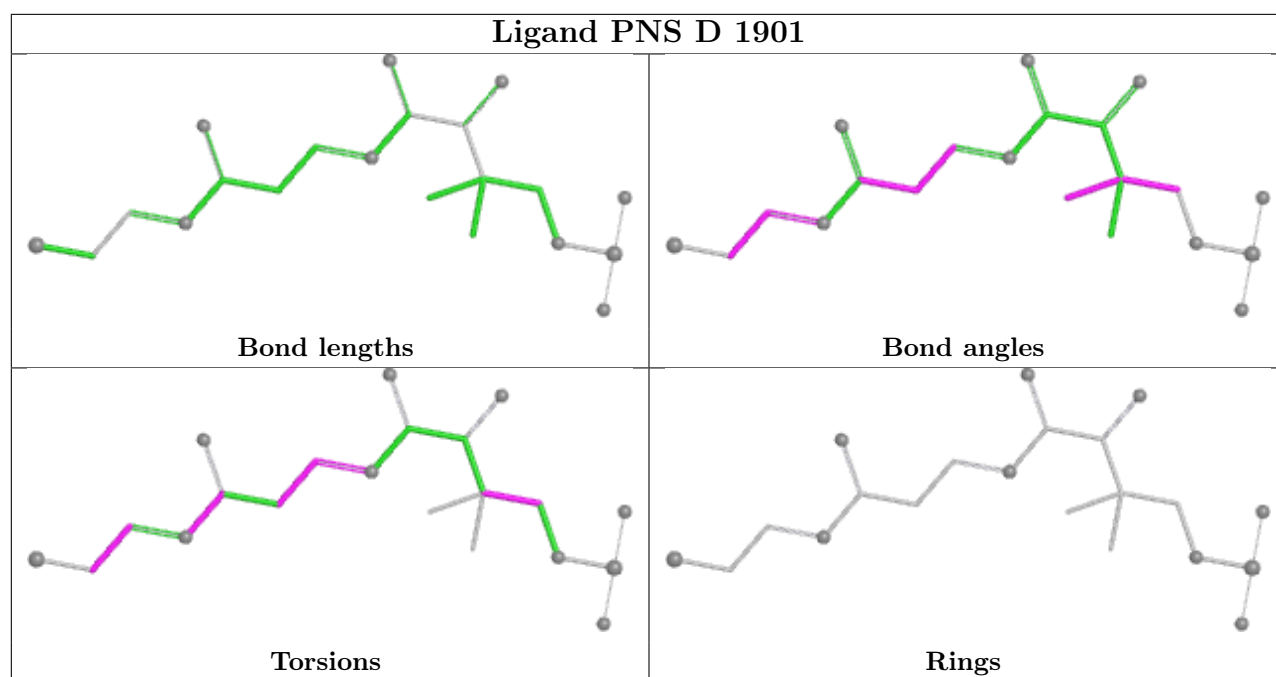
There are no ring outliers.

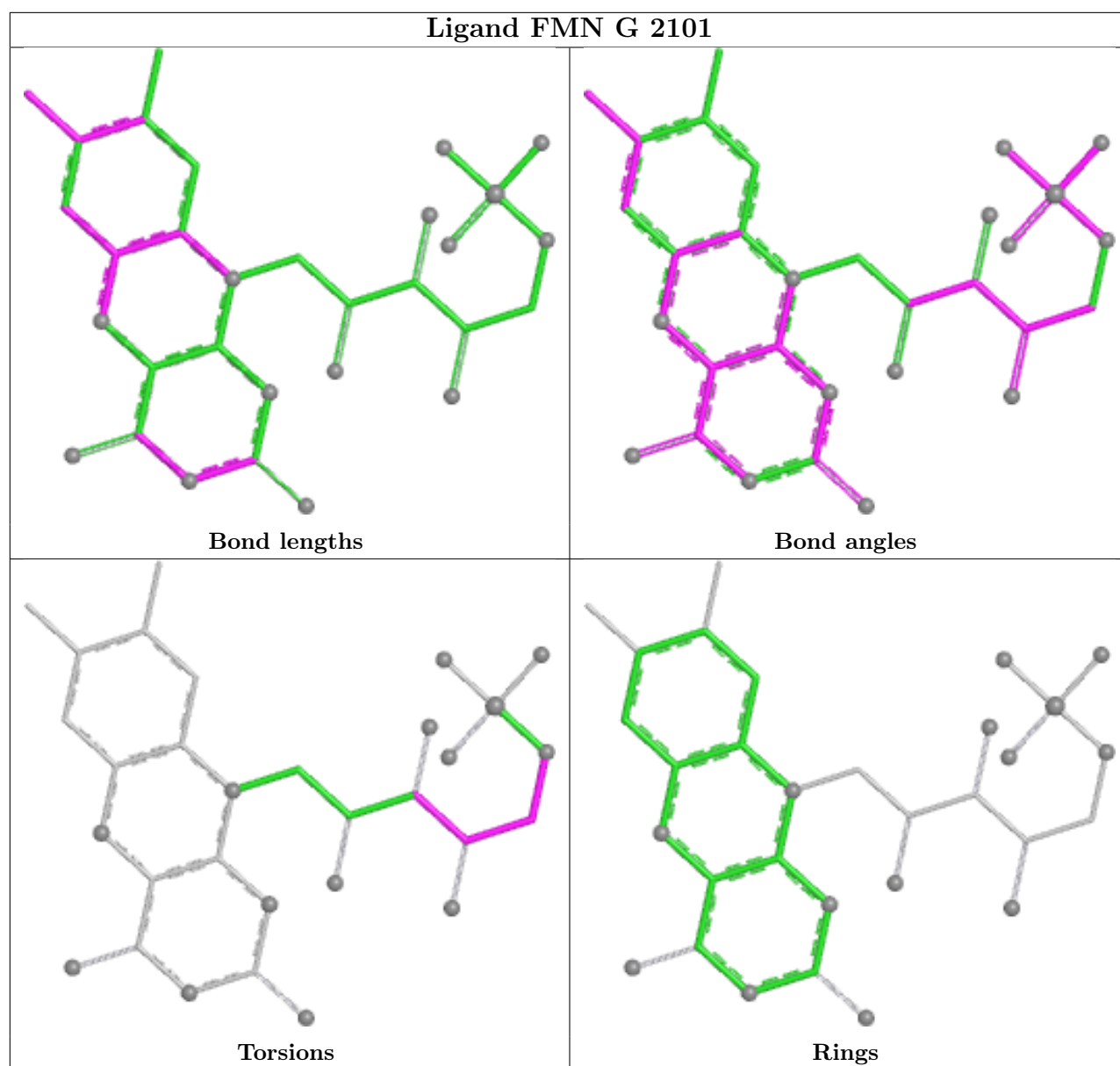
12 monomers are involved in 31 short contacts:

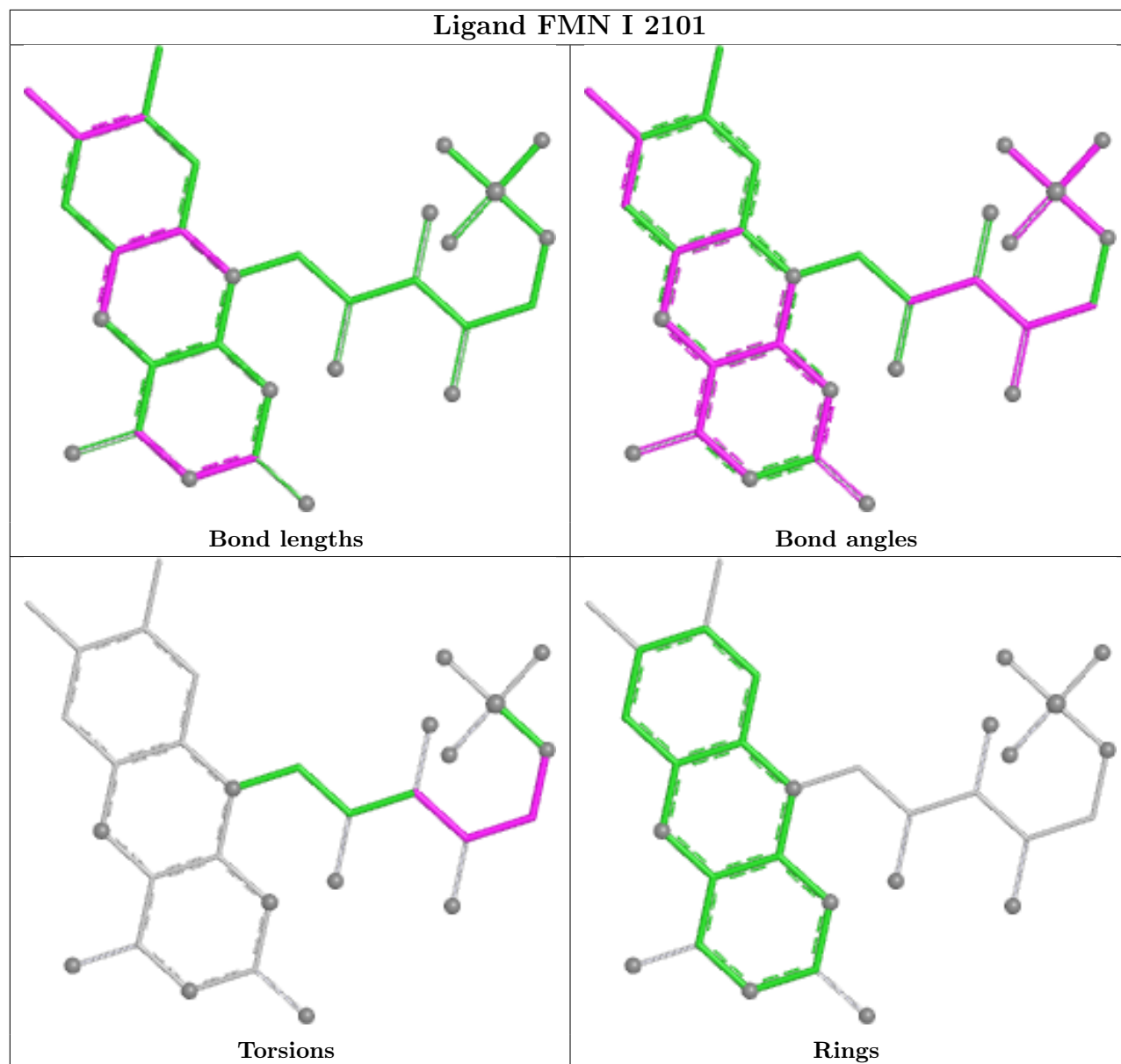
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2101	FMN	2	0
4	D	1901	PNS	3	0
4	F	1901	PNS	3	0
5	G	2101	FMN	2	0
5	I	2101	FMN	2	0
4	C	1901	PNS	3	0
4	B	1901	PNS	4	0
4	A	1901	PNS	3	0
5	L	2101	FMN	2	0
4	E	1901	PNS	3	0
5	H	2101	FMN	2	0
5	K	2101	FMN	2	0

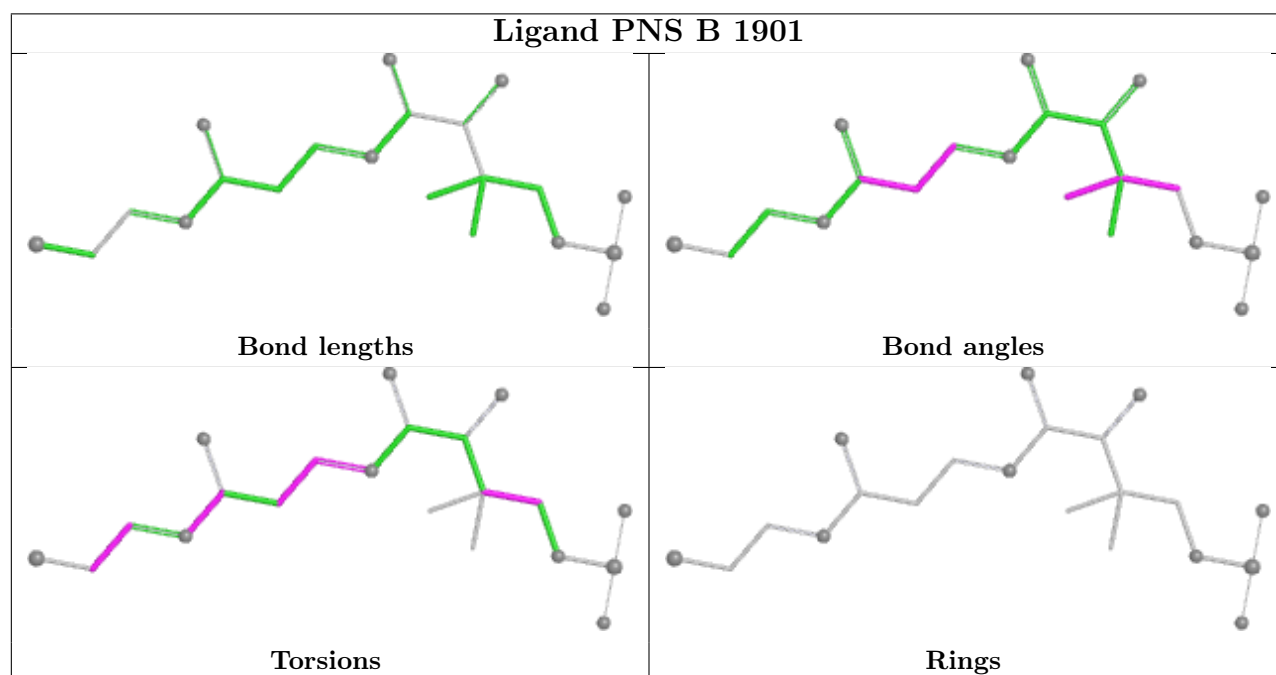
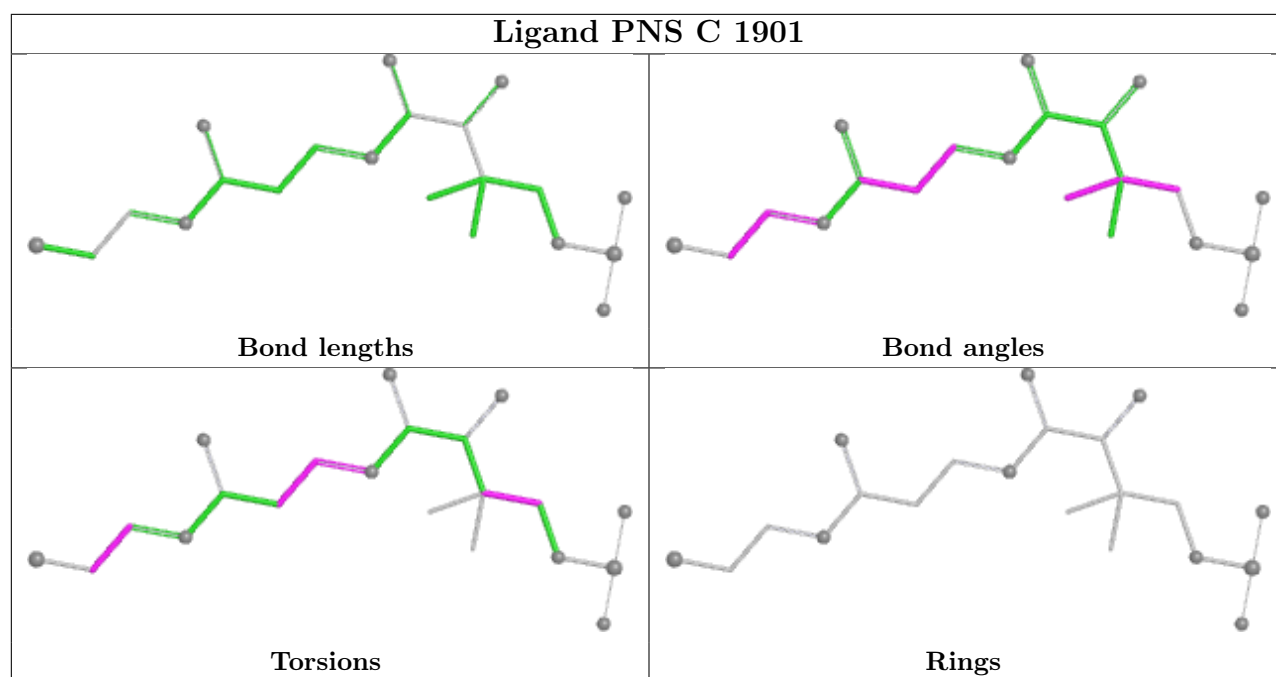
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

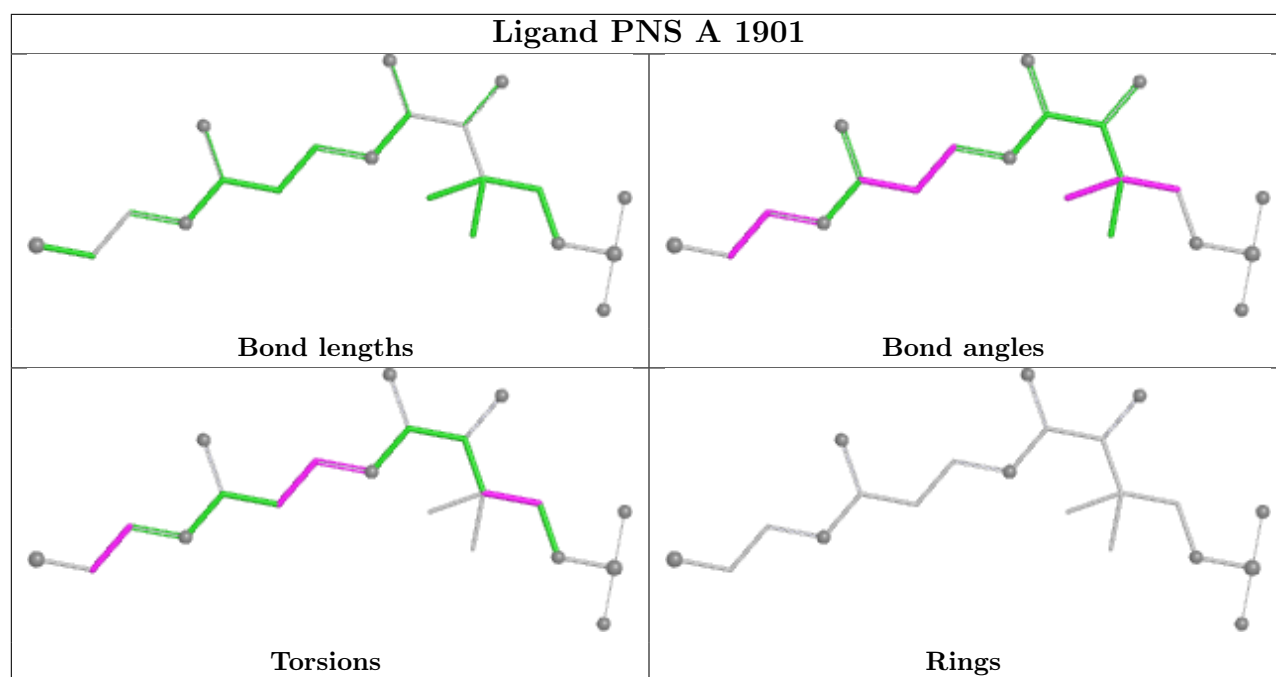


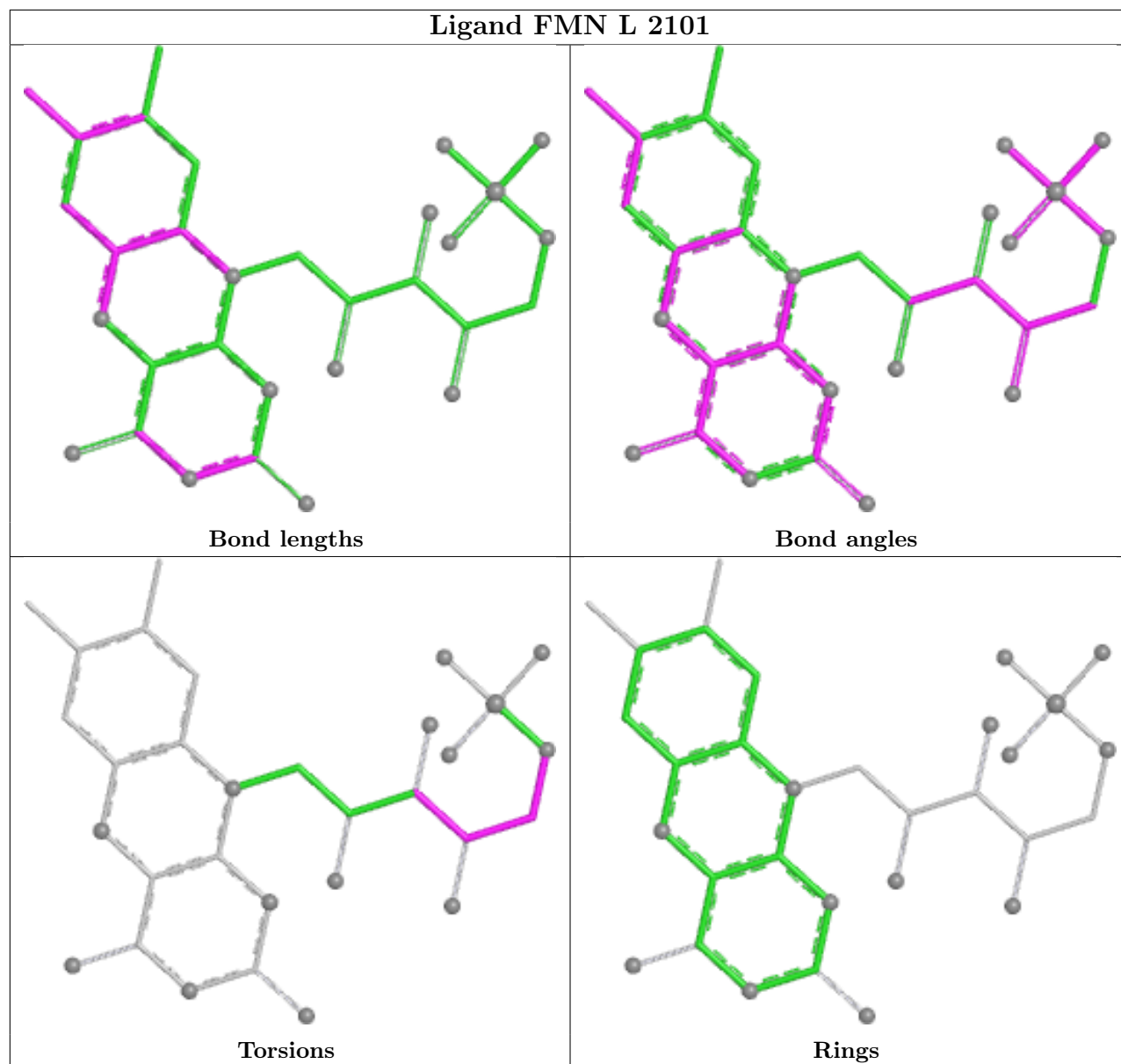


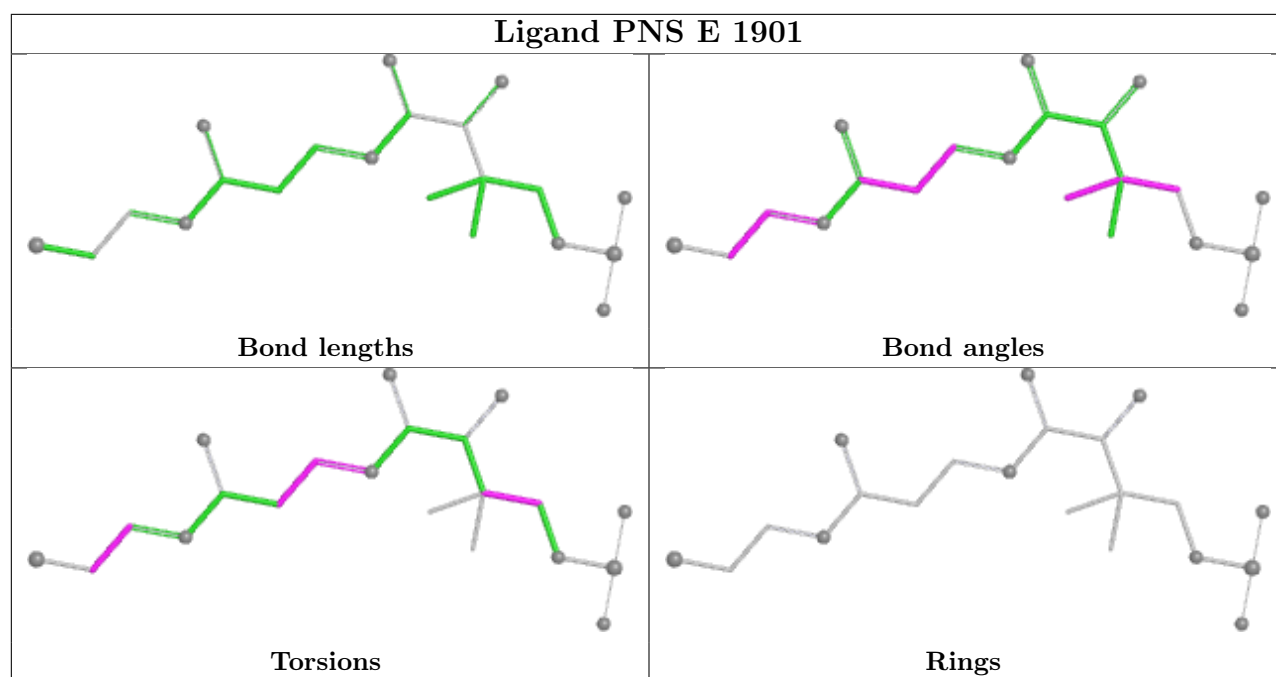


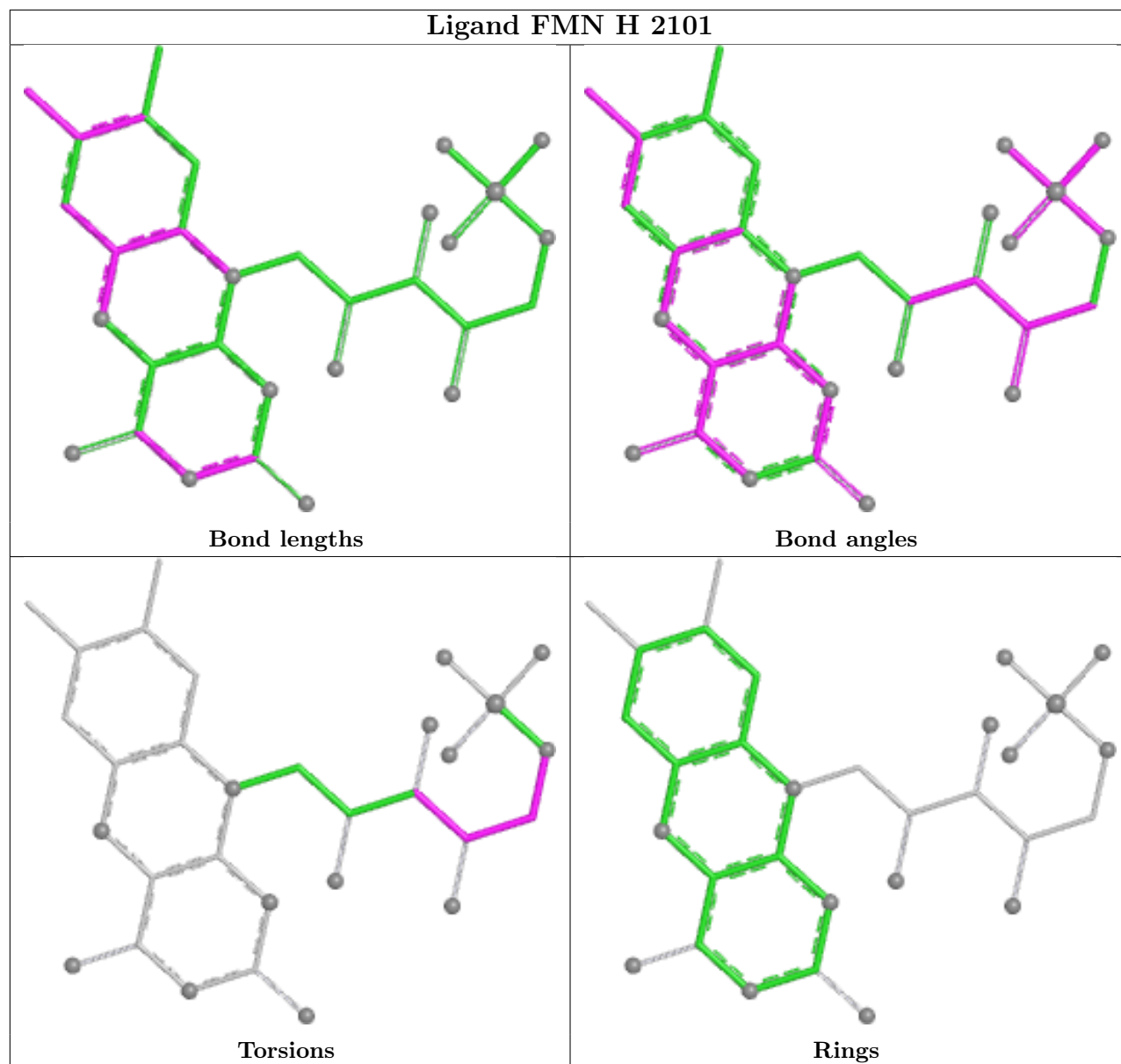


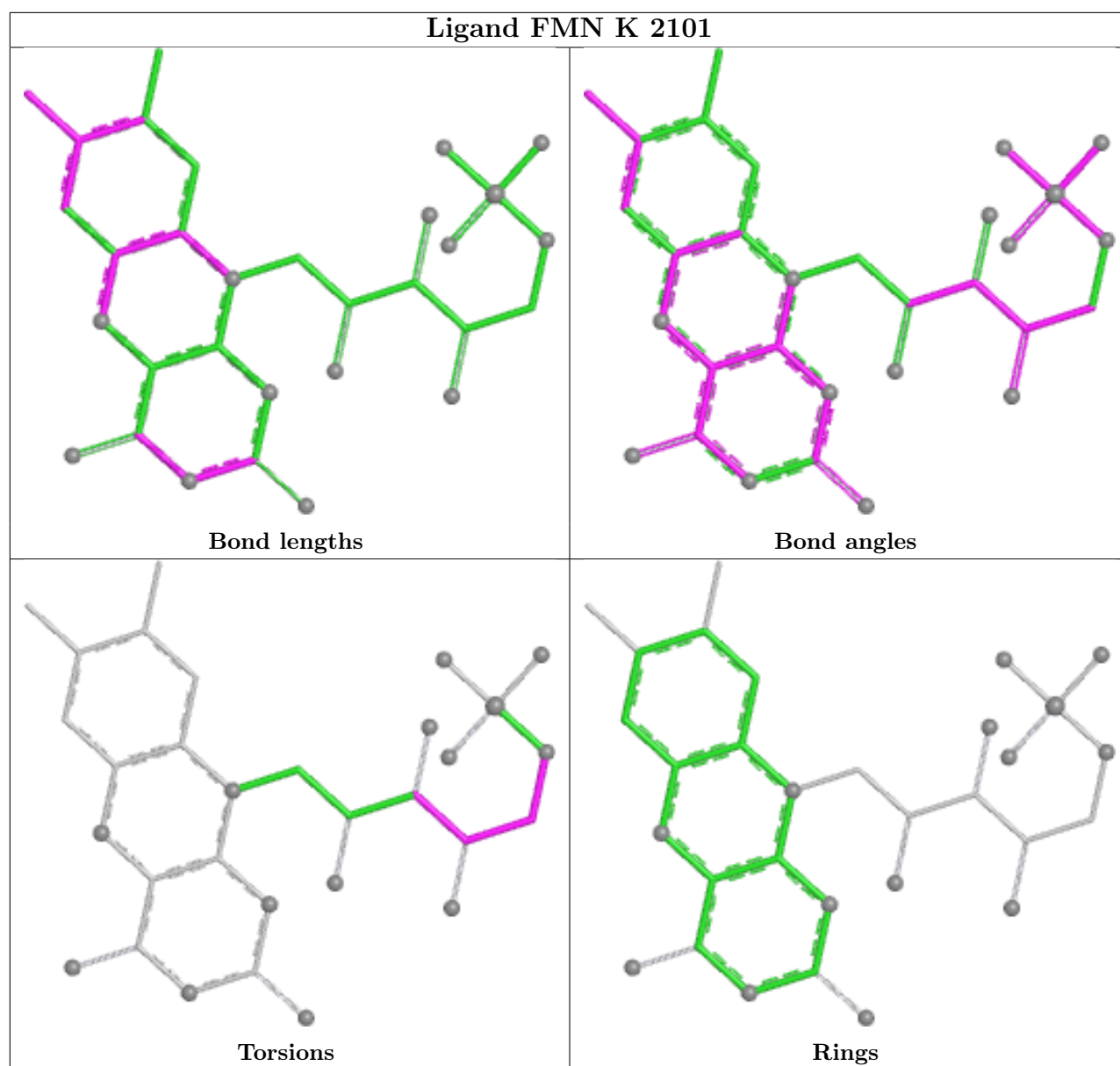












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

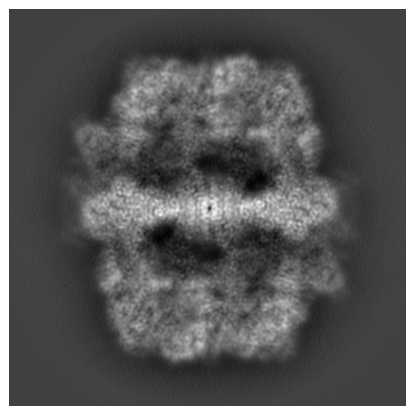
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4577. These allow visual inspection of the internal detail of the map and identification of artifacts.

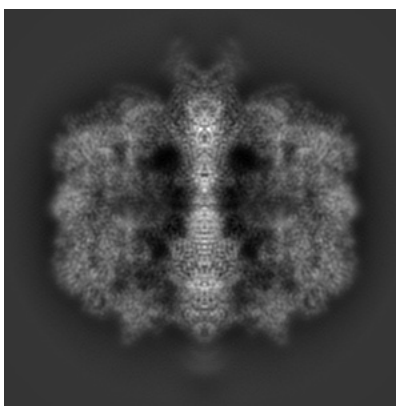
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

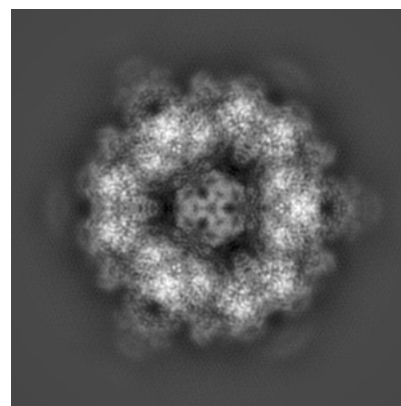
6.1.1 Primary map



X

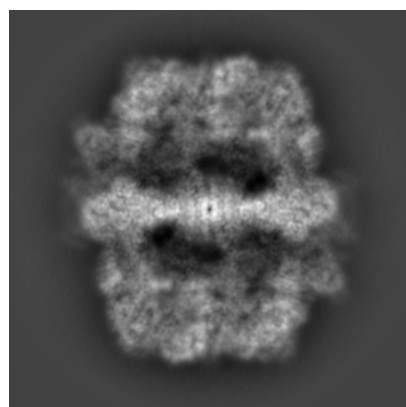


Y

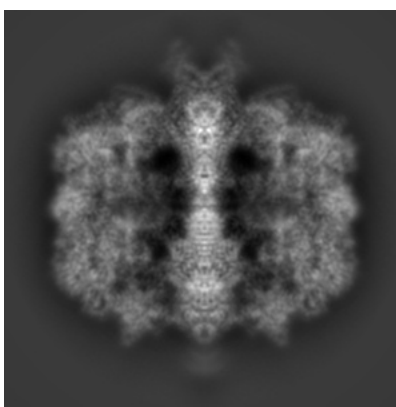


Z

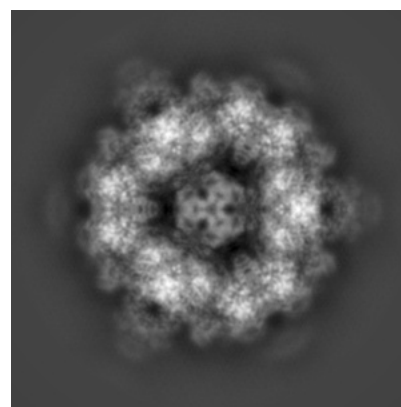
6.1.2 Raw map



X



Y

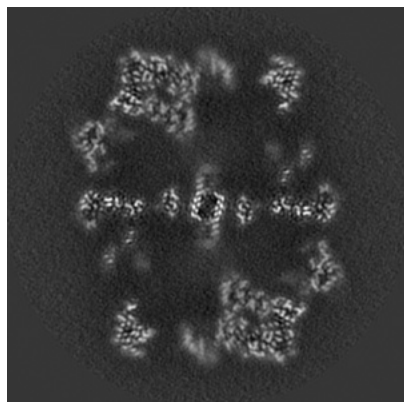


Z

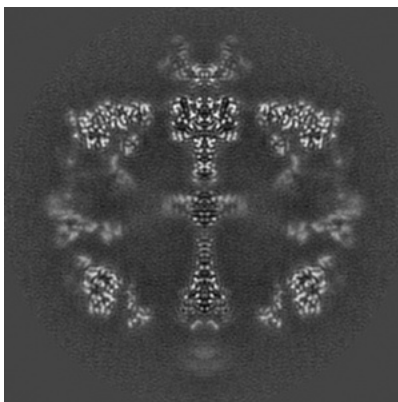
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

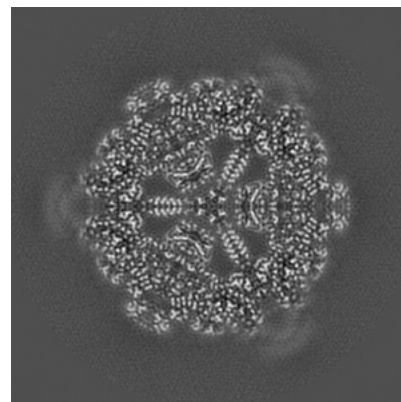
6.2.1 Primary map



X Index: 160

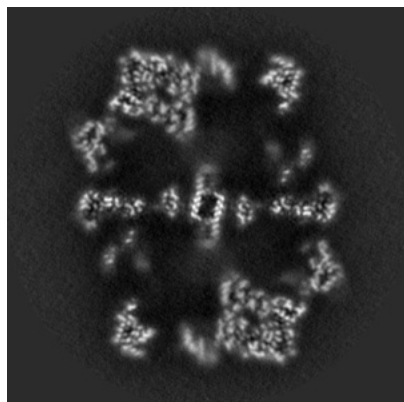


Y Index: 160

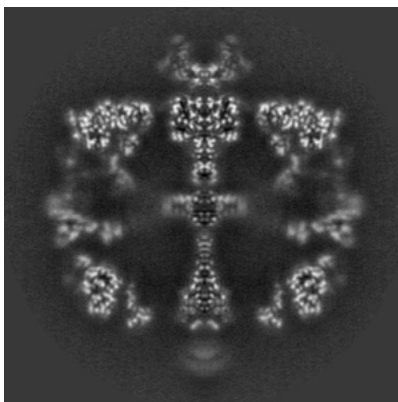


Z Index: 160

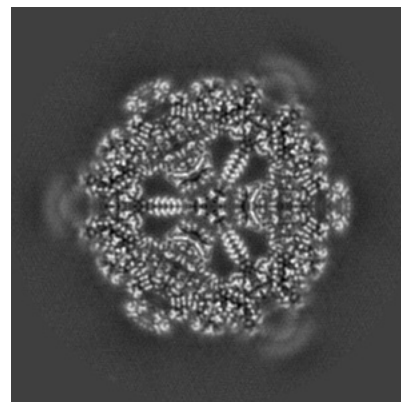
6.2.2 Raw map



X Index: 160



Y Index: 160

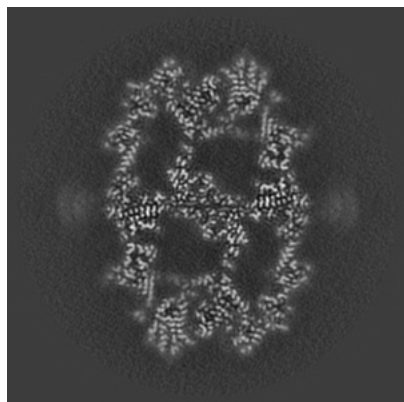


Z Index: 160

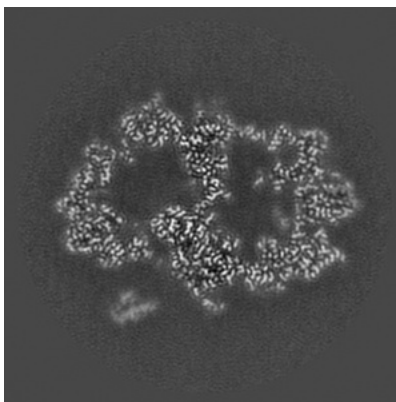
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

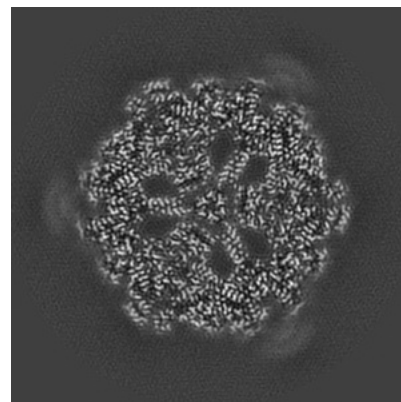
6.3.1 Primary map



X Index: 215

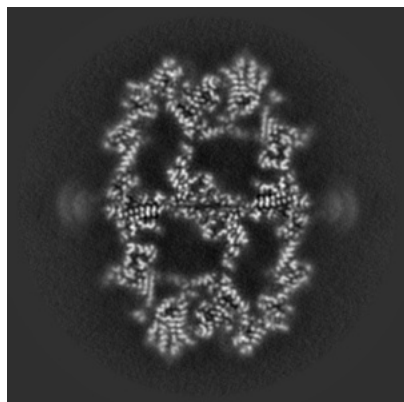


Y Index: 99

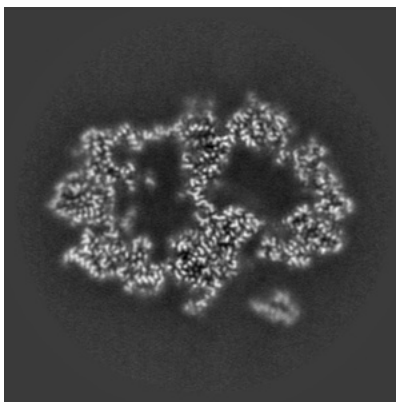


Z Index: 162

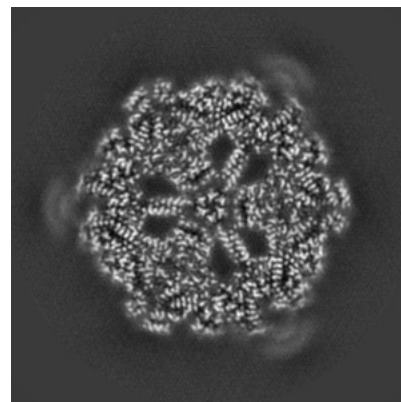
6.3.2 Raw map



X Index: 215



Y Index: 220

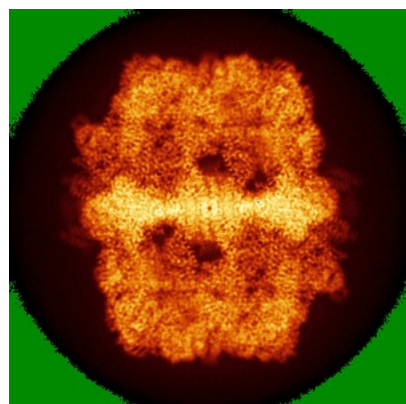


Z Index: 158

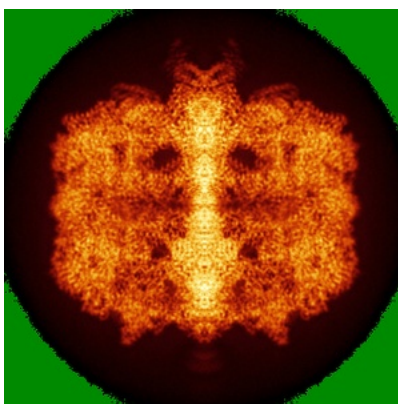
The images above show the largest variance slices of the map in three orthogonal directions.

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

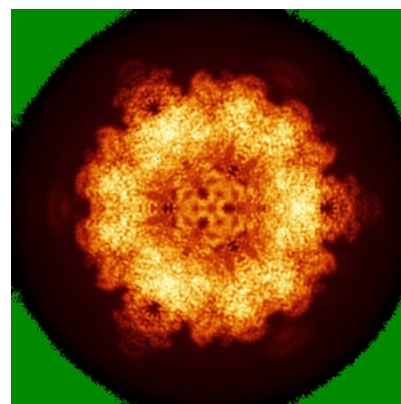
6.4.1 Primary map



X

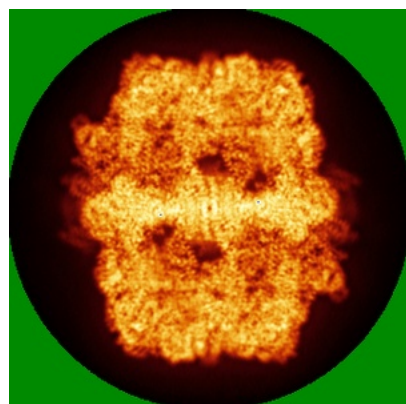


Y

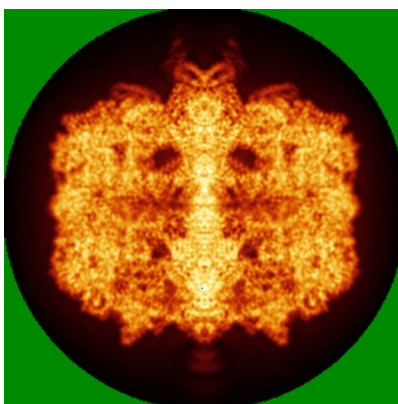


Z

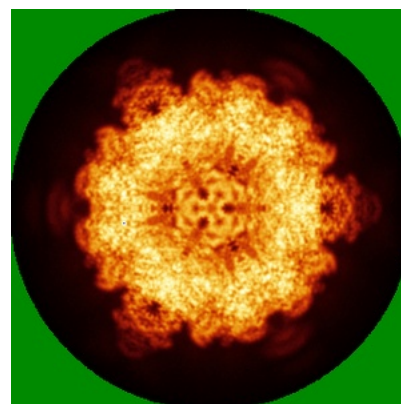
6.4.2 Raw map



X



Y

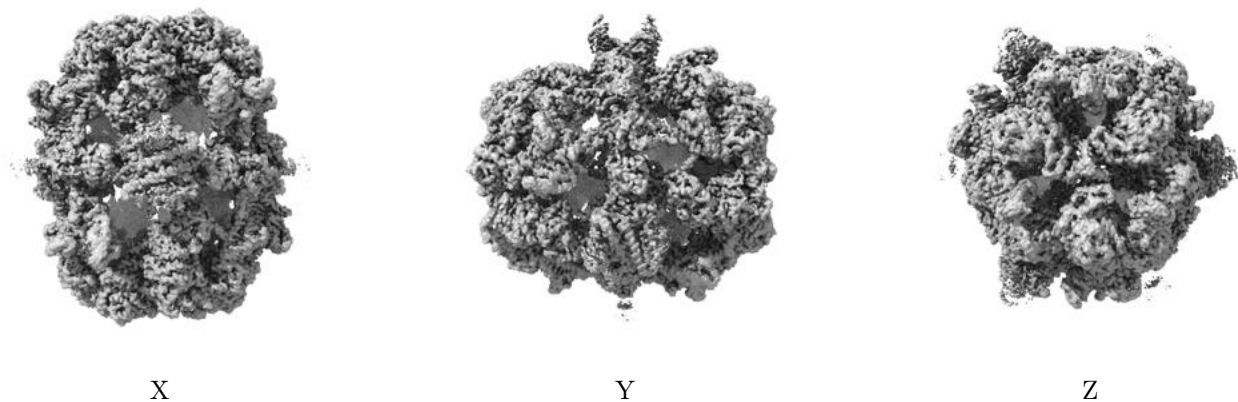


Z

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

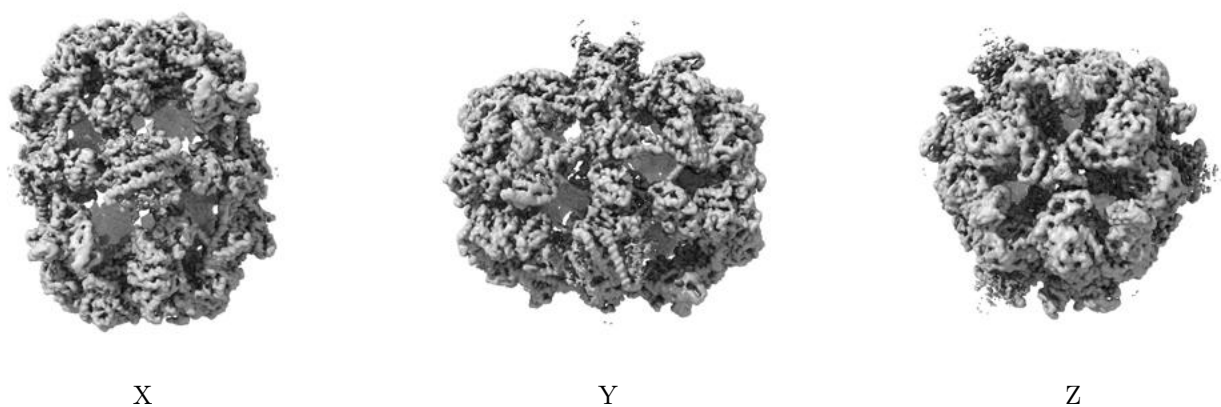
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

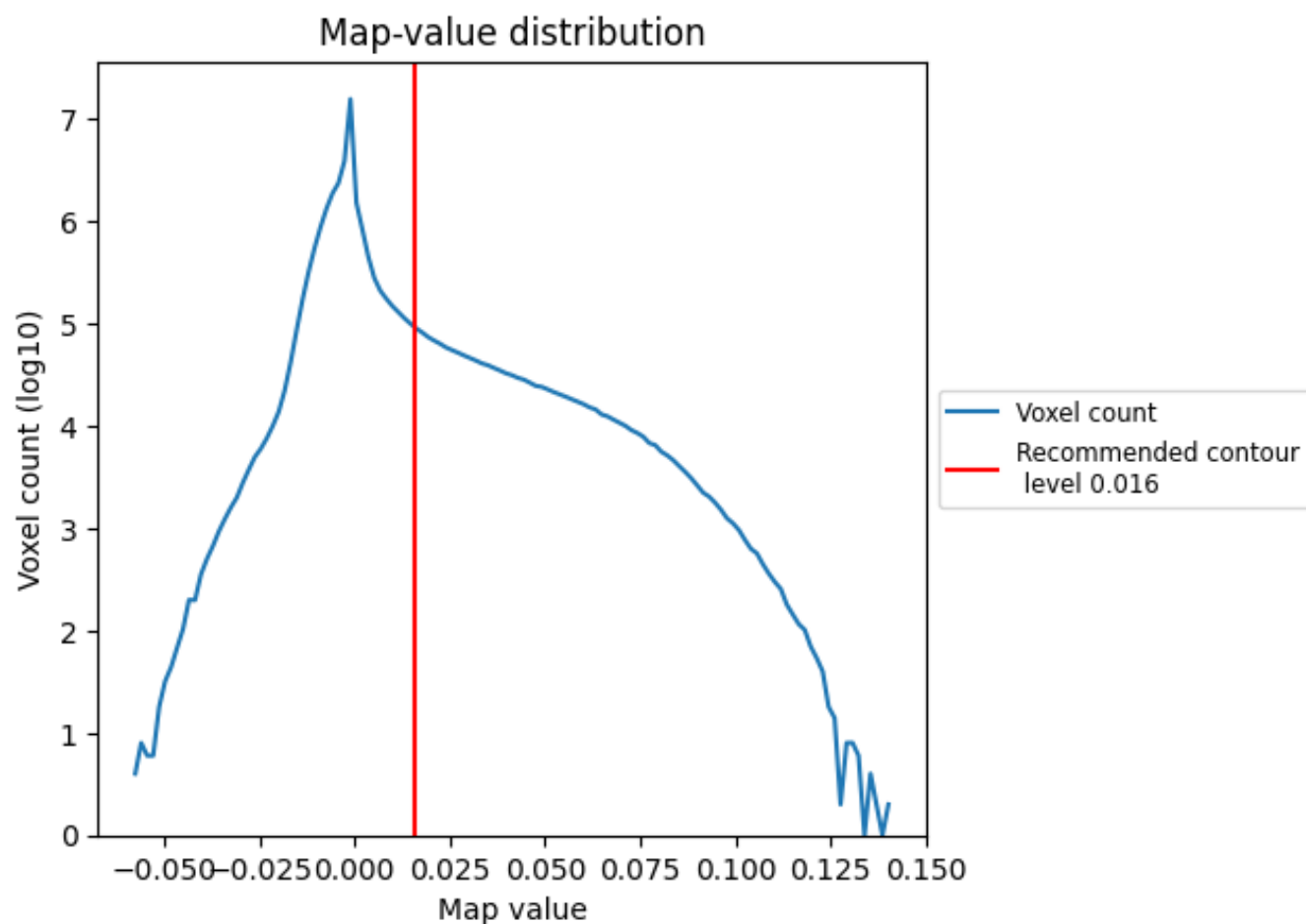
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

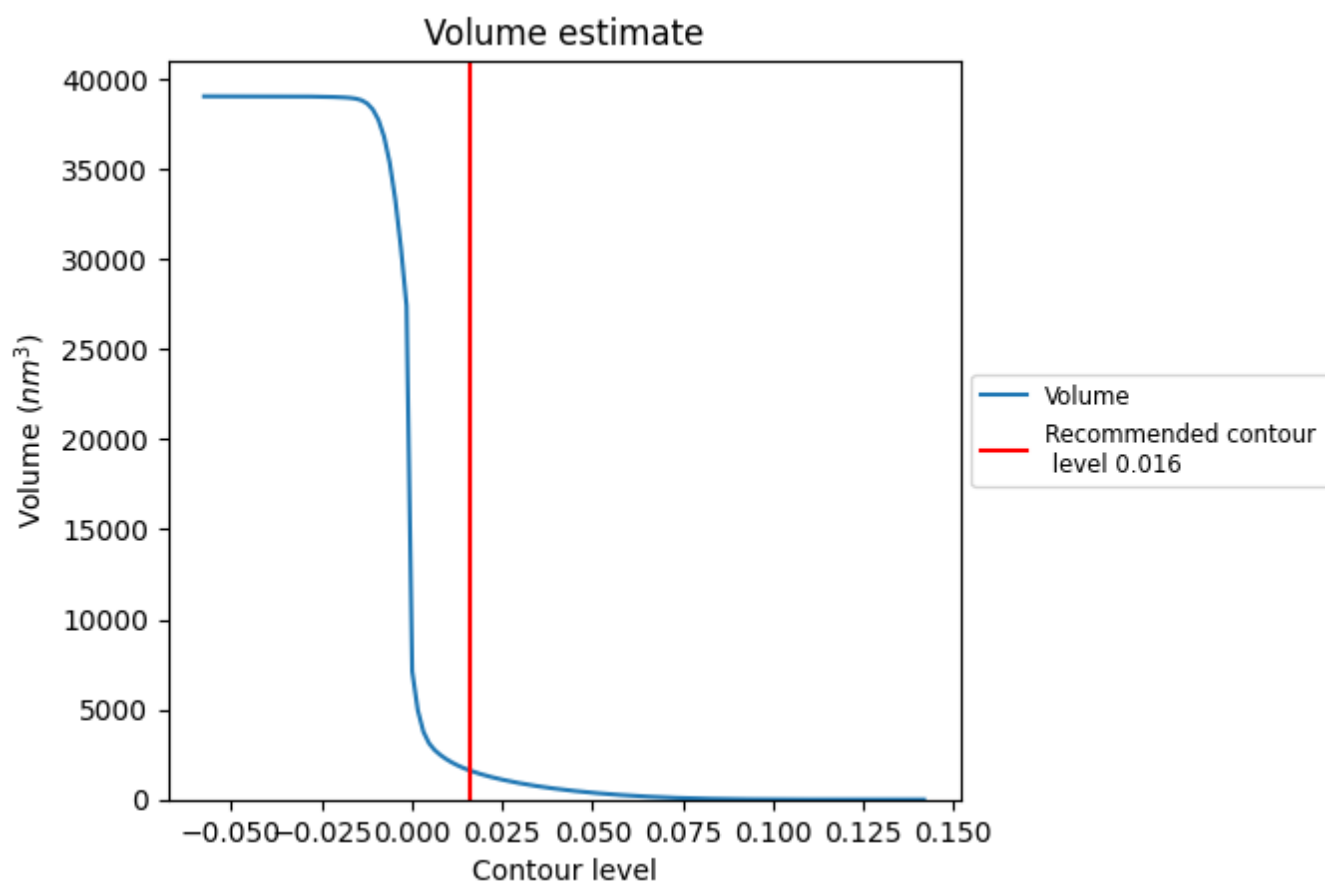
This section contains the results of statistical analysis of the map.

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.

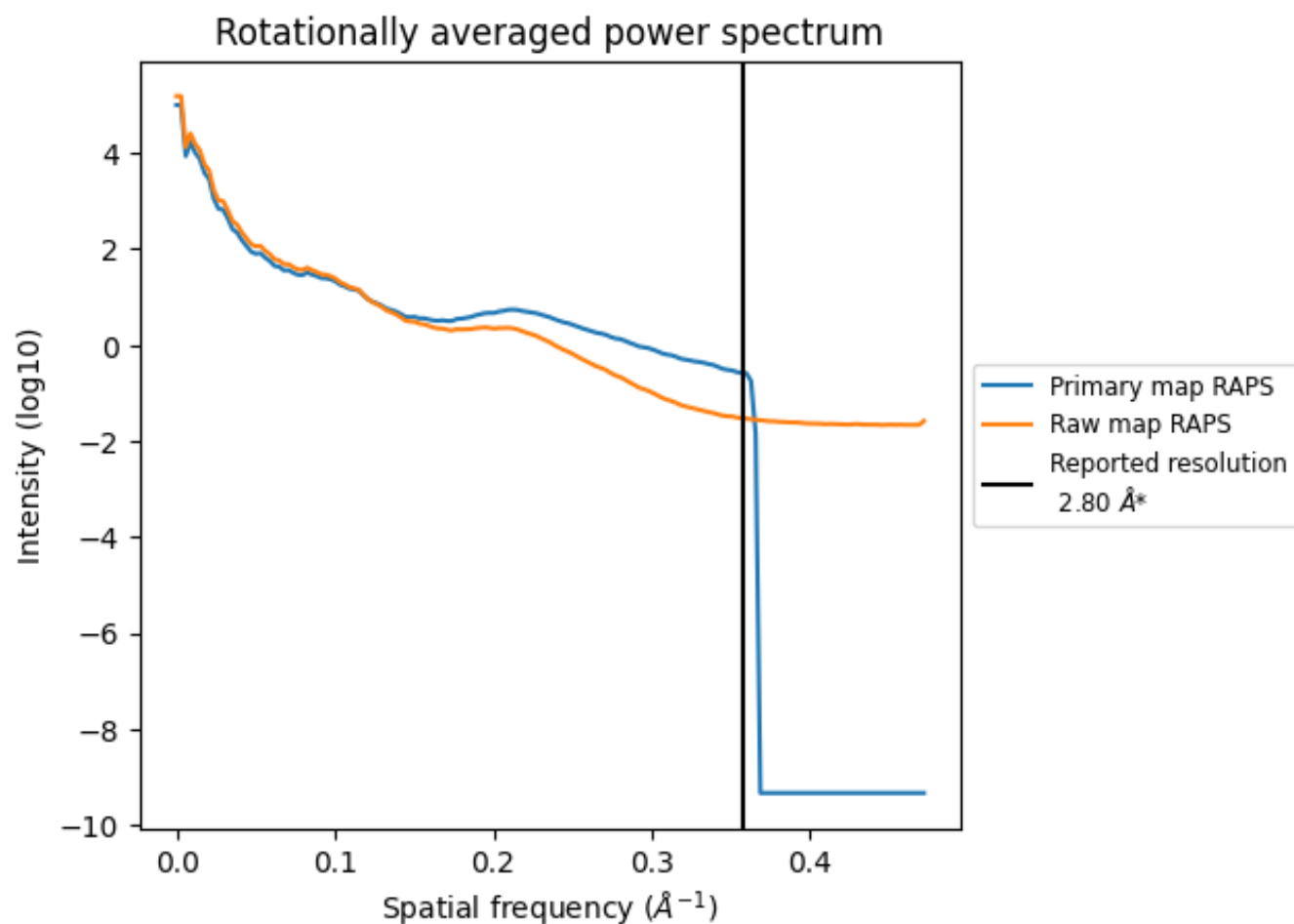
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1616 nm^3 ; this corresponds to an approximate mass of 1460 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 ⓘ

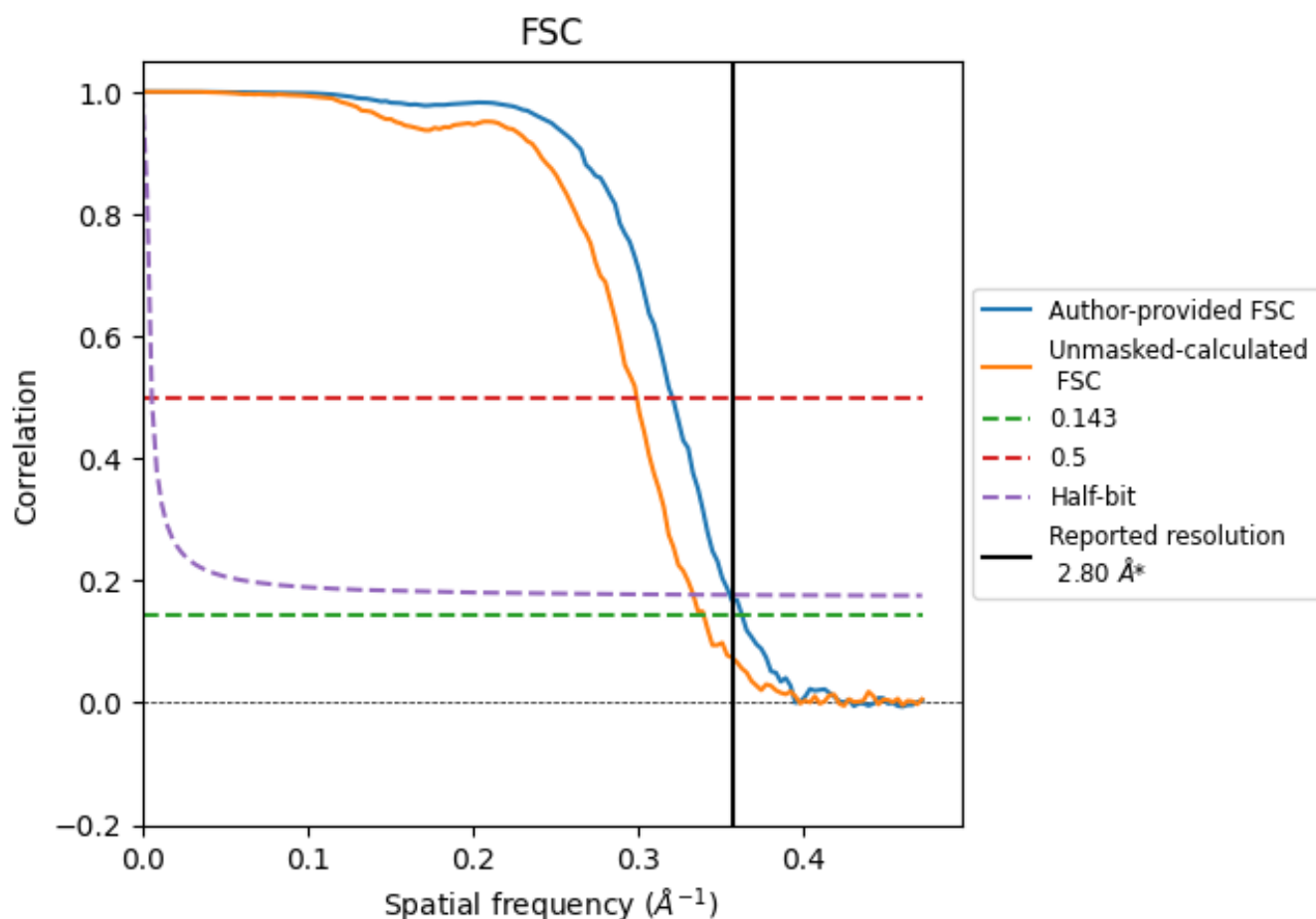


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

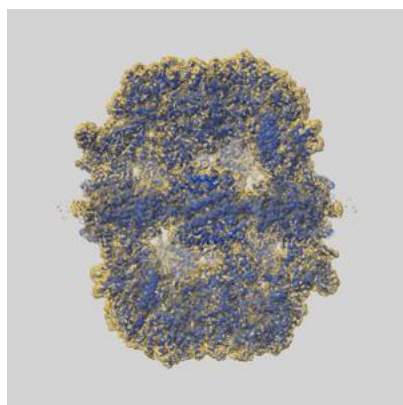
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.12	2.81
Unmasked-calculated*	2.94	3.34	3.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

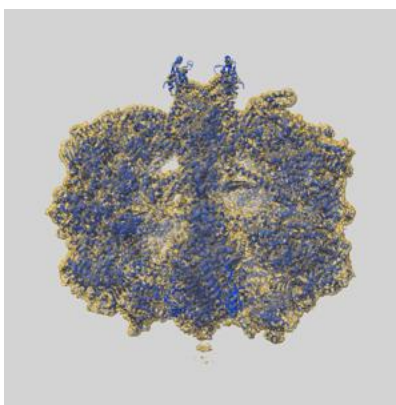
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4577 and PDB model 6QL5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

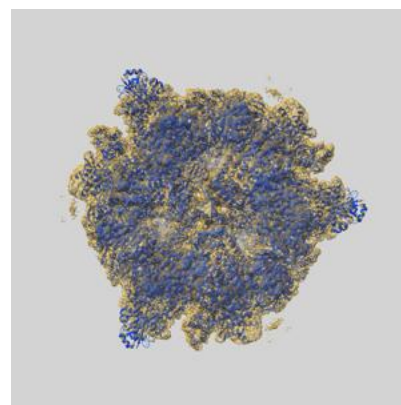
9.1 Map-model overlay [i](#)



X



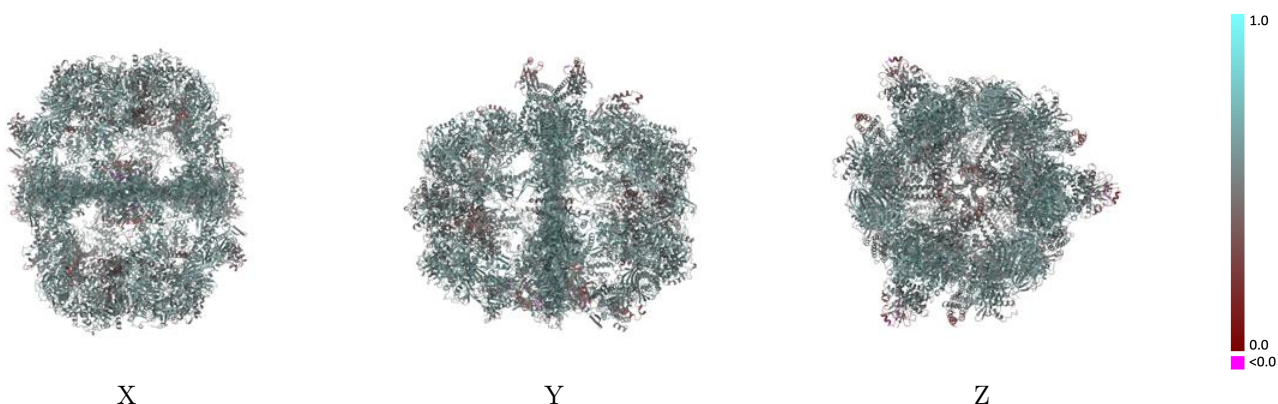
Y



Z

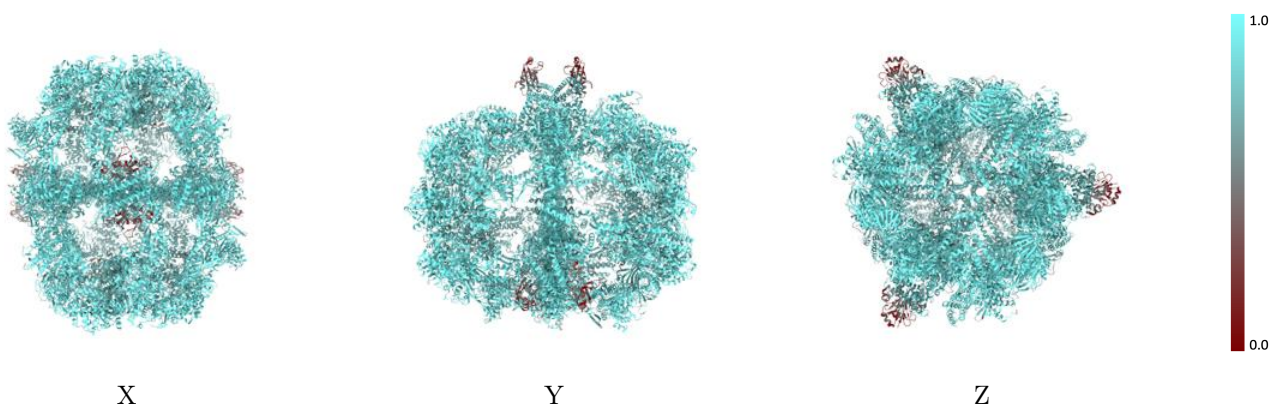
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



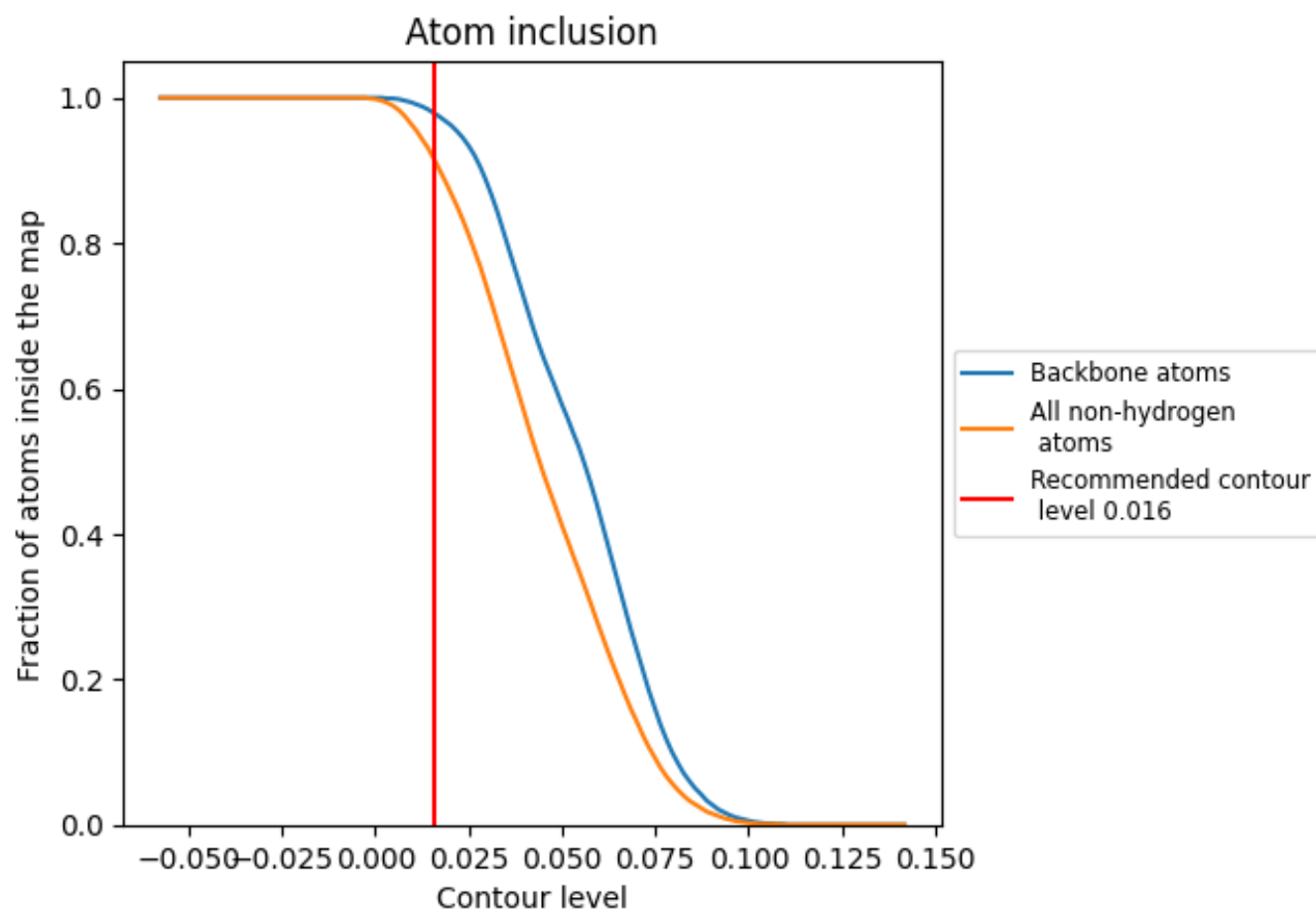
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.5530
A	0.8870	0.5610
B	0.8880	0.5610
C	0.8870	0.5620
D	0.8880	0.5620
E	0.8870	0.5620
F	0.8870	0.5610
G	0.9390	0.5490
H	0.9390	0.5490
I	0.9400	0.5480
J	0.9400	0.5490
K	0.9400	0.5490
L	0.9390	0.5490
M	0.8430	0.5150
N	0.8300	0.5160
O	0.8300	0.5140
P	0.8340	0.5140
Q	0.8330	0.5130
R	0.8360	0.5150

1.0

0.0

<0.0