



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:20 AM UTC

PDB ID : 6JSI / pdb_00006jsi
EMDB ID : EMD-9882
Title : Co-purified Fatty Acid Synthase
Authors : Qiu, S.W.; Liu, S.
Deposited on : 2019-04-08
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

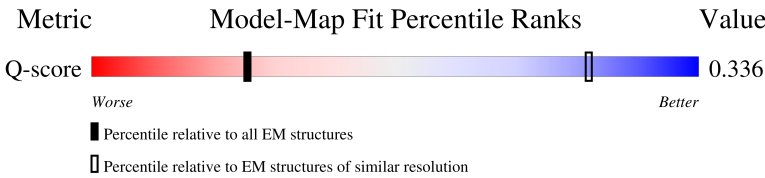
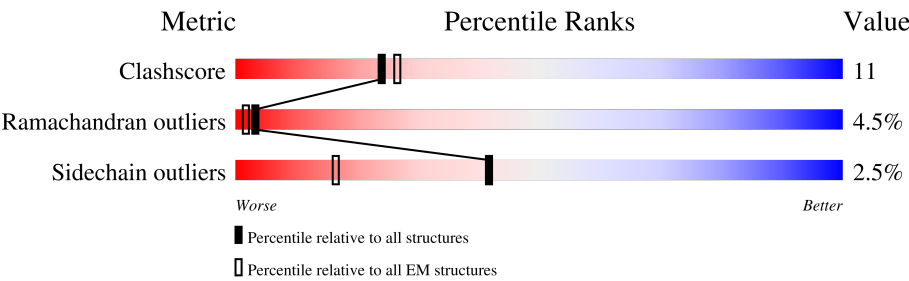
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

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	B	2051	
1	F	2051	
1	G	2051	
2	A	1887	

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Mol	Chain	Length	Quality of chain
2	D	1887	5%52%15%•30%
2	E	1887	5%52%15%•30%
3	C	71	•68%30%••
3	H	71	6%69%28%••
3	I	71	•69%28%••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 62820 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 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		
1	F	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		
1	G	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1321	Total	C	N	O	S	0	0
			8587	5349	1534	1673	31		
2	D	1321	Total	C	N	O	S	0	0
			8587	5349	1534	1673	31		
2	E	1321	Total	C	N	O	S	0	0
			8587	5349	1534	1673	31		

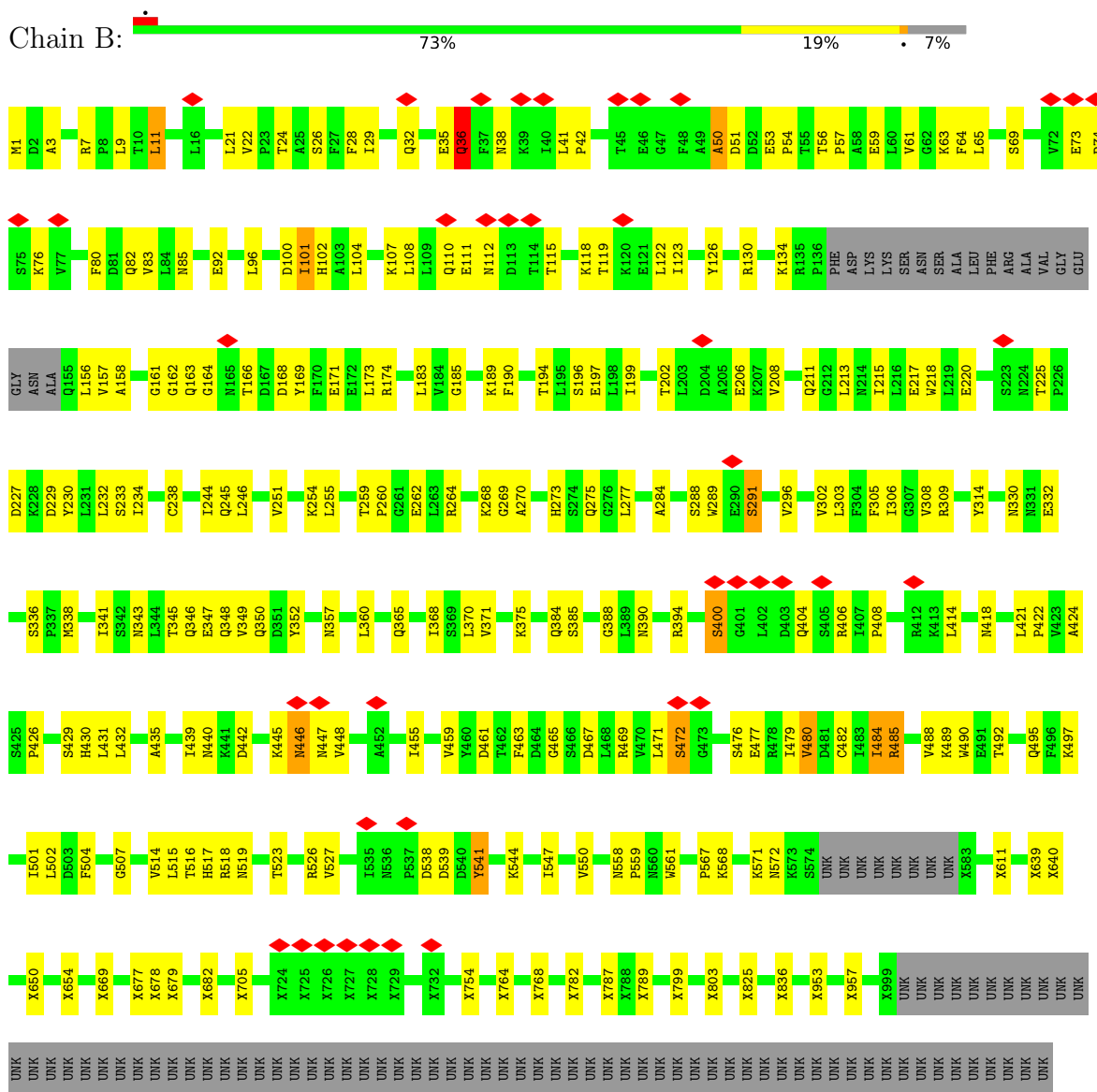
- Molecule 3 is a protein called Fatty acid synthase subunit alpha.

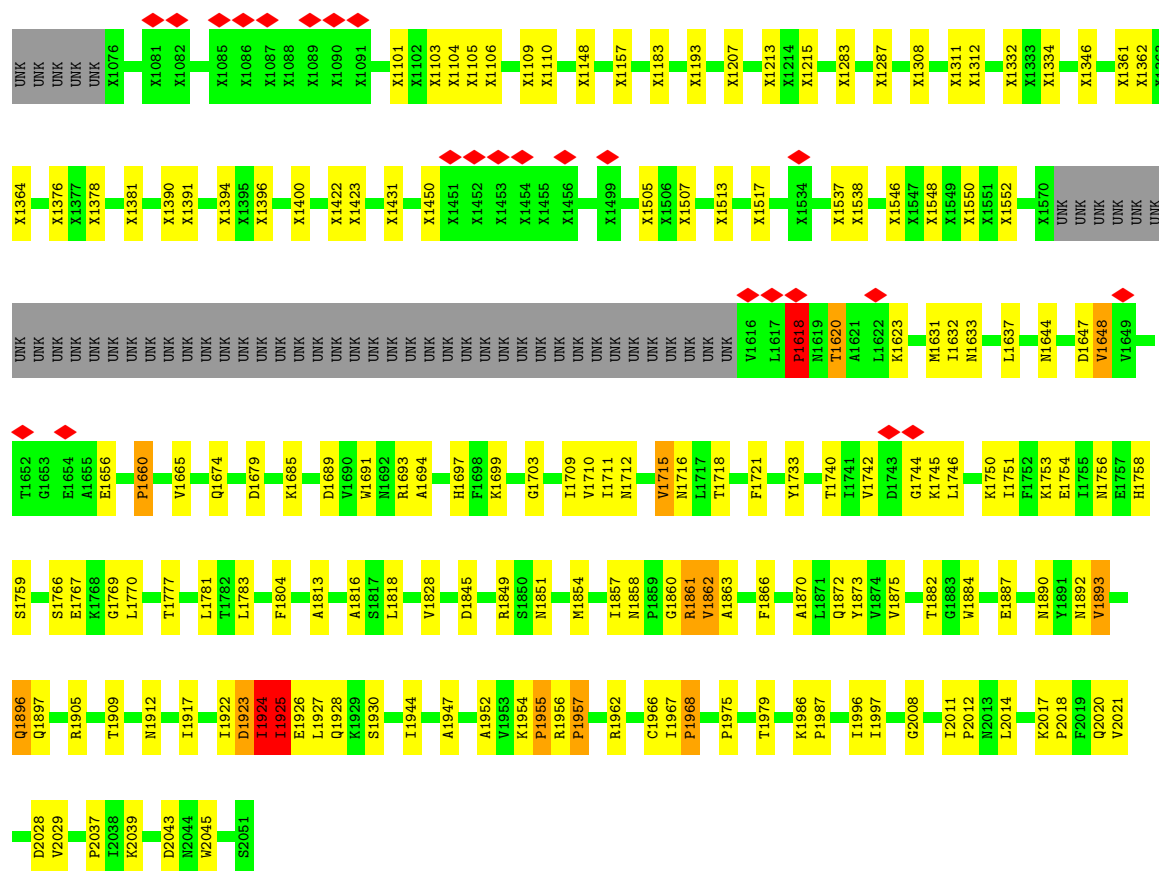
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	71	Total	C	N	O	S	0	0
			607	376	109	121	1		
3	H	71	Total	C	N	O	S	0	0
			607	376	109	121	1		
3	I	71	Total	C	N	O	S	0	0
			607	376	109	121	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

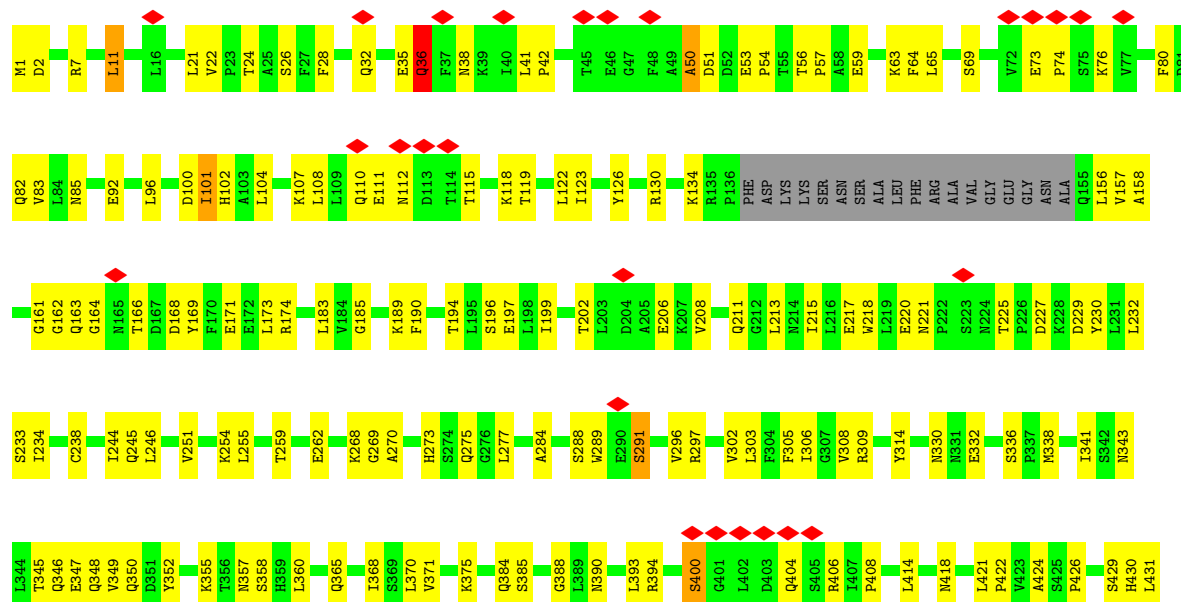
• Molecule 1: Fatty acid synthase subunit beta



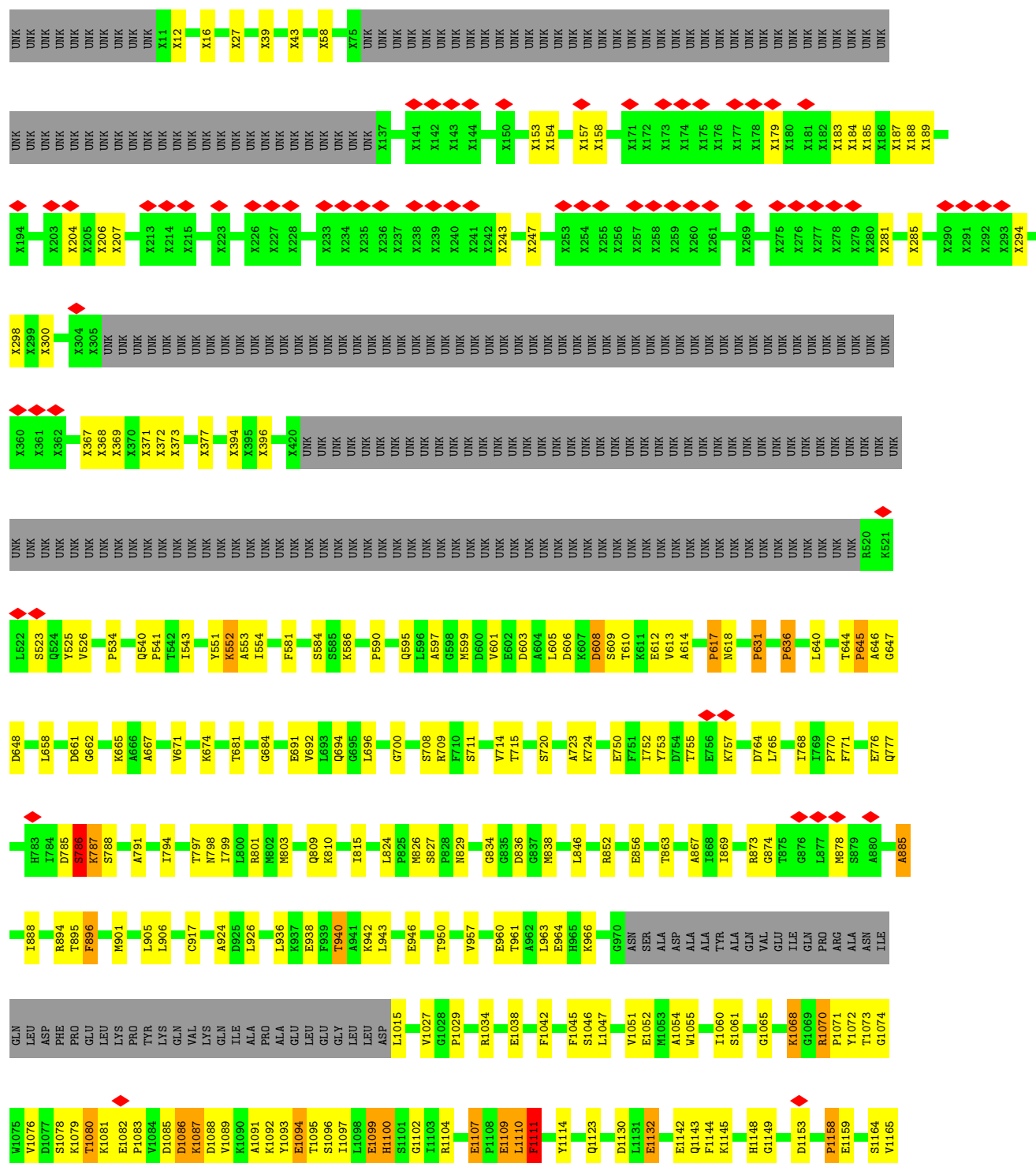


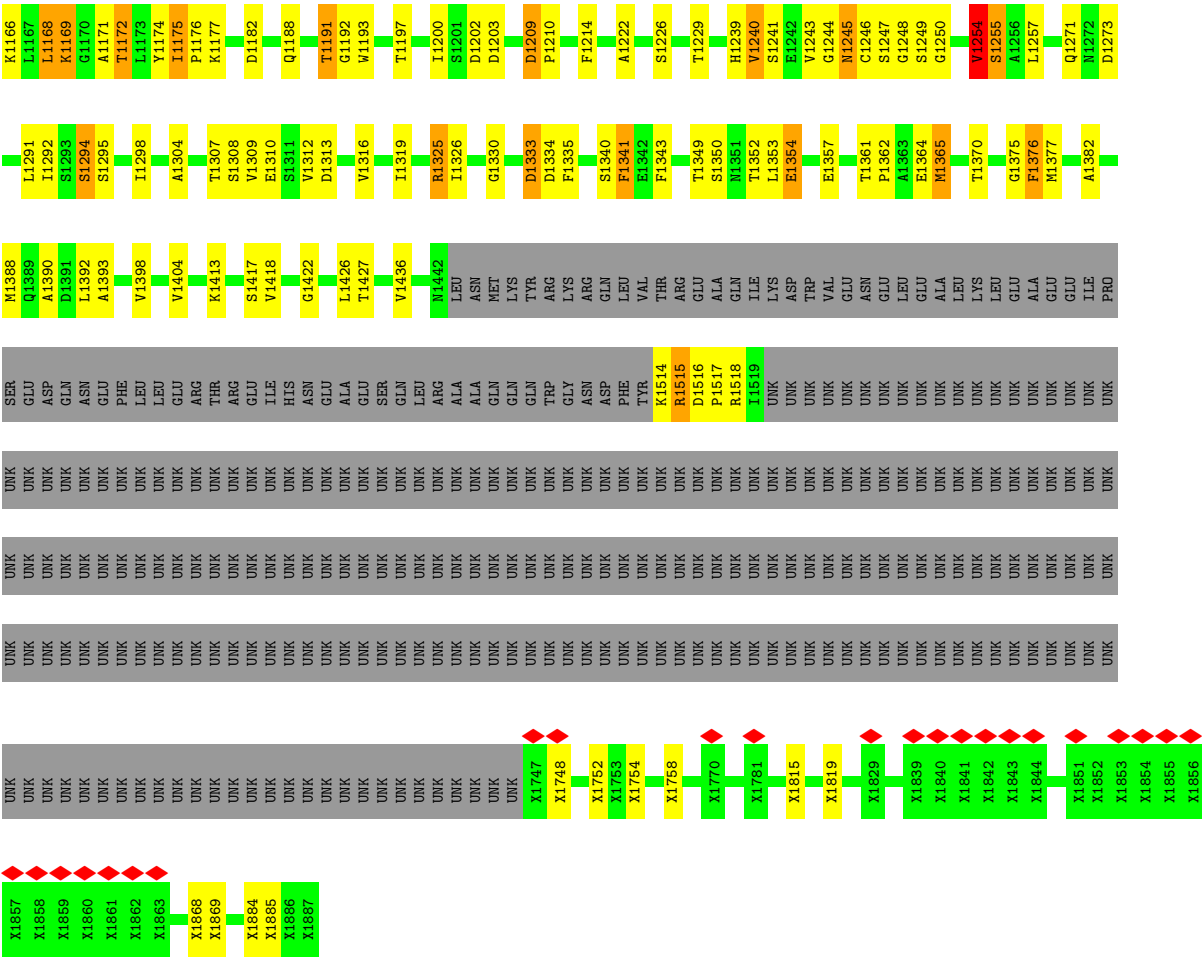
● Molecule 1: Fatty acid synthase subunit beta

Chain F: 73% 19% 7%

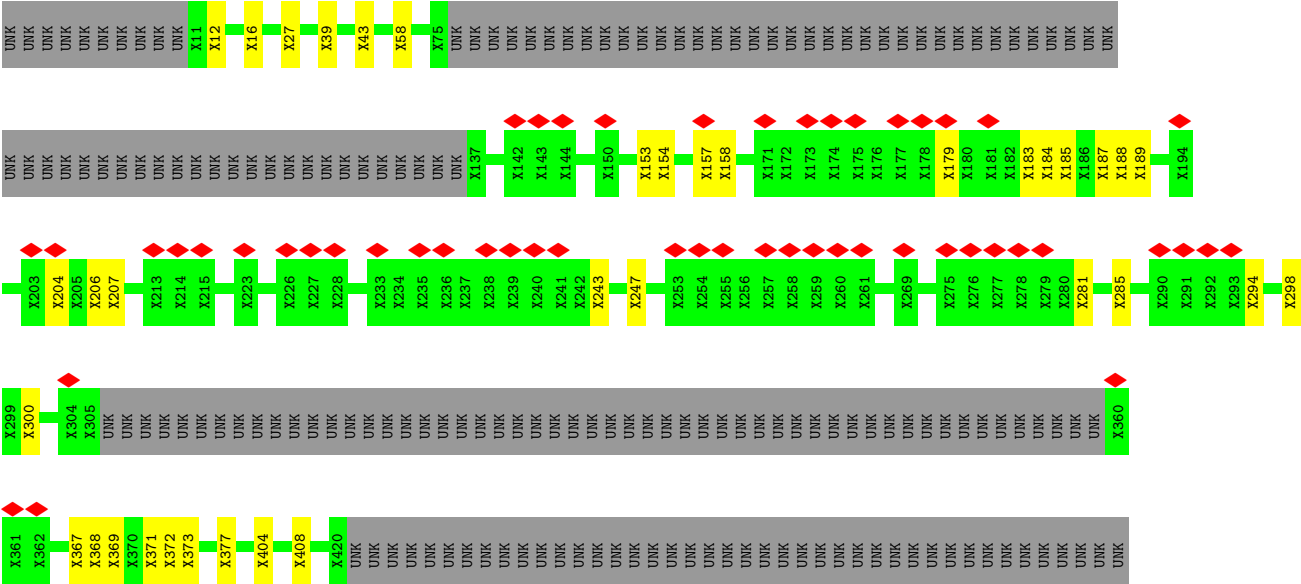


N1912	H1758	P1660	UNK	X1378	UNK	UNK	UNK	X669	F504	S429	I341	I234	L84
I1917	S1759	V1665	UNK	X1381	UNK	UNK	UNK	X677	G507	H430	S942	C238	N85
I1922	E1767	Q1674	UNK	X1390	UNK	UNK	UNK	X678	V514	L431	N343	Q244	E92
I1924	K1768	Q1674	UNK	X1391	UNK	UNK	UNK	X679	L515	L432	L344	Q245	L96
I1925	G1769	D1679	UNK	X1394	UNK	UNK	UNK	X682	L516	A435	T345	Q246	D100
E1926	L1770	K1682	UNK	X1395	UNK	UNK	UNK	X705	H517	I439	Q346	D167	I101
L1927	L1783	T1683	UNK	X1396	UNK	UNK	UNK	X705	H518	N440	Q347	Y169	H102
Q1928	F1804	S1684	UNK	X1400	UNK	UNK	UNK	X724	N519	D442	Q350	K254	A103
K1929	A1813	Q1688	UNK	X1422	UNK	UNK	UNK	X725	T523	K445	Y352	L255	L104
S1930	A1816	D1689	UNK	X1423	UNK	UNK	UNK	X726	R526	N446	N357	T259	K107
I1944	S1817	V1690	UNK	X1431	UNK	UNK	UNK	X727	V527	N447	L360	P260	L108
A1947	L1818	H1691	UNK	X1450	UNK	UNK	UNK	X728	T535	V448	L183	G261	L189
A1952	V1828	H1692	UNK	X1451	UNK	UNK	UNK	X729	N536	A452	Q365	L263	Q110
V1953	D1845	A1694	UNK	X1452	UNK	UNK	UNK	X732	P537	I455	T368	G185	E111
K1954	H1697	R1693	UNK	X1453	UNK	UNK	UNK	X754	D538	T455	S969	G189	N112
P1955	F1698	A1694	UNK	X1454	UNK	UNK	UNK	X764	D539	V459	L370	A270	D113
R1956	K1699	H1697	UNK	X1455	UNK	UNK	UNK	X768	B540	Y460	V371	T194	T114
P1957	S1850	F1698	UNK	X1456	UNK	UNK	UNK	X782	Y541	D461	K375	L195	T115
R1962	M1851	G1703	UNK	X1499	UNK	UNK	UNK	X787	K544	T462	K375	H273	K118
C1966	M1854	I1709	UNK	X1505	UNK	UNK	UNK	X788	V550	F463	Q384	S274	T119
I1967	T1857	V1710	UNK	X1506	UNK	UNK	UNK	X789	N558	G465	S385	Q275	K120
P1968	N1858	H1711	UNK	X1507	UNK	UNK	UNK	X799	P559	D467	Q388	L277	E121
P1975	P1859	N1712	UNK	X1513	UNK	UNK	UNK	X803	N560	R469	G388	A284	I123
G1860	G1860	V1715	UNK	X1517	UNK	UNK	UNK	X825	N561	R470	L389	S288	Y126
R1861	R1861	N1716	UNK	X1534	UNK	UNK	UNK	X836	Y566	L471	N390	E206	R130
V1862	L1717	L1717	UNK	X1537	UNK	UNK	UNK	X836	P567	S472	R394	E290	K134
A1863	T1718	T1718	UNK	X1538	UNK	UNK	UNK	X853	K568	G401	S400	S291	R135
F1866	F1721	F1721	UNK	X1546	UNK	UNK	UNK	X857	K571	L402	G401	V296	F136
A1870	R1728	R1728	UNK	X1547	UNK	UNK	UNK	X857	N572	D403	L402	Q211	PHE
Q1871	N1732	N1732	UNK	X1548	UNK	UNK	UNK	X857	K573	L303	D403	G212	ASP
Y1873	Y1733	Y1733	UNK	X1550	UNK	UNK	UNK	X857	S574	Q404	Q404	L213	LYS
T1740	T1740	T1740	UNK	X1551	UNK	UNK	UNK	X857	S574	S405	S405	L214	LYS
I1741	I1741	I1741	UNK	X1552	UNK	UNK	UNK	X857	S574	R406	R406	L215	SER
V1742	V1742	V1742	UNK	X1553	UNK	UNK	UNK	X857	S574	I407	I407	L216	SER
D1743	D1743	D1743	UNK	X1554	UNK	UNK	UNK	X857	S574	C482	C482	L217	ASN
G1744	G1744	G1744	UNK	X1555	UNK	UNK	UNK	X857	S574	I484	I484	L218	SER
K1745	K1745	K1745	UNK	X1556	UNK	UNK	UNK	X857	S574	R485	R485	L219	ALA
L1746	L1746	L1746	UNK	X1557	UNK	UNK	UNK	X857	S574	V488	V488	E220	LEU
K1750	K1750	K1750	UNK	X1570	UNK	UNK	UNK	X857	S574	K489	K489	N221	PHE
I1751	I1751	I1751	UNK	UNK	UNK	UNK	UNK	X857	S574	W490	W490	P222	ALA
F1752	F1752	F1752	UNK	UNK	UNK	UNK	UNK	X857	S574	E491	E491	S223	VAL
K1753	K1753	K1753	UNK	UNK	UNK	UNK	UNK	X857	S574	T492	T492	N224	GLY
E1754	E1754	E1754	UNK	UNK	UNK	UNK	UNK	X857	S574	Q495	Q495	T225	GLY
I1755	I1755	I1755	UNK	UNK	UNK	UNK	UNK	X857	S574	F496	F496	D227	ASN
N1756	N1756	N1756	UNK	UNK	UNK	UNK	UNK	X857	S574	K497	K497	K228	ALA
E1757	E1757	E1757	UNK	UNK	UNK	UNK	UNK	X857	S574	X639	X639	D229	ALA
E1656	E1656	E1656	UNK	UNK	UNK	UNK	UNK	X857	S574	X640	X640	Y230	L156
			UNK	UNK	UNK	UNK	UNK	UNK	UNK	X650	X650	L231	V157
			UNK	UNK	UNK	UNK	UNK	UNK	UNK	X654	X654	L232	A158
			UNK	UNK	UNK	UNK	UNK	UNK	UNK			S233	

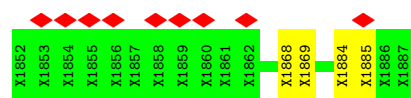




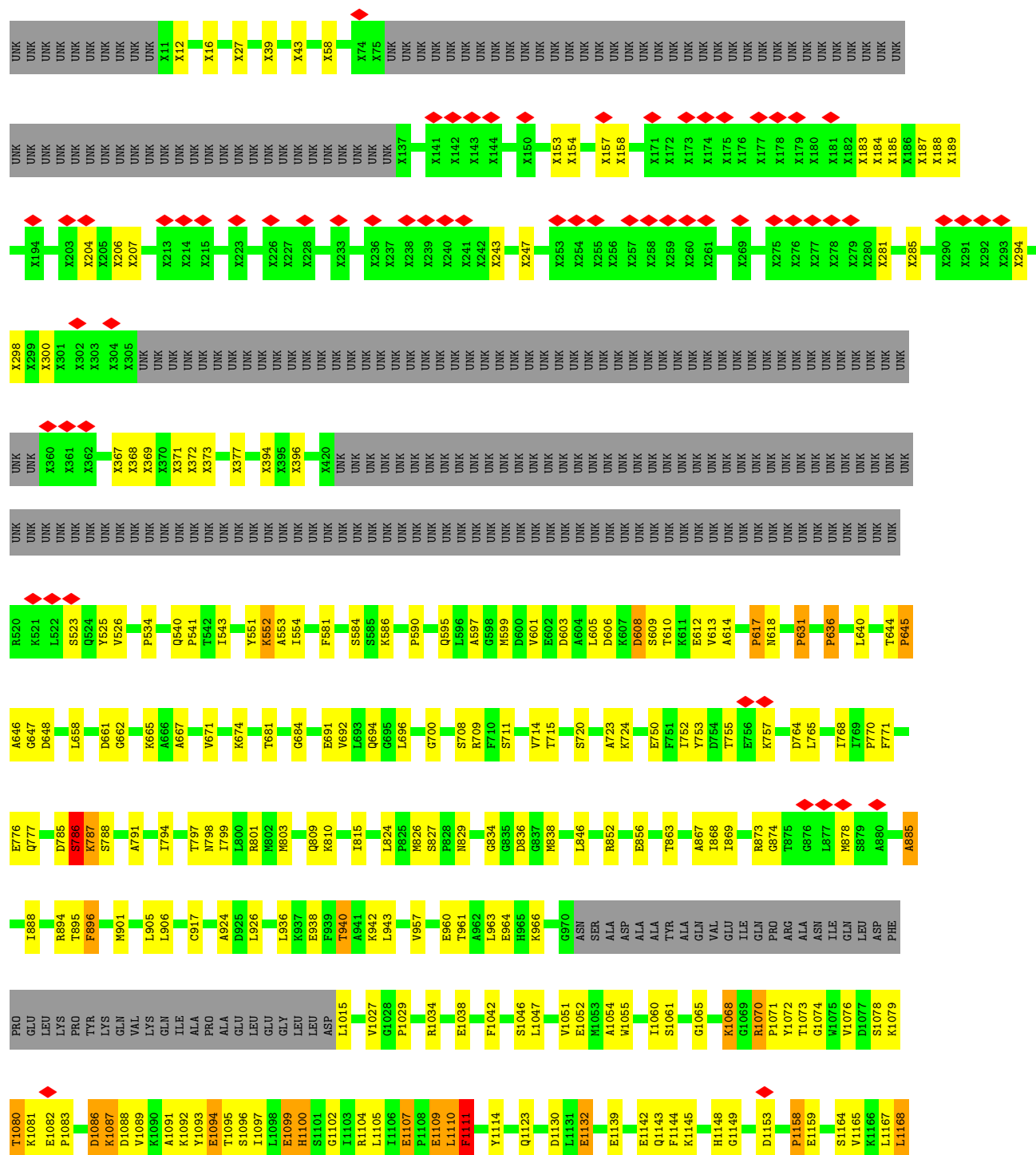
● Molecule 2: Fatty acid synthase subunit alpha

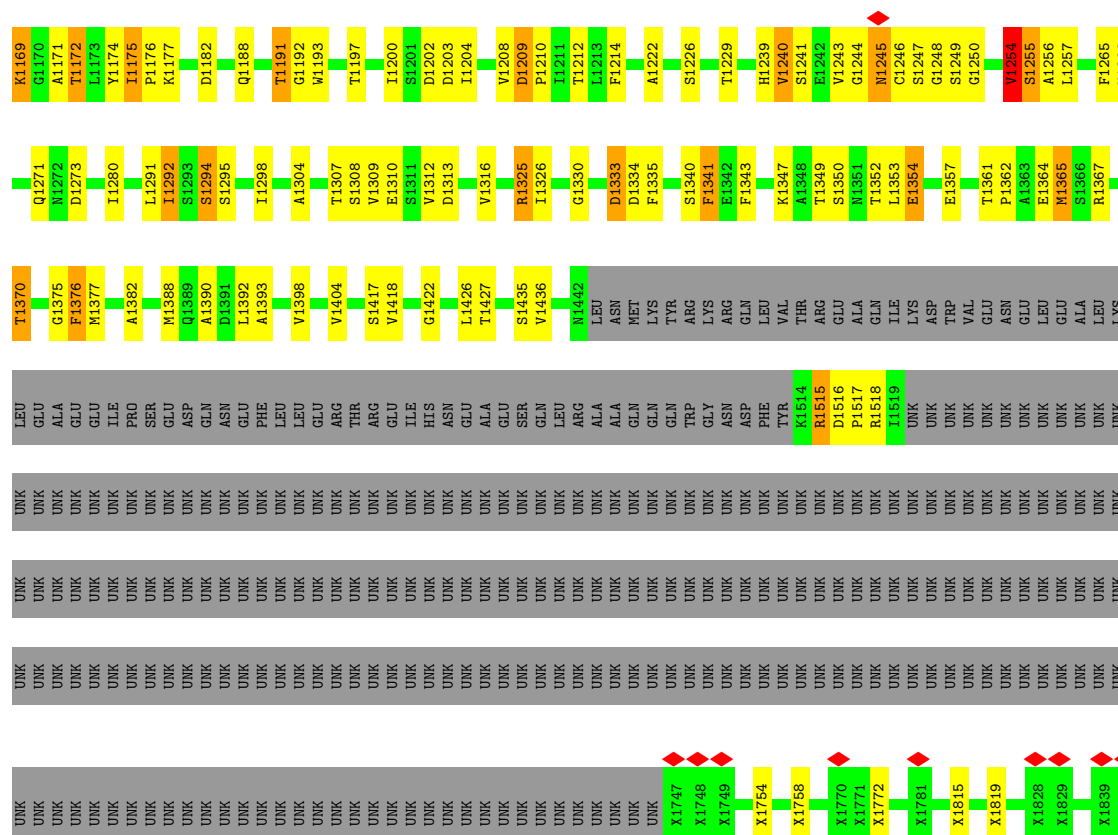






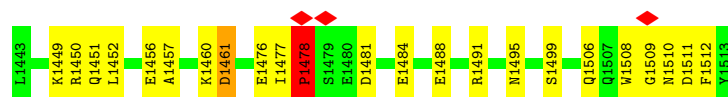
● Molecule 2: Fatty acid synthase subunit alpha





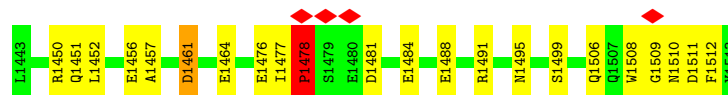
• Molecule 3: Fatty acid synthase subunit alpha

Chain C: 68% 30%



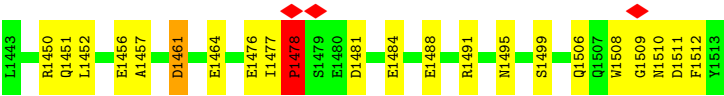
• Molecule 3: Fatty acid synthase subunit alpha

Chain H: 6% 69% 28%



• Molecule 3: Fatty acid synthase subunit alpha

Chain I: 69% 28%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	3692	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 ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.160	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0215	Depositor
Map size (Å)	453.6, 453.6, 453.6	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.40	0/7308	0.92	32/9952 (0.3%)
1	F	0.40	0/7308	0.92	32/9952 (0.3%)
1	G	0.40	0/7308	0.93	32/9952 (0.3%)
2	A	0.46	0/6518	1.03	35/8839 (0.4%)
2	D	0.46	0/6518	1.03	37/8839 (0.4%)
2	E	0.46	0/6518	1.03	35/8839 (0.4%)
3	C	0.38	0/616	0.88	4/828 (0.5%)
3	H	0.38	0/616	0.88	4/828 (0.5%)
3	I	0.38	0/616	0.88	4/828 (0.5%)
All	All	0.43	0/43326	0.97	215/58857 (0.4%)

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	B	0	19
1	F	0	19
1	G	0	19
2	A	0	26
2	D	0	27
2	E	0	27
3	C	0	2
3	H	0	2
3	I	0	2
All	All	0	143

There are no bond length outliers.

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1987	PRO	N-CA-CB	11.28	111.31	101.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1987	PRO	N-CA-CB	11.27	111.29	101.83
1	G	1987	PRO	N-CA-CB	11.24	111.28	101.83
1	B	1975	PRO	N-CA-CB	8.84	111.58	103.19
1	G	1975	PRO	N-CA-CB	8.83	111.58	103.19
1	F	1975	PRO	N-CA-CB	8.79	111.54	103.19
2	E	1169	LYS	N-CA-C	8.55	121.36	110.33
2	D	1169	LYS	N-CA-C	8.51	121.31	110.33
2	A	1169	LYS	N-CA-C	8.50	121.30	110.33
1	G	36	GLN	CA-CB-CG	8.18	130.45	114.10
1	F	36	GLN	CA-CB-CG	8.17	130.44	114.10
1	B	36	GLN	CA-CB-CG	8.16	130.41	114.10
2	A	645	PRO	N-CA-CB	7.75	111.39	103.25
2	E	645	PRO	N-CA-CB	7.73	111.36	103.25
2	D	645	PRO	N-CA-CB	7.68	111.32	103.25
2	D	541	PRO	N-CA-CB	7.57	109.91	103.17
2	A	541	PRO	N-CA-CB	7.56	109.90	103.17
1	B	1923	ASP	CA-C-N	7.54	135.53	121.97
1	B	1923	ASP	C-N-CA	7.54	135.53	121.97
1	G	1923	ASP	CA-C-N	7.54	135.53	121.97
1	G	1923	ASP	C-N-CA	7.54	135.53	121.97
2	E	541	PRO	N-CA-CB	7.54	109.88	103.17
1	F	1923	ASP	CA-C-N	7.53	135.52	121.97
1	F	1923	ASP	C-N-CA	7.53	135.52	121.97
1	B	559	PRO	N-CA-CB	7.52	111.14	103.25
1	G	1968	PRO	N-CA-CB	7.51	111.14	103.25
1	B	1968	PRO	N-CA-CB	7.51	111.13	103.25
1	G	559	PRO	N-CA-CB	7.50	111.12	103.25
1	F	559	PRO	N-CA-CB	7.48	111.11	103.25
1	F	1968	PRO	N-CA-CB	7.48	111.10	103.25
1	B	1957	PRO	N-CA-CB	7.34	110.96	103.25
1	F	1957	PRO	N-CA-CB	7.33	110.95	103.25
1	G	1957	PRO	N-CA-CB	7.31	110.93	103.25
2	A	636	PRO	N-CA-CB	7.30	110.92	103.25
1	F	2012	PRO	N-CA-CB	7.29	110.93	102.76
1	G	2012	PRO	N-CA-CB	7.28	110.92	102.76
2	E	636	PRO	N-CA-CB	7.28	110.89	103.25
2	D	636	PRO	N-CA-CB	7.27	110.88	103.25
1	B	1924	ILE	CA-C-N	7.25	135.03	121.97
1	B	1924	ILE	C-N-CA	7.25	135.03	121.97
1	G	1924	ILE	CA-C-N	7.25	135.02	121.97
1	G	1924	ILE	C-N-CA	7.25	135.02	121.97
1	B	2012	PRO	N-CA-CB	7.25	110.88	102.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1924	ILE	CA-C-N	7.23	134.99	121.97
1	F	1924	ILE	C-N-CA	7.23	134.99	121.97
1	F	476	SER	CA-C-N	7.17	135.24	121.54
1	F	476	SER	C-N-CA	7.17	135.24	121.54
1	G	2018	PRO	N-CA-CB	7.16	110.39	103.51
1	G	476	SER	CA-C-N	7.16	135.22	121.54
1	G	476	SER	C-N-CA	7.16	135.22	121.54
1	B	1857	ILE	CA-C-N	7.16	133.37	121.92
1	B	1857	ILE	C-N-CA	7.16	133.37	121.92
1	B	2018	PRO	N-CA-CB	7.15	110.38	103.51
1	F	1857	ILE	CA-C-N	7.14	133.35	121.92
1	F	1857	ILE	C-N-CA	7.14	133.35	121.92
1	G	1857	ILE	CA-C-N	7.14	133.35	121.92
1	G	1857	ILE	C-N-CA	7.14	133.35	121.92
1	F	2018	PRO	N-CA-CB	7.13	110.36	103.51
1	B	476	SER	CA-C-N	7.13	135.15	121.54
1	B	476	SER	C-N-CA	7.13	135.15	121.54
2	E	543	ILE	N-CA-C	-7.09	104.82	111.48
2	D	543	ILE	N-CA-C	-7.07	104.84	111.48
2	A	543	ILE	N-CA-C	-7.06	104.84	111.48
1	G	2014	LEU	N-CA-C	-7.02	103.78	114.16
1	B	2014	LEU	N-CA-C	-7.01	103.79	114.16
2	A	590	PRO	N-CA-CB	7.00	110.60	102.33
1	F	2014	LEU	N-CA-C	-7.00	103.79	114.16
1	G	1618	PRO	N-CA-CB	6.99	110.59	103.25
1	F	1618	PRO	N-CA-CB	6.99	110.58	103.25
1	B	1618	PRO	N-CA-CB	6.97	110.57	103.25
2	E	590	PRO	N-CA-CB	6.97	110.56	102.33
2	D	590	PRO	N-CA-CB	6.97	110.56	102.33
1	B	2037	PRO	N-CA-CB	6.85	110.78	103.52
1	G	2037	PRO	N-CA-CB	6.84	110.77	103.52
1	G	1955	PRO	N-CA-CB	6.83	110.42	103.25
1	B	1955	PRO	N-CA-CB	6.82	110.41	103.25
1	F	2037	PRO	N-CA-CB	6.81	110.74	103.52
1	B	1660	PRO	N-CA-CB	6.80	110.39	103.25
1	G	1660	PRO	N-CA-CB	6.79	110.38	103.25
1	F	1955	PRO	N-CA-CB	6.79	110.38	103.25
1	F	1660	PRO	N-CA-CB	6.77	110.36	103.25
2	D	1240	VAL	N-CA-C	-6.77	104.73	111.77
2	E	1240	VAL	N-CA-C	-6.74	104.76	111.77
2	A	1240	VAL	N-CA-C	-6.73	104.77	111.77
2	A	1370	THR	CA-C-N	6.65	134.24	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1370	THR	C-N-CA	6.65	134.24	121.54
2	D	1158	PRO	CA-C-N	6.64	134.22	121.54
2	D	1158	PRO	C-N-CA	6.64	134.22	121.54
2	D	1370	THR	CA-C-N	6.63	134.20	121.54
2	D	1370	THR	C-N-CA	6.63	134.20	121.54
2	E	1158	PRO	CA-C-N	6.62	134.19	121.54
2	E	1158	PRO	C-N-CA	6.62	134.19	121.54
2	A	1158	PRO	CA-C-N	6.62	134.19	121.54
2	A	1158	PRO	C-N-CA	6.62	134.19	121.54
2	D	1191	THR	N-CA-C	6.62	116.73	108.19
2	E	1370	THR	CA-C-N	6.62	134.18	121.54
2	E	1370	THR	C-N-CA	6.62	134.18	121.54
2	A	1191	THR	N-CA-C	6.61	116.72	108.19
2	E	1191	THR	N-CA-C	6.58	116.68	108.19
2	D	534	PRO	N-CA-CB	6.55	110.46	103.52
2	E	534	PRO	N-CA-CB	6.55	110.46	103.52
2	A	534	PRO	N-CA-CB	6.54	110.45	103.52
2	D	1245	ASN	N-CA-C	6.40	118.58	110.33
2	A	1245	ASN	N-CA-C	6.39	118.57	110.33
2	A	631	PRO	N-CA-CB	6.38	109.95	103.25
2	E	1245	ASN	N-CA-C	6.38	118.56	110.33
2	D	631	PRO	N-CA-CB	6.36	109.93	103.25
1	B	36	GLN	CB-CG-CD	6.36	123.41	112.60
1	F	36	GLN	CB-CG-CD	6.36	123.41	112.60
2	A	1398	VAL	CA-C-N	6.35	142.24	127.00
2	A	1398	VAL	C-N-CA	6.35	142.24	127.00
1	G	36	GLN	CB-CG-CD	6.35	123.39	112.60
2	E	1398	VAL	CA-C-N	6.35	142.24	127.00
2	E	1398	VAL	C-N-CA	6.35	142.24	127.00
2	E	631	PRO	N-CA-CB	6.33	109.89	103.25
2	D	1398	VAL	CA-C-N	6.32	142.16	127.00
2	D	1398	VAL	C-N-CA	6.32	142.16	127.00
2	D	1304	ALA	CA-C-N	6.27	133.52	121.54
2	D	1304	ALA	C-N-CA	6.27	133.52	121.54
1	F	1623	LYS	N-CA-C	6.26	117.73	108.60
1	G	1623	LYS	N-CA-C	6.21	117.67	108.60
1	B	1623	LYS	N-CA-C	6.21	117.67	108.60
2	E	1175	ILE	CA-C-N	6.19	141.86	127.00
2	E	1175	ILE	C-N-CA	6.19	141.86	127.00
2	A	1175	ILE	CA-C-N	6.18	141.83	127.00
2	A	1175	ILE	C-N-CA	6.18	141.83	127.00
3	H	1476	GLU	CA-C-N	6.18	133.56	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1476	GLU	C-N-CA	6.18	133.56	122.13
2	D	1175	ILE	CA-C-N	6.18	141.82	127.00
2	D	1175	ILE	C-N-CA	6.18	141.82	127.00
3	C	1476	GLU	CA-C-N	6.15	133.51	122.13
3	C	1476	GLU	C-N-CA	6.15	133.51	122.13
2	A	617	PRO	N-CA-CB	6.15	109.71	103.25
3	I	1476	GLU	CA-C-N	6.15	133.51	122.13
3	I	1476	GLU	C-N-CA	6.15	133.51	122.13
2	E	617	PRO	N-CA-CB	6.11	109.67	103.25
2	E	1376	PHE	CA-C-N	6.11	133.21	121.54
2	E	1376	PHE	C-N-CA	6.11	133.21	121.54
2	A	1376	PHE	CA-C-N	6.10	133.19	121.54
2	A	1376	PHE	C-N-CA	6.10	133.19	121.54
2	D	617	PRO	N-CA-CB	6.08	109.64	103.25
2	D	1376	PHE	CA-C-N	6.08	133.16	121.54
2	D	1376	PHE	C-N-CA	6.08	133.16	121.54
2	E	551	TYR	N-CA-C	-6.00	105.79	113.23
2	A	551	TYR	N-CA-C	-5.98	105.82	113.23
2	D	551	TYR	N-CA-C	-5.97	105.83	113.23
3	H	1478	PRO	CA-C-N	5.95	132.91	121.54
3	H	1478	PRO	C-N-CA	5.95	132.91	121.54
3	C	1478	PRO	CA-C-N	5.94	132.88	121.54
3	C	1478	PRO	C-N-CA	5.94	132.88	121.54
3	I	1478	PRO	CA-C-N	5.92	132.85	121.54
3	I	1478	PRO	C-N-CA	5.92	132.85	121.54
1	G	472	SER	N-CA-C	-5.91	105.38	112.58
1	F	472	SER	N-CA-C	-5.90	105.38	112.58
1	F	1925	ILE	N-CA-C	5.90	121.61	109.34
1	B	1925	ILE	N-CA-C	5.89	121.59	109.34
1	G	1925	ILE	N-CA-C	5.88	121.58	109.34
1	B	472	SER	N-CA-C	-5.87	105.42	112.58
2	E	1175	ILE	C-N-CD	-5.77	107.90	120.60
2	A	1175	ILE	C-N-CD	-5.77	107.91	120.60
2	D	1175	ILE	C-N-CD	-5.75	107.94	120.60
1	B	406	ARG	CA-CB-CG	5.75	125.60	114.10
1	G	1620	THR	N-CA-C	5.73	116.79	107.23
1	F	406	ARG	CA-CB-CG	5.72	125.55	114.10
1	B	1620	THR	N-CA-C	5.72	116.78	107.23
1	F	1620	THR	N-CA-C	5.72	116.78	107.23
1	G	406	ARG	CA-CB-CG	5.72	125.54	114.10
1	B	1861	ARG	CA-C-N	5.54	131.94	121.97
1	B	1861	ARG	C-N-CA	5.54	131.94	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1861	ARG	CA-C-N	5.53	131.92	121.97
1	G	1861	ARG	C-N-CA	5.53	131.92	121.97
1	F	1861	ARG	CA-C-N	5.51	131.89	121.97
1	F	1861	ARG	C-N-CA	5.51	131.89	121.97
2	A	1093	TYR	CA-C-N	5.49	132.03	121.54
2	A	1093	TYR	C-N-CA	5.49	132.03	121.54
2	E	1093	TYR	CA-C-N	5.46	131.97	121.54
2	E	1093	TYR	C-N-CA	5.46	131.97	121.54
2	D	1093	TYR	CA-C-N	5.45	131.95	121.54
2	D	1093	TYR	C-N-CA	5.45	131.95	121.54
1	B	233	SER	CA-C-N	5.37	124.63	120.33
1	B	233	SER	C-N-CA	5.37	124.63	120.33
2	E	1109	GLU	CA-C-N	5.37	131.79	121.54
2	E	1109	GLU	C-N-CA	5.37	131.79	121.54
2	A	1109	GLU	CA-C-N	5.36	131.78	121.54
2	A	1109	GLU	C-N-CA	5.36	131.78	121.54
2	D	1109	GLU	CA-C-N	5.35	131.76	121.54
2	D	1109	GLU	C-N-CA	5.35	131.76	121.54
1	G	233	SER	CA-C-N	5.35	124.61	120.33
1	G	233	SER	C-N-CA	5.35	124.61	120.33
2	A	1110	LEU	CA-C-N	5.29	131.64	121.54
2	A	1110	LEU	C-N-CA	5.29	131.64	121.54
2	E	1110	LEU	CA-C-N	5.28	131.63	121.54
2	E	1110	LEU	C-N-CA	5.28	131.63	121.54
2	D	1110	LEU	CA-C-N	5.27	131.61	121.54
2	D	1110	LEU	C-N-CA	5.27	131.61	121.54
1	F	233	SER	CA-C-N	5.27	124.55	120.33
1	F	233	SER	C-N-CA	5.27	124.55	120.33
2	A	1398	VAL	C-N-CD	-5.21	109.14	120.60
2	E	1398	VAL	C-N-CD	-5.20	109.15	120.60
1	F	567	PRO	N-CA-CB	5.18	110.25	103.42
2	D	1398	VAL	C-N-CD	-5.17	109.22	120.60
1	G	567	PRO	N-CA-CB	5.16	110.23	103.42
1	B	567	PRO	N-CA-CB	5.13	110.20	103.42
2	A	1202	ASP	CA-C-N	5.05	131.18	121.54
2	A	1202	ASP	C-N-CA	5.05	131.18	121.54
2	E	1174	TYR	N-CA-C	5.05	118.35	111.39
2	D	1202	ASP	CA-C-N	5.04	131.16	121.54
2	D	1202	ASP	C-N-CA	5.04	131.16	121.54
2	E	1202	ASP	CA-C-N	5.04	131.16	121.54
2	E	1202	ASP	C-N-CA	5.04	131.16	121.54
2	E	1175	ILE	N-CA-C	-5.03	98.01	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1175	ILE	N-CA-C	-5.03	98.02	108.88
2	A	1174	TYR	N-CA-C	5.02	118.32	111.39
2	D	1175	ILE	N-CA-C	-5.01	98.06	108.88
2	D	1174	TYR	N-CA-C	5.01	118.30	111.39

There are no chirality outliers.

All (143) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1046	SER	Peptide
2	A	1070	ARG	Peptide
2	A	1082	GLU	Peptide
2	A	1086	ASP	Peptide
2	A	1087	LYS	Peptide
2	A	1094	GLU	Peptide
2	A	1099	GLU	Peptide
2	A	1107	GLU	Peptide
2	A	1110	LEU	Peptide
2	A	1111	PHE	Peptide
2	A	1132	GLU	Peptide
2	A	1168	LEU	Peptide
2	A	1171	ALA	Peptide
2	A	1177	LYS	Peptide
2	A	1203	ASP	Peptide
2	A	1209	ASP	Peptide
2	A	1244	GLY	Peptide
2	A	1254	VAL	Peptide
2	A	1325	ARG	Peptide
2	A	1341	PHE	Peptide
2	A	1354	GLU	Peptide
2	A	1422	GLY	Peptide
2	A	1515	ARG	Peptide
2	A	684	GLY	Peptide
2	A	786	SER	Peptide
2	A	896	PHE	Peptide
1	B	11	LEU	Peptide
1	B	1207	UNK	Peptide
1	B	1715	VAL	Peptide
1	B	1746	LEU	Peptide
1	B	1756	ASN	Peptide
1	B	1858	ASN	Peptide
1	B	1861	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	1862	VAL	Peptide
1	B	1896	GLN	Peptide
1	B	1912	ASN	Peptide
1	B	1922	ILE	Peptide
1	B	1924	ILE	Peptide
1	B	446	ASN	Peptide
1	B	471	LEU	Peptide
1	B	484	ILE	Peptide
1	B	485	ARG	Peptide
1	B	50	ALA	Peptide
1	B	74	PRO	Peptide
1	B	76	LYS	Peptide
3	C	1477	ILE	Peptide
3	C	1478	PRO	Peptide
2	D	1046	SER	Peptide
2	D	1070	ARG	Peptide
2	D	1082	GLU	Peptide
2	D	1086	ASP	Peptide
2	D	1087	LYS	Peptide
2	D	1094	GLU	Peptide
2	D	1099	GLU	Peptide
2	D	1107	GLU	Peptide
2	D	1110	LEU	Peptide
2	D	1111	PHE	Peptide
2	D	1132	GLU	Peptide
2	D	1168	LEU	Peptide
2	D	1171	ALA	Peptide
2	D	1177	LYS	Peptide
2	D	1203	ASP	Peptide
2	D	1209	ASP	Peptide
2	D	1244	GLY	Peptide
2	D	1254	VAL	Peptide
2	D	1292	ILE	Peptide
2	D	1325	ARG	Peptide
2	D	1341	PHE	Peptide
2	D	1354	GLU	Peptide
2	D	1422	GLY	Peptide
2	D	1515	ARG	Peptide
2	D	684	GLY	Peptide
2	D	786	SER	Peptide
2	D	896	PHE	Peptide
2	E	1046	SER	Peptide

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Mol	Chain	Res	Type	Group
2	E	1070	ARG	Peptide
2	E	1082	GLU	Peptide
2	E	1086	ASP	Peptide
2	E	1087	LYS	Peptide
2	E	1094	GLU	Peptide
2	E	1099	GLU	Peptide
2	E	1107	GLU	Peptide
2	E	1110	LEU	Peptide
2	E	1111	PHE	Peptide
2	E	1132	GLU	Peptide
2	E	1168	LEU	Peptide
2	E	1171	ALA	Peptide
2	E	1177	LYS	Peptide
2	E	1203	ASP	Peptide
2	E	1209	ASP	Peptide
2	E	1244	GLY	Peptide
2	E	1254	VAL	Peptide
2	E	1292	ILE	Peptide
2	E	1325	ARG	Peptide
2	E	1341	PHE	Peptide
2	E	1354	GLU	Peptide
2	E	1422	GLY	Peptide
2	E	1515	ARG	Peptide
2	E	684	GLY	Peptide
2	E	786	SER	Peptide
2	E	896	PHE	Peptide
1	F	11	LEU	Peptide
1	F	1207	UNK	Peptide
1	F	1715	VAL	Peptide
1	F	1746	LEU	Peptide
1	F	1756	ASN	Peptide
1	F	1858	ASN	Peptide
1	F	1861	ARG	Peptide
1	F	1862	VAL	Peptide
1	F	1896	GLN	Peptide
1	F	1912	ASN	Peptide
1	F	1922	ILE	Peptide
1	F	1924	ILE	Peptide
1	F	446	ASN	Peptide
1	F	471	LEU	Peptide
1	F	484	ILE	Peptide
1	F	485	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	F	50	ALA	Peptide
1	F	74	PRO	Peptide
1	F	76	LYS	Peptide
1	G	11	LEU	Peptide
1	G	1207	UNK	Peptide
1	G	1715	VAL	Peptide
1	G	1746	LEU	Peptide
1	G	1756	ASN	Peptide
1	G	1858	ASN	Peptide
1	G	1861	ARG	Peptide
1	G	1862	VAL	Peptide
1	G	1896	GLN	Peptide
1	G	1912	ASN	Peptide
1	G	1922	ILE	Peptide
1	G	1924	ILE	Peptide
1	G	446	ASN	Peptide
1	G	471	LEU	Peptide
1	G	484	ILE	Peptide
1	G	485	ARG	Peptide
1	G	50	ALA	Peptide
1	G	74	PRO	Peptide
1	G	76	LYS	Peptide
3	H	1477	ILE	Peptide
3	H	1478	PRO	Peptide
3	I	1477	ILE	Peptide
3	I	1478	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	11746	0	7740	206	0
1	F	11746	0	7741	214	0
1	G	11746	0	7742	208	0
2	A	8587	0	6479	166	0
2	D	8587	0	6479	164	0
2	E	8587	0	6479	169	0
3	C	607	0	580	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	607	0	580	11	0
3	I	607	0	580	11	0
All	All	62820	0	44400	1154	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 11.

All (1154) 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)
1:F:163:GLN:HG2	1:F:275:GLN:HG3	1.74	0.70
1:F:238:CYS:HB2	1:F:303:LEU:HD12	1.74	0.69
1:G:163:GLN:HG2	1:G:275:GLN:HG3	1.74	0.69
1:B:163:GLN:HG2	1:B:275:GLN:HG3	1.74	0.68
1:B:238:CYS:HB2	1:B:303:LEU:HD12	1.74	0.68
1:G:238:CYS:HB2	1:G:303:LEU:HD12	1.74	0.68
1:B:32:GLN:HA	1:B:35:GLU:HB2	1.79	0.65
1:B:1863:ALA:HA	1:B:1866:PHE:HB2	1.78	0.65
1:G:1863:ALA:HA	1:G:1866:PHE:HB2	1.78	0.65
2:A:894:ARG:HE	2:A:895:THR:H	1.45	0.64
1:G:32:GLN:HA	1:G:35:GLU:HB2	1.79	0.64
2:D:1254:VAL:HG23	2:D:1257:LEU:HB3	1.80	0.64
2:E:963:LEU:HA	2:E:966:LYS:HG2	1.80	0.64
2:E:1175:ILE:HG12	2:E:1176:PRO:HA	1.79	0.64
2:E:1254:VAL:HG23	2:E:1257:LEU:HB3	1.80	0.64
2:A:1248:GLY:HA2	2:A:1330:GLY:HA3	1.79	0.64
1:F:32:GLN:HA	1:F:35:GLU:HB2	1.79	0.64
1:F:1863:ALA:HA	1:F:1866:PHE:HB2	1.78	0.64
2:D:1248:GLY:HA2	2:D:1330:GLY:HA3	1.79	0.64
2:D:963:LEU:HA	2:D:966:LYS:HG2	1.80	0.64
2:E:1248:GLY:HA2	2:E:1330:GLY:HA3	1.79	0.63
2:A:1175:ILE:HG12	2:A:1176:PRO:HA	1.80	0.63
2:E:894:ARG:HE	2:E:895:THR:H	1.45	0.63
2:D:894:ARG:HE	2:D:895:THR:H	1.45	0.63
2:D:1197:THR:HG23	2:D:1200:ILE:HG22	1.81	0.63
1:B:461:ASP:H	1:B:465:GLY:HA2	1.64	0.62
2:A:1254:VAL:HG23	2:A:1257:LEU:HB3	1.80	0.62
1:B:38:ASN:HA	1:B:41:LEU:HG	1.82	0.62
1:F:1860:GLY:H	1:F:1863:ALA:HB2	1.64	0.62
2:E:1197:THR:HG23	2:E:1200:ILE:HG22	1.81	0.62
2:A:963:LEU:HA	2:A:966:LYS:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1175:ILE:HG12	2:D:1176:PRO:HA	1.80	0.62
1:G:38:ASN:HA	1:G:41:LEU:HG	1.82	0.62
1:G:1860:GLY:H	1:G:1863:ALA:HB2	1.64	0.62
2:A:1197:THR:HG23	2:A:1200:ILE:HG22	1.81	0.62
1:F:461:ASP:H	1:F:465:GLY:HA2	1.64	0.62
1:F:479:ILE:HG13	1:F:480:VAL:HG12	1.82	0.62
1:G:479:ILE:HG13	1:G:480:VAL:HG12	1.82	0.62
1:G:1546:UNK:O	1:G:1550:UNK:N	2.33	0.61
3:I:1484:GLU:O	3:I:1488:GLU:N	2.33	0.61
1:F:1699:LYS:HA	1:F:1703:GLY:HA2	1.82	0.61
1:B:479:ILE:HG13	1:B:480:VAL:HG12	1.82	0.61
1:F:199:ILE:HG12	1:F:206:GLU:HG3	1.81	0.61
1:B:517:HIS:NE2	1:B:538:ASP:OD1	2.34	0.61
1:B:1699:LYS:HA	1:B:1703:GLY:HA2	1.82	0.61
3:H:1484:GLU:O	3:H:1488:GLU:N	2.33	0.61
1:B:199:ILE:HG12	1:B:206:GLU:HG3	1.81	0.61
1:B:1860:GLY:H	1:B:1863:ALA:HB2	1.64	0.61
2:A:1142:GLU:OE1	2:A:1143:GLN:NE2	2.33	0.61
2:A:863:THR:HG21	2:A:917:CYS:HB3	1.83	0.61
1:G:461:ASP:H	1:G:465:GLY:HA2	1.64	0.61
1:F:517:HIS:NE2	1:F:538:ASP:OD1	2.34	0.61
1:F:1546:UNK:O	1:F:1550:UNK:N	2.33	0.61
1:B:1546:UNK:O	1:B:1550:UNK:N	2.33	0.61
1:F:38:ASN:HA	1:F:41:LEU:HG	1.81	0.61
1:G:199:ILE:HG12	1:G:206:GLU:HG3	1.81	0.61
3:C:1484:GLU:O	3:C:1488:GLU:N	2.33	0.61
1:G:1699:LYS:HA	1:G:1703:GLY:HA2	1.82	0.61
2:D:1142:GLU:OE1	2:D:1143:GLN:NE2	2.34	0.60
2:E:1142:GLU:OE1	2:E:1143:GLN:NE2	2.34	0.60
1:G:517:HIS:NE2	1:G:538:ASP:OD1	2.34	0.60
2:E:863:THR:HG21	2:E:917:CYS:HB3	1.83	0.60
1:F:126:TYR:OH	1:F:130:ARG:NH1	2.35	0.60
1:G:126:TYR:OH	1:G:130:ARG:NH1	2.35	0.60
1:G:1718:THR:HB	1:G:1770:LEU:HD22	1.83	0.60
1:B:126:TYR:OH	1:B:130:ARG:NH1	2.35	0.60
2:D:863:THR:HG21	2:D:917:CYS:HB3	1.83	0.60
2:D:281:UNK:O	2:D:285:UNK:N	2.35	0.59
1:F:157:VAL:HB	1:F:501:ILE:HG12	1.84	0.59
1:B:157:VAL:HB	1:B:501:ILE:HG12	1.84	0.59
2:A:281:UNK:O	2:A:285:UNK:N	2.35	0.59
2:A:1271:GLN:NE2	2:A:1273:ASP:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1271:GLN:NE2	2:E:1273:ASP:O	2.36	0.59
2:E:1312:VAL:O	2:E:1316:VAL:N	2.35	0.59
1:F:1718:THR:HB	1:F:1770:LEU:HD22	1.83	0.59
2:E:281:UNK:O	2:E:285:UNK:N	2.35	0.59
1:B:259:THR:HG23	1:B:262:GLU:H	1.67	0.59
1:B:157:VAL:HG13	1:B:269:GLY:HA3	1.84	0.59
2:A:750:GLU:OE2	2:A:809:GLN:NE2	2.36	0.59
1:F:157:VAL:HG13	1:F:269:GLY:HA3	1.84	0.59
1:F:259:THR:HG23	1:F:262:GLU:H	1.67	0.59
1:G:259:THR:HG23	1:G:262:GLU:H	1.67	0.59
1:G:246:LEU:HD11	1:G:296:VAL:HG22	1.85	0.59
1:B:1718:THR:HB	1:B:1770:LEU:HD22	1.84	0.58
1:G:345:THR:OG1	1:G:348:GLN:NE2	2.36	0.58
2:E:1307:THR:OG1	2:E:1308:SER:N	2.35	0.58
1:F:1882:THR:HA	1:F:1893:VAL:HA	1.85	0.58
2:A:1307:THR:OG1	2:A:1308:SER:N	2.35	0.58
1:F:345:THR:OG1	1:F:348:GLN:NE2	2.36	0.58
2:E:1436:VAL:O	2:E:1518:ARG:NH1	2.36	0.58
2:A:1436:VAL:O	2:A:1518:ARG:NH1	2.36	0.58
1:F:440:ASN:ND2	1:F:477:GLU:OE1	2.36	0.58
2:D:1307:THR:OG1	2:D:1308:SER:N	2.35	0.58
1:G:157:VAL:HB	1:G:501:ILE:HG12	1.84	0.58
1:B:343:ASN:HA	1:B:375:LYS:HB3	1.86	0.58
2:E:1868:UNK:HA	2:E:1885:UNK:HA	1.85	0.58
2:D:1094:GLU:H	2:D:1097:ILE:HG22	1.69	0.58
2:E:750:GLU:OE2	2:E:809:GLN:NE2	2.36	0.58
2:D:1271:GLN:NE2	2:D:1273:ASP:O	2.36	0.58
2:A:1294:SER:OG	2:A:1295:SER:N	2.36	0.58
2:A:1868:UNK:HA	2:A:1885:UNK:HA	1.85	0.58
1:G:1742:VAL:HG22	1:G:1744:GLY:H	1.69	0.58
1:B:330:ASN:ND2	1:B:332:GLU:OE2	2.37	0.58
1:B:345:THR:OG1	1:B:348:GLN:NE2	2.36	0.58
1:F:246:LEU:HD11	1:F:296:VAL:HG22	1.86	0.58
1:G:440:ASN:ND2	1:G:477:GLU:OE1	2.36	0.58
1:F:59:GLU:O	1:F:63:LYS:N	2.36	0.57
2:D:1436:VAL:O	2:D:1518:ARG:NH1	2.36	0.57
1:G:467:ASP:OD2	1:G:469:ARG:NH2	2.37	0.57
1:B:246:LEU:HD11	1:B:296:VAL:HG22	1.86	0.57
1:B:440:ASN:ND2	1:B:477:GLU:OE1	2.36	0.57
1:F:1715:VAL:HA	1:F:1769:GLY:HA2	1.86	0.57
2:D:1312:VAL:O	2:D:1316:VAL:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1390:UNK:O	1:B:1423:UNK:N	2.37	0.57
2:D:1868:UNK:HA	2:D:1885:UNK:HA	1.85	0.57
1:G:1715:VAL:HA	1:G:1769:GLY:HA2	1.86	0.57
1:G:1882:THR:HA	1:G:1893:VAL:HA	1.85	0.57
1:B:1715:VAL:HA	1:B:1769:GLY:HA2	1.86	0.57
2:A:1094:GLU:H	2:A:1097:ILE:HG22	1.69	0.57
1:G:157:VAL:HG13	1:G:269:GLY:HA3	1.84	0.57
1:G:1390:UNK:O	1:G:1423:UNK:N	2.37	0.57
2:E:826:MET:HE1	2:E:846:LEU:HB2	1.85	0.57
1:B:1750:LYS:O	1:B:1753:LYS:NZ	2.37	0.57
1:B:1882:THR:HA	1:B:1893:VAL:HA	1.85	0.57
1:F:1390:UNK:O	1:F:1423:UNK:N	2.37	0.57
2:D:826:MET:HE1	2:D:846:LEU:HB2	1.85	0.57
2:A:826:MET:HE1	2:A:846:LEU:HB2	1.85	0.57
1:F:1742:VAL:HG22	1:F:1744:GLY:H	1.69	0.57
1:G:1740:THR:HB	1:G:1751:ILE:HD12	1.87	0.57
2:E:1094:GLU:H	2:E:1097:ILE:HG22	1.69	0.57
1:B:678:UNK:O	1:B:682:UNK:N	2.38	0.57
1:F:343:ASN:HA	1:F:375:LYS:HB3	1.86	0.57
1:F:1740:THR:HB	1:F:1751:ILE:HD12	1.87	0.57
1:B:59:GLU:O	1:B:63:LYS:N	2.36	0.57
1:B:232:LEU:HD21	1:B:422:PRO:HB2	1.87	0.57
1:F:330:ASN:ND2	1:F:332:GLU:OE2	2.37	0.57
1:F:467:ASP:OD2	1:F:469:ARG:NH2	2.37	0.57
2:E:852:ARG:NH1	2:E:856:GLU:OE1	2.38	0.57
1:B:467:ASP:OD2	1:B:469:ARG:NH2	2.37	0.56
2:A:1312:VAL:O	2:A:1316:VAL:N	2.35	0.56
1:G:1:MET:N	1:G:11:LEU:O	2.38	0.56
1:G:343:ASN:HA	1:G:375:LYS:HB3	1.86	0.56
1:B:1538:UNK:O	1:B:1618:PRO:N	2.39	0.56
1:G:400:SER:O	1:G:400:SER:OG	2.23	0.56
1:G:678:UNK:O	1:G:682:UNK:N	2.38	0.56
1:G:1422:UNK:O	1:G:1450:UNK:N	2.38	0.56
2:E:1034:ARG:NH2	2:E:1052:GLU:OE2	2.39	0.56
1:B:1422:UNK:O	1:B:1450:UNK:N	2.38	0.56
1:B:1740:THR:HB	1:B:1751:ILE:HD12	1.87	0.56
1:B:1742:VAL:HG22	1:B:1744:GLY:H	1.69	0.56
1:F:442:ASP:HA	1:F:445:LYS:HD2	1.88	0.56
1:F:1422:UNK:O	1:F:1450:UNK:N	2.38	0.56
1:G:1674:GLN:NE2	1:G:1710:VAL:O	2.39	0.56
2:E:755:THR:HG22	2:E:757:LYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MET:N	1:F:11:LEU:O	2.38	0.56
2:D:1034:ARG:NH2	2:D:1052:GLU:OE2	2.38	0.56
1:G:232:LEU:HD21	1:G:422:PRO:HB2	1.88	0.56
1:G:1538:UNK:O	1:G:1618:PRO:N	2.39	0.56
1:B:461:ASP:HB2	1:B:465:GLY:HA2	1.88	0.56
2:A:1034:ARG:NH2	2:A:1052:GLU:OE2	2.39	0.56
1:F:1538:UNK:O	1:F:1618:PRO:N	2.39	0.56
2:D:852:ARG:NH1	2:D:856:GLU:OE1	2.38	0.56
2:E:785:ASP:OD1	2:E:785:ASP:N	2.39	0.56
1:B:1644:ASN:H	1:B:1648:VAL:H	1.54	0.56
1:B:1674:GLN:NE2	1:B:1710:VAL:O	2.39	0.56
1:B:1689:ASP:OD2	1:B:1693:ARG:NH2	2.39	0.56
1:G:349:VAL:HA	1:G:352:TYR:HD1	1.71	0.56
1:G:1689:ASP:OD2	1:G:1693:ARG:NH2	2.39	0.56
1:F:108:LEU:HD13	1:F:119:THR:HG23	1.87	0.56
1:F:232:LEU:HD21	1:F:422:PRO:HB2	1.87	0.56
1:B:115:THR:O	1:B:119:THR:OG1	2.24	0.56
1:F:1644:ASN:H	1:F:1648:VAL:H	1.54	0.56
1:G:330:ASN:ND2	1:G:332:GLU:OE2	2.37	0.56
1:G:115:THR:O	1:G:119:THR:OG1	2.24	0.56
1:B:1311:UNK:HA	1:B:1362:UNK:HA	1.88	0.56
1:F:678:UNK:O	1:F:682:UNK:N	2.38	0.56
2:D:750:GLU:OE2	2:D:809:GLN:NE2	2.36	0.56
1:G:59:GLU:O	1:G:63:LYS:N	2.36	0.56
1:G:1721:PHE:O	1:G:1733:TYR:OH	2.24	0.56
1:B:1:MET:N	1:B:11:LEU:O	2.38	0.55
1:F:461:ASP:HB2	1:F:465:GLY:HA2	1.88	0.55
1:F:1689:ASP:OD2	1:F:1693:ARG:NH2	2.39	0.55
2:D:153:UNK:O	2:D:157:UNK:N	2.39	0.55
1:G:1644:ASN:H	1:G:1648:VAL:H	1.54	0.55
1:B:349:VAL:HA	1:B:352:TYR:HD1	1.71	0.55
2:A:1209:ASP:N	2:A:1209:ASP:OD1	2.39	0.55
2:D:755:THR:HG22	2:D:757:LYS:H	1.71	0.55
2:E:1209:ASP:OD1	2:E:1209:ASP:N	2.39	0.55
1:B:442:ASP:HA	1:B:445:LYS:HD2	1.88	0.55
2:A:373:UNK:O	2:A:377:UNK:N	2.39	0.55
2:A:852:ARG:NH1	2:A:856:GLU:OE1	2.38	0.55
1:F:349:VAL:HA	1:F:352:TYR:HD1	1.71	0.55
1:F:1674:GLN:NE2	1:F:1710:VAL:O	2.39	0.55
2:D:1815:UNK:O	2:D:1819:UNK:N	2.40	0.55
1:G:211:GLN:HE22	1:G:230:TYR:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:461:ASP:HB2	1:G:465:GLY:HA2	1.88	0.55
1:G:1311:UNK:HA	1:G:1362:UNK:HA	1.89	0.55
1:B:108:LEU:HD13	1:B:119:THR:HG23	1.88	0.55
1:B:1721:PHE:O	1:B:1733:TYR:OH	2.24	0.55
1:F:115:THR:O	1:F:119:THR:OG1	2.24	0.55
2:E:1073:THR:OG1	2:E:1074:GLY:N	2.40	0.55
2:A:755:THR:HG22	2:A:757:LYS:H	1.71	0.55
2:D:1073:THR:OG1	2:D:1074:GLY:N	2.40	0.55
2:D:1209:ASP:OD1	2:D:1209:ASP:N	2.39	0.55
1:G:7:ARG:HB3	1:G:54:PRO:HG3	1.89	0.55
1:G:442:ASP:HA	1:G:445:LYS:HD2	1.88	0.55
1:B:211:GLN:HE22	1:B:230:TYR:HB3	1.71	0.55
1:B:370:LEU:HG	1:B:488:VAL:HB	1.89	0.55
1:B:568:LYS:H	1:B:572:ASN:H	1.55	0.55
2:E:153:UNK:O	2:E:157:UNK:N	2.39	0.55
1:F:1311:UNK:HA	1:F:1362:UNK:HA	1.89	0.55
1:F:1721:PHE:O	1:F:1733:TYR:OH	2.24	0.55
2:E:1815:UNK:O	2:E:1819:UNK:N	2.40	0.55
1:B:7:ARG:HB3	1:B:54:PRO:HG3	1.89	0.55
2:A:1815:UNK:O	2:A:1819:UNK:N	2.40	0.55
1:F:568:LYS:H	1:F:572:ASN:H	1.55	0.55
2:D:720:SER:O	2:D:724:LYS:N	2.40	0.55
2:D:785:ASP:OD1	2:D:785:ASP:N	2.39	0.55
2:E:896:PHE:HE1	2:E:901:MET:HB3	1.72	0.55
2:A:369:UNK:O	2:A:373:UNK:N	2.40	0.55
1:G:108:LEU:HD13	1:G:119:THR:HG23	1.88	0.55
2:E:373:UNK:O	2:E:377:UNK:N	2.39	0.55
1:B:50:ALA:HB2	1:B:118:LYS:HE2	1.89	0.54
2:D:373:UNK:O	2:D:377:UNK:N	2.39	0.54
2:D:786:SER:OG	2:D:787:LYS:N	2.40	0.54
1:G:370:LEU:HG	1:G:488:VAL:HB	1.89	0.54
2:E:827:SER:OG	2:E:829:ASN:OD1	2.25	0.54
2:E:1294:SER:OG	2:E:1295:SER:N	2.36	0.54
2:A:786:SER:OG	2:A:787:LYS:N	2.40	0.54
2:A:1073:THR:OG1	2:A:1074:GLY:N	2.40	0.54
1:F:50:ALA:HB2	1:F:118:LYS:HE2	1.89	0.54
1:F:211:GLN:HE22	1:F:230:TYR:HB3	1.71	0.54
1:F:370:LEU:HG	1:F:488:VAL:HB	1.89	0.54
1:B:1758:HIS:CD2	1:B:1759:SER:H	2.26	0.54
2:A:153:UNK:O	2:A:157:UNK:N	2.39	0.54
1:G:568:LYS:H	1:G:572:ASN:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:VAL:O	1:B:484:ILE:N	2.39	0.54
1:F:173:LEU:HD12	1:F:244:ILE:HG12	1.90	0.54
2:D:896:PHE:HE1	2:D:901:MET:HB3	1.72	0.54
2:E:786:SER:OG	2:E:787:LYS:N	2.40	0.54
2:E:1132:GLU:HB3	2:E:1172:THR:HG23	1.90	0.54
1:B:1505:UNK:O	1:B:1507:UNK:N	2.41	0.54
2:D:938:GLU:O	2:D:942:LYS:N	2.40	0.54
3:H:1450:ARG:HB3	3:H:1508:TRP:HE1	1.73	0.54
2:E:938:GLU:O	2:E:942:LYS:N	2.40	0.54
2:A:938:GLU:O	2:A:942:LYS:N	2.40	0.54
1:F:82:GLN:HE22	1:F:85:ASN:HD22	1.56	0.54
2:D:154:UNK:O	2:D:158:UNK:N	2.41	0.54
2:E:369:UNK:O	2:E:373:UNK:N	2.40	0.54
2:A:27:UNK:O	2:A:58:UNK:N	2.42	0.54
2:A:896:PHE:HE1	2:A:901:MET:HB3	1.72	0.54
2:A:1145:LYS:O	2:A:1149:GLY:N	2.34	0.54
2:D:369:UNK:O	2:D:373:UNK:N	2.40	0.54
1:G:185:GLY:O	1:G:189:LYS:NZ	2.41	0.54
2:E:1078:SER:OG	2:E:1079:LYS:N	2.41	0.54
1:B:173:LEU:HD12	1:B:244:ILE:HG12	1.90	0.53
1:F:7:ARG:HB3	1:F:54:PRO:HG3	1.89	0.53
1:F:1505:UNK:O	1:F:1507:UNK:N	2.41	0.53
2:D:1333:ASP:OD1	2:D:1333:ASP:N	2.41	0.53
1:F:185:GLY:O	1:F:189:LYS:NZ	2.41	0.53
1:F:1283:UNK:O	1:F:1287:UNK:N	2.41	0.53
1:F:1758:HIS:CD2	1:F:1759:SER:H	2.26	0.53
2:D:1061:SER:HB2	2:D:1081:LYS:HD2	1.90	0.53
1:G:173:LEU:HD12	1:G:244:ILE:HG12	1.89	0.53
2:A:154:UNK:O	2:A:158:UNK:N	2.41	0.53
2:A:1061:SER:HB2	2:A:1081:LYS:HD2	1.90	0.53
2:E:27:UNK:O	2:E:58:UNK:N	2.41	0.53
2:E:1109:GLU:HA	2:E:1188:GLN:HB2	1.90	0.53
1:F:107:LYS:HA	1:F:110:GLN:HE21	1.74	0.53
1:G:50:ALA:HB2	1:G:118:LYS:HE2	1.89	0.53
1:G:480:VAL:O	1:G:484:ILE:N	2.39	0.53
1:G:527:VAL:HG11	1:G:544:LYS:HB2	1.91	0.53
2:E:1164:SER:OG	2:E:1165:VAL:N	2.41	0.53
2:E:1333:ASP:N	2:E:1333:ASP:OD1	2.41	0.53
2:E:1350:SER:HA	2:E:1375:GLY:HA3	1.89	0.53
1:B:107:LYS:HA	1:B:110:GLN:HE21	1.74	0.53
1:B:185:GLY:O	1:B:189:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1679:ASP:N	1:B:1679:ASP:OD1	2.41	0.53
2:A:1350:SER:HA	2:A:1375:GLY:HA3	1.89	0.53
3:C:1450:ARG:HB3	3:C:1508:TRP:HE1	1.73	0.53
2:D:1109:GLU:HA	2:D:1188:GLN:HB2	1.90	0.53
1:G:158:ALA:HB3	1:G:270:ALA:HA	1.91	0.53
1:G:1283:UNK:O	1:G:1287:UNK:N	2.41	0.53
2:E:1100:HIS:O	2:E:1104:ARG:N	2.40	0.53
1:B:400:SER:O	1:B:400:SER:OG	2.23	0.53
1:B:404:GLN:HA	1:B:408:PRO:HB3	1.90	0.53
1:B:1283:UNK:O	1:B:1287:UNK:N	2.41	0.53
1:G:107:LYS:HA	1:G:110:GLN:HE21	1.74	0.53
1:G:1758:HIS:CD2	1:G:1759:SER:H	2.26	0.53
2:E:154:UNK:O	2:E:158:UNK:N	2.41	0.53
1:B:82:GLN:HE22	1:B:85:ASN:HD22	1.56	0.53
1:F:404:GLN:HA	1:F:408:PRO:HB3	1.90	0.53
1:G:1505:UNK:O	1:G:1507:UNK:N	2.41	0.53
1:B:65:LEU:HD21	1:B:83:VAL:HG23	1.91	0.53
1:F:492:THR:HA	1:F:495:GLN:HE21	1.74	0.53
2:D:1294:SER:OG	2:D:1295:SER:N	2.36	0.53
1:B:1766:SER:OG	1:B:1767:GLU:N	2.42	0.53
2:A:827:SER:OG	2:A:829:ASN:OD1	2.25	0.53
2:A:1078:SER:OG	2:A:1079:LYS:N	2.41	0.53
1:F:527:VAL:HG11	1:F:544:LYS:HB2	1.91	0.53
1:B:273:HIS:O	1:B:277:LEU:N	2.43	0.52
2:D:957:VAL:O	2:D:961:THR:OG1	2.25	0.52
1:B:518:ARG:NH2	1:B:519:ASN:OD1	2.41	0.52
2:A:1333:ASP:OD1	2:A:1333:ASP:N	2.41	0.52
3:C:1491:ARG:O	3:C:1495:ASN:ND2	2.42	0.52
1:F:273:HIS:O	1:F:277:LEU:N	2.43	0.52
2:D:1350:SER:HA	2:D:1375:GLY:HA3	1.89	0.52
3:H:1491:ARG:O	3:H:1495:ASN:ND2	2.42	0.52
1:G:492:THR:HA	1:G:495:GLN:HE21	1.74	0.52
1:G:1334:UNK:HA	1:G:1381:UNK:HA	1.91	0.52
2:A:960:GLU:O	2:A:964:GLU:N	2.39	0.52
2:D:786:SER:O	2:D:788:SER:N	2.42	0.52
2:D:827:SER:OG	2:D:829:ASN:OD1	2.25	0.52
1:G:357:ASN:O	1:G:365:GLN:NE2	2.42	0.52
3:I:1491:ARG:O	3:I:1495:ASN:ND2	2.42	0.52
2:D:27:UNK:O	2:D:58:UNK:N	2.42	0.52
1:G:539:ASP:N	1:G:539:ASP:OD1	2.42	0.52
2:A:1132:GLU:HB3	2:A:1172:THR:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1334:UNK:HA	1:F:1381:UNK:HA	1.91	0.52
2:D:367:UNK:O	2:D:371:UNK:N	2.43	0.52
1:G:404:GLN:HA	1:G:408:PRO:HB3	1.90	0.52
1:G:518:ARG:NH2	1:G:519:ASN:OD1	2.41	0.52
2:E:720:SER:O	2:E:724:LYS:N	2.40	0.52
2:E:960:GLU:O	2:E:964:GLU:N	2.39	0.52
1:F:65:LEU:HD21	1:F:83:VAL:HG23	1.91	0.52
1:F:539:ASP:OD1	1:F:539:ASP:N	2.42	0.52
2:D:1132:GLU:HB3	2:D:1172:THR:HG23	1.90	0.52
1:G:65:LEU:HD21	1:G:83:VAL:HG23	1.91	0.52
2:A:1109:GLU:HA	2:A:1188:GLN:HB2	1.90	0.52
1:G:1766:SER:OG	1:G:1767:GLU:N	2.42	0.52
2:E:1061:SER:HB2	2:E:1081:LYS:HD2	1.90	0.52
1:B:346:GLN:HG2	1:B:347:GLU:HG2	1.92	0.52
1:B:492:THR:HA	1:B:495:GLN:HE21	1.74	0.52
1:B:527:VAL:HG11	1:B:544:LYS:HB2	1.91	0.52
1:B:1334:UNK:HA	1:B:1381:UNK:HA	1.91	0.52
2:E:752:ILE:HG23	2:E:753:TYR:HD1	1.75	0.52
2:E:786:SER:O	2:E:788:SER:N	2.42	0.52
1:B:1332:UNK:HA	1:B:1346:UNK:HA	1.92	0.52
2:A:367:UNK:O	2:A:371:UNK:N	2.43	0.52
2:A:720:SER:O	2:A:724:LYS:N	2.40	0.52
1:G:82:GLN:HE22	1:G:85:ASN:HD22	1.56	0.52
1:G:273:HIS:O	1:G:277:LEU:N	2.43	0.52
2:E:936:LEU:O	2:E:940:THR:OG1	2.28	0.52
2:A:39:UNK:O	2:A:43:UNK:N	2.43	0.52
2:A:1515:ARG:HG2	2:A:1516:ASP:H	1.75	0.52
2:D:752:ILE:HG23	2:D:753:TYR:HD1	1.75	0.52
3:H:1506:GLN:O	3:H:1511:ASP:N	2.43	0.52
1:G:161:GLY:N	1:G:245:GLN:OE1	2.41	0.52
2:E:1144:PHE:O	2:E:1148:HIS:N	2.43	0.52
1:F:259:THR:HA	1:F:289:TRP:HE1	1.75	0.51
2:D:1144:PHE:O	2:D:1148:HIS:N	2.43	0.51
1:B:158:ALA:HB3	1:B:270:ALA:HA	1.91	0.51
2:D:1100:HIS:O	2:D:1104:ARG:N	2.40	0.51
1:G:1332:UNK:HA	1:G:1346:UNK:HA	1.92	0.51
1:F:346:GLN:HG2	1:F:347:GLU:HG2	1.92	0.51
1:F:1766:SER:OG	1:F:1767:GLU:N	2.42	0.51
2:D:39:UNK:O	2:D:43:UNK:N	2.43	0.51
2:E:869:ILE:HG22	2:E:926:LEU:HD22	1.93	0.51
2:E:1111:PHE:HB2	2:E:1114:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:786:SER:O	2:A:788:SER:N	2.42	0.51
2:A:869:ILE:HG22	2:A:926:LEU:HD22	1.92	0.51
1:F:357:ASN:O	1:F:365:GLN:NE2	2.41	0.51
2:D:1078:SER:OG	2:D:1079:LYS:N	2.41	0.51
2:D:1164:SER:OG	2:D:1165:VAL:N	2.41	0.51
2:E:367:UNK:O	2:E:371:UNK:N	2.43	0.51
3:I:1450:ARG:HB3	3:I:1508:TRP:HE1	1.73	0.51
1:B:302:VAL:O	1:B:306:ILE:N	2.43	0.51
1:B:461:ASP:HB3	1:B:463:PHE:H	1.75	0.51
1:B:539:ASP:OD1	1:B:539:ASP:N	2.42	0.51
2:A:936:LEU:O	2:A:940:THR:OG1	2.28	0.51
2:A:1144:PHE:O	2:A:1148:HIS:N	2.43	0.51
1:F:158:ALA:HB3	1:F:270:ALA:HA	1.91	0.51
2:D:799:ILE:HG22	2:D:803:MET:HE1	1.93	0.51
2:D:1111:PHE:HB2	2:D:1114:TYR:HB2	1.92	0.51
1:G:1213:UNK:O	1:G:1215:UNK:N	2.43	0.51
2:E:799:ILE:HG22	2:E:803:MET:HE1	1.93	0.51
1:B:1712:ASN:OD1	1:B:1712:ASN:N	2.43	0.51
3:C:1506:GLN:O	3:C:1511:ASP:N	2.43	0.51
1:F:461:ASP:HB3	1:F:463:PHE:H	1.75	0.51
1:G:346:GLN:HG2	1:G:347:GLU:HG2	1.92	0.51
3:I:1506:GLN:O	3:I:1511:ASP:N	2.43	0.51
2:A:1362:PRO:HA	2:A:1365:MET:HE2	1.93	0.51
1:F:953:UNK:O	1:F:957:UNK:N	2.44	0.51
1:F:1213:UNK:O	1:F:1215:UNK:N	2.43	0.51
1:G:259:THR:HA	1:G:289:TRP:HE1	1.75	0.51
1:G:1712:ASN:OD1	1:G:1712:ASN:N	2.43	0.51
2:E:1362:PRO:HA	2:E:1365:MET:HE2	1.93	0.51
1:B:1213:UNK:O	1:B:1215:UNK:N	2.43	0.51
2:A:1111:PHE:HB2	2:A:1114:TYR:HB2	1.92	0.51
1:F:347:GLU:HA	1:F:350:GLN:HB3	1.93	0.51
1:G:2039:LYS:O	1:G:2043:ASP:N	2.44	0.51
1:B:953:UNK:O	1:B:957:UNK:N	2.44	0.51
2:A:1100:HIS:O	2:A:1104:ARG:N	2.40	0.51
1:G:157:VAL:O	1:G:502:LEU:N	2.44	0.51
1:G:347:GLU:HA	1:G:350:GLN:HB3	1.93	0.51
2:E:39:UNK:O	2:E:43:UNK:N	2.43	0.51
2:E:1239:HIS:HB2	2:E:1241:SER:H	1.76	0.51
1:B:1106:UNK:O	1:B:1110:UNK:N	2.44	0.50
1:F:480:VAL:O	1:F:484:ILE:N	2.39	0.50
2:D:681:THR:HB	2:D:771:PHE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:461:ASP:HB3	1:G:463:PHE:H	1.75	0.50
1:B:259:THR:HA	1:B:289:TRP:HE1	1.75	0.50
2:A:752:ILE:HG23	2:A:753:TYR:HD1	1.75	0.50
1:F:217:GLU:HA	1:F:220:GLU:HB2	1.93	0.50
1:F:1106:UNK:O	1:F:1110:UNK:N	2.44	0.50
1:G:1679:ASP:N	1:G:1679:ASP:OD1	2.41	0.50
2:E:691:GLU:OE1	2:E:694:GLN:NE2	2.44	0.50
2:E:1772:UNK:HA	3:I:1464:GLU:HG2	1.94	0.50
1:B:104:LEU:HA	1:B:107:LYS:HB2	1.93	0.50
1:B:217:GLU:HA	1:B:220:GLU:HB2	1.93	0.50
2:A:1326:ILE:HD12	2:A:1388:MET:HG2	1.94	0.50
1:F:1679:ASP:OD1	1:F:1679:ASP:N	2.41	0.50
2:D:691:GLU:OE1	2:D:694:GLN:NE2	2.44	0.50
2:D:1362:PRO:HA	2:D:1365:MET:HE2	1.93	0.50
2:D:1515:ARG:HG2	2:D:1516:ASP:H	1.75	0.50
1:G:104:LEU:HA	1:G:107:LYS:HB2	1.93	0.50
1:G:390:ASN:O	1:G:394:ARG:N	2.45	0.50
1:G:953:UNK:O	1:G:957:UNK:N	2.44	0.50
1:B:161:GLY:N	1:B:245:GLN:OE1	2.41	0.50
2:A:1361:THR:HB	2:A:1364:GLU:HB2	1.93	0.50
1:F:1394:UNK:O	1:F:1396:UNK:N	2.45	0.50
2:D:1361:THR:HB	2:D:1364:GLU:HB2	1.93	0.50
1:B:126:TYR:O	1:B:130:ARG:N	2.44	0.50
1:B:338:MET:HG3	1:B:421:LEU:HD12	1.94	0.50
1:B:1381:UNK:O	1:B:1431:UNK:N	2.45	0.50
2:A:1417:SER:OG	2:A:1418:VAL:N	2.45	0.50
1:F:157:VAL:O	1:F:502:LEU:N	2.44	0.50
2:D:1210:PRO:HB2	2:D:1255:SER:HB2	1.94	0.50
2:D:1349:THR:O	2:D:1376:PHE:N	2.45	0.50
1:G:126:TYR:O	1:G:130:ARG:N	2.44	0.50
2:A:799:ILE:HG22	2:A:803:MET:HE1	1.93	0.50
1:F:338:MET:HG3	1:F:421:LEU:HD12	1.94	0.50
2:D:1027:VAL:HB	2:D:1382:ALA:HB3	1.94	0.50
1:G:217:GLU:HA	1:G:220:GLU:HB2	1.93	0.50
1:B:1394:UNK:O	1:B:1396:UNK:N	2.45	0.50
2:A:1239:HIS:HB2	2:A:1241:SER:H	1.76	0.50
1:F:1332:UNK:HA	1:F:1346:UNK:HA	1.92	0.50
2:D:1340:SER:OG	2:D:1341:PHE:N	2.45	0.50
1:G:1106:UNK:O	1:G:1110:UNK:N	2.44	0.50
2:E:1515:ARG:HG2	2:E:1516:ASP:H	1.75	0.50
1:B:1905:ARG:O	1:B:1909:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2039:LYS:O	1:B:2043:ASP:N	2.44	0.50
2:A:1015:LEU:HD23	3:C:1510:ASN:HD21	1.77	0.50
2:A:1210:PRO:HB2	2:A:1255:SER:HB2	1.94	0.50
1:F:309:ARG:HB3	1:F:435:ALA:HB1	1.94	0.50
2:E:681:THR:HB	2:E:771:PHE:H	1.76	0.50
2:A:691:GLU:OE1	2:A:694:GLN:NE2	2.44	0.50
2:A:785:ASP:OD1	2:A:785:ASP:N	2.39	0.50
1:F:104:LEU:HA	1:F:107:LYS:HB2	1.93	0.50
1:F:518:ARG:NH2	1:F:519:ASN:OD1	2.41	0.50
2:D:1239:HIS:HB2	2:D:1241:SER:H	1.76	0.50
1:G:338:MET:HG3	1:G:421:LEU:HD12	1.94	0.50
2:A:1027:VAL:HB	2:A:1382:ALA:HB3	1.93	0.49
1:G:1394:UNK:O	1:G:1396:UNK:N	2.45	0.49
1:B:390:ASN:O	1:B:394:ARG:N	2.45	0.49
1:F:1381:UNK:O	1:F:1431:UNK:N	2.45	0.49
2:D:936:LEU:O	2:D:940:THR:OG1	2.28	0.49
2:E:1027:VAL:HB	2:E:1382:ALA:HB3	1.94	0.49
1:B:357:ASN:O	1:B:365:GLN:NE2	2.42	0.49
2:A:1349:THR:O	2:A:1376:PHE:N	2.45	0.49
1:F:1396:UNK:O	1:F:1400:UNK:N	2.46	0.49
1:G:1381:UNK:O	1:G:1431:UNK:N	2.45	0.49
1:B:157:VAL:O	1:B:502:LEU:N	2.44	0.49
1:B:347:GLU:HA	1:B:350:GLN:HB3	1.93	0.49
1:B:514:VAL:HG23	1:B:515:LEU:HD12	1.93	0.49
1:B:764:UNK:O	1:B:768:UNK:N	2.46	0.49
2:A:1340:SER:OG	2:A:1341:PHE:N	2.45	0.49
1:F:514:VAL:HG23	1:F:515:LEU:HD12	1.93	0.49
1:F:1712:ASN:OD1	1:F:1712:ASN:N	2.43	0.49
1:F:2039:LYS:O	1:F:2043:ASP:N	2.44	0.49
2:D:869:ILE:HG22	2:D:926:LEU:HD22	1.92	0.49
2:D:1310:GLU:OE1	2:D:1310:GLU:N	2.45	0.49
1:G:764:UNK:O	1:G:768:UNK:N	2.46	0.49
2:E:1245:ASN:HB3	2:E:1298:ILE:HG12	1.94	0.49
2:D:798:ASN:HA	2:D:801:ARG:HH21	1.77	0.49
1:G:330:ASN:HB3	1:G:332:GLU:HG3	1.95	0.49
2:A:768:ILE:HG22	2:A:770:PRO:HD3	1.95	0.49
2:A:1869:UNK:N	2:A:1884:UNK:O	2.46	0.49
1:F:390:ASN:O	1:F:394:ARG:N	2.45	0.49
1:G:514:VAL:HG23	1:G:515:LEU:HD12	1.93	0.49
1:G:1396:UNK:O	1:G:1400:UNK:N	2.46	0.49
1:F:126:TYR:O	1:F:130:ARG:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:TRP:HE1	1:F:516:THR:HG22	1.78	0.49
2:D:1326:ILE:HD12	2:D:1388:MET:HG2	1.94	0.49
2:E:798:ASN:HA	2:E:801:ARG:HH21	1.77	0.49
2:E:1326:ILE:HD12	2:E:1388:MET:HG2	1.93	0.49
1:B:309:ARG:HB3	1:B:435:ALA:HB1	1.94	0.49
2:A:681:THR:HB	2:A:771:PHE:H	1.77	0.49
2:A:1325:ARG:HH11	2:A:1392:LEU:HD11	1.77	0.49
3:H:1509:GLY:H	3:H:1512:PHE:HB2	1.78	0.49
2:E:692:VAL:HA	2:E:906:LEU:HD21	1.95	0.49
2:E:1078:SER:HA	2:E:1088:ASP:HB3	1.95	0.49
2:E:1210:PRO:HB2	2:E:1255:SER:HB2	1.94	0.49
2:E:1340:SER:OG	2:E:1341:PHE:N	2.45	0.49
1:B:330:ASN:HB3	1:B:332:GLU:HG3	1.95	0.49
1:B:1396:UNK:O	1:B:1400:UNK:N	2.46	0.49
3:C:1509:GLY:H	3:C:1512:PHE:HB2	1.78	0.49
1:F:302:VAL:O	1:F:306:ILE:N	2.43	0.49
1:G:1750:LYS:O	1:G:1753:LYS:NZ	2.37	0.49
2:E:1325:ARG:HH11	2:E:1392:LEU:HD11	1.78	0.49
2:E:1361:THR:HB	2:E:1364:GLU:HB2	1.94	0.49
2:E:1417:SER:OG	2:E:1418:VAL:N	2.45	0.49
3:I:1509:GLY:H	3:I:1512:PHE:HB2	1.78	0.49
2:A:1078:SER:HA	2:A:1088:ASP:HB3	1.94	0.49
1:F:161:GLY:N	1:F:245:GLN:OE1	2.41	0.49
2:D:692:VAL:HA	2:D:906:LEU:HD21	1.95	0.49
2:D:1869:UNK:N	2:D:1884:UNK:O	2.46	0.49
3:H:1451:GLN:NE2	3:H:1456:GLU:OE2	2.46	0.49
1:G:1854:MET:HB2	1:G:1952:ALA:HB3	1.95	0.49
2:A:692:VAL:HA	2:A:906:LEU:HD21	1.95	0.48
1:F:764:UNK:O	1:F:768:UNK:N	2.46	0.48
1:G:1813:ALA:HA	1:G:1816:ALA:HB3	1.95	0.48
1:B:1813:ALA:HA	1:B:1816:ALA:HB3	1.95	0.48
2:A:1245:ASN:HB3	2:A:1298:ILE:HG12	1.94	0.48
1:F:1905:ARG:O	1:F:1909:THR:OG1	2.29	0.48
1:G:490:TRP:HE1	1:G:516:THR:HG22	1.78	0.48
2:E:243:UNK:O	2:E:247:UNK:N	2.46	0.48
2:E:1326:ILE:HG23	2:E:1388:MET:HG2	1.95	0.48
1:B:1884:TRP:H	1:B:1892:ASN:HD22	1.61	0.48
3:C:1451:GLN:NE2	3:C:1456:GLU:OE2	2.46	0.48
1:F:1872:GLN:HA	1:F:1875:VAL:HG22	1.95	0.48
2:D:243:UNK:O	2:D:247:UNK:N	2.46	0.48
2:D:960:GLU:O	2:D:964:GLU:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1051:VAL:HA	2:D:1054:ALA:HB3	1.95	0.48
1:G:50:ALA:HB1	1:G:56:THR:HB	1.95	0.48
1:G:1872:GLN:HA	1:G:1875:VAL:HG22	1.95	0.48
2:E:368:UNK:O	2:E:372:UNK:N	2.47	0.48
2:E:768:ILE:HG22	2:E:770:PRO:HD3	1.94	0.48
2:E:1015:LEU:HD23	3:I:1510:ASN:HD21	1.77	0.48
2:D:824:LEU:HD21	2:D:846:LEU:HD22	1.96	0.48
2:D:1078:SER:HA	2:D:1088:ASP:HB3	1.95	0.48
2:D:1099:GLU:O	2:D:1102:GLY:N	2.37	0.48
2:D:1245:ASN:HB3	2:D:1298:ILE:HG12	1.94	0.48
1:G:221:ASN:O	1:G:225:THR:OG1	2.26	0.48
1:G:1308:UNK:HA	1:G:1364:UNK:HA	1.96	0.48
2:E:1349:THR:O	2:E:1376:PHE:N	2.45	0.48
1:B:50:ALA:HB1	1:B:56:THR:HB	1.95	0.48
1:B:1308:UNK:HA	1:B:1364:UNK:HA	1.96	0.48
1:F:190:PHE:O	1:F:194:THR:OG1	2.25	0.48
1:F:218:TRP:O	1:F:225:THR:OG1	2.31	0.48
2:D:644:THR:O	2:D:647:GLY:N	2.47	0.48
2:D:1145:LYS:O	2:D:1149:GLY:N	2.34	0.48
2:E:1869:UNK:N	2:E:1884:UNK:O	2.46	0.48
3:I:1451:GLN:NE2	3:I:1456:GLU:OE2	2.46	0.48
2:D:1325:ARG:HH11	2:D:1392:LEU:HD11	1.78	0.48
1:G:309:ARG:HB3	1:G:435:ALA:HB1	1.94	0.48
1:B:640:UNK:H	1:B:669:UNK:HA	1.79	0.48
2:A:368:UNK:O	2:A:372:UNK:N	2.47	0.48
2:A:798:ASN:HA	2:A:801:ARG:HH21	1.77	0.48
1:F:330:ASN:HB3	1:F:332:GLU:HG3	1.95	0.48
1:F:1854:MET:HB2	1:F:1952:ALA:HB3	1.95	0.48
1:G:218:TRP:O	1:G:225:THR:OG1	2.31	0.48
2:E:644:THR:O	2:E:647:GLY:N	2.47	0.48
2:E:1435:SER:O	2:E:1435:SER:OG	2.31	0.48
1:B:110:GLN:HG3	1:B:111:GLU:HG3	1.96	0.48
2:A:243:UNK:O	2:A:247:UNK:N	2.46	0.48
2:A:826:MET:HG2	2:A:867:ALA:H	1.79	0.48
2:A:1310:GLU:OE1	2:A:1310:GLU:N	2.45	0.48
2:A:1326:ILE:HG23	2:A:1388:MET:HG2	1.95	0.48
1:F:102:HIS:HE1	1:F:123:ILE:HD13	1.79	0.48
1:B:56:THR:HA	1:B:122:LEU:HD21	1.96	0.48
1:B:1390:UNK:N	1:B:1423:UNK:O	2.47	0.48
1:B:1854:MET:HB2	1:B:1952:ALA:HB3	1.95	0.48
1:F:56:THR:HA	1:F:122:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:711:SER:H	2:D:714:VAL:HB	1.79	0.48
2:D:1390:ALA:HA	2:D:1393:ALA:HB3	1.96	0.48
2:E:826:MET:HG2	2:E:867:ALA:H	1.78	0.48
1:B:1537:UNK:O	1:B:1620:THR:N	2.47	0.48
1:F:467:ASP:OD1	1:F:469:ARG:NE	2.47	0.48
2:D:768:ILE:HG22	2:D:770:PRO:HD3	1.94	0.48
1:G:92:GLU:HA	1:G:96:LEU:HD21	1.96	0.48
2:E:1065:GLY:HA3	2:E:1068:LYS:NZ	2.29	0.48
2:E:1145:LYS:O	2:E:1149:GLY:N	2.34	0.48
1:B:490:TRP:HE1	1:B:516:THR:HG22	1.78	0.47
2:A:957:VAL:O	2:A:961:THR:OG1	2.25	0.47
1:F:754:UNK:N	1:F:782:UNK:O	2.47	0.47
2:D:1417:SER:OG	2:D:1418:VAL:N	2.45	0.47
1:G:183:LEU:HD22	1:G:254:LYS:HB3	1.96	0.47
1:G:1537:UNK:O	1:G:1620:THR:N	2.47	0.47
2:E:294:UNK:O	2:E:298:UNK:N	2.47	0.47
1:B:218:TRP:O	1:B:225:THR:OG1	2.31	0.47
1:B:384:GLN:O	1:B:388:GLY:N	2.47	0.47
1:B:754:UNK:N	1:B:782:UNK:O	2.47	0.47
1:B:1927:LEU:O	1:B:1930:SER:OG	2.32	0.47
2:A:644:THR:O	2:A:647:GLY:N	2.47	0.47
1:F:110:GLN:HG3	1:F:111:GLU:HG3	1.96	0.47
1:F:21:LEU:O	1:F:24:THR:OG1	2.25	0.47
1:F:1537:UNK:O	1:F:1620:THR:N	2.47	0.47
2:D:1065:GLY:HA3	2:D:1068:LYS:NZ	2.29	0.47
1:G:102:HIS:HE1	1:G:123:ILE:HD13	1.79	0.47
1:G:1390:UNK:N	1:G:1423:UNK:O	2.47	0.47
2:E:1130:ASP:OD1	2:E:1130:ASP:N	2.48	0.47
1:B:51:ASP:HA	1:B:57:PRO:HD3	1.96	0.47
1:B:1694:ALA:HB1	1:B:1828:VAL:HG21	1.97	0.47
1:F:400:SER:O	1:F:400:SER:OG	2.23	0.47
1:F:1390:UNK:N	1:F:1423:UNK:O	2.47	0.47
1:G:110:GLN:HG3	1:G:111:GLU:HG3	1.96	0.47
3:I:1452:LEU:HD23	3:I:1456:GLU:HG3	1.97	0.47
1:B:190:PHE:O	1:B:194:THR:OG1	2.25	0.47
1:F:431:LEU:HG	1:F:432:LEU:HG	1.96	0.47
3:H:1452:LEU:HD23	3:H:1456:GLU:HG3	1.97	0.47
1:G:467:ASP:OD1	1:G:469:ARG:NE	2.47	0.47
1:G:502:LEU:HD13	1:G:504:PHE:HE2	1.79	0.47
1:G:1884:TRP:H	1:G:1892:ASN:HD22	1.61	0.47
1:B:183:LEU:HD22	1:B:254:LYS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:183:UNK:O	2:A:187:UNK:N	2.48	0.47
2:A:1099:GLU:O	2:A:1102:GLY:N	2.37	0.47
1:F:336:SER:O	1:F:338:MET:N	2.46	0.47
1:F:640:UNK:H	1:F:669:UNK:HA	1.79	0.47
1:F:1694:ALA:HB1	1:F:1828:VAL:HG21	1.97	0.47
2:D:1326:ILE:HG23	2:D:1388:MET:HG2	1.95	0.47
1:G:1694:ALA:HB1	1:G:1828:VAL:HG21	1.97	0.47
1:G:1927:LEU:O	1:G:1930:SER:OG	2.32	0.47
2:E:1390:ALA:HA	2:E:1393:ALA:HB3	1.96	0.47
1:B:92:GLU:HA	1:B:96:LEU:HD21	1.96	0.47
1:B:100:ASP:O	1:B:102:HIS:N	2.48	0.47
1:B:164:GLY:O	1:B:169:TYR:OH	2.29	0.47
1:B:431:LEU:HG	1:B:432:LEU:HG	1.97	0.47
1:B:502:LEU:HD13	1:B:504:PHE:HE2	1.79	0.47
1:B:1872:GLN:HA	1:B:1875:VAL:HG22	1.95	0.47
1:F:164:GLY:O	1:F:169:TYR:OH	2.28	0.47
1:F:1308:UNK:HA	1:F:1364:UNK:HA	1.96	0.47
2:D:183:UNK:O	2:D:187:UNK:N	2.48	0.47
2:D:368:UNK:O	2:D:372:UNK:N	2.47	0.47
1:G:56:THR:HA	1:G:122:LEU:HD21	1.96	0.47
1:G:190:PHE:O	1:G:194:THR:OG1	2.25	0.47
1:G:640:UNK:H	1:G:669:UNK:HA	1.79	0.47
1:G:677:UNK:O	1:G:679:UNK:N	2.48	0.47
1:G:1851:ASN:O	1:G:1896:GLN:NE2	2.48	0.47
2:E:1354:GLU:H	2:E:1357:GLU:H	1.62	0.47
1:B:82:GLN:OE1	1:B:134:LYS:NZ	2.45	0.47
2:A:1051:VAL:HA	2:A:1054:ALA:HB3	1.96	0.47
1:F:1105:UNK:O	1:F:1109:UNK:N	2.48	0.47
1:F:1851:ASN:O	1:F:1896:GLN:NE2	2.48	0.47
2:D:294:UNK:O	2:D:298:UNK:N	2.47	0.47
2:D:597:ALA:H	2:D:610:THR:HA	1.80	0.47
2:D:1354:GLU:H	2:D:1357:GLU:H	1.62	0.47
1:G:100:ASP:O	1:G:102:HIS:N	2.48	0.47
1:B:102:HIS:HE1	1:B:123:ILE:HD13	1.79	0.47
1:B:268:LYS:NZ	1:B:497:LYS:O	2.42	0.47
2:A:586:LYS:HA	2:A:671:VAL:H	1.80	0.47
2:A:1130:ASP:OD1	2:A:1130:ASP:N	2.48	0.47
3:C:1452:LEU:HD23	3:C:1456:GLU:HG3	1.97	0.47
1:F:227:ASP:OD1	1:F:227:ASP:N	2.48	0.47
1:F:314:TYR:HB2	1:F:432:LEU:HD21	1.97	0.47
1:F:527:VAL:HG13	1:F:541:TYR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:826:MET:HG2	2:D:867:ALA:H	1.78	0.47
1:G:754:UNK:N	1:G:782:UNK:O	2.47	0.47
2:E:183:UNK:O	2:E:187:UNK:N	2.48	0.47
2:A:294:UNK:O	2:A:298:UNK:N	2.47	0.47
2:A:599:MET:O	2:A:608:ASP:N	2.48	0.47
2:A:640:LEU:HA	2:A:924:ALA:HA	1.97	0.47
2:A:824:LEU:HD21	2:A:846:LEU:HD22	1.96	0.47
1:F:650:UNK:O	1:F:654:UNK:N	2.48	0.47
2:D:753:TYR:OH	2:D:764:ASP:O	2.33	0.47
2:E:552:LYS:O	2:E:554:ILE:N	2.48	0.47
2:E:711:SER:H	2:E:714:VAL:HB	1.79	0.47
1:B:650:UNK:O	1:B:654:UNK:N	2.48	0.46
2:A:661:ASP:O	2:A:665:LYS:N	2.48	0.46
2:A:1304:ALA:HA	2:A:1307:THR:HB	1.97	0.46
1:F:50:ALA:HB1	1:F:56:THR:HB	1.95	0.46
1:F:100:ASP:O	1:F:102:HIS:N	2.48	0.46
1:F:183:LEU:HD22	1:F:254:LYS:HB3	1.95	0.46
1:F:1884:TRP:H	1:F:1892:ASN:HD22	1.62	0.46
2:D:185:UNK:O	2:D:189:UNK:N	2.48	0.46
1:G:51:ASP:HA	1:G:57:PRO:HD3	1.96	0.46
2:E:957:VAL:O	2:E:961:THR:OG1	2.25	0.46
2:E:1099:GLU:O	2:E:1102:GLY:N	2.37	0.46
2:E:1304:ALA:HA	2:E:1307:THR:HB	1.97	0.46
1:B:467:ASP:OD1	1:B:469:ARG:NE	2.47	0.46
1:B:527:VAL:HG13	1:B:541:TYR:HA	1.98	0.46
2:A:1214:PHE:HB3	2:A:1382:ALA:HB2	1.98	0.46
1:F:51:ASP:HA	1:F:57:PRO:HD3	1.96	0.46
1:F:502:LEU:HD13	1:F:504:PHE:HE2	1.79	0.46
2:D:586:LYS:HA	2:D:671:VAL:H	1.80	0.46
2:D:834:GLY:O	2:D:836:ASP:N	2.48	0.46
1:G:227:ASP:OD1	1:G:227:ASP:N	2.48	0.46
2:E:640:LEU:HA	2:E:924:ALA:HA	1.97	0.46
2:E:824:LEU:HD21	2:E:846:LEU:HD22	1.96	0.46
2:E:1038:GLU:O	2:E:1042:PHE:N	2.45	0.46
2:E:1051:VAL:HA	2:E:1054:ALA:HB3	1.96	0.46
1:B:1851:ASN:O	1:B:1896:GLN:NE2	2.48	0.46
2:A:1065:GLY:HA3	2:A:1068:LYS:NZ	2.29	0.46
2:A:1070:ARG:O	2:A:1072:TYR:N	2.49	0.46
2:A:1390:ALA:HA	2:A:1393:ALA:HB3	1.96	0.46
1:F:1813:ALA:HA	1:F:1816:ALA:HB3	1.95	0.46
2:E:885:ALA:HA	2:E:888:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1310:GLU:OE1	2:E:1310:GLU:N	2.45	0.46
1:F:384:GLN:O	1:F:388:GLY:N	2.46	0.46
1:G:430:HIS:O	1:G:485:ARG:NH1	2.48	0.46
1:G:1105:UNK:O	1:G:1109:UNK:N	2.48	0.46
1:G:1905:ARG:O	1:G:1909:THR:OG1	2.29	0.46
2:E:834:GLY:O	2:E:836:ASP:N	2.48	0.46
2:E:1070:ARG:O	2:E:1072:TYR:N	2.49	0.46
2:A:184:UNK:O	2:A:188:UNK:N	2.49	0.46
2:A:185:UNK:O	2:A:189:UNK:N	2.48	0.46
1:F:92:GLU:HA	1:F:96:LEU:HD21	1.96	0.46
1:F:677:UNK:O	1:F:679:UNK:N	2.48	0.46
1:G:260:PRO:O	1:G:264:ARG:N	2.44	0.46
1:G:341:ILE:HA	1:G:418:ASN:HD22	1.80	0.46
2:E:185:UNK:O	2:E:189:UNK:N	2.48	0.46
2:E:1214:PHE:HB3	2:E:1382:ALA:HB2	1.98	0.46
1:B:677:UNK:O	1:B:679:UNK:N	2.48	0.46
2:A:711:SER:H	2:A:714:VAL:HB	1.79	0.46
1:F:107:LYS:HA	1:F:110:GLN:HG2	1.97	0.46
1:F:1927:LEU:O	1:F:1930:SER:OG	2.32	0.46
1:G:82:GLN:OE1	1:G:134:LYS:NZ	2.45	0.46
1:G:302:VAL:O	1:G:306:ILE:N	2.43	0.46
2:E:184:UNK:O	2:E:188:UNK:N	2.49	0.46
2:A:552:LYS:O	2:A:554:ILE:N	2.48	0.46
2:D:1754:UNK:O	2:D:1758:UNK:N	2.49	0.46
1:G:429:SER:H	1:G:484:ILE:HD12	1.80	0.46
1:G:431:LEU:HG	1:G:432:LEU:HG	1.96	0.46
1:B:227:ASP:N	1:B:227:ASP:OD1	2.48	0.46
2:A:1354:GLU:H	2:A:1357:GLU:H	1.62	0.46
1:F:82:GLN:OE1	1:F:134:LYS:NZ	2.45	0.46
1:F:1101:UNK:O	1:F:1103:UNK:N	2.49	0.46
2:E:661:ASP:O	2:E:665:LYS:N	2.48	0.46
1:B:314:TYR:HB2	1:B:432:LEU:HD21	1.97	0.46
1:F:341:ILE:HA	1:F:418:ASN:HD22	1.80	0.46
2:D:661:ASP:O	2:D:665:LYS:N	2.48	0.46
2:D:1304:ALA:HA	2:D:1307:THR:HB	1.97	0.46
1:G:1101:UNK:O	1:G:1103:UNK:N	2.49	0.46
2:E:586:LYS:HA	2:E:671:VAL:H	1.80	0.46
2:E:597:ALA:H	2:E:610:THR:HA	1.80	0.46
2:E:1076:VAL:HB	2:E:1087:LYS:HD3	1.98	0.46
2:A:1086:ASP:OD1	2:A:1086:ASP:N	2.47	0.46
2:A:1246:CYS:SG	2:A:1247:SER:N	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:SER:H	1:F:484:ILE:HD12	1.80	0.46
1:F:1870:ALA:HA	1:F:1873:TYR:HD2	1.81	0.46
2:D:552:LYS:O	2:D:554:ILE:N	2.48	0.46
2:D:1076:VAL:HB	2:D:1087:LYS:HD3	1.98	0.46
2:D:1214:PHE:HB3	2:D:1382:ALA:HB2	1.98	0.46
1:G:234:ILE:HG12	1:G:424:ALA:HB3	1.98	0.46
1:G:314:TYR:HB2	1:G:432:LEU:HD21	1.97	0.46
2:E:1246:CYS:SG	2:E:1247:SER:N	2.89	0.46
1:B:430:HIS:O	1:B:485:ARG:NH1	2.49	0.45
2:A:597:ALA:H	2:A:610:THR:HA	1.80	0.45
2:A:810:LYS:HG2	2:A:815:ILE:HD11	1.99	0.45
2:A:1754:UNK:O	2:A:1758:UNK:N	2.49	0.45
1:F:430:HIS:O	1:F:485:ARG:NH1	2.49	0.45
2:D:184:UNK:O	2:D:188:UNK:N	2.49	0.45
2:D:873:ARG:HG3	2:D:874:GLY:H	1.82	0.45
1:G:107:LYS:HA	1:G:110:GLN:HG2	1.97	0.45
1:G:650:UNK:O	1:G:654:UNK:N	2.48	0.45
1:B:1105:UNK:O	1:B:1109:UNK:N	2.48	0.45
2:D:1514:LYS:HB3	2:D:1515:ARG:H	1.57	0.45
1:G:336:SER:O	1:G:338:MET:N	2.46	0.45
2:E:1148:HIS:NE2	2:E:1153:ASP:OD1	2.48	0.45
2:E:1280:ILE:HD12	2:E:1280:ILE:HA	1.82	0.45
2:A:1029:PRO:HA	2:A:1193:TRP:HZ2	1.81	0.45
2:A:1076:VAL:HB	2:A:1087:LYS:HD3	1.98	0.45
2:A:1148:HIS:NE2	2:A:1153:ASP:OD1	2.49	0.45
1:F:22:VAL:O	1:F:26:SER:N	2.50	0.45
1:F:497:LYS:HD3	1:F:497:LYS:HA	1.82	0.45
1:F:825:UNK:N	1:F:836:UNK:O	2.50	0.45
1:F:1750:LYS:O	1:F:1753:LYS:NZ	2.37	0.45
1:G:229:ASP:N	1:G:229:ASP:OD1	2.50	0.45
1:G:825:UNK:N	1:G:836:UNK:O	2.50	0.45
2:E:873:ARG:HG3	2:E:874:GLY:H	1.82	0.45
1:B:429:SER:H	1:B:484:ILE:HD12	1.80	0.45
2:A:1309:VAL:O	2:A:1313:ASP:N	2.48	0.45
2:D:1038:GLU:O	2:D:1042:PHE:N	2.45	0.45
2:D:1222:ALA:O	2:D:1226:SER:OG	2.33	0.45
1:G:21:LEU:O	1:G:24:THR:OG1	2.25	0.45
1:G:527:VAL:HG13	1:G:541:TYR:HA	1.97	0.45
1:B:107:LYS:HA	1:B:110:GLN:HG2	1.97	0.45
1:B:194:THR:HA	1:B:197:GLU:HB2	1.99	0.45
2:A:1222:ALA:O	2:A:1226:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:LEU:HD11	1:F:502:LEU:HG	1.99	0.45
2:D:599:MET:O	2:D:608:ASP:N	2.48	0.45
2:D:885:ALA:HA	2:D:888:ILE:HD11	1.98	0.45
2:D:1029:PRO:HA	2:D:1193:TRP:HZ2	1.81	0.45
2:D:1070:ARG:O	2:D:1072:TYR:N	2.49	0.45
1:G:1104:UNK:O	1:G:1106:UNK:N	2.50	0.45
1:G:1513:UNK:O	1:G:1517:UNK:N	2.50	0.45
1:G:1870:ALA:HA	1:G:1873:TYR:HD2	1.81	0.45
2:E:720:SER:HA	2:E:723:ALA:HB3	1.99	0.45
2:E:1254:VAL:O	2:E:1256:ALA:N	2.35	0.45
1:B:69:SER:OG	1:B:80:PHE:O	2.35	0.45
2:A:753:TYR:OH	2:A:764:ASP:O	2.33	0.45
1:F:426:PRO:HG2	1:F:432:LEU:HD11	1.99	0.45
2:D:640:LEU:HA	2:D:924:ALA:HA	1.97	0.45
1:G:69:SER:OG	1:G:80:PHE:O	2.35	0.45
1:B:1870:ALA:HA	1:B:1873:TYR:HD2	1.81	0.45
1:F:1513:UNK:O	1:F:1517:UNK:N	2.50	0.45
2:D:12:UNK:O	2:D:16:UNK:N	2.50	0.45
1:G:156:LEU:HD11	1:G:502:LEU:HG	1.99	0.45
1:G:799:UNK:O	1:G:803:UNK:N	2.50	0.45
1:B:799:UNK:O	1:B:803:UNK:N	2.50	0.45
2:A:885:ALA:HA	2:A:888:ILE:HD11	1.98	0.45
2:A:1123:GLN:N	2:A:1182:ASP:O	2.49	0.45
1:F:69:SER:OG	1:F:80:PHE:O	2.35	0.45
2:D:810:LYS:HG2	2:D:815:ILE:HD11	1.99	0.45
1:B:260:PRO:O	1:B:264:ARG:N	2.44	0.45
1:B:336:SER:O	1:B:338:MET:N	2.46	0.45
1:B:1101:UNK:O	1:B:1103:UNK:N	2.49	0.45
1:B:1513:UNK:O	1:B:1517:UNK:N	2.50	0.45
2:A:873:ARG:HG3	2:A:874:GLY:H	1.82	0.45
1:F:1923:ASP:HB3	1:F:1924:ILE:H	1.50	0.45
2:D:1015:LEU:HD23	3:H:1510:ASN:HD21	1.82	0.45
1:G:120:LYS:HA	1:G:120:LYS:HD2	1.78	0.45
2:E:12:UNK:O	2:E:16:UNK:N	2.50	0.45
2:E:753:TYR:OH	2:E:764:ASP:O	2.33	0.45
1:B:156:LEU:HD11	1:B:502:LEU:HG	1.99	0.45
2:A:584:SER:H	2:A:674:LYS:HZ2	1.63	0.45
2:A:834:GLY:O	2:A:836:ASP:N	2.48	0.45
1:F:284:ALA:HB3	1:F:455:ILE:HG12	1.99	0.45
1:F:799:UNK:O	1:F:803:UNK:N	2.50	0.45
2:D:1130:ASP:OD1	2:D:1130:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1246:CYS:SG	2:D:1247:SER:N	2.89	0.45
1:G:426:PRO:HG2	1:G:432:LEU:HD11	1.99	0.45
2:E:1352:THR:OG1	2:E:1353:LEU:N	2.50	0.45
1:B:284:ALA:HB3	1:B:455:ILE:HG12	1.99	0.44
1:B:341:ILE:HA	1:B:418:ASN:HD22	1.80	0.44
1:B:426:PRO:HG2	1:B:432:LEU:HD11	1.99	0.44
2:A:1352:THR:OG1	2:A:1353:LEU:N	2.50	0.44
2:A:1436:VAL:H	2:A:1518:ARG:HH22	1.65	0.44
1:F:104:LEU:HA	1:F:107:LYS:HD3	1.99	0.44
1:F:268:LYS:NZ	1:F:497:LYS:O	2.42	0.44
1:F:1104:UNK:O	1:F:1106:UNK:N	2.50	0.44
2:D:1086:ASP:OD1	2:D:1086:ASP:N	2.47	0.44
2:D:1426:LEU:HG	2:D:1427:THR:HG23	1.99	0.44
2:D:1436:VAL:H	2:D:1518:ARG:HH22	1.65	0.44
1:G:32:GLN:O	1:G:36:GLN:N	2.39	0.44
1:G:384:GLN:O	1:G:388:GLY:N	2.47	0.44
2:E:599:MET:O	2:E:608:ASP:N	2.48	0.44
2:E:1426:LEU:HG	2:E:1427:THR:HG23	1.99	0.44
1:B:309:ARG:HA	1:B:309:ARG:HD3	1.71	0.44
1:G:1689:ASP:O	1:G:1693:ARG:N	2.51	0.44
2:E:584:SER:H	2:E:674:LYS:HZ2	1.64	0.44
2:E:810:LYS:HG2	2:E:815:ILE:HD11	1.99	0.44
2:E:1029:PRO:HA	2:E:1193:TRP:HZ2	1.81	0.44
2:E:1754:UNK:O	2:E:1758:UNK:N	2.49	0.44
2:A:12:UNK:O	2:A:16:UNK:N	2.50	0.44
2:A:1426:LEU:HG	2:A:1427:THR:HG23	1.99	0.44
1:F:1694:ALA:HA	1:F:1697:HIS:HB3	1.99	0.44
2:D:1280:ILE:HD12	2:D:1280:ILE:HA	1.82	0.44
1:B:234:ILE:HG12	1:B:424:ALA:HB3	1.98	0.44
1:B:1104:UNK:O	1:B:1106:UNK:N	2.49	0.44
1:B:1391:UNK:HA	1:B:1422:UNK:HA	1.99	0.44
1:B:1689:ASP:O	1:B:1693:ARG:N	2.50	0.44
1:B:1694:ALA:HA	1:B:1697:HIS:HB3	1.99	0.44
1:F:1745:LYS:HD2	1:F:1745:LYS:HA	1.77	0.44
2:D:584:SER:H	2:D:674:LYS:HZ2	1.64	0.44
1:G:1312:UNK:N	1:G:1361:UNK:O	2.51	0.44
1:B:825:UNK:N	1:B:836:UNK:O	2.49	0.44
1:B:1548:UNK:O	1:B:1552:UNK:N	2.51	0.44
2:A:1514:LYS:HB3	2:A:1515:ARG:H	1.57	0.44
1:F:118:LYS:HA	1:F:118:LYS:HD2	1.90	0.44
2:D:1291:LEU:HD23	2:D:1291:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HA	1:B:107:LYS:HD3	1.99	0.44
2:A:720:SER:HA	2:A:723:ALA:HB3	1.99	0.44
1:F:1183:UNK:HA	1:F:1193:UNK:HA	2.00	0.44
2:D:1123:GLN:HB2	2:D:1182:ASP:HB3	2.00	0.44
2:D:1341:PHE:N	2:D:1343:PHE:O	2.48	0.44
2:D:1772:UNK:HA	3:H:1464:GLU:HG2	2.00	0.44
2:A:1099:GLU:HB3	2:A:1100:HIS:H	1.70	0.44
1:F:234:ILE:HG12	1:F:424:ALA:HB3	1.98	0.44
1:F:1391:UNK:HA	1:F:1422:UNK:HA	1.99	0.44
2:D:1265:PHE:HB3	2:D:1266:LYS:HZ2	1.83	0.44
2:E:1436:VAL:H	2:E:1518:ARG:HH22	1.65	0.44
1:B:22:VAL:O	1:B:26:SER:N	2.50	0.44
2:A:1191:THR:HB	2:A:1192:GLY:H	1.55	0.44
1:G:194:THR:HA	1:G:197:GLU:HB2	1.99	0.44
1:B:1884:TRP:O	1:B:1892:ASN:ND2	2.51	0.44
1:F:194:THR:HA	1:F:197:GLU:HB2	1.99	0.44
1:F:1884:TRP:O	1:F:1892:ASN:ND2	2.51	0.44
2:D:1204:ILE:HD13	2:D:1204:ILE:HA	1.90	0.44
2:D:1326:ILE:H	2:D:1326:ILE:HG12	1.53	0.44
1:G:284:ALA:HB3	1:G:455:ILE:HG12	1.99	0.44
1:G:501:ILE:HB	1:G:526:ARG:HB3	2.00	0.44
1:G:1694:ALA:HA	1:G:1697:HIS:HB3	1.99	0.44
1:F:446:ASN:O	1:F:448:VAL:N	2.51	0.43
2:E:204:UNK:O	2:E:206:UNK:N	2.51	0.43
1:B:229:ASP:OD1	1:B:229:ASP:N	2.50	0.43
1:F:1548:UNK:O	1:F:1552:UNK:N	2.51	0.43
2:D:1254:VAL:O	2:D:1256:ALA:N	2.35	0.43
2:D:1517:PRO:HG2	2:D:1518:ARG:HE	1.83	0.43
1:G:326:ASP:OD2	1:G:394:ARG:NH1	2.42	0.43
1:G:446:ASN:O	1:G:448:VAL:N	2.51	0.43
1:G:1548:UNK:O	1:G:1552:UNK:N	2.51	0.43
1:B:1312:UNK:N	1:B:1361:UNK:O	2.51	0.43
2:A:1123:GLN:HB2	2:A:1182:ASP:HB3	2.00	0.43
2:A:1164:SER:OG	2:A:1165:VAL:N	2.41	0.43
1:F:1689:ASP:O	1:F:1693:ARG:N	2.51	0.43
1:G:104:LEU:HA	1:G:107:LYS:HD3	1.99	0.43
2:E:1517:PRO:HG2	2:E:1518:ARG:HE	1.83	0.43
1:B:168:ASP:OD1	1:B:168:ASP:N	2.51	0.43
1:B:288:SER:OG	1:B:291:SER:N	2.42	0.43
3:C:1449:LYS:HB3	3:C:1449:LYS:HE2	1.78	0.43
1:F:1777:THR:O	1:F:1781:LEU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:644:THR:O	2:D:646:ALA:N	2.51	0.43
2:D:1095:THR:HA	2:D:1099:GLU:HG3	2.01	0.43
3:H:1457:ALA:O	3:H:1461:ASP:N	2.52	0.43
1:G:288:SER:OG	1:G:291:SER:N	2.42	0.43
1:G:787:UNK:O	1:G:789:UNK:N	2.52	0.43
3:I:1457:ALA:O	3:I:1461:ASP:N	2.52	0.43
2:A:644:THR:O	2:A:646:ALA:N	2.51	0.43
2:A:658:LEU:O	2:A:662:GLY:N	2.51	0.43
2:D:720:SER:HA	2:D:723:ALA:HB3	1.99	0.43
2:D:801:ARG:HE	2:D:801:ARG:HB2	1.60	0.43
2:D:1352:THR:OG1	2:D:1353:LEU:N	2.50	0.43
1:G:1376:UNK:O	1:G:1378:UNK:N	2.52	0.43
2:E:1060:ILE:HA	2:E:1079:LYS:HA	2.00	0.43
2:E:1079:LYS:HG3	2:E:1080:THR:HG22	2.01	0.43
1:B:21:LEU:O	1:B:24:THR:OG1	2.25	0.43
1:B:305:PHE:HA	1:B:308:VAL:HG12	2.01	0.43
1:B:501:ILE:HB	1:B:526:ARG:HB3	2.00	0.43
2:A:791:ALA:HA	2:A:794:ILE:HG22	2.01	0.43
1:F:1376:UNK:O	1:F:1378:UNK:N	2.52	0.43
2:D:1148:HIS:NE2	2:D:1153:ASP:OD1	2.48	0.43
2:E:1265:PHE:HB3	2:E:1266:LYS:HZ2	1.84	0.43
2:D:791:ALA:HA	2:D:794:ILE:HG22	2.01	0.43
2:E:644:THR:O	2:E:646:ALA:N	2.51	0.43
2:E:708:SER:OG	2:E:709:ARG:N	2.52	0.43
2:E:1095:THR:HA	2:E:1099:GLU:HG3	2.01	0.43
2:A:1316:VAL:HG21	2:A:1404:VAL:HG11	2.01	0.43
2:D:204:UNK:O	2:D:206:UNK:N	2.51	0.43
2:D:658:LEU:O	2:D:662:GLY:N	2.51	0.43
1:G:309:ARG:HD3	1:G:309:ARG:HA	1.71	0.43
1:G:1391:UNK:HA	1:G:1422:UNK:HA	1.99	0.43
2:E:791:ALA:HA	2:E:794:ILE:HG22	2.01	0.43
1:B:254:LYS:HE2	1:B:289:TRP:HH2	1.84	0.43
1:B:446:ASN:O	1:B:448:VAL:N	2.51	0.43
1:B:1376:UNK:O	1:B:1378:UNK:N	2.52	0.43
2:A:1095:THR:HA	2:A:1099:GLU:HG3	2.01	0.43
3:C:1457:ALA:O	3:C:1461:ASP:N	2.52	0.43
2:E:696:LEU:O	2:E:700:GLY:N	2.52	0.43
2:E:826:MET:N	2:E:867:ALA:O	2.37	0.43
1:B:158:ALA:H	1:B:270:ALA:H	1.66	0.43
1:B:208:VAL:HG11	1:B:308:VAL:HG23	2.01	0.43
1:F:171:GLU:HA	1:F:174:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:PHE:HA	1:F:308:VAL:HG12	2.01	0.43
1:F:501:ILE:HB	1:F:526:ARG:HB3	2.00	0.43
1:F:787:UNK:O	1:F:789:UNK:N	2.52	0.43
2:D:1060:ILE:HA	2:D:1079:LYS:HA	2.00	0.43
2:D:1096:SER:H	2:D:1099:GLU:HB2	1.84	0.43
1:G:171:GLU:HA	1:G:174:ARG:HB3	2.00	0.43
1:G:360:LEU:HD11	1:G:385:SER:HB3	2.01	0.43
1:G:1884:TRP:O	1:G:1892:ASN:ND2	2.51	0.43
2:E:711:SER:O	2:E:715:THR:OG1	2.30	0.43
1:B:787:UNK:O	1:B:789:UNK:N	2.52	0.42
2:A:901:MET:H	2:A:901:MET:HG3	1.64	0.42
2:D:204:UNK:O	2:D:207:UNK:N	2.52	0.42
1:G:22:VAL:O	1:G:26:SER:N	2.50	0.42
1:G:158:ALA:H	1:G:270:ALA:H	1.66	0.42
1:G:208:VAL:HG11	1:G:308:VAL:HG23	2.01	0.42
2:E:1123:GLN:HB2	2:E:1182:ASP:HB3	2.00	0.42
2:E:1291:LEU:HD23	2:E:1291:LEU:HA	1.82	0.42
1:B:196:SER:OG	1:B:213:LEU:O	2.37	0.42
1:B:360:LEU:HD11	1:B:385:SER:HB3	2.01	0.42
1:B:1685:LYS:HA	1:B:1685:LYS:HD3	1.85	0.42
2:A:1060:ILE:HA	2:A:1079:LYS:HA	2.00	0.42
1:F:309:ARG:HG3	1:F:439:ILE:HB	2.01	0.42
1:G:251:VAL:O	1:G:255:LEU:N	2.51	0.42
1:G:254:LYS:HE2	1:G:289:TRP:HH2	1.84	0.42
1:G:1183:UNK:HA	1:G:1193:UNK:HA	2.00	0.42
1:G:1699:LYS:H	1:G:1699:LYS:HG2	1.60	0.42
2:E:658:LEU:O	2:E:662:GLY:N	2.51	0.42
2:E:1316:VAL:HG21	2:E:1404:VAL:HG11	2.01	0.42
2:E:1341:PHE:N	2:E:1343:PHE:O	2.48	0.42
1:B:3:ALA:N	1:B:9:LEU:O	2.50	0.42
1:B:1183:UNK:HA	1:B:1193:UNK:HA	2.00	0.42
1:B:1691:TRP:CE2	1:B:1783:LEU:HG	2.54	0.42
1:F:229:ASP:OD1	1:F:229:ASP:N	2.50	0.42
2:D:1111:PHE:HD1	2:D:1111:PHE:HA	1.72	0.42
1:G:196:SER:OG	1:G:213:LEU:O	2.37	0.42
1:G:305:PHE:HA	1:G:308:VAL:HG12	2.01	0.42
2:E:1086:ASP:N	2:E:1086:ASP:OD1	2.47	0.42
2:E:1309:VAL:O	2:E:1313:ASP:N	2.48	0.42
2:A:708:SER:OG	2:A:709:ARG:N	2.52	0.42
2:A:1079:LYS:HG3	2:A:1080:THR:HG22	2.01	0.42
1:F:297:ARG:HD2	1:F:297:ARG:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:LEU:HD23	1:F:393:LEU:HA	1.86	0.42
1:G:268:LYS:NZ	1:G:497:LYS:O	2.42	0.42
1:G:309:ARG:HG3	1:G:439:ILE:HB	2.01	0.42
1:G:371:VAL:HB	1:G:489:LYS:HA	2.01	0.42
2:E:1191:THR:HB	2:E:1192:GLY:H	1.55	0.42
1:B:611:UNK:N	1:B:639:UNK:O	2.53	0.42
1:B:1804:PHE:HE1	1:B:1818:LEU:HG	1.84	0.42
1:B:1845:ASP:CG	1:B:1849:ARG:HB2	2.44	0.42
2:A:1517:PRO:HG2	2:A:1518:ARG:HE	1.83	0.42
1:F:158:ALA:H	1:F:270:ALA:H	1.66	0.42
1:F:211:GLN:NE2	1:F:230:TYR:O	2.53	0.42
1:F:1312:UNK:N	1:F:1361:UNK:O	2.51	0.42
2:D:696:LEU:O	2:D:700:GLY:N	2.52	0.42
1:G:1691:TRP:CE2	1:G:1783:LEU:HG	2.55	0.42
1:G:1845:ASP:CG	1:G:1849:ARG:HB2	2.44	0.42
2:E:204:UNK:O	2:E:207:UNK:N	2.53	0.42
1:B:171:GLU:HA	1:B:174:ARG:HB3	2.01	0.42
1:B:309:ARG:HG3	1:B:439:ILE:HB	2.01	0.42
1:B:1148:UNK:HA	1:B:1157:UNK:HA	2.02	0.42
2:A:204:UNK:O	2:A:206:UNK:N	2.51	0.42
2:A:696:LEU:O	2:A:700:GLY:N	2.52	0.42
2:A:711:SER:O	2:A:715:THR:OG1	2.30	0.42
1:F:221:ASN:O	1:F:225:THR:OG1	2.26	0.42
1:G:1148:UNK:HA	1:G:1157:UNK:HA	2.02	0.42
1:B:32:GLN:O	1:B:36:GLN:N	2.39	0.42
1:B:1923:ASP:HB3	1:B:1924:ILE:H	1.50	0.42
2:A:1413:LYS:HA	2:A:1413:LYS:HD2	1.95	0.42
2:D:777:GLN:N	2:D:777:GLN:OE1	2.52	0.42
2:E:1334:ASP:OD1	2:E:1335:PHE:N	2.53	0.42
1:B:1777:THR:O	1:B:1781:LEU:N	2.48	0.42
2:A:204:UNK:O	2:A:207:UNK:N	2.52	0.42
2:A:777:GLN:OE1	2:A:777:GLN:N	2.52	0.42
1:F:360:LEU:HD11	1:F:385:SER:HB3	2.01	0.42
1:F:490:TRP:O	1:F:493:THR:OG1	2.28	0.42
2:D:708:SER:OG	2:D:709:ARG:N	2.52	0.42
2:E:777:GLN:OE1	2:E:777:GLN:N	2.52	0.42
2:E:1096:SER:H	2:E:1099:GLU:HB2	1.84	0.42
2:E:1222:ALA:O	2:E:1226:SER:OG	2.33	0.42
1:B:28:PHE:HB3	1:B:64:PHE:HE2	1.85	0.42
1:B:29:ILE:HD12	1:B:29:ILE:HA	1.89	0.42
2:A:1096:SER:H	2:A:1099:GLU:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:GLN:O	1:F:36:GLN:N	2.39	0.42
1:F:162:GLY:HA3	1:F:275:GLN:HB2	2.02	0.42
1:F:196:SER:OG	1:F:213:LEU:O	2.37	0.42
2:D:1309:VAL:O	2:D:1313:ASP:N	2.48	0.42
1:G:1804:PHE:HE1	1:G:1818:LEU:HG	1.84	0.42
2:E:1249:SER:OG	2:E:1250:GLY:N	2.53	0.42
1:B:1745:LYS:HD2	1:B:1745:LYS:HA	1.77	0.42
1:F:168:ASP:OD1	1:F:168:ASP:N	2.51	0.42
1:F:288:SER:OG	1:F:291:SER:N	2.42	0.42
1:F:371:VAL:HB	1:F:489:LYS:HA	2.01	0.42
1:F:502:LEU:HD23	1:F:502:LEU:HA	1.90	0.42
1:F:1691:TRP:CE2	1:F:1783:LEU:HG	2.54	0.42
1:F:1833:TYR:O	1:F:1837:THR:OG1	2.28	0.42
2:D:1079:LYS:HG3	2:D:1080:THR:HG22	2.01	0.42
2:E:1168:LEU:HG	2:E:1169:LYS:HG2	2.02	0.42
2:E:1204:ILE:HD13	2:E:1204:ILE:HA	1.90	0.42
2:A:801:ARG:HE	2:A:801:ARG:HB2	1.60	0.41
1:F:28:PHE:HB3	1:F:64:PHE:HE2	1.85	0.41
1:F:1804:PHE:HE1	1:F:1818:LEU:HG	1.84	0.41
2:D:711:SER:O	2:D:715:THR:OG1	2.30	0.41
1:G:156:LEU:HD12	1:G:156:LEU:HA	1.87	0.41
2:A:298:UNK:O	2:A:300:UNK:N	2.54	0.41
2:A:1076:VAL:HG11	2:A:1089:VAL:HA	2.02	0.41
1:F:611:UNK:N	1:F:639:UNK:O	2.53	0.41
1:F:1845:ASP:CG	1:F:1849:ARG:HB2	2.44	0.41
2:D:1316:VAL:HG21	2:D:1404:VAL:HG11	2.01	0.41
2:D:1334:ASP:OD1	2:D:1335:PHE:N	2.53	0.41
2:E:1076:VAL:HG11	2:E:1089:VAL:HA	2.02	0.41
2:E:1347:LYS:HD3	2:E:1347:LYS:HA	1.93	0.41
2:A:765:LEU:HD23	2:A:765:LEU:HA	1.88	0.41
2:A:1249:SER:OG	2:A:1250:GLY:N	2.53	0.41
1:G:211:GLN:NE2	1:G:230:TYR:O	2.53	0.41
1:G:611:UNK:N	1:G:639:UNK:O	2.53	0.41
2:E:1111:PHE:HD1	2:E:1111:PHE:HA	1.72	0.41
2:D:946:GLU:O	2:D:950:THR:N	2.52	0.41
2:D:1076:VAL:HG11	2:D:1089:VAL:HA	2.02	0.41
2:E:1308:SER:O	2:E:1308:SER:OG	2.37	0.41
2:E:1349:THR:HA	2:E:1376:PHE:CE1	2.55	0.41
1:B:251:VAL:O	1:B:255:LEU:N	2.51	0.41
1:B:1925:ILE:HA	1:B:1928:GLN:HB2	2.02	0.41
1:F:208:VAL:HG11	1:F:308:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:LYS:HE2	1:F:289:TRP:HH2	1.84	0.41
1:F:1148:UNK:HA	1:F:1157:UNK:HA	2.02	0.41
2:D:298:UNK:O	2:D:300:UNK:N	2.54	0.41
1:G:162:GLY:HA3	1:G:275:GLN:HB2	2.02	0.41
2:E:1167:LEU:HD23	2:E:1167:LEU:HA	1.90	0.41
2:E:1869:UNK:O	2:E:1884:UNK:N	2.53	0.41
1:B:1709:ILE:HD12	1:B:1770:LEU:HD23	2.03	0.41
2:A:826:MET:N	2:A:867:ALA:O	2.37	0.41
1:F:53:GLU:HG3	1:F:112:ASN:HB3	2.03	0.41
2:A:179:UNK:H	1:G:705:UNK:HA	1.86	0.41
2:A:394:UNK:O	2:A:396:UNK:N	2.54	0.41
1:F:1699:LYS:H	1:F:1699:LYS:HG2	1.60	0.41
2:D:1168:LEU:HG	2:D:1169:LYS:HG2	2.02	0.41
1:G:485:ARG:HD2	1:G:485:ARG:HA	1.85	0.41
1:B:211:GLN:NE2	1:B:230:TYR:O	2.53	0.41
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.94	0.41
1:B:215:ILE:HA	1:B:218:TRP:CD2	2.56	0.41
2:A:946:GLU:O	2:A:950:THR:N	2.52	0.41
2:A:1869:UNK:O	2:A:1884:UNK:N	2.54	0.41
1:F:215:ILE:HA	1:F:218:TRP:CD2	2.56	0.41
1:F:485:ARG:HD2	1:F:485:ARG:HA	1.85	0.41
2:D:1051:VAL:O	2:D:1055:TRP:N	2.54	0.41
2:D:1167:LEU:HD23	2:D:1167:LEU:HA	1.90	0.41
2:D:1349:THR:HA	2:D:1376:PHE:CE1	2.55	0.41
1:G:28:PHE:HB3	1:G:64:PHE:HE2	1.85	0.41
1:B:166:THR:HG21	1:B:507:GLY:HA3	2.02	0.41
2:A:776:GLU:CD	2:A:838:MET:H	2.28	0.41
2:A:1045:PHE:HD1	2:A:1045:PHE:HA	1.78	0.41
2:A:1085:ASP:OD2	2:A:1085:ASP:N	2.50	0.41
2:A:1319:ILE:HD13	2:A:1325:ARG:HA	2.03	0.41
2:A:1748:UNK:O	2:A:1752:UNK:N	2.54	0.41
3:C:1457:ALA:HA	3:C:1460:LYS:HB3	2.03	0.41
1:F:1630:GLY:N	1:F:1637:LEU:O	2.54	0.41
1:F:1709:ILE:HD12	1:F:1770:LEU:HD23	2.03	0.41
1:F:1728:ARG:HB3	1:F:1732:ASN:HD22	1.85	0.41
2:D:1249:SER:OG	2:D:1250:GLY:N	2.53	0.41
2:D:1748:UNK:O	2:D:1752:UNK:N	2.54	0.41
3:H:1481:ASP:HB3	3:H:1484:GLU:HB3	2.02	0.41
1:G:166:THR:HG21	1:G:507:GLY:HA3	2.02	0.41
1:G:168:ASP:OD1	1:G:168:ASP:N	2.51	0.41
1:G:407:ILE:HG22	1:G:410:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1630:GLY:N	1:G:1637:LEU:O	2.54	0.41
1:G:1925:ILE:HA	1:G:1928:GLN:HB2	2.02	0.41
2:E:776:GLU:CD	2:E:838:MET:H	2.29	0.41
1:B:29:ILE:HG12	1:B:61:VAL:HG22	2.03	0.41
2:A:1038:GLU:O	2:A:1042:PHE:N	2.45	0.41
1:F:1:MET:HB3	1:F:2:ASP:H	1.70	0.41
1:F:211:GLN:NE2	1:F:230:TYR:HB3	2.36	0.41
1:F:1857:ILE:HG22	1:F:1891:TYR:HB2	2.03	0.41
2:D:1205:ILE:HA	2:D:1208:VAL:HG22	2.03	0.41
1:G:211:GLN:NE2	1:G:230:TYR:HB3	2.36	0.41
1:G:1684:SER:O	1:G:1688:GLN:N	2.54	0.41
2:E:298:UNK:O	2:E:300:UNK:N	2.54	0.41
2:E:1139:GLU:HB3	2:E:1168:LEU:HD22	2.03	0.41
3:I:1481:ASP:HB3	3:I:1484:GLU:HB3	2.02	0.41
1:B:53:GLU:HG3	1:B:112:ASN:HB3	2.03	0.40
1:B:162:GLY:HA3	1:B:275:GLN:HB2	2.02	0.40
1:B:705:UNK:HA	2:D:179:UNK:H	1.86	0.40
1:B:1887:GLU:HB2	1:B:1890:ASN:HB3	2.03	0.40
2:A:1349:THR:HA	2:A:1376:PHE:CE1	2.55	0.40
1:F:1925:ILE:HA	1:F:1928:GLN:HB2	2.03	0.40
1:G:164:GLY:O	1:G:169:TYR:OH	2.28	0.40
1:G:215:ILE:HA	1:G:218:TRP:CD2	2.56	0.40
1:G:1709:ILE:HD12	1:G:1770:LEU:HD23	2.03	0.40
2:E:1208:VAL:O	2:E:1212:THR:OG1	2.28	0.40
1:B:371:VAL:HB	1:B:489:LYS:HA	2.01	0.40
1:B:1753:LYS:O	1:B:1754:GLU:HG3	2.21	0.40
2:A:1291:LEU:HA	2:A:1291:LEU:HD23	1.82	0.40
3:C:1481:ASP:HB3	3:C:1484:GLU:HB3	2.02	0.40
1:F:251:VAL:O	1:F:255:LEU:N	2.51	0.40
1:F:355:LYS:O	1:F:358:SER:OG	2.29	0.40
1:F:1691:TRP:HE1	1:F:1784:MET:HA	1.87	0.40
2:D:1869:UNK:O	2:D:1884:UNK:N	2.53	0.40
1:G:1753:LYS:O	1:G:1754:GLU:HG3	2.21	0.40
2:E:1326:ILE:H	2:E:1326:ILE:HG12	1.53	0.40
2:A:1051:VAL:O	2:A:1055:TRP:N	2.54	0.40
1:F:174:ARG:NH2	1:F:218:TRP:O	2.49	0.40
1:G:225:THR:HA	1:G:226:PRO:HD3	1.94	0.40
1:G:502:LEU:HD23	1:G:502:LEU:HA	1.90	0.40
2:E:752:ILE:HD13	2:E:765:LEU:HD11	2.04	0.40
2:E:826:MET:HB2	2:E:868:ILE:HA	2.03	0.40
2:A:1166:LYS:HD2	2:A:1166:LYS:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1341:PHE:N	2:A:1343:PHE:O	2.48	0.40
1:F:166:THR:HG21	1:F:507:GLY:HA3	2.02	0.40
2:D:404:UNK:O	2:D:408:UNK:N	2.55	0.40
2:D:1367:ARG:HB3	2:D:1370:THR:HG21	2.04	0.40
1:G:481:ASP:O	1:G:485:ARG:N	2.55	0.40
1:G:1728:ARG:HB3	1:G:1732:ASN:HD22	1.86	0.40
2:E:394:UNK:O	2:E:396:UNK:N	2.54	0.40
2:E:1367:ARG:HB3	2:E:1370:THR:HG21	2.04	0.40
1:B:469:ARG:HH11	1:B:469:ARG:HD3	1.75	0.40
1:B:1674:GLN:NE2	1:B:1711:ILE:O	2.54	0.40
2:A:1168:LEU:HG	2:A:1169:LYS:HG2	2.02	0.40
2:A:1334:ASP:OD1	2:A:1335:PHE:N	2.53	0.40
1:F:1674:GLN:NE2	1:F:1711:ILE:O	2.54	0.40
1:F:1684:SER:O	1:F:1688:GLN:N	2.54	0.40
2:E:1051:VAL:O	2:E:1055:TRP:N	2.54	0.40
2:E:1105:LEU:HD23	2:E:1105:LEU:HA	1.87	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	B	986/2051 (48%)	739 (75%)	202 (20%)	45 (5%)	2	17
1	F	986/2051 (48%)	739 (75%)	202 (20%)	45 (5%)	2	17
1	G	986/2051 (48%)	740 (75%)	201 (20%)	45 (5%)	2	17
2	A	879/1887 (47%)	606 (69%)	231 (26%)	42 (5%)	2	16
2	D	879/1887 (47%)	606 (69%)	231 (26%)	42 (5%)	2	16
2	E	879/1887 (47%)	606 (69%)	231 (26%)	42 (5%)	2	16
3	C	69/71 (97%)	53 (77%)	16 (23%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	69/71 (97%)	53 (77%)	16 (23%)	0	100	100
3	I	69/71 (97%)	54 (78%)	15 (22%)	0	100	100
All	All	5802/12027 (48%)	4196 (72%)	1345 (23%)	261 (4%)	3	17

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	447	ASN
1	B	558	ASN
1	B	1618	PRO
1	B	1862	VAL
1	B	1925	ILE
1	B	1955	PRO
1	B	1956	ARG
1	B	1957	PRO
1	B	1986	LYS
1	B	2011	ILE
1	B	2017	LYS
2	A	617	PRO
2	A	636	PRO
2	A	645	PRO
2	A	787	LYS
2	A	1111	PHE
2	A	1159	GLU
2	A	1255	SER
1	F	447	ASN
1	F	558	ASN
1	F	1618	PRO
1	F	1862	VAL
1	F	1925	ILE
1	F	1955	PRO
1	F	1956	ARG
1	F	1957	PRO
1	F	1986	LYS
1	F	2017	LYS
2	D	617	PRO
2	D	636	PRO
2	D	645	PRO
2	D	787	LYS
2	D	1111	PHE
2	D	1159	GLU

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Mol	Chain	Res	Type
2	D	1255	SER
1	G	447	ASN
1	G	558	ASN
1	G	1618	PRO
1	G	1862	VAL
1	G	1925	ILE
1	G	1955	PRO
1	G	1956	ARG
1	G	1957	PRO
1	G	1986	LYS
1	G	2011	ILE
1	G	2017	LYS
2	E	617	PRO
2	E	636	PRO
2	E	645	PRO
2	E	787	LYS
2	E	1111	PHE
2	E	1159	GLU
2	E	1255	SER
1	B	101	ILE
1	B	547	ILE
1	B	550	VAL
1	B	1632	ILE
1	B	1637	LEU
1	B	1660	PRO
1	B	1924	ILE
1	B	1966	CYS
1	B	1968	PRO
1	B	1996	ILE
1	B	2008	GLY
1	B	2029	VAL
1	B	2045	TRP
2	A	525	TYR
2	A	526	VAL
2	A	552	LYS
2	A	553	ALA
2	A	603	ASP
2	A	605	LEU
2	A	614	ALA
2	A	618	ASN
2	A	648	ASP
2	A	667	ALA

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Mol	Chain	Res	Type
2	A	1092	LYS
2	A	1100	HIS
2	A	1158	PRO
2	A	1172	THR
1	F	101	ILE
1	F	547	ILE
1	F	550	VAL
1	F	1632	ILE
1	F	1637	LEU
1	F	1660	PRO
1	F	1924	ILE
1	F	1966	CYS
1	F	1968	PRO
1	F	1996	ILE
1	F	2008	GLY
1	F	2011	ILE
1	F	2029	VAL
1	F	2045	TRP
2	D	525	TYR
2	D	526	VAL
2	D	552	LYS
2	D	553	ALA
2	D	603	ASP
2	D	605	LEU
2	D	614	ALA
2	D	618	ASN
2	D	648	ASP
2	D	667	ALA
2	D	1092	LYS
2	D	1100	HIS
2	D	1158	PRO
2	D	1172	THR
1	G	101	ILE
1	G	547	ILE
1	G	550	VAL
1	G	1632	ILE
1	G	1637	LEU
1	G	1660	PRO
1	G	1924	ILE
1	G	1966	CYS
1	G	1968	PRO
1	G	1996	ILE

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Mol	Chain	Res	Type
1	G	2008	GLY
1	G	2029	VAL
1	G	2045	TRP
2	E	525	TYR
2	E	526	VAL
2	E	553	ALA
2	E	603	ASP
2	E	605	LEU
2	E	614	ALA
2	E	618	ASN
2	E	648	ASP
2	E	667	ALA
2	E	1092	LYS
2	E	1100	HIS
2	E	1158	PRO
2	E	1172	THR
1	B	571	LYS
1	B	1656	GLU
1	B	1947	ALA
1	B	1954	LYS
1	B	1962	ARG
1	B	2028	ASP
2	A	606	ASP
2	A	612	GLU
2	A	631	PRO
2	A	1083	PRO
2	A	1377	MET
1	F	571	LYS
1	F	1656	GLU
1	F	1947	ALA
1	F	1954	LYS
1	F	1962	ARG
1	F	2028	ASP
2	D	606	ASP
2	D	612	GLU
2	D	631	PRO
2	D	1083	PRO
2	D	1377	MET
1	G	571	LYS
1	G	1656	GLU
1	G	1947	ALA
1	G	1954	LYS

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Mol	Chain	Res	Type
1	G	1962	ARG
1	G	2028	ASP
2	E	552	LYS
2	E	606	ASP
2	E	612	GLU
2	E	631	PRO
2	E	1083	PRO
2	E	1377	MET
1	B	561	TRP
1	B	1631	MET
1	B	1716	ASN
1	B	1979	THR
1	B	2020	GLN
1	B	2021	VAL
2	A	523	SER
2	A	595	GLN
2	A	609	SER
2	A	786	SER
2	A	885	ALA
2	A	1047	LEU
2	A	1080	THR
1	F	561	TRP
1	F	1631	MET
1	F	1716	ASN
1	F	1979	THR
1	F	2020	GLN
1	F	2021	VAL
2	D	523	SER
2	D	595	GLN
2	D	609	SER
2	D	786	SER
2	D	885	ALA
2	D	1047	LEU
2	D	1080	THR
1	G	561	TRP
1	G	1631	MET
1	G	1716	ASN
1	G	1979	THR
1	G	2020	GLN
1	G	2021	VAL
2	E	523	SER
2	E	595	GLN

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Mol	Chain	Res	Type
2	E	608	ASP
2	E	609	SER
2	E	786	SER
2	E	885	ALA
2	E	1047	LEU
2	E	1080	THR
1	B	1633	ASN
1	B	1897	GLN
1	B	1944	ILE
2	A	608	ASP
2	A	613	VAL
2	A	1091	ALA
2	A	1365	MET
1	F	1633	ASN
1	F	1897	GLN
1	F	1944	ILE
2	D	608	ASP
2	D	613	VAL
2	D	1091	ALA
2	D	1365	MET
1	G	1633	ASN
1	G	1897	GLN
1	G	1944	ILE
2	E	613	VAL
2	E	1091	ALA
2	E	1365	MET
1	B	1647	ASP
2	A	581	PHE
2	A	1071	PRO
1	F	1647	ASP
2	D	581	PHE
2	D	1071	PRO
1	G	1647	ASP
2	E	581	PHE
2	E	1071	PRO
1	B	1665	VAL
1	B	1967	ILE
2	A	540	GLN
2	A	1107	GLU
1	F	1665	VAL
1	F	1967	ILE
2	D	540	GLN

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Mol	Chain	Res	Type
2	D	1107	GLU
1	G	1665	VAL
1	G	1967	ILE
2	E	540	GLN
2	E	1107	GLU
1	B	42	PRO
1	B	1648	VAL
1	F	42	PRO
1	F	1648	VAL
1	G	42	PRO
1	G	1648	VAL
1	B	1997	ILE
2	A	601	VAL
1	F	1997	ILE
2	D	601	VAL
1	G	1997	ILE
2	E	601	VAL

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	B	690/877 (79%)	672 (97%)	18 (3%)	40	61
1	F	690/877 (79%)	672 (97%)	18 (3%)	40	61
1	G	690/877 (79%)	672 (97%)	18 (3%)	40	61
2	A	610/845 (72%)	597 (98%)	13 (2%)	47	65
2	D	610/845 (72%)	597 (98%)	13 (2%)	47	65
2	E	610/845 (72%)	597 (98%)	13 (2%)	47	65
3	C	64/64 (100%)	61 (95%)	3 (5%)	23	45
3	H	64/64 (100%)	61 (95%)	3 (5%)	23	45
3	I	64/64 (100%)	61 (95%)	3 (5%)	23	45
All	All	4092/5358 (76%)	3990 (98%)	102 (2%)	42	62

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	GLN
1	B	73	GLU
1	B	101	ILE
1	B	202	THR
1	B	291	SER
1	B	368	ILE
1	B	400	SER
1	B	414	LEU
1	B	459	VAL
1	B	472	SER
1	B	480	VAL
1	B	482	CYS
1	B	523	THR
1	B	541	TYR
1	B	1893	VAL
1	B	1917	ILE
1	B	1924	ILE
1	B	1926	GLU
2	A	797	THR
2	A	878	MET
2	A	905	LEU
2	A	940	THR
2	A	943	LEU
2	A	1068	LYS
2	A	1229	THR
2	A	1240	VAL
2	A	1243	VAL
2	A	1254	VAL
2	A	1292	ILE
2	A	1294	SER
2	A	1333	ASP
3	C	1461	ASP
3	C	1478	PRO
3	C	1499	SER
1	F	36	GLN
1	F	73	GLU
1	F	101	ILE
1	F	202	THR
1	F	291	SER
1	F	368	ILE
1	F	400	SER
1	F	414	LEU

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Mol	Chain	Res	Type
1	F	459	VAL
1	F	472	SER
1	F	480	VAL
1	F	482	CYS
1	F	523	THR
1	F	541	TYR
1	F	1893	VAL
1	F	1917	ILE
1	F	1924	ILE
1	F	1926	GLU
2	D	797	THR
2	D	878	MET
2	D	905	LEU
2	D	940	THR
2	D	943	LEU
2	D	1068	LYS
2	D	1229	THR
2	D	1240	VAL
2	D	1243	VAL
2	D	1254	VAL
2	D	1292	ILE
2	D	1294	SER
2	D	1333	ASP
3	H	1461	ASP
3	H	1478	PRO
3	H	1499	SER
1	G	36	GLN
1	G	73	GLU
1	G	101	ILE
1	G	202	THR
1	G	291	SER
1	G	368	ILE
1	G	400	SER
1	G	414	LEU
1	G	459	VAL
1	G	472	SER
1	G	480	VAL
1	G	482	CYS
1	G	523	THR
1	G	541	TYR
1	G	1893	VAL
1	G	1917	ILE

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Mol	Chain	Res	Type
1	G	1924	ILE
1	G	1926	GLU
2	E	797	THR
2	E	878	MET
2	E	905	LEU
2	E	940	THR
2	E	943	LEU
2	E	1068	LYS
2	E	1229	THR
2	E	1240	VAL
2	E	1243	VAL
2	E	1254	VAL
2	E	1292	ILE
2	E	1294	SER
2	E	1333	ASP
3	I	1461	ASP
3	I	1478	PRO
3	I	1499	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	ASN
1	B	110	GLN
1	B	248	HIS
1	B	273	HIS
1	B	348	GLN
1	B	350	GLN
1	B	354	ASN
1	B	440	ASN
1	B	495	GLN
1	B	1674	GLN
1	B	1696	ASN
1	B	1872	GLN
1	B	1892	ASN
1	B	1896	GLN
1	B	1939	HIS
2	A	694	GLN
2	A	698	GLN
2	A	798	ASN
2	A	860	ASN
2	A	1066	ASN

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Mol	Chain	Res	Type
2	A	1271	GLN
2	A	1276	GLN
2	A	1351	ASN
3	C	1495	ASN
3	C	1510	ASN
1	F	85	ASN
1	F	110	GLN
1	F	125	ASN
1	F	248	HIS
1	F	273	HIS
1	F	348	GLN
1	F	350	GLN
1	F	354	ASN
1	F	440	ASN
1	F	495	GLN
1	F	1674	GLN
1	F	1696	ASN
1	F	1872	GLN
1	F	1892	ASN
1	F	1896	GLN
1	F	1939	HIS
2	D	694	GLN
2	D	698	GLN
2	D	798	ASN
2	D	860	ASN
2	D	882	ASN
2	D	1066	ASN
2	D	1271	GLN
2	D	1276	GLN
2	D	1351	ASN
3	H	1495	ASN
3	H	1510	ASN
1	G	85	ASN
1	G	110	GLN
1	G	248	HIS
1	G	273	HIS
1	G	348	GLN
1	G	350	GLN
1	G	354	ASN
1	G	495	GLN
1	G	1674	GLN
1	G	1696	ASN

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Mol	Chain	Res	Type
1	G	1892	ASN
1	G	1896	GLN
1	G	1939	HIS
2	E	694	GLN
2	E	698	GLN
2	E	798	ASN
2	E	860	ASN
2	E	1066	ASN
2	E	1271	GLN
2	E	1276	GLN
2	E	1351	ASN
3	I	1494	HIS
3	I	1495	ASN
3	I	1510	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

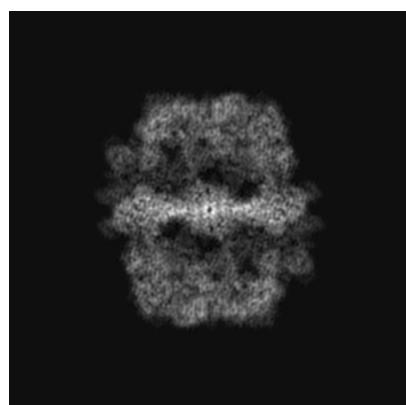
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9882. These allow visual inspection of the internal detail of the map and identification of artifacts.

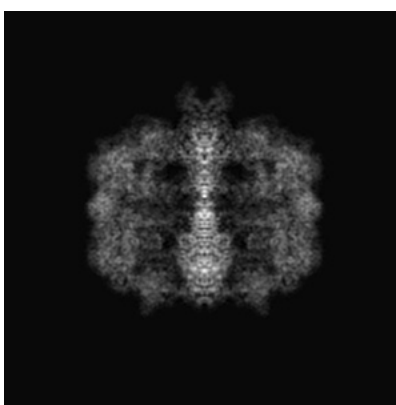
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

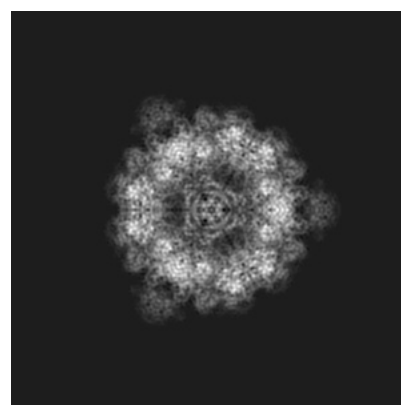
6.1.1 Primary map



X



Y



Z

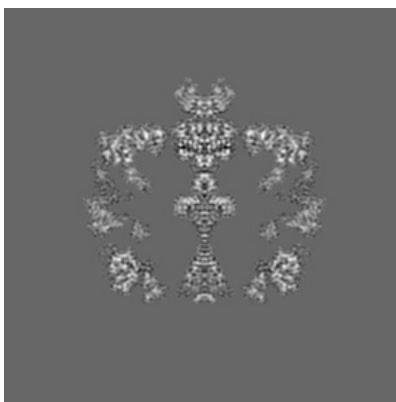
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

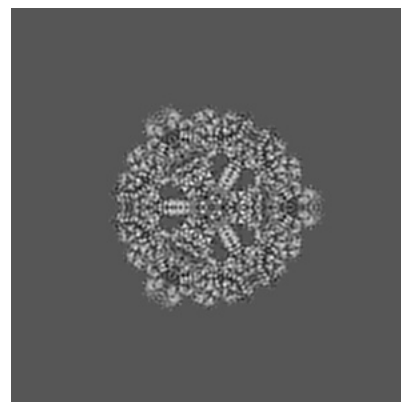
6.2.1 Primary map



X Index: 168



Y Index: 168

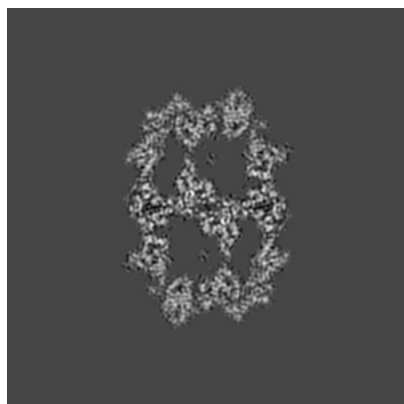


Z Index: 168

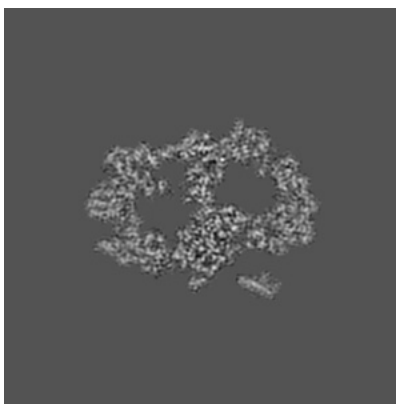
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

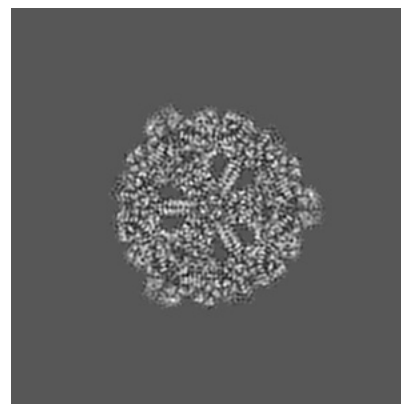
6.3.1 Primary map



X Index: 213



Y Index: 218

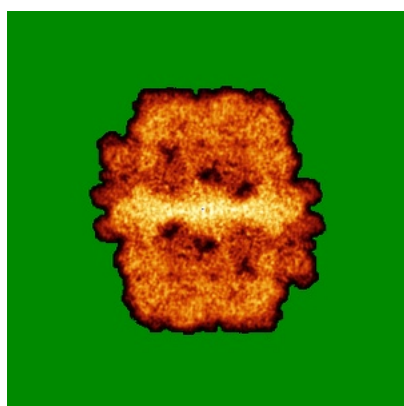


Z Index: 167

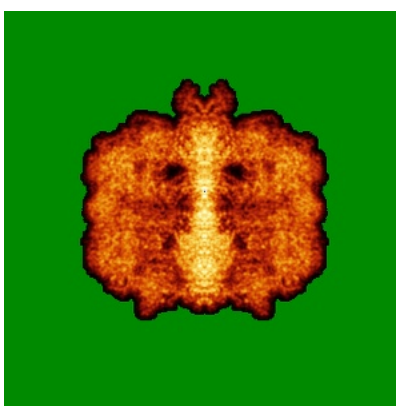
The images above show the largest variance slices of the map in three orthogonal directions.

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

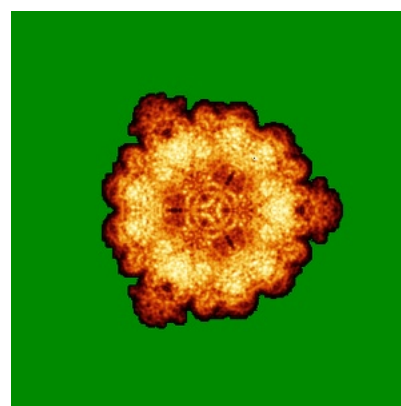
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

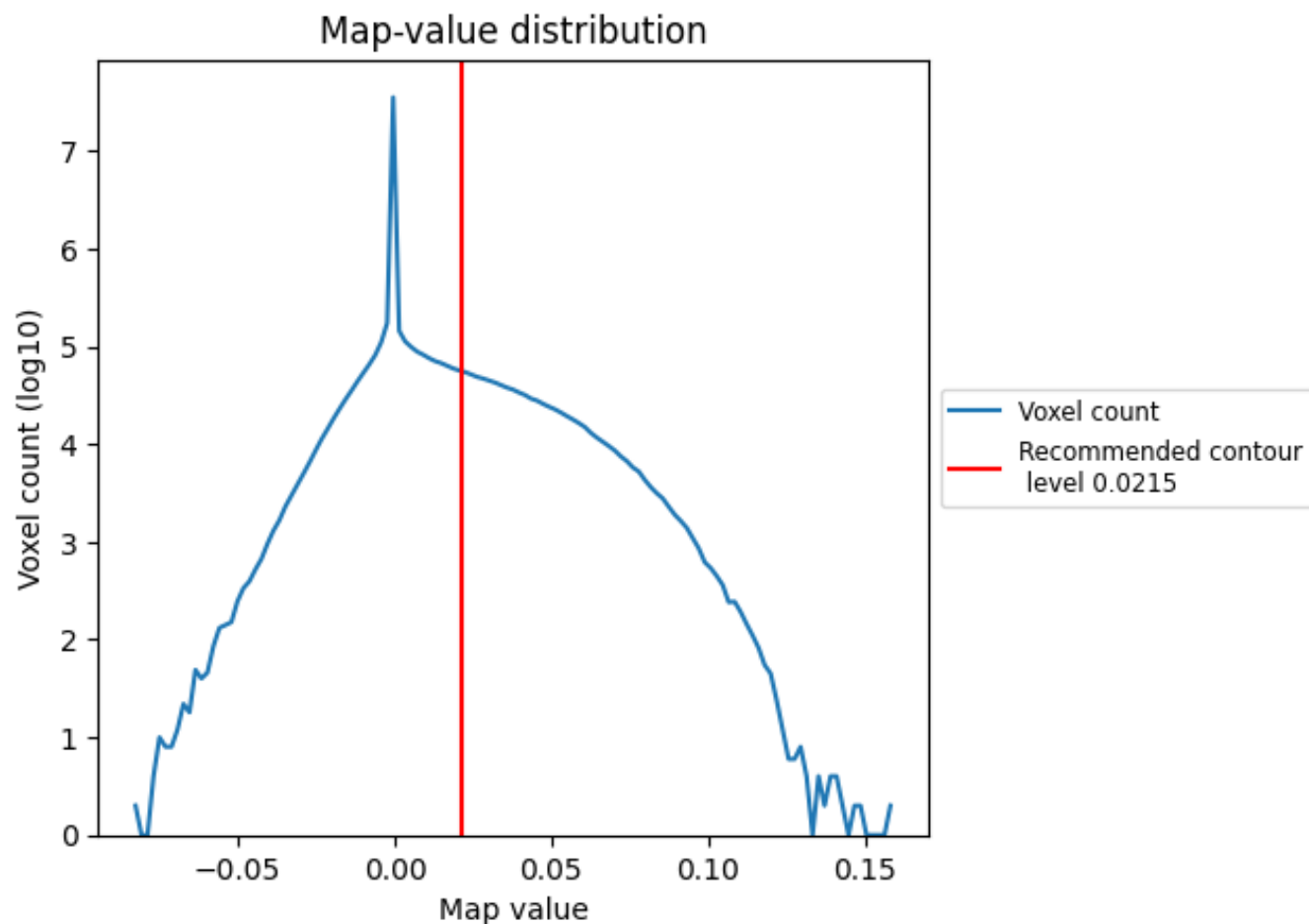
6.6 Mask visualisation

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

7 Map analysis [i](#)

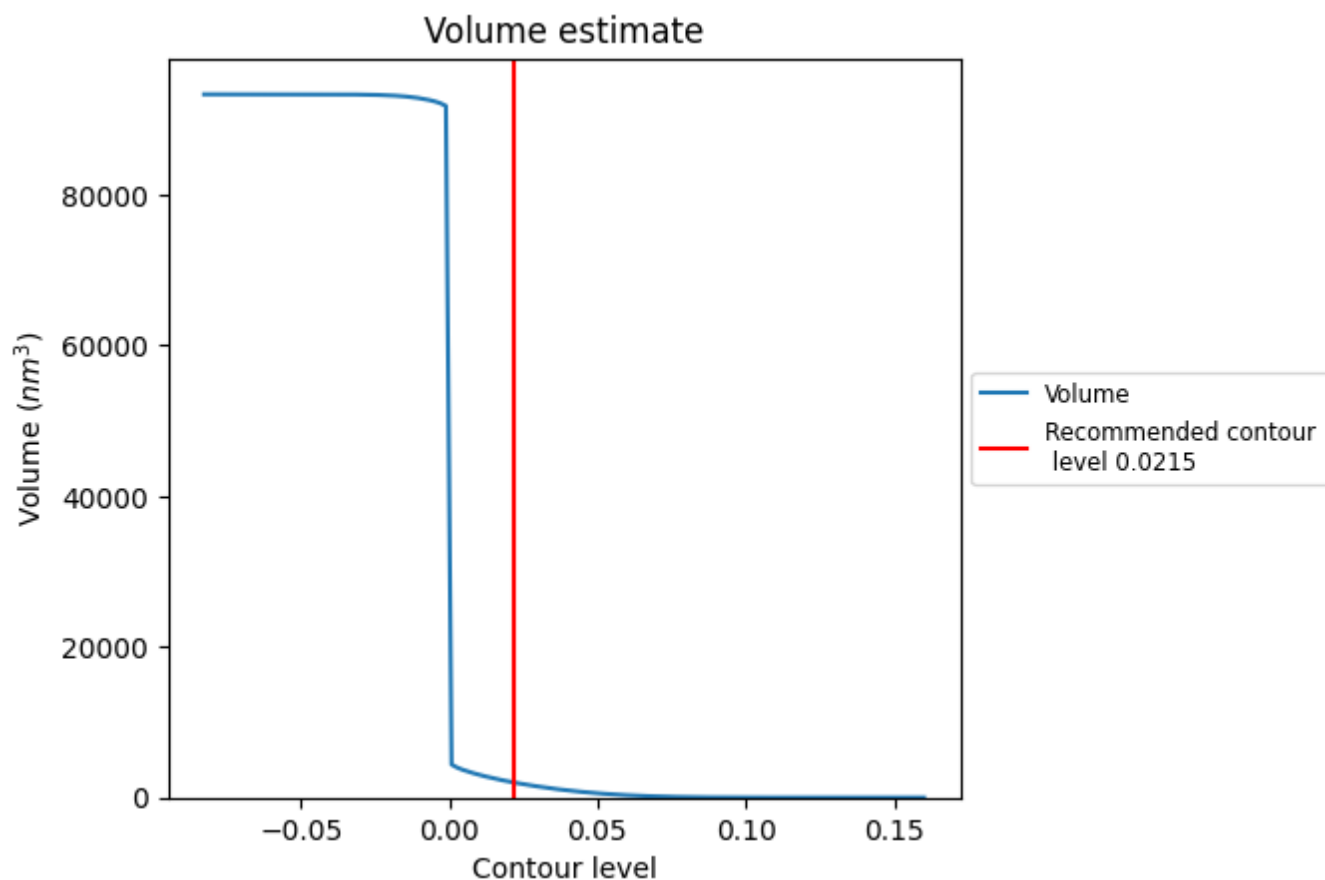
This section contains the results of statistical analysis of the map.

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.

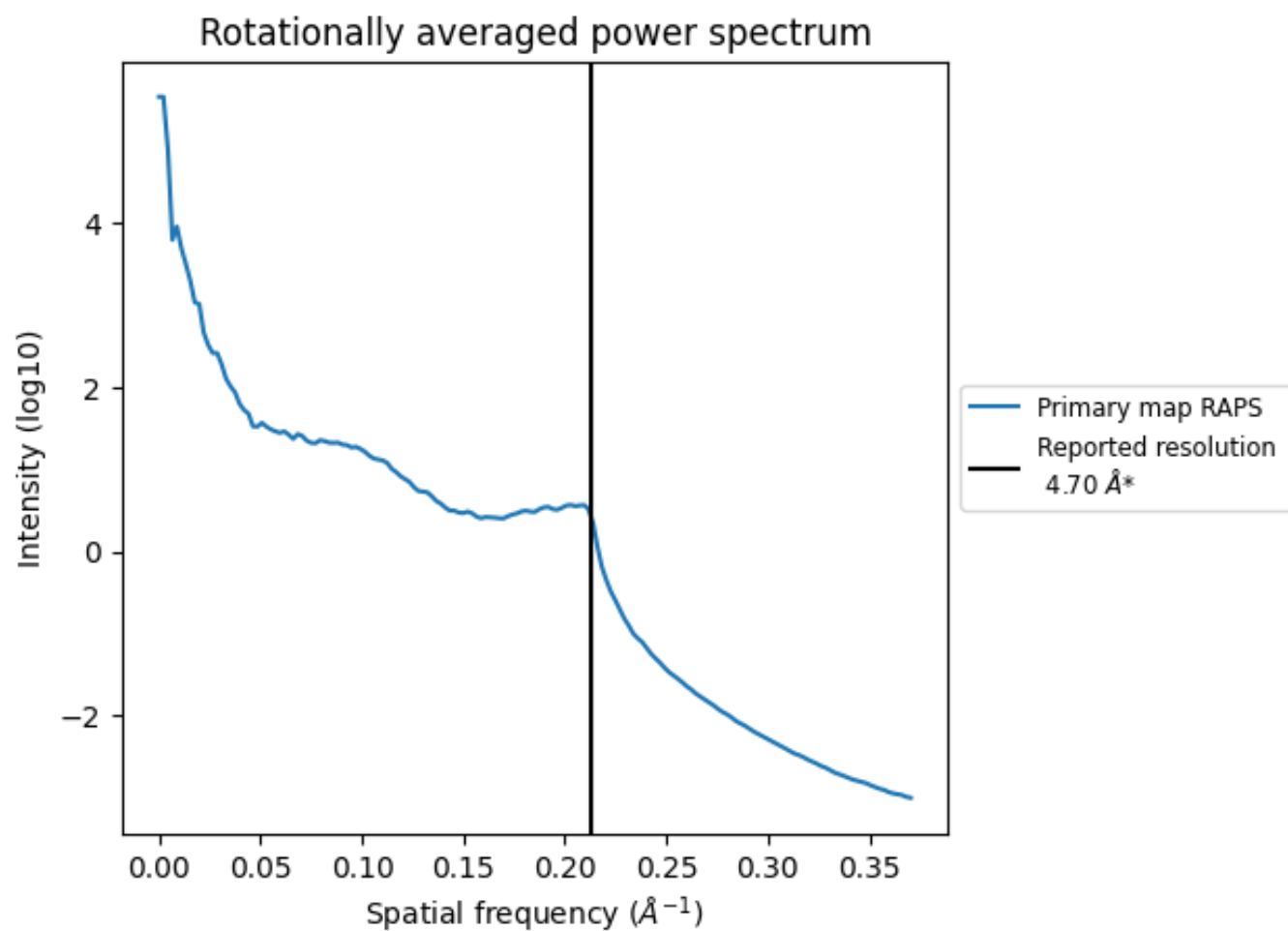
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2026 nm³; this corresponds to an approximate mass of 1830 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 0.213 Å⁻¹

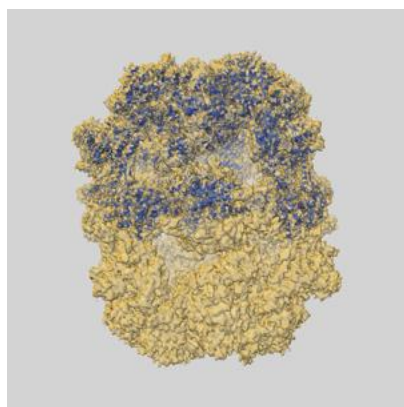
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

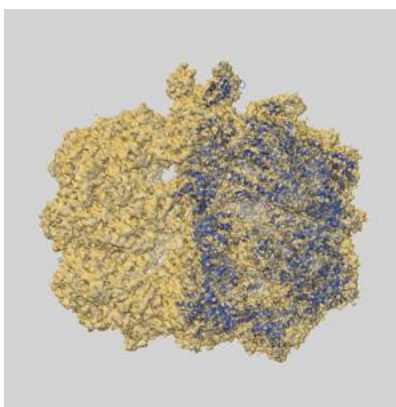
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9882 and PDB model 6JSI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

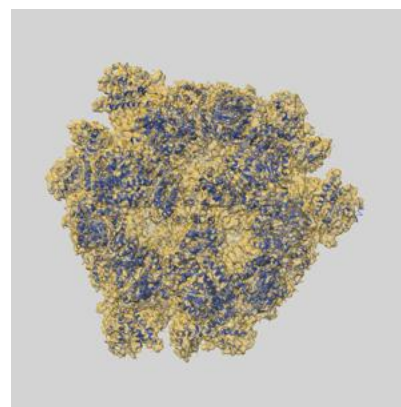
9.1 Map-model overlay [i](#)



X



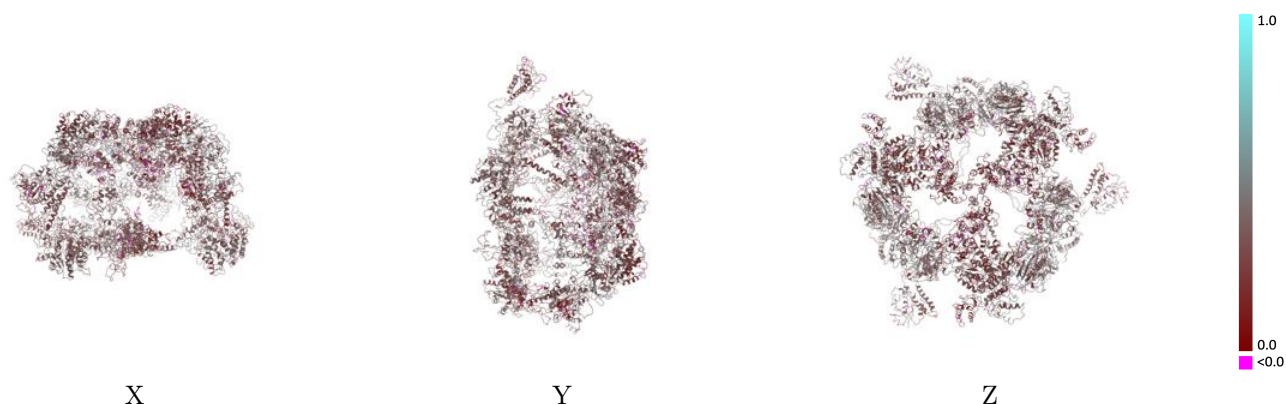
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0215 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](#)

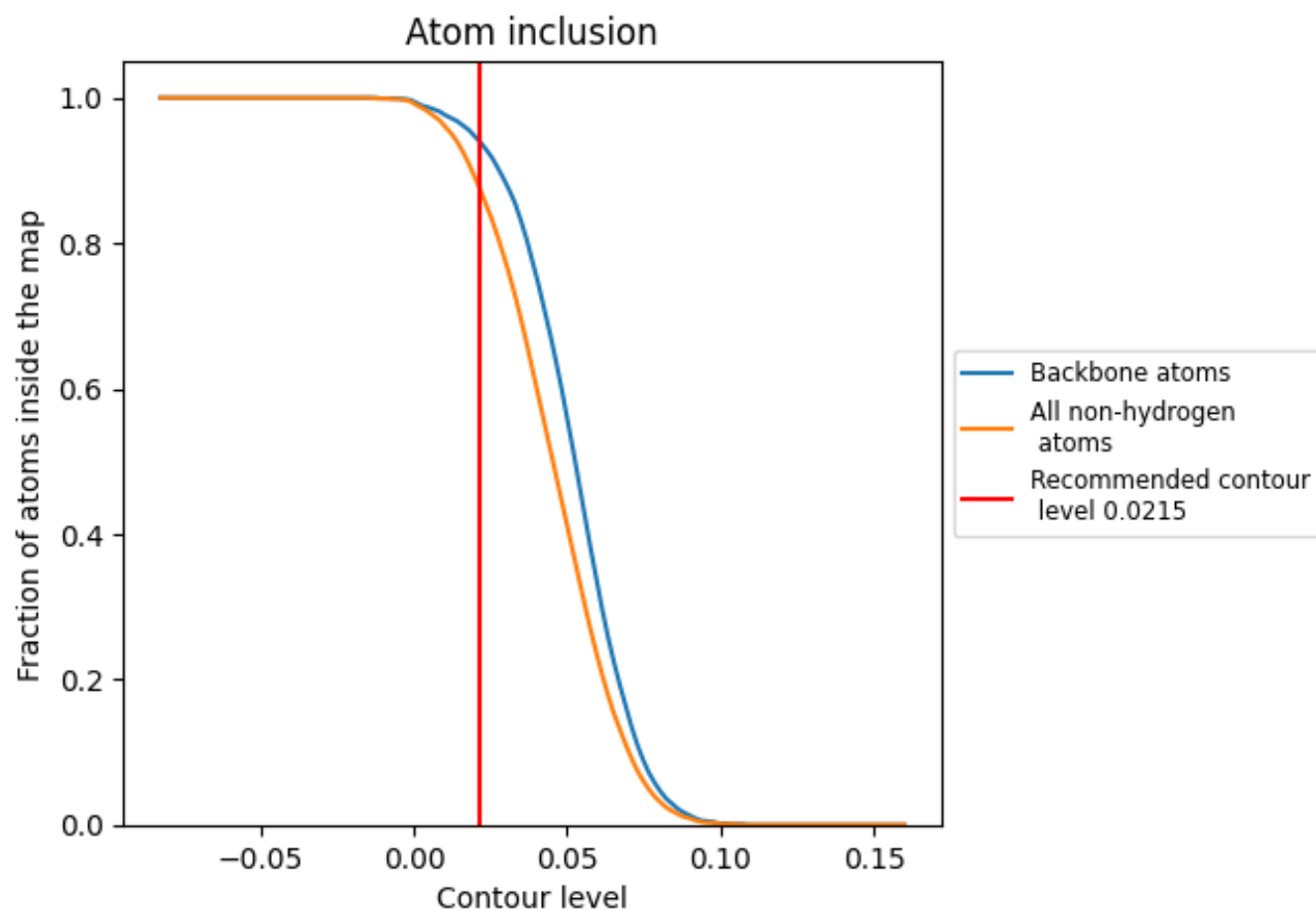


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.0215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8760	0.3360
A	0.8620	0.3400
B	0.8870	0.3360
C	0.8260	0.2770
D	0.8650	0.3390
E	0.8660	0.3410
F	0.8870	0.3360
G	0.8880	0.3360
H	0.8240	0.2760
I	0.8260	0.2790

1.0

0.0

<0.0