



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:33 AM UTC

PDB ID : 8ZU8 / pdb_00008zu8
EMDB ID : EMD-60481
Title : Human PIEZO1-A1988V
Authors : Zhang, M.F.
Deposited on : 2024-06-08
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

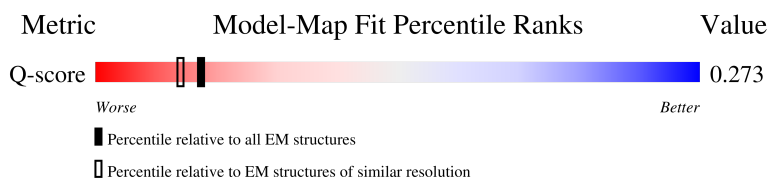
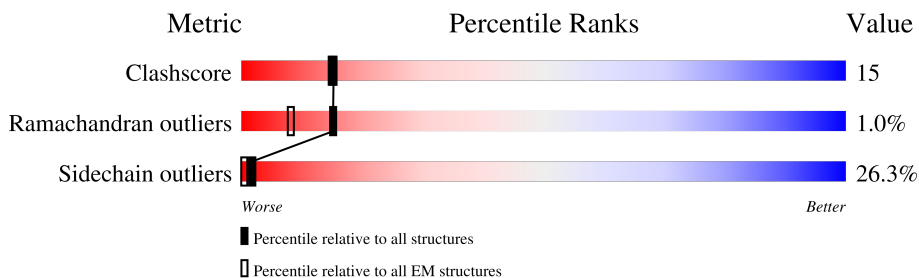
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	A	1952	
1	B	1952	
1	C	1952	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 31401 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.

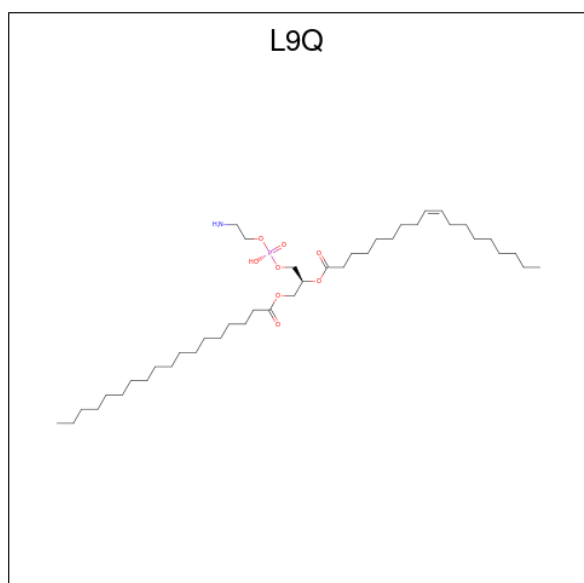
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1279	Total	C	N	O	S	0	0
			10418	6910	1721	1726	61		
1	B	1279	Total	C	N	O	S	0	0
			10418	6910	1721	1726	61		
1	C	1279	Total	C	N	O	S	0	0
			10412	6907	1718	1726	61		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1988	VAL	ALA	engineered mutation	UNP Q92508
B	1988	VAL	ALA	engineered mutation	UNP Q92508
C	1988	VAL	ALA	engineered mutation	UNP Q92508

- Molecule 2 is (1S)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxymethyl)ethyl (9Z)-octadec-9-enoate (CCD ID: L9Q) (formula: C₄₁H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).

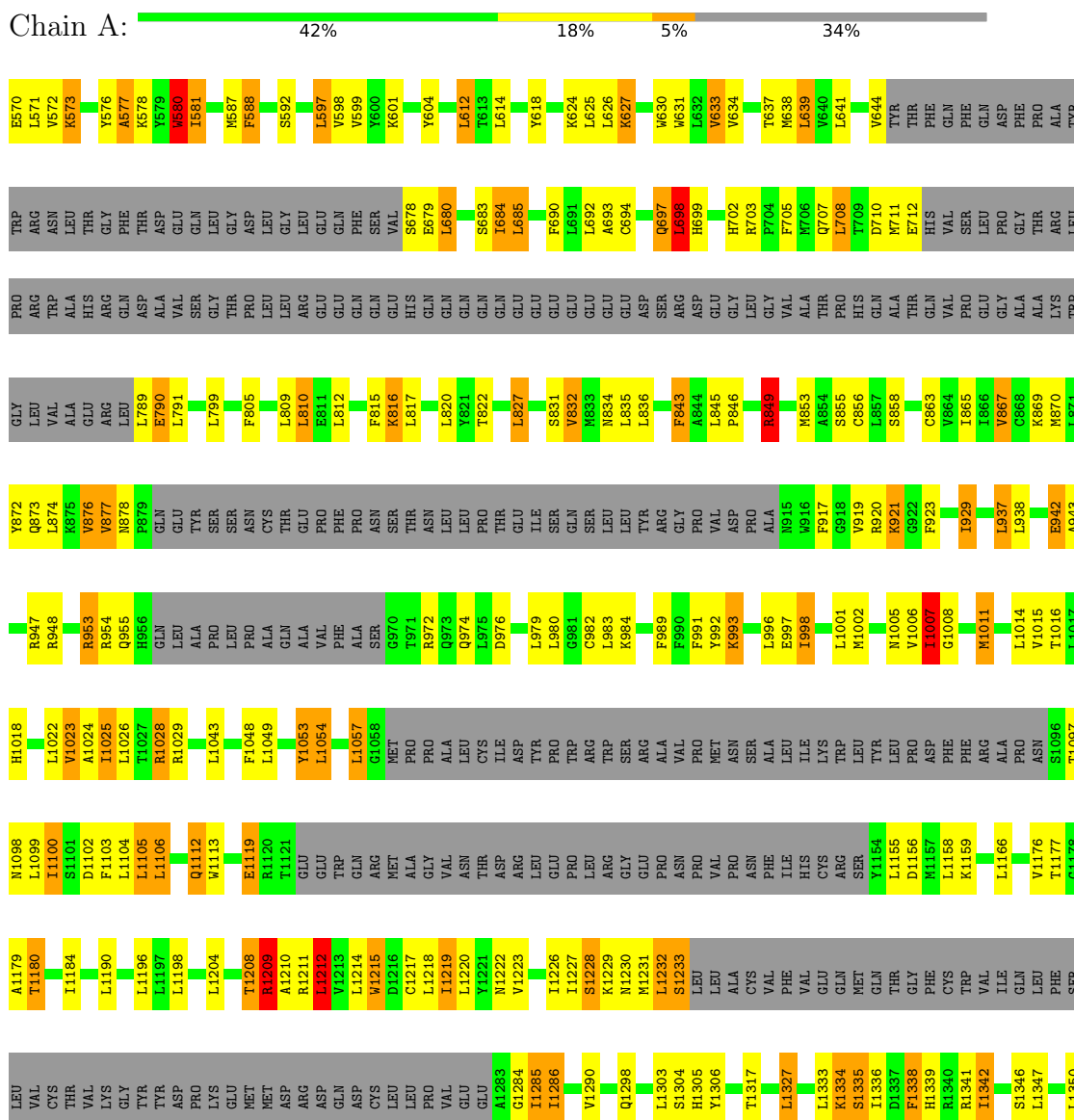


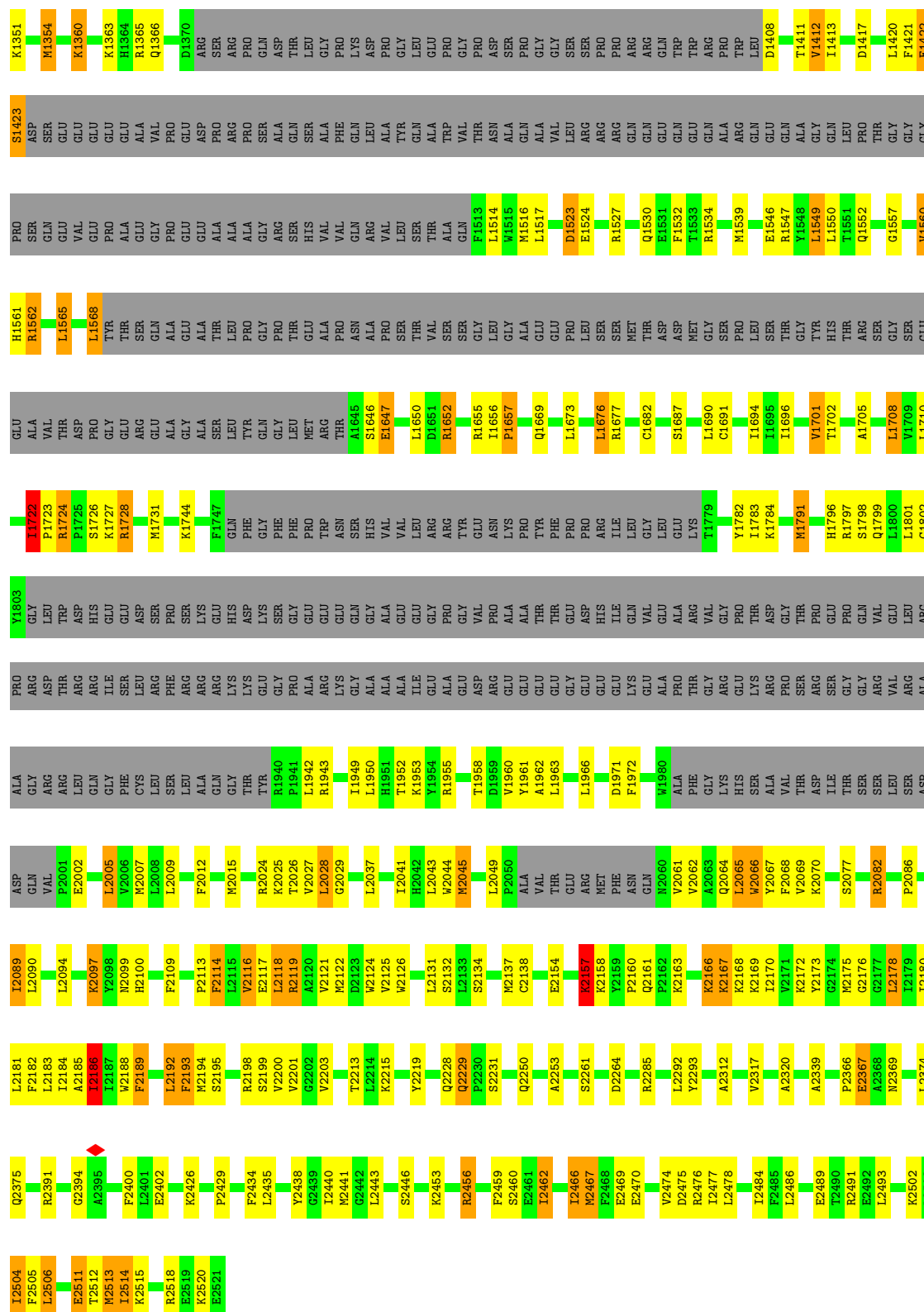
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 51	C 41	N 1	O 8	P 1	0
2	B	1	Total 51	C 41	N 1	O 8	P 1	0
2	C	1	Total 51	C 41	N 1	O 8	P 1	0

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: Piezo-type mechanosensitive ion channel component 1

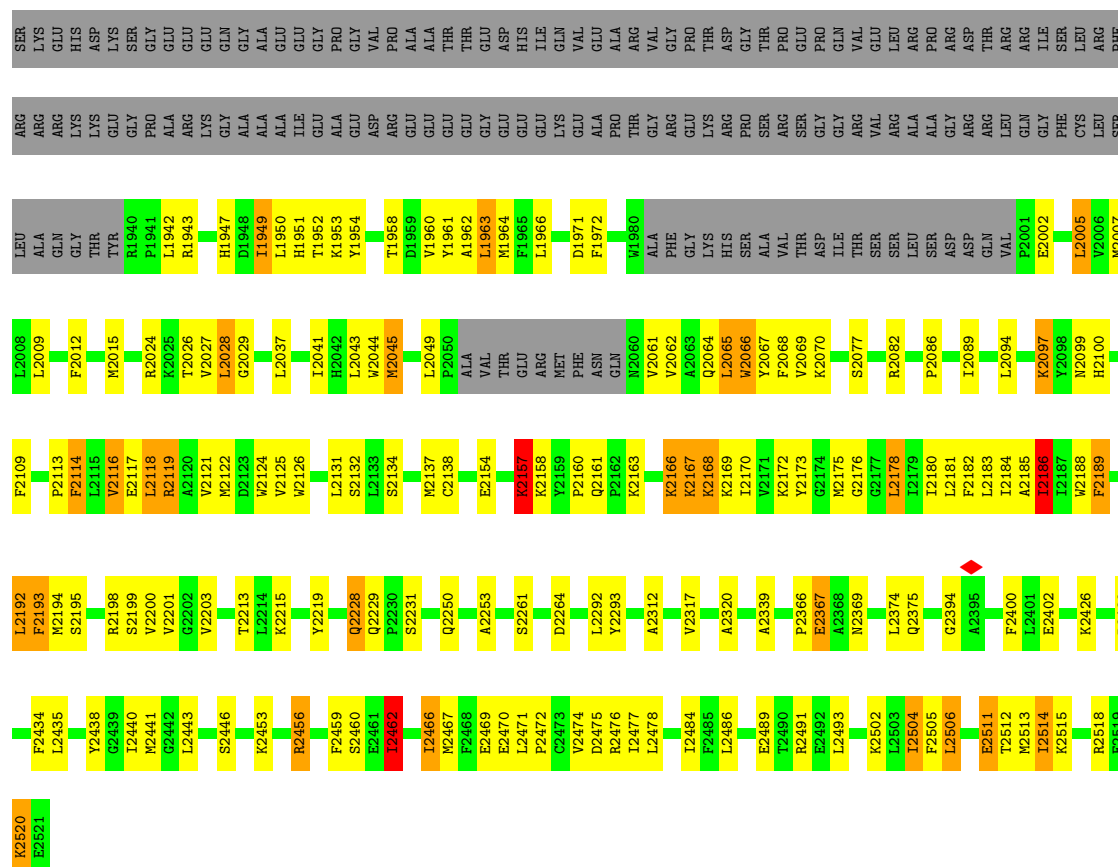




- Molecule 1: Piezo-type mechanosensitive ion channel component 1

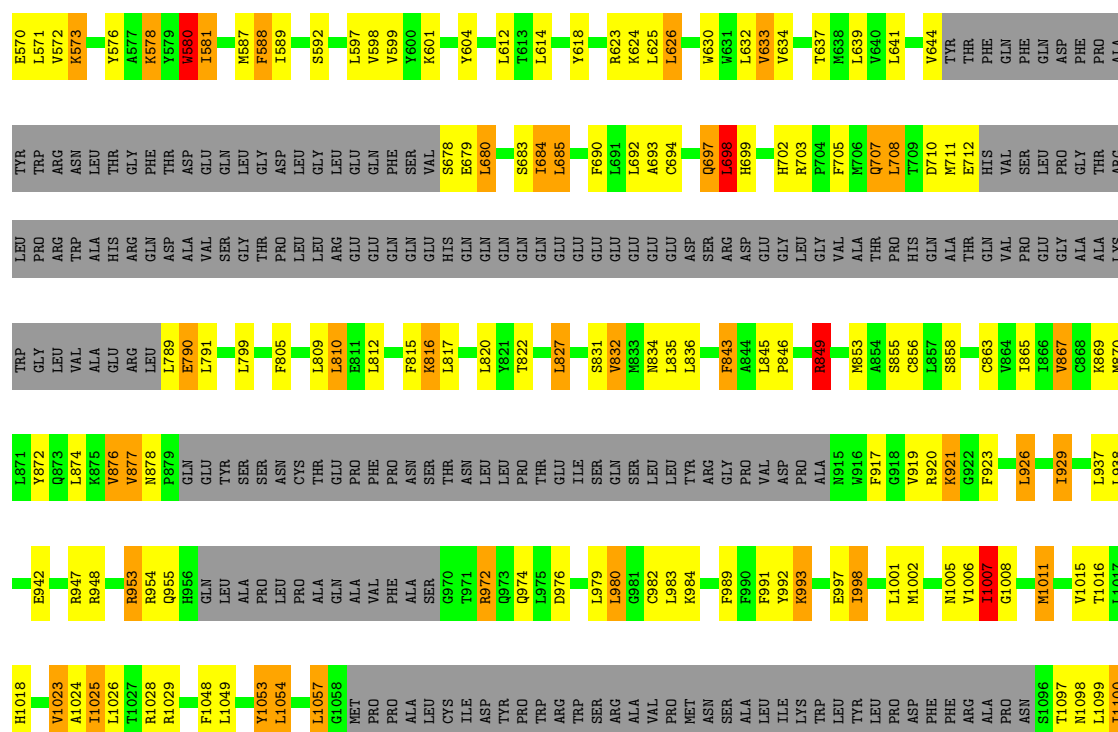
Chain B: 43% 17% 5% 34%





• Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain C: 43% 17% 5% 34%



F2434	M2194	P2113	L2008	LEU	ARG	SER	M1731	ALA	ALA	PRO	PRO	D1370	Tyr	L1184	S1101
L2435	S2195	F2114	L2009	SER	PHE	LEU	K1744	GLY	GLU	GLU	GLU	D1370	ASP	L1190	D1102
Y2438	R2198	L2115	F2012	ALA	ARG	ALA	K1744	ALA	ALA	ASP	PRO	ARG	PRO	L1103	F1103
V2440	S2199	E2116	M2015	GLN	ARG	LEU	F1747	LEU	ALA	LEU	ARG	PRO	GLY	L1106	L1104
M2441	V2201	R2119	L2024	THR	LYS	GLN	F1747	GLN	ALA	PRO	PRO	PRO	MET	L1204	L1105
G2442	G2203	K2120	R2024	TYR	GLY	PHE	F1747	GLY	GLY	ASP	SER	ASP	MET	L1204	L1106
L2443	V2121	V2121	K2025	TYR	LYS	GLY	F1747	GLY	ARG	GLY	GLN	ASP	ASP	Q1112	Q1112
T2213	G2123	G2123	V2027	GLY	GLY	PHE	F1747	GLY	THR	GLN	ALA	THR	ASP	W1113	W1113
L2214	L2124	L2124	V2027	ALA	ALA	PHE	F1747	GLY	GLY	GLN	ALA	THR	ASP	R1209	R1209
K2215	G2125	G2125	L2028	ALA	ALA	GLY	F1747	GLY	VAL	VAL	ALA	GLY	ASP	A1210	A1210
Y2219	V2125	V2125	G2029	LYS	LYS	GLU	F1747	THR	ASN	VAL	PHE	PRO	ASP	R1210	R1210
Q2228	W2126	W2126	L2037	GLY	GLY	GLN	F1747	S1645	ALA	GLN	GLN	LYS	ASP	R1212	R1212
Q2229	L2131	L2131	L2041	ALA	ALA	GLY	F1747	E1647	PRO	VAL	VAL	PRO	LEU	V1213	V1213
S2230	S2132	S2132	H2041	LYS	LYS	ALA	F1747	E1647	SER	THR	TYR	GLY	PRO	W1214	W1214
S2231	L2133	L2133	H2042	ILE	ILE	GLU	F1747	D1650	THR	THR	GLN	LEU	GLY	I1219	I1219
S2231	S2134	S2134	L2043	GLU	GLU	GLY	F1747	D1651	VAL	VAL	ALA	GLY	GLY	L1220	L1220
Q2250	W2137	W2137	W2044	ALA	ALA	PRO	F1747	R1652	SER	THR	THR	PRO	GLY	W1223	W1223
A2253	C2138	C2138	M2045	ASP	ASP	VAL	F1747	R1655	GLY	THR	VAL	PRO	GLY	I1226	I1226
S2261	E2154	E2154	L2049	GLU	GLU	ALA	F1747	P1657	GLY	GLY	ALA	PRO	ASP	I1227	I1227
E2470	K2157	K2157	P2050	GLU	GLU	ALA	F1747	P1657	GLY	GLY	ALA	PRO	ASP	S1228	S1228
D2264	R2158	R2158	VAL	VAL	VAL	THR	F1747	Q1669	GLU	GLY	VAL	GLY	GLY	K1229	K1229
P2472	Y2159	Y2159	GLU	GLU	GLU	THR	F1747	L1673	PRO	LEU	ARG	SER	LEU	M1231	M1231
R2285	L2160	L2160	THR	THR	THR	ASP	F1747	L1676	SER	ARG	ARG	PRO	PRO	L1232	L1232
C2473	Q2161	Q2161	MET	MET	MET	ASP	F1747	R1677	SER	ARG	ARG	PRO	LEU	S1233	S1233
V2474	P2162	P2162	PHE	PHE	PHE	ILE	F1747	C1682	THR	GLN	GLN	ARG	ARG	LEU	LEU
D2475	K2163	K2163	ASN	ASN	ASN	LEU	F1747	C1682	THR	GLN	GLN	ARG	ARG	GLY	GLY
R2476	L2166	L2166	GLN	GLN	GLN	GLY	F1747	S1687	ASP	GLU	GLU	GLN	GLY	ALA	ALA
T2477	K2167	K2167	N2060	ALA	ALA	VAL	F1747	S1687	ASP	GLU	GLU	TRP	TRP	CYS	CYS
T2484	R2167	R2167	V2061	PHE	PRO	ALA	F1747	F1532	ASP	GLY	GLY	TRP	TRP	VAL	VAL
F2485	K2168	K2168	A2063	GLY	THR	ALA	F1747	F1532	ASP	GLY	GLY	TRP	TRP	PHE	PHE
L2486	L2170	L2170	Q2064	LYS	ARG	VAL	F1747	R1534	GLY	GLN	GLN	ARG	ARG	VAL	VAL
E2489	V2171	V2171	W2066	HIS	GLY	PRO	F1747	M1539	PRO	ARG	ARG	TRP	TRP	GLU	GLU
T2490	K2172	K2172	L2065	SER	LYS	THR	F1747	E1546	THR	GLN	GLN	LEU	LEU	ASN	ASN
R2491	Y2173	Y2173	Y2067	ALA	ARG	ASP	F1747	R1547	THR	GLY	GLY	GLN	GLN	ILE	ILE
E2492	G2174	G2174	F2068	VAL	PRO	GLY	F1747	R1548	GLY	ALA	ALA	THR	THR	THR	THR
L2493	R2175	R2175	V2069	THR	SER	THR	F1747	L1549	TYR	GLY	GLY	GLY	GLY	CYS	CYS
K2502	G2176	G2176	K2070	ASP	ARG	PRO	F1747	L1550	HIS	THR	LEU	I1413	I1341	ARG	ARG
L2503	G2177	G2177	S2077	ILE	SER	GLY	F1747	T1551	THR	THR	PRO	D1417	I1342	SER	SER
L2504	L2178	L2178	R2082	THR	GLY	PRO	F1747	Q1552	ARG	GLY	THR	D1417	I1342	Y1154	Y1154
F2505	T2180	T2180	R2082	SER	GLY	GLN	F1747	G1557	GLY	THR	THR	L1420	S1346	L1155	L1155
L2506	L2181	L2181	P2086	LEU	VAL	VAL	F1747	G1557	GLY	GLY	GLY	F1421	S1346	M1157	M1157
E2511	F2182	F2182	P2086	SER	ARG	ARG	F1747	V1560	GLY	GLY	GLY	E1422	S1346	L1158	L1158
T2512	L2183	L2183	I2089	ASP	ALA	ALA	F1747	R1561	GLY	PRO	PRO	S1423	K1351	K1159	K1159
M2513	L2184	L2184	L2094	ASP	GLY	GLY	F1747	R1562	VAL	SER	SER	ASP	M1354	PHE	PHE
L2514	G2186	G2186	L2094	VAL	ARG	ARG	F1747	R1565	THR	GLN	GLN	GLY	M1354	LEU	LEU
K2515	L2187	L2187	K2097	VAL	ARG	THR	F1747	L1565	VAL	VAL	VAL	GLY	M1354	VAL	VAL
E2518	V2188	V2188	Y2096	P2001	ARG	ARG	F1747	L1568	PRO	GLY	GLY	GLY	K1360	CYS	CYS
E2519	F2189	F2189	W2006	E2002	LEU	THR	F1747	L1568	GLY	GLY	GLY	GLY	K1360	THR	THR
K2520	L2192	L2192	H2100	L2005	GLN	ARG	F1747	T1726	TYR	PRO	PRO	GLY	K1363	VAL	VAL
	F2193	F2193		W2007	PHE	ILE	F1747	R1727	THR	ALA	ALA	GLY	H1364	LYS	LYS
					SER	SER	F1747	R1728	ARG	GLY	GLY	ALA	T1180	GLY	GLY
					LEU	ASP	F1747		GLU	ASP	VAL	VAL	Q1366	TYR	TYR

EMD-60481

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.525	Depositor
Minimum map value	-0.286	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	434.688, 434.688, 434.688	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.849, 0.849, 0.849	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: L9Q

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	2/10678 (0.0%)	0.98	52/14479 (0.4%)
1	B	0.74	1/10678 (0.0%)	0.98	50/14479 (0.3%)
1	C	0.74	1/10672 (0.0%)	0.98	50/14472 (0.3%)
All	All	0.74	4/32028 (0.0%)	0.98	152/43430 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	ALA	C-O	-6.54	1.15	1.24
1	B	2099	ASN	CA-C	-5.62	1.50	1.53
1	C	2099	ASN	CA-C	-5.55	1.50	1.53
1	A	2099	ASN	CA-C	-5.50	1.50	1.53

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	684	ILE	N-CA-C	-10.51	103.39	111.90
1	B	684	ILE	N-CA-C	-10.48	103.41	111.90
1	A	684	ILE	N-CA-C	-10.47	103.42	111.90
1	A	1025	ILE	N-CA-C	-10.24	103.60	111.90
1	C	1025	ILE	N-CA-C	-10.22	103.62	111.90
1	B	1025	ILE	N-CA-C	-10.20	103.64	111.90
1	C	2466	ILE	N-CA-C	-9.95	101.78	113.42
1	B	2466	ILE	N-CA-C	-9.94	101.80	113.42
1	A	2466	ILE	N-CA-C	-9.93	101.81	113.42
1	A	2506	LEU	N-CA-C	-9.65	101.05	113.12
1	C	2506	LEU	N-CA-C	-9.65	101.06	113.12
1	B	2506	LEU	N-CA-C	-9.64	101.07	113.12
1	C	1177	THR	N-CA-C	-9.23	102.15	113.41
1	A	1177	THR	N-CA-C	-9.22	102.16	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1177	THR	N-CA-C	-9.22	102.16	113.41
1	C	1054	LEU	N-CA-C	-8.40	101.90	112.90
1	A	1054	LEU	N-CA-C	-8.39	101.91	112.90
1	B	1054	LEU	N-CA-C	-8.38	101.92	112.90
1	C	1098	ASN	N-CA-C	-8.30	102.35	114.39
1	A	1098	ASN	N-CA-C	-8.29	102.36	114.39
1	B	1098	ASN	N-CA-C	-8.29	102.38	114.39
1	C	923	PHE	CA-C-N	-7.47	111.08	120.79
1	C	923	PHE	C-N-CA	-7.47	111.08	120.79
1	C	2484	ILE	N-CA-C	-7.45	103.19	110.72
1	B	2484	ILE	N-CA-C	-7.40	103.25	110.72
1	A	2484	ILE	N-CA-C	-7.40	103.25	110.72
1	C	1057	LEU	N-CA-C	-7.37	104.82	113.88
1	B	1057	LEU	N-CA-C	-7.36	104.82	113.88
1	A	1057	LEU	N-CA-C	-7.36	104.83	113.88
1	A	2493	LEU	N-CA-C	7.31	121.64	112.87
1	C	2493	LEU	N-CA-C	7.31	121.64	112.87
1	B	2493	LEU	N-CA-C	7.30	121.63	112.87
1	C	1119	GLU	N-CA-C	-7.11	104.08	112.89
1	A	1119	GLU	N-CA-C	-7.08	104.11	112.89
1	B	1119	GLU	N-CA-C	-7.08	104.12	112.89
1	B	1722	ILE	CA-C-N	-7.05	111.03	119.84
1	B	1722	ILE	C-N-CA	-7.05	111.03	119.84
1	A	834	ASN	N-CA-C	-6.94	104.00	113.30
1	C	834	ASN	N-CA-C	-6.93	104.01	113.30
1	B	834	ASN	N-CA-C	-6.92	104.03	113.30
1	B	1412	VAL	N-CA-C	-6.91	105.87	111.81
1	A	1412	VAL	N-CA-C	-6.89	105.89	111.81
1	C	1412	VAL	N-CA-C	-6.88	105.89	111.81
1	B	634	VAL	N-CA-C	-6.80	102.87	110.62
1	A	1724	ARG	CA-C-N	-6.75	112.70	119.93
1	A	1724	ARG	C-N-CA	-6.75	112.70	119.93
1	C	1180	THR	N-CA-C	-6.60	105.77	113.88
1	A	1180	THR	N-CA-C	-6.59	105.78	113.88
1	B	1180	THR	N-CA-C	-6.57	105.80	113.88
1	B	923	PHE	CA-C-N	-6.56	112.27	120.79
1	B	923	PHE	C-N-CA	-6.56	112.27	120.79
1	C	1724	ARG	CA-C-N	-6.56	112.92	119.93
1	C	1724	ARG	C-N-CA	-6.56	112.92	119.93
1	A	1290	VAL	N-CA-C	-6.51	103.98	110.62
1	B	2157	LYS	N-CA-C	-6.51	105.88	113.88
1	C	2157	LYS	N-CA-C	-6.50	105.88	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2157	LYS	N-CA-C	-6.50	105.89	113.88
1	C	1290	VAL	N-CA-C	-6.47	104.02	110.62
1	B	1290	VAL	N-CA-C	-6.47	104.02	110.62
1	B	843	PHE	N-CA-C	-6.47	103.67	113.89
1	C	843	PHE	N-CA-C	-6.46	103.67	113.89
1	A	843	PHE	N-CA-C	-6.46	103.69	113.89
1	B	1708	LEU	N-CA-C	-6.45	105.95	113.88
1	C	1708	LEU	N-CA-C	-6.44	105.96	113.88
1	B	1106	LEU	N-CA-C	-6.43	104.92	112.89
1	A	1106	LEU	N-CA-C	-6.42	104.93	112.89
1	A	1708	LEU	N-CA-C	-6.41	105.99	113.88
1	C	1106	LEU	N-CA-C	-6.40	104.95	112.89
1	A	923	PHE	CA-C-N	-6.35	112.54	120.79
1	A	923	PHE	C-N-CA	-6.35	112.54	120.79
1	A	1212	LEU	N-CA-C	6.30	118.23	111.36
1	B	2394	GLY	N-CA-C	-6.08	106.53	115.72
1	A	2394	GLY	N-CA-C	-6.08	106.55	115.72
1	C	2394	GLY	N-CA-C	-6.06	106.57	115.72
1	A	1722	ILE	CA-C-N	-6.03	112.31	119.84
1	A	1722	ILE	C-N-CA	-6.03	112.31	119.84
1	A	1024	ALA	N-CA-C	-6.00	104.79	114.09
1	B	1024	ALA	N-CA-C	-5.99	104.81	114.09
1	B	2462	ILE	N-CA-C	-5.98	106.49	112.17
1	A	2462	ILE	N-CA-C	-5.98	106.49	112.17
1	C	1018	HIS	N-CA-C	-5.98	104.85	111.36
1	C	1024	ALA	N-CA-C	-5.97	104.83	114.09
1	B	1018	HIS	N-CA-C	-5.97	104.85	111.36
1	A	1018	HIS	N-CA-C	-5.96	104.86	111.36
1	C	1210	ALA	N-CA-C	5.96	117.78	111.28
1	C	2462	ILE	N-CA-C	-5.96	106.51	112.17
1	B	1305	HIS	N-CA-C	-5.92	106.02	113.72
1	C	1305	HIS	N-CA-C	-5.92	106.02	113.72
1	A	1305	HIS	N-CA-C	-5.92	106.03	113.72
1	C	2513	MET	N-CA-C	-5.91	105.90	113.23
1	B	2513	MET	N-CA-C	-5.91	105.91	113.23
1	A	2513	MET	N-CA-C	-5.89	105.92	113.23
1	C	827	LEU	N-CA-C	-5.84	106.32	113.50
1	B	827	LEU	N-CA-C	-5.84	106.32	113.50
1	A	827	LEU	N-CA-C	-5.82	106.34	113.50
1	C	1097	THR	N-CA-C	-5.77	103.60	111.56
1	B	2099	ASN	CB-CA-C	-5.75	108.07	116.53
1	B	1097	THR	N-CA-C	-5.75	103.63	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2099	ASN	CB-CA-C	-5.75	108.08	116.53
1	A	1097	THR	N-CA-C	-5.74	103.64	111.56
1	C	2099	ASN	CB-CA-C	-5.74	108.10	116.53
1	A	1166	LEU	N-CA-C	-5.71	106.96	114.04
1	C	1166	LEU	N-CA-C	-5.71	106.96	114.04
1	B	2375	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	B	1166	LEU	N-CA-C	-5.69	106.99	114.04
1	C	2375	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	C	1722	ILE	CA-C-N	-5.66	112.77	119.84
1	C	1722	ILE	C-N-CA	-5.66	112.77	119.84
1	A	2375	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	B	1726	SER	N-CA-C	5.61	117.15	110.19
1	A	1726	SER	N-CA-C	5.59	117.12	110.19
1	C	1726	SER	N-CA-C	5.59	117.12	110.19
1	C	1705	ALA	N-CA-C	-5.58	106.30	114.39
1	A	1705	ALA	N-CA-C	-5.58	106.30	114.39
1	B	1705	ALA	N-CA-C	-5.57	106.31	114.39
1	C	1029	ARG	N-CA-C	5.55	119.80	113.19
1	A	1029	ARG	N-CA-C	5.53	119.77	113.19
1	C	1557	GLY	N-CA-C	-5.52	107.40	115.63
1	B	1029	ARG	N-CA-C	5.52	119.76	113.19
1	B	1557	GLY	N-CA-C	-5.52	107.40	115.63
1	C	1113	TRP	N-CA-C	-5.52	106.05	112.89
1	A	1557	GLY	N-CA-C	-5.52	107.41	115.63
1	B	1113	TRP	N-CA-C	-5.51	106.05	112.89
1	A	1113	TRP	N-CA-C	-5.51	106.06	112.89
1	C	1284	GLY	N-CA-C	5.44	120.73	111.16
1	B	1284	GLY	N-CA-C	5.44	120.73	111.16
1	A	1284	GLY	N-CA-C	5.44	120.73	111.16
1	C	1011	MET	N-CA-C	5.37	118.98	111.90
1	A	1011	MET	N-CA-C	5.36	118.97	111.90
1	B	1011	MET	N-CA-C	5.35	118.97	111.90
1	B	849	ARG	N-CA-C	-5.30	106.98	113.50
1	C	849	ARG	N-CA-C	-5.30	106.98	113.50
1	A	849	ARG	N-CA-C	-5.28	107.01	113.50
1	A	2229	GLN	CA-C-N	-5.26	113.11	118.85
1	A	2229	GLN	C-N-CA	-5.26	113.11	118.85
1	B	2375	GLN	CA-C-N	5.14	124.81	119.56
1	B	2375	GLN	C-N-CA	5.14	124.81	119.56
1	C	2186	ILE	N-CA-C	-5.14	107.97	112.90
1	A	2186	ILE	N-CA-C	-5.13	107.98	112.90
1	A	2375	GLN	CA-C-N	5.13	124.79	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2375	GLN	C-N-CA	5.13	124.79	119.56
1	C	2375	GLN	CA-C-N	5.13	124.79	119.56
1	C	2375	GLN	C-N-CA	5.13	124.79	119.56
1	B	2186	ILE	N-CA-C	-5.11	107.99	112.90
1	A	815	PHE	N-CA-C	-5.10	105.90	111.82
1	C	815	PHE	N-CA-C	-5.09	105.92	111.82
1	B	815	PHE	N-CA-C	-5.09	105.92	111.82
1	B	1724	ARG	CA-C-N	-5.09	114.49	119.93
1	B	1724	ARG	C-N-CA	-5.09	114.49	119.93
1	B	1411	THR	N-CA-C	-5.03	106.56	113.30
1	C	1411	THR	N-CA-C	-5.03	106.56	113.30
1	A	1411	THR	N-CA-C	-5.02	106.57	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10418	0	10650	354	0
1	B	10418	0	10650	343	0
1	C	10412	0	10639	338	0
2	A	51	0	79	20	0
2	B	51	0	79	20	0
2	C	51	0	79	19	0
All	All	31401	0	32176	946	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (946) 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:A:2157:LYS:CB	1:A:2157:LYS:NZ	1.70	1.45
1:C:2193:PHE:HD1	1:C:2194:MET:N	1.11	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2193:PHE:HD1	1:B:2194:MET:N	1.11	1.42
1:C:2028:LEU:CD1	1:C:2028:LEU:C	1.78	1.42
1:B:2028:LEU:CD1	1:B:2028:LEU:C	1.78	1.40
1:C:2028:LEU:C	1:C:2028:LEU:HD13	1.31	1.40
1:A:2193:PHE:HD1	1:A:2194:MET:N	1.11	1.39
1:C:2028:LEU:HD12	1:C:2029:GLY:N	1.39	1.38
1:C:2157:LYS:NZ	1:C:2157:LYS:CB	1.70	1.38
1:A:2028:LEU:CD1	1:A:2028:LEU:C	1.78	1.36
1:A:2028:LEU:HD12	1:A:2029:GLY:N	1.39	1.36
1:B:2028:LEU:HD12	1:B:2029:GLY:N	1.39	1.33
1:B:2114:PHE:CD1	1:C:2183:LEU:HD22	1.63	1.33
1:A:2193:PHE:CD1	1:A:2194:MET:N	1.96	1.32
1:B:2193:PHE:CD1	1:B:2194:MET:N	1.96	1.32
1:C:2193:PHE:CD1	1:C:2194:MET:N	1.96	1.32
1:A:2183:LEU:HD22	1:C:2114:PHE:CD1	1.64	1.32
1:B:2157:LYS:NZ	1:B:2157:LYS:CB	1.70	1.32
1:A:2114:PHE:CD1	1:B:2183:LEU:HD22	1.63	1.31
1:B:2028:LEU:C	1:B:2028:LEU:HD13	1.31	1.30
1:A:587:MET:HE1	1:A:693:ALA:CB	1.64	1.28
1:B:2193:PHE:HD1	1:B:2193:PHE:C	1.42	1.27
1:C:587:MET:HE1	1:C:693:ALA:CB	1.64	1.26
1:B:587:MET:HE1	1:B:693:ALA:CB	1.64	1.26
1:A:2193:PHE:HD1	1:A:2193:PHE:C	1.42	1.25
1:A:2028:LEU:O	1:A:2028:LEU:HD13	1.09	1.24
1:C:2193:PHE:HD1	1:C:2193:PHE:C	1.42	1.24
2:C:2601:L9Q:O31	2:C:2601:L9Q:H15	1.34	1.24
1:C:2028:LEU:HD13	1:C:2028:LEU:O	1.09	1.23
2:B:2601:L9Q:O31	2:B:2601:L9Q:H15	1.34	1.23
1:A:2028:LEU:C	1:A:2028:LEU:HD13	1.31	1.23
1:B:2028:LEU:HD13	1:B:2028:LEU:O	1.09	1.22
2:A:2601:L9Q:O31	2:A:2601:L9Q:H15	1.34	1.22
1:B:1783:ILE:O	1:B:1783:ILE:HG22	1.37	1.17
1:A:2193:PHE:CE1	1:A:2194:MET:HG2	1.82	1.15
1:C:2157:LYS:NZ	1:C:2157:LYS:HB3	1.41	1.14
1:C:2193:PHE:CE1	1:C:2194:MET:HG2	1.82	1.13
1:B:2193:PHE:CE1	1:B:2194:MET:HG2	1.82	1.13
1:A:587:MET:HE1	1:A:693:ALA:HB3	1.14	1.13
1:A:1023:VAL:CG1	1:A:1023:VAL:O	1.97	1.12
1:B:587:MET:HE1	1:B:693:ALA:HB3	1.14	1.12
1:B:2137:MET:SD	1:C:2459:PHE:HE1	1.71	1.12
1:A:2125:VAL:CG1	1:B:2173:TYR:CD1	2.33	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2137:MET:SD	1:B:2459:PHE:HE1	1.71	1.11
1:A:2173:TYR:CD1	1:C:2125:VAL:CG1	2.33	1.11
1:A:2459:PHE:HE1	1:C:2137:MET:SD	1.71	1.11
1:B:1023:VAL:O	1:B:1023:VAL:CG1	1.97	1.11
1:B:2125:VAL:CG1	1:C:2173:TYR:CD1	2.33	1.10
1:C:1023:VAL:CG1	1:C:1023:VAL:O	1.97	1.10
1:A:1783:ILE:HG22	1:A:1783:ILE:O	1.37	1.09
1:C:1783:ILE:HG22	1:C:1783:ILE:O	1.37	1.09
1:A:2193:PHE:CD1	1:A:2193:PHE:C	2.18	1.08
1:C:929:ILE:O	1:C:929:ILE:CG2	2.02	1.08
1:B:2157:LYS:NZ	1:B:2157:LYS:HB3	1.41	1.07
1:A:2137:MET:SD	1:B:2459:PHE:CE1	2.47	1.07
1:A:2459:PHE:CE1	1:C:2137:MET:SD	2.47	1.07
1:C:2193:PHE:CD1	1:C:2193:PHE:C	2.18	1.07
1:A:2114:PHE:CE1	1:B:2183:LEU:HD22	1.89	1.07
1:A:2192:LEU:HB2	1:C:2005:LEU:HD11	1.37	1.07
1:C:587:MET:HE1	1:C:693:ALA:HB3	1.14	1.06
1:A:2157:LYS:NZ	1:A:2157:LYS:HB2	1.41	1.06
1:B:2114:PHE:CE1	1:C:2183:LEU:HD22	1.89	1.06
1:B:2137:MET:SD	1:C:2459:PHE:CE1	2.47	1.06
1:A:2183:LEU:HD22	1:C:2114:PHE:CE1	1.90	1.06
1:B:929:ILE:CG2	1:B:929:ILE:O	2.02	1.06
1:A:2173:TYR:CE1	1:C:2125:VAL:HG12	1.91	1.05
1:C:587:MET:SD	1:C:690:PHE:HA	1.96	1.05
1:A:587:MET:SD	1:A:690:PHE:HA	1.96	1.05
1:A:929:ILE:O	1:A:929:ILE:CG2	2.02	1.05
1:B:2005:LEU:HD11	1:C:2192:LEU:HB2	1.37	1.05
1:B:587:MET:SD	1:B:690:PHE:HA	1.96	1.04
1:B:2157:LYS:NZ	1:B:2157:LYS:HB2	1.41	1.04
1:A:2005:LEU:HD11	1:B:2192:LEU:HB2	1.37	1.04
1:A:2125:VAL:HG12	1:B:2173:TYR:CE1	1.91	1.04
1:A:2157:LYS:NZ	1:A:2157:LYS:HB3	1.41	1.04
1:B:2125:VAL:HG12	1:C:2173:TYR:CE1	1.91	1.04
1:C:2157:LYS:NZ	1:C:2157:LYS:HB2	1.41	1.03
1:C:2193:PHE:HE1	1:C:2194:MET:HG2	1.13	1.03
1:C:1023:VAL:O	1:C:1023:VAL:HG13	1.59	1.03
1:B:1338:PHE:CE1	1:B:1339:HIS:CD2	2.48	1.01
1:B:1562:ARG:CD	1:B:1565:LEU:HD12	1.90	1.01
1:A:1053:TYR:O	1:A:1053:TYR:CD1	2.14	1.01
1:B:1053:TYR:O	1:B:1053:TYR:CD1	2.14	1.01
1:B:2193:PHE:CD1	1:B:2193:PHE:C	2.18	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2193:PHE:HE1	1:B:2194:MET:HG2	1.13	1.01
1:C:1562:ARG:CD	1:C:1565:LEU:HD12	1.90	1.01
1:C:1053:TYR:O	1:C:1053:TYR:CD1	2.14	1.00
1:A:1562:ARG:CD	1:A:1565:LEU:HD12	1.90	1.00
1:B:1338:PHE:HD1	1:B:1339:HIS:N	1.60	1.00
1:C:1338:PHE:CE1	1:C:1339:HIS:CD2	2.48	1.00
1:C:1338:PHE:HD1	1:C:1339:HIS:N	1.60	1.00
1:A:1338:PHE:HD1	1:A:1339:HIS:N	1.60	1.00
1:B:2114:PHE:CE1	1:C:2183:LEU:CD2	2.45	1.00
1:A:863:CYS:O	1:A:867:VAL:HG23	1.61	1.00
1:A:1338:PHE:CE1	1:A:1339:HIS:CD2	2.48	1.00
1:A:2183:LEU:CD2	1:C:2114:PHE:CE1	2.45	0.99
1:B:929:ILE:O	1:B:929:ILE:HG22	1.62	0.99
1:A:2193:PHE:HE1	1:A:2194:MET:HG2	1.13	0.99
1:A:929:ILE:O	1:A:929:ILE:HG22	1.62	0.99
1:B:863:CYS:O	1:B:867:VAL:HG23	1.61	0.99
1:B:1338:PHE:CD1	1:B:1339:HIS:N	2.31	0.99
1:C:2505:PHE:O	1:C:2505:PHE:CD1	2.16	0.98
1:A:2114:PHE:CE1	1:B:2183:LEU:CD2	2.45	0.98
1:B:2193:PHE:CE1	1:B:2194:MET:CG	2.47	0.98
1:A:1338:PHE:CD1	1:A:1339:HIS:N	2.31	0.98
1:B:1023:VAL:O	1:B:1023:VAL:HG13	1.59	0.98
1:C:1338:PHE:CD1	1:C:1339:HIS:N	2.31	0.98
1:A:2193:PHE:CE1	1:A:2194:MET:CG	2.47	0.98
1:C:2193:PHE:CE1	1:C:2194:MET:CG	2.47	0.98
1:C:863:CYS:O	1:C:867:VAL:HG23	1.61	0.97
1:B:2505:PHE:O	1:B:2505:PHE:CD1	2.16	0.97
1:A:2173:TYR:CE1	1:C:2125:VAL:CG1	2.48	0.97
1:B:2114:PHE:HD1	1:C:2183:LEU:HD22	1.20	0.97
1:B:2125:VAL:CG1	1:C:2173:TYR:CE1	2.48	0.97
1:A:1023:VAL:O	1:A:1023:VAL:HG13	1.59	0.97
1:A:2505:PHE:O	1:A:2505:PHE:CD1	2.16	0.97
1:A:1338:PHE:HE1	1:A:1339:HIS:CD2	1.83	0.96
1:B:1342:ILE:N	1:B:1342:ILE:HD13	1.80	0.96
1:C:1338:PHE:HE1	1:C:1339:HIS:CD2	1.84	0.96
1:A:2125:VAL:CG1	1:B:2173:TYR:CE1	2.48	0.96
1:C:1783:ILE:O	1:C:1783:ILE:CG2	2.12	0.95
1:A:1342:ILE:HD13	1:A:1342:ILE:N	1.80	0.95
1:C:929:ILE:O	1:C:929:ILE:HG22	1.62	0.94
1:B:1338:PHE:HE1	1:B:1339:HIS:CD2	1.83	0.94
1:A:2028:LEU:CD1	1:A:2029:GLY:N	2.10	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2601:L9Q:O31	2:A:2601:L9Q:C15	2.16	0.94
2:C:2601:L9Q:O31	2:C:2601:L9Q:C15	2.16	0.93
1:A:1783:ILE:O	1:A:1783:ILE:CG2	2.12	0.93
2:B:2601:L9Q:O31	2:B:2601:L9Q:C15	2.16	0.93
1:C:1342:ILE:HD13	1:C:1342:ILE:N	1.80	0.93
1:B:2028:LEU:CD1	1:B:2029:GLY:N	2.10	0.93
1:C:2157:LYS:HB2	1:C:2157:LYS:HZ1	1.27	0.92
1:A:2183:LEU:HD22	1:C:2114:PHE:HD1	1.20	0.92
1:A:2113:PRO:O	1:A:2114:PHE:HB2	1.69	0.92
1:A:846:PRO:HG3	1:A:1106:LEU:HD11	1.52	0.92
1:B:846:PRO:HG3	1:B:1106:LEU:HD11	1.52	0.91
1:B:2157:LYS:HB2	1:B:2157:LYS:HZ1	1.24	0.91
1:A:1562:ARG:HD3	1:A:1565:LEU:HD12	1.51	0.91
1:B:2113:PRO:O	1:B:2114:PHE:HB2	1.69	0.91
1:A:2173:TYR:CD1	1:C:2125:VAL:HG11	2.04	0.91
2:B:2601:L9Q:H14A	2:B:2601:L9Q:H40	1.52	0.91
1:A:2114:PHE:HD1	1:B:2183:LEU:HD22	1.20	0.91
1:B:1562:ARG:HD3	1:B:1565:LEU:HD12	1.51	0.90
2:C:2601:L9Q:H40	2:C:2601:L9Q:H14A	1.52	0.90
1:A:2173:TYR:HD1	1:C:2125:VAL:HG11	1.35	0.90
1:A:2125:VAL:HG11	1:B:2173:TYR:HD1	1.35	0.90
1:C:2028:LEU:CD1	1:C:2029:GLY:N	2.10	0.90
1:C:2113:PRO:O	1:C:2114:PHE:HB2	1.69	0.90
2:A:2601:L9Q:H22A	2:A:2601:L9Q:O11	1.72	0.90
2:A:2601:L9Q:H40	2:A:2601:L9Q:H14A	1.52	0.90
1:A:1338:PHE:CD1	1:A:1338:PHE:C	2.50	0.89
1:B:2125:VAL:HG11	1:C:2173:TYR:CD1	2.04	0.89
2:B:2601:L9Q:H22A	2:B:2601:L9Q:O11	1.72	0.89
1:C:1338:PHE:CD1	1:C:1338:PHE:C	2.50	0.89
1:C:1562:ARG:HD3	1:C:1565:LEU:HD12	1.51	0.89
2:C:2601:L9Q:H22A	2:C:2601:L9Q:O11	1.72	0.89
1:B:1783:ILE:O	1:B:1783:ILE:CG2	2.12	0.89
1:C:846:PRO:HG3	1:C:1106:LEU:HD11	1.52	0.89
1:B:2125:VAL:HG11	1:C:2173:TYR:HD1	1.35	0.89
1:A:2125:VAL:HG11	1:B:2173:TYR:CD1	2.04	0.88
1:B:1338:PHE:CD1	1:B:1338:PHE:C	2.50	0.88
1:B:1656:ILE:HG23	1:B:1657:PRO:HD2	1.56	0.87
1:A:2173:TYR:CE1	1:C:2126:TRP:CZ3	2.63	0.87
1:B:2126:TRP:CZ3	1:C:2173:TYR:CE1	2.63	0.87
1:B:2126:TRP:CZ3	1:C:2173:TYR:OH	2.27	0.87
1:A:2126:TRP:CZ3	1:B:2173:TYR:CE1	2.63	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2118:LEU:HD21	1:C:2180:ILE:HG23	1.57	0.87
1:C:1656:ILE:HG23	1:C:1657:PRO:HD2	1.56	0.87
2:A:2601:L9Q:H32	2:A:2601:L9Q:H25	1.56	0.86
2:C:2601:L9Q:H25	2:C:2601:L9Q:H32	1.55	0.86
1:A:2180:ILE:HG23	1:C:2118:LEU:HD21	1.57	0.86
1:A:2173:TYR:OH	1:C:2126:TRP:CZ3	2.27	0.86
1:A:2126:TRP:CZ3	1:B:2173:TYR:OH	2.27	0.86
2:B:2601:L9Q:H25	2:B:2601:L9Q:H32	1.55	0.86
1:A:1656:ILE:HG23	1:A:1657:PRO:HD2	1.56	0.86
1:A:2118:LEU:HD21	1:B:2180:ILE:HG23	1.57	0.85
1:C:587:MET:CE	1:C:693:ALA:HB3	2.05	0.84
1:B:2028:LEU:HD12	1:B:2029:GLY:CA	2.08	0.84
1:C:2028:LEU:CD1	1:C:2028:LEU:O	2.03	0.83
1:C:2028:LEU:HD12	1:C:2029:GLY:CA	2.08	0.83
1:A:604:TYR:OH	1:A:637:THR:HA	1.79	0.82
1:B:1560:VAL:HG12	1:B:1560:VAL:O	1.79	0.82
1:A:2028:LEU:HD12	1:A:2029:GLY:CA	2.08	0.82
1:A:2192:LEU:HB2	1:C:2005:LEU:CD1	2.10	0.82
1:B:604:TYR:OH	1:B:637:THR:HA	1.79	0.82
1:C:604:TYR:OH	1:C:637:THR:HA	1.79	0.81
1:A:874:LEU:HB2	1:A:877:VAL:CG2	2.10	0.81
1:B:874:LEU:HB2	1:B:877:VAL:CG2	2.10	0.81
1:C:2193:PHE:HD1	1:C:2194:MET:CA	1.94	0.81
1:B:2005:LEU:CD1	1:C:2192:LEU:HB2	2.10	0.81
2:C:2601:L9Q:H14A	2:C:2601:L9Q:C40	2.11	0.81
1:B:2193:PHE:HD1	1:B:2194:MET:CA	1.94	0.81
2:B:2601:L9Q:H14A	2:B:2601:L9Q:C40	2.11	0.81
1:A:1023:VAL:O	1:A:1023:VAL:HG12	1.80	0.80
1:A:1210:ALA:O	1:A:1211:ARG:C	2.23	0.80
1:A:2193:PHE:HD1	1:A:2194:MET:CA	1.94	0.80
1:C:1560:VAL:HG12	1:C:1560:VAL:O	1.79	0.80
1:A:1560:VAL:HG12	1:A:1560:VAL:O	1.79	0.80
1:A:2312:ALA:HB2	1:B:2366:PRO:HD2	1.63	0.80
1:C:874:LEU:HB2	1:C:877:VAL:CG2	2.10	0.80
1:C:1023:VAL:O	1:C:1023:VAL:HG12	1.80	0.80
1:A:863:CYS:O	1:A:867:VAL:CG2	2.29	0.80
1:A:2173:TYR:CZ	1:C:2126:TRP:CZ3	2.69	0.80
1:B:2114:PHE:CD1	1:C:2183:LEU:CD2	2.56	0.80
1:A:587:MET:CE	1:A:693:ALA:HB3	2.06	0.80
1:B:1656:ILE:HG23	1:B:1657:PRO:CD	2.12	0.80
1:A:2183:LEU:CD2	1:C:2114:PHE:HE1	1.92	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2601:L9Q:H14A	2:A:2601:L9Q:C40	2.11	0.80
1:B:863:CYS:O	1:B:867:VAL:CG2	2.29	0.80
1:B:1023:VAL:O	1:B:1023:VAL:HG12	1.80	0.80
1:B:1342:ILE:HD13	1:B:1342:ILE:H	1.45	0.80
1:B:2126:TRP:CZ3	1:C:2173:TYR:CZ	2.69	0.80
1:A:2005:LEU:CD1	1:B:2192:LEU:HB2	2.10	0.80
1:A:2126:TRP:CZ3	1:B:2173:TYR:CZ	2.69	0.80
1:A:1656:ILE:HG23	1:A:1657:PRO:CD	2.12	0.79
1:C:863:CYS:O	1:C:867:VAL:CG2	2.29	0.79
1:A:2028:LEU:CD1	1:A:2028:LEU:O	2.03	0.79
1:B:2114:PHE:HE1	1:C:2183:LEU:CD2	1.92	0.79
1:A:1342:ILE:HD13	1:A:1342:ILE:H	1.45	0.79
1:B:2065:LEU:O	1:B:2066:TRP:C	2.25	0.78
1:A:2065:LEU:O	1:A:2066:TRP:C	2.25	0.78
1:C:1656:ILE:HG23	1:C:1657:PRO:CD	2.12	0.78
1:A:2193:PHE:CD1	1:A:2194:MET:CA	2.66	0.78
1:C:2193:PHE:CD1	1:C:2194:MET:CA	2.66	0.78
1:B:992:TYR:OH	1:B:1119:GLU:HG2	1.84	0.78
1:A:992:TYR:OH	1:A:1119:GLU:HG2	1.84	0.78
1:A:2114:PHE:HE1	1:B:2183:LEU:CD2	1.92	0.78
1:B:2312:ALA:HB2	1:C:2366:PRO:HD2	1.63	0.77
1:C:1342:ILE:HD13	1:C:1342:ILE:H	1.46	0.77
1:C:2065:LEU:O	1:C:2066:TRP:C	2.25	0.77
1:C:992:TYR:OH	1:C:1119:GLU:HG2	1.84	0.77
1:C:1701:VAL:HG12	1:C:1702:THR:N	1.99	0.77
1:A:1338:PHE:O	1:A:1342:ILE:CD1	2.34	0.76
1:B:1338:PHE:O	1:B:1342:ILE:CD1	2.34	0.76
1:B:2193:PHE:CD1	1:B:2194:MET:CA	2.67	0.76
1:C:1338:PHE:O	1:C:1342:ILE:CD1	2.34	0.76
1:B:1701:VAL:HG12	1:B:1702:THR:N	1.99	0.76
1:A:1701:VAL:HG12	1:A:1702:THR:N	1.99	0.76
1:B:2028:LEU:CD1	1:B:2028:LEU:O	2.02	0.76
1:A:2125:VAL:HG12	1:B:2173:TYR:HE1	1.48	0.75
1:A:1053:TYR:CD1	1:A:1053:TYR:C	2.64	0.75
1:B:2126:TRP:HZ3	1:C:2173:TYR:OH	1.68	0.75
1:C:1053:TYR:CD1	1:C:1053:TYR:C	2.64	0.75
1:B:929:ILE:O	1:B:929:ILE:HG23	1.87	0.75
1:C:929:ILE:O	1:C:929:ILE:HG23	1.87	0.75
1:B:587:MET:CE	1:B:693:ALA:HB3	2.06	0.75
2:C:2601:L9Q:C40	2:C:2601:L9Q:C14	2.63	0.75
1:A:2173:TYR:OH	1:C:2126:TRP:HZ3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1562:ARG:HD2	1:C:1565:LEU:HD12	1.69	0.75
1:C:1562:ARG:CD	1:C:1565:LEU:CD1	2.64	0.75
1:C:2505:PHE:O	1:C:2505:PHE:HD1	1.69	0.74
1:A:1562:ARG:HD2	1:A:1565:LEU:HD12	1.69	0.74
1:B:1562:ARG:CD	1:B:1565:LEU:CD1	2.65	0.74
1:B:1053:TYR:CD1	1:B:1053:TYR:C	2.64	0.74
1:A:2114:PHE:HE1	1:B:2183:LEU:HD23	1.53	0.73
1:A:1562:ARG:CD	1:A:1565:LEU:CD1	2.64	0.73
1:A:2183:LEU:HD23	1:C:2114:PHE:HE1	1.53	0.73
1:B:2125:VAL:HG12	1:C:2173:TYR:HE1	1.48	0.73
1:B:2114:PHE:CE1	1:C:2183:LEU:HD23	2.24	0.73
1:B:2505:PHE:O	1:B:2505:PHE:HD1	1.69	0.73
1:C:2320:ALA:HA	1:C:2366:PRO:HA	1.71	0.73
1:A:2126:TRP:HZ3	1:B:2173:TYR:OH	1.68	0.72
1:A:2505:PHE:O	1:A:2505:PHE:HD1	1.69	0.72
1:A:929:ILE:O	1:A:929:ILE:HG23	1.87	0.72
1:A:2114:PHE:CE1	1:B:2183:LEU:HD23	2.24	0.72
1:B:1208:THR:O	1:B:1209:ARG:C	2.31	0.72
1:C:1016:THR:HG22	1:C:1230:ASN:HD21	1.53	0.72
1:B:2320:ALA:HA	1:B:2366:PRO:HA	1.71	0.72
1:A:1016:THR:HG22	1:A:1230:ASN:HD21	1.53	0.72
1:B:1016:THR:HG22	1:B:1230:ASN:HD21	1.53	0.72
2:A:2601:L9Q:H16	2:A:2601:L9Q:H41	1.73	0.71
1:B:2189:PHE:CD1	1:B:2189:PHE:C	2.69	0.71
2:C:2601:L9Q:H16	2:C:2601:L9Q:H41	1.73	0.71
1:A:1208:THR:O	1:A:1209:ARG:C	2.31	0.71
1:A:2189:PHE:CD1	1:A:2189:PHE:C	2.69	0.71
1:C:2189:PHE:CD1	1:C:2189:PHE:C	2.69	0.70
1:A:577:ALA:O	1:A:705:PHE:HD1	1.74	0.70
1:B:1562:ARG:HD2	1:B:1565:LEU:HD12	1.69	0.70
1:B:2114:PHE:HE1	1:C:2183:LEU:HD23	1.53	0.70
2:B:2601:L9Q:H41	2:B:2601:L9Q:H16	1.73	0.70
1:B:2125:VAL:HG13	1:C:2173:TYR:CD1	2.27	0.70
1:A:2173:TYR:HE1	1:C:2125:VAL:HG12	1.48	0.70
1:C:1208:THR:O	1:C:1209:ARG:C	2.31	0.70
1:C:581:ILE:HA	1:C:697:GLN:NE2	2.07	0.70
1:A:1338:PHE:O	1:A:1342:ILE:HD11	1.92	0.69
1:C:1421:PHE:HZ	1:C:2502:LYS:O	1.75	0.69
1:C:2186:ILE:HG22	1:C:2186:ILE:O	1.92	0.69
1:B:991:PHE:HE1	1:B:998:ILE:CG2	2.05	0.69
2:B:2601:L9Q:C40	2:B:2601:L9Q:H16	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:PHE:HZ	1:A:2502:LYS:O	1.75	0.69
1:A:991:PHE:HE1	1:A:998:ILE:CG2	2.05	0.69
1:B:581:ILE:HA	1:B:697:GLN:NE2	2.07	0.69
1:B:1338:PHE:O	1:B:1342:ILE:HD11	1.92	0.69
1:B:1421:PHE:HZ	1:B:2502:LYS:O	1.75	0.69
2:C:2601:L9Q:C40	2:C:2601:L9Q:H16	2.23	0.69
2:A:2601:L9Q:C40	2:A:2601:L9Q:H16	2.23	0.69
1:B:2028:LEU:CD1	1:B:2029:GLY:CA	2.69	0.69
1:C:2028:LEU:CD1	1:C:2029:GLY:CA	2.69	0.69
1:C:991:PHE:HE1	1:C:998:ILE:CG2	2.05	0.69
1:C:1338:PHE:O	1:C:1342:ILE:HD11	1.92	0.68
1:A:581:ILE:HA	1:A:697:GLN:NE2	2.07	0.68
1:A:2183:LEU:HD23	1:C:2114:PHE:CE1	2.24	0.68
1:A:2186:ILE:O	1:A:2186:ILE:HG22	1.92	0.68
1:A:587:MET:HE1	1:A:693:ALA:HB2	1.72	0.68
2:A:2601:L9Q:C40	2:A:2601:L9Q:C16	2.69	0.68
1:C:1961:TYR:O	1:C:1962:ALA:C	2.37	0.68
1:B:2186:ILE:HG22	1:B:2186:ILE:O	1.92	0.67
1:A:1961:TYR:O	1:A:1962:ALA:C	2.37	0.67
1:B:2186:ILE:O	1:B:2186:ILE:CG2	2.43	0.67
1:A:2028:LEU:CD1	1:A:2029:GLY:CA	2.70	0.67
1:A:1342:ILE:N	1:A:1342:ILE:CD1	2.53	0.67
1:A:2173:TYR:CD1	1:C:2125:VAL:HG13	2.27	0.66
1:A:2186:ILE:O	1:A:2186:ILE:CG2	2.43	0.66
1:A:2125:VAL:HG13	1:B:2173:TYR:CD1	2.27	0.66
1:C:2065:LEU:O	1:C:2067:TYR:N	2.29	0.66
1:A:1562:ARG:HD3	1:A:1565:LEU:CD1	2.25	0.66
1:A:2065:LEU:O	1:A:2067:TYR:N	2.29	0.66
1:B:2065:LEU:O	1:B:2067:TYR:N	2.29	0.65
2:B:2601:L9Q:C40	2:B:2601:L9Q:C14	2.63	0.65
1:A:2193:PHE:HE1	1:A:2194:MET:CG	1.96	0.65
1:C:2186:ILE:O	1:C:2186:ILE:CG2	2.43	0.65
1:B:805:PHE:CD1	1:B:805:PHE:C	2.73	0.65
1:A:2012:PHE:CE2	1:B:2184:ILE:HG12	2.32	0.65
1:B:1210:ALA:O	1:B:1211:ARG:C	2.39	0.65
1:B:2012:PHE:CE2	1:C:2184:ILE:HG12	2.32	0.64
1:C:2113:PRO:O	1:C:2114:PHE:CB	2.43	0.64
1:A:2184:ILE:HG12	1:C:2012:PHE:CE2	2.32	0.64
1:B:874:LEU:HB2	1:B:877:VAL:HG21	1.80	0.64
1:A:805:PHE:C	1:A:805:PHE:CD1	2.73	0.63
1:B:587:MET:HE1	1:B:693:ALA:HB2	1.72	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:MET:HE1	1:C:693:ALA:HB2	1.72	0.63
1:A:1568:LEU:HG	1:A:1652:ARG:HG3	1.81	0.63
1:B:1961:TYR:O	1:B:1962:ALA:C	2.37	0.63
1:A:2113:PRO:O	1:A:2114:PHE:CB	2.43	0.63
1:C:805:PHE:CD1	1:C:805:PHE:C	2.73	0.63
1:C:874:LEU:HB2	1:C:877:VAL:HG21	1.80	0.63
1:A:2005:LEU:CD1	1:B:2188:TRP:HE1	2.12	0.63
1:A:2188:TRP:HE1	1:C:2005:LEU:CD1	2.12	0.62
1:B:2005:LEU:CD1	1:C:2188:TRP:HE1	2.12	0.62
1:A:874:LEU:HB2	1:A:877:VAL:HG21	1.80	0.62
1:B:2005:LEU:HG	1:C:2188:TRP:HE1	1.65	0.62
1:A:2005:LEU:HG	1:B:2188:TRP:HE1	1.65	0.62
1:B:1562:ARG:HD3	1:B:1565:LEU:CD1	2.25	0.62
1:B:2125:VAL:CG1	1:C:2173:TYR:HD1	1.93	0.62
1:B:2113:PRO:O	1:B:2114:PHE:CB	2.43	0.62
1:A:2188:TRP:HE1	1:C:2005:LEU:HG	1.65	0.62
1:C:581:ILE:HB	1:C:697:GLN:NE2	2.15	0.62
1:A:581:ILE:HB	1:A:697:GLN:NE2	2.15	0.61
1:B:581:ILE:HB	1:B:697:GLN:NE2	2.15	0.61
1:B:1568:LEU:HG	1:B:1652:ARG:HG3	1.81	0.61
1:C:1103:PHE:O	1:C:1104:LEU:C	2.43	0.61
1:A:581:ILE:HA	1:A:697:GLN:HE21	1.65	0.61
1:B:581:ILE:HA	1:B:697:GLN:HE21	1.65	0.61
1:A:2193:PHE:CE1	1:A:2194:MET:HG3	2.36	0.61
1:C:1568:LEU:HG	1:C:1652:ARG:HG3	1.81	0.61
1:B:1560:VAL:O	1:B:1560:VAL:CG1	2.49	0.61
1:B:1342:ILE:N	1:B:1342:ILE:CD1	2.53	0.60
2:C:2601:L9Q:H16	2:C:2601:L9Q:C41	2.31	0.60
1:B:1338:PHE:CD1	1:B:1339:HIS:CD2	2.89	0.60
1:C:581:ILE:HA	1:C:697:GLN:HE21	1.65	0.60
1:C:1338:PHE:CD1	1:C:1339:HIS:CD2	2.89	0.60
2:A:2601:L9Q:H16	2:A:2601:L9Q:C41	2.31	0.60
1:B:2137:MET:SD	1:C:2459:PHE:CD1	2.95	0.60
1:B:587:MET:CE	1:B:693:ALA:CB	2.59	0.60
2:C:2601:L9Q:H32	2:C:2601:L9Q:C25	2.31	0.60
1:A:876:VAL:O	1:A:876:VAL:CG2	2.50	0.60
1:A:1338:PHE:CD1	1:A:1339:HIS:CD2	2.89	0.60
2:B:2601:L9Q:C40	2:B:2601:L9Q:C16	2.69	0.60
1:C:1656:ILE:CG2	1:C:1657:PRO:CD	2.79	0.60
1:A:1560:VAL:O	1:A:1560:VAL:CG1	2.49	0.59
1:A:1656:ILE:CG2	1:A:1657:PRO:CD	2.79	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1656:ILE:CG2	1:B:1657:PRO:CD	2.79	0.59
2:B:2601:L9Q:H16	2:B:2601:L9Q:C41	2.31	0.59
1:C:1562:ARG:HD3	1:C:1565:LEU:CD1	2.25	0.59
1:A:2183:LEU:CD2	1:C:2114:PHE:CD1	2.56	0.59
1:B:876:VAL:CG2	1:B:876:VAL:O	2.50	0.59
1:B:1103:PHE:O	1:B:1104:LEU:C	2.43	0.59
1:A:1103:PHE:O	1:A:1104:LEU:C	2.43	0.59
1:B:2312:ALA:HB2	1:C:2366:PRO:CD	2.33	0.59
1:C:876:VAL:CG2	1:C:876:VAL:O	2.50	0.59
1:A:1212:LEU:HD11	1:A:1303:LEU:HD11	1.85	0.59
1:A:1423:SER:O	1:A:1423:SER:OG	2.20	0.58
1:C:587:MET:CE	1:C:693:ALA:CB	2.59	0.58
1:C:1334:LYS:HG3	1:C:1335:SER:N	2.18	0.58
1:A:2114:PHE:CD1	1:B:2183:LEU:CD2	2.56	0.58
2:A:2601:L9Q:H32	2:A:2601:L9Q:C25	2.31	0.58
1:A:2137:MET:SD	1:B:2459:PHE:CD1	2.95	0.58
1:A:2317:VAL:HG21	1:A:2366:PRO:HD3	1.84	0.58
1:C:1423:SER:O	1:C:1423:SER:OG	2.20	0.58
1:A:2173:TYR:HE1	1:C:2126:TRP:CZ3	2.21	0.58
1:C:1728:ARG:NH1	1:C:1728:ARG:HG2	2.18	0.58
1:A:2459:PHE:CD1	1:C:2137:MET:SD	2.95	0.57
1:B:630:TRP:HB2	1:B:698:LEU:CD1	2.34	0.57
1:B:1728:ARG:HG2	1:B:1728:ARG:NH1	2.18	0.57
1:A:578:LYS:HD2	1:A:708:LEU:HG	1.86	0.57
1:B:580:TRP:HE1	1:B:697:GLN:HB2	1.70	0.57
2:B:2601:L9Q:H32	2:B:2601:L9Q:C25	2.31	0.57
1:B:2193:PHE:CE1	1:B:2194:MET:HG3	2.36	0.57
1:C:1560:VAL:O	1:C:1560:VAL:CG1	2.49	0.57
1:C:580:TRP:HE1	1:C:697:GLN:HB2	1.70	0.57
1:C:991:PHE:HE1	1:C:998:ILE:HG21	1.70	0.57
1:B:1212:LEU:HD11	1:B:1303:LEU:HD11	1.87	0.57
1:A:580:TRP:HE1	1:A:697:GLN:HB2	1.70	0.57
1:A:1728:ARG:NH1	1:A:1728:ARG:HG2	2.18	0.57
1:A:2028:LEU:CD1	1:A:2029:GLY:HA2	2.35	0.57
1:A:630:TRP:O	1:A:633:VAL:HB	2.04	0.57
1:B:870:MET:C	1:B:872:TYR:H	2.13	0.57
1:B:874:LEU:CB	1:B:877:VAL:CG2	2.82	0.57
1:A:991:PHE:HE1	1:A:998:ILE:HG21	1.70	0.56
1:C:633:VAL:HG11	1:C:694:CYS:SG	2.45	0.56
1:A:1334:LYS:HG3	1:A:1335:SER:N	2.18	0.56
1:C:2193:PHE:CE1	1:C:2194:MET:HG3	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1701:VAL:CG1	1:A:1702:THR:N	2.69	0.56
1:A:2178:LEU:CD2	1:A:2182:PHE:CZ	2.89	0.56
1:C:630:TRP:O	1:C:633:VAL:HB	2.05	0.56
1:C:874:LEU:CB	1:C:877:VAL:CG2	2.82	0.56
1:B:2126:TRP:CZ3	1:C:2173:TYR:HE1	2.21	0.56
1:C:2028:LEU:CD1	1:C:2029:GLY:HA2	2.34	0.56
1:A:2312:ALA:HB2	1:B:2366:PRO:CD	2.33	0.56
1:B:805:PHE:CD1	1:B:805:PHE:O	2.59	0.56
1:B:2005:LEU:CD1	1:C:2188:TRP:NE1	2.68	0.56
1:A:581:ILE:CA	1:A:697:GLN:NE2	2.69	0.56
1:A:805:PHE:CD1	1:A:805:PHE:O	2.59	0.56
1:A:2005:LEU:CD1	1:B:2188:TRP:NE1	2.68	0.56
1:A:2188:TRP:NE1	1:C:2005:LEU:CD1	2.68	0.56
1:B:2178:LEU:CD2	1:B:2182:PHE:CZ	2.89	0.56
1:C:805:PHE:CD1	1:C:805:PHE:O	2.59	0.56
1:C:870:MET:C	1:C:872:TYR:H	2.13	0.56
1:C:2178:LEU:CD2	1:C:2182:PHE:CZ	2.89	0.56
1:A:2172:LYS:HA	1:C:2124:TRP:CZ3	2.41	0.55
1:B:2124:TRP:CZ3	1:C:2172:LYS:HA	2.41	0.55
1:C:1971:ASP:O	1:C:1972:PHE:C	2.49	0.55
1:A:1523:ASP:HB3	1:A:1527:ARG:HH21	1.71	0.55
1:A:2317:VAL:HG11	1:A:2366:PRO:HG3	1.88	0.55
1:B:1423:SER:O	1:B:1423:SER:OG	2.20	0.55
1:A:2124:TRP:CZ3	1:B:2172:LYS:HA	2.41	0.55
1:B:991:PHE:HE1	1:B:998:ILE:HG21	1.70	0.55
1:B:581:ILE:CA	1:B:697:GLN:NE2	2.69	0.55
1:B:1523:ASP:HB3	1:B:1527:ARG:HH21	1.71	0.55
1:A:870:MET:C	1:A:872:TYR:H	2.13	0.55
1:B:1971:ASP:O	1:B:1972:PHE:C	2.49	0.55
1:B:2028:LEU:CD1	1:B:2029:GLY:HA2	2.34	0.55
1:C:1523:ASP:HB3	1:C:1527:ARG:HH21	1.72	0.55
1:B:1687:SER:HB2	1:B:1796:HIS:ND1	2.22	0.55
1:B:2126:TRP:HZ3	1:C:2173:TYR:CZ	2.23	0.54
1:C:581:ILE:CA	1:C:697:GLN:NE2	2.69	0.54
1:A:2126:TRP:CZ3	1:B:2173:TYR:HE1	2.21	0.54
1:A:1971:ASP:O	1:A:1972:PHE:C	2.50	0.54
2:B:2601:L9Q:O11	2:B:2601:L9Q:C22	2.52	0.54
1:B:1215:TRP:HE1	1:B:1298:GLN:HB3	1.72	0.54
1:A:1728:ARG:HG2	1:A:1728:ARG:HH11	1.73	0.54
1:C:1342:ILE:N	1:C:1342:ILE:CD1	2.53	0.54
2:A:2601:L9Q:O11	2:A:2601:L9Q:C22	2.52	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1334:LYS:HG3	1:B:1335:SER:N	2.18	0.54
1:A:2173:TYR:HD1	1:C:2125:VAL:CG1	1.93	0.54
1:A:2466:ILE:HG23	1:A:2470:GLU:HG3	1.90	0.54
1:B:1728:ARG:HG2	1:B:1728:ARG:HH11	1.73	0.53
1:A:1103:PHE:O	1:A:1105:LEU:N	2.42	0.53
1:B:2466:ILE:HG23	1:B:2470:GLU:HG3	1.89	0.53
1:C:2065:LEU:C	1:C:2067:TYR:N	2.66	0.53
1:A:587:MET:CE	1:A:693:ALA:CB	2.59	0.53
1:A:2188:TRP:HE1	1:C:2005:LEU:CG	2.21	0.53
1:C:1728:ARG:HG2	1:C:1728:ARG:HH11	1.73	0.53
1:A:874:LEU:CB	1:A:877:VAL:CG2	2.82	0.53
1:C:1053:TYR:C	1:C:1053:TYR:HD1	2.16	0.53
1:C:1687:SER:HB2	1:C:1796:HIS:ND1	2.22	0.53
1:C:2466:ILE:HG23	1:C:2470:GLU:HG3	1.90	0.53
1:A:577:ALA:O	1:A:705:PHE:CD1	2.60	0.53
1:A:641:LEU:HB2	1:A:684:ILE:HG23	1.91	0.53
1:A:1053:TYR:O	1:A:1053:TYR:HD1	1.88	0.53
1:A:1687:SER:HB2	1:A:1796:HIS:ND1	2.22	0.53
1:A:2317:VAL:CG1	1:A:2366:PRO:HG3	2.38	0.53
1:C:1103:PHE:O	1:C:1105:LEU:N	2.42	0.53
1:C:1338:PHE:HE1	1:C:1339:HIS:CG	2.27	0.53
1:B:641:LEU:HB2	1:B:684:ILE:HG23	1.91	0.52
1:B:1215:TRP:NE1	1:B:1298:GLN:HB3	2.25	0.52
1:B:1103:PHE:O	1:B:1105:LEU:N	2.42	0.52
1:B:2065:LEU:C	1:B:2067:TYR:N	2.66	0.52
1:A:2005:LEU:CG	1:B:2188:TRP:HE1	2.21	0.52
1:C:641:LEU:HB2	1:C:684:ILE:HG23	1.91	0.52
2:C:2601:L9Q:H25	2:C:2601:L9Q:C32	2.35	0.52
1:A:1408:ASP:OD1	1:B:2160:PRO:HB3	2.10	0.52
1:B:992:TYR:CZ	1:B:1119:GLU:HG2	2.45	0.52
1:B:2005:LEU:CG	1:C:2188:TRP:HE1	2.21	0.52
1:A:630:TRP:HB2	1:A:698:LEU:CD1	2.39	0.52
1:A:1215:TRP:HE1	1:A:1298:GLN:HB3	1.74	0.52
1:A:992:TYR:CZ	1:A:1119:GLU:HG2	2.45	0.52
1:A:1656:ILE:CG2	1:A:1657:PRO:HD2	2.35	0.51
1:C:1215:TRP:HE1	1:C:1298:GLN:HB3	1.76	0.51
1:B:832:VAL:HG23	1:B:917:PHE:HA	1.92	0.51
1:B:627:LYS:HA	1:B:630:TRP:HD1	1.75	0.51
1:B:1408:ASP:OD1	1:C:2160:PRO:HB3	2.10	0.51
1:A:1728:ARG:HH11	1:A:1728:ARG:CG	2.24	0.51
1:B:630:TRP:O	1:B:633:VAL:HB	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:992:TYR:CZ	1:C:1119:GLU:HG2	2.45	0.51
1:C:1656:ILE:CG2	1:C:1657:PRO:HD2	2.35	0.51
1:A:1053:TYR:C	1:A:1053:TYR:HD1	2.16	0.51
1:A:2160:PRO:HB3	1:C:1408:ASP:OD1	2.10	0.51
1:B:1053:TYR:O	1:B:1053:TYR:CG	2.62	0.51
1:B:1728:ARG:HH11	1:B:1728:ARG:CG	2.24	0.51
1:C:1342:ILE:H	1:C:1342:ILE:CD1	2.09	0.51
1:A:2065:LEU:C	1:A:2067:TYR:N	2.66	0.51
1:C:832:VAL:HG23	1:C:917:PHE:HA	1.92	0.51
1:A:989:PHE:HB3	1:A:992:TYR:HB3	1.93	0.50
1:C:1338:PHE:HD1	1:C:1339:HIS:H	1.56	0.50
1:A:633:VAL:HG11	1:A:694:CYS:SG	2.51	0.50
1:C:1338:PHE:O	1:C:1342:ILE:HG12	2.12	0.50
1:A:1338:PHE:O	1:A:1342:ILE:HG12	2.12	0.50
1:B:604:TYR:HH	1:B:637:THR:HA	1.76	0.50
1:B:1338:PHE:O	1:B:1342:ILE:HG12	2.12	0.50
2:C:2601:L9Q:O11	2:C:2601:L9Q:C22	2.52	0.50
1:A:2025:LYS:HE2	1:A:2089:ILE:HG12	1.93	0.50
1:A:2400:PHE:HB3	1:A:2402:GLU:HG3	1.93	0.50
1:B:1690:LEU:O	1:B:1691:CYS:C	2.55	0.50
1:C:1049:LEU:HD13	1:C:1102:ASP:HB3	1.93	0.50
1:A:633:VAL:HG12	1:A:634:VAL:N	2.27	0.50
1:A:832:VAL:HG23	1:A:917:PHE:HA	1.92	0.50
1:A:1049:LEU:HD13	1:A:1102:ASP:HB3	1.93	0.50
1:B:1049:LEU:HD13	1:B:1102:ASP:HB3	1.93	0.50
1:C:989:PHE:HB3	1:C:992:TYR:HB3	1.93	0.50
1:C:578:LYS:HD2	1:C:708:LEU:HG	1.94	0.50
1:A:2167:LYS:HE3	1:C:2132:SER:HA	1.94	0.50
1:B:2400:PHE:HB3	1:B:2402:GLU:HG3	1.93	0.50
1:C:1728:ARG:HH11	1:C:1728:ARG:CG	2.24	0.50
1:A:2065:LEU:O	1:A:2068:PHE:N	2.45	0.49
1:A:2132:SER:HA	1:B:2167:LYS:HE3	1.94	0.49
1:B:604:TYR:OH	1:B:637:THR:CA	2.57	0.49
1:C:2193:PHE:CD1	1:C:2194:MET:HA	2.47	0.49
1:C:2193:PHE:HE1	1:C:2194:MET:CG	1.96	0.49
1:B:2132:SER:HA	1:C:2167:LYS:HE3	1.94	0.49
1:A:1338:PHE:CD1	1:A:1339:HIS:CA	2.95	0.49
1:C:865:ILE:HG22	1:C:869:LYS:HD2	1.94	0.49
1:C:1338:PHE:CD1	1:C:1339:HIS:CA	2.95	0.49
1:C:2065:LEU:O	1:C:2068:PHE:N	2.45	0.49
1:C:2400:PHE:HB3	1:C:2402:GLU:HG3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2125:VAL:CG1	1:B:2173:TYR:HD1	1.93	0.49
2:A:2601:L9Q:H25	2:A:2601:L9Q:C32	2.35	0.49
1:B:2097:LYS:HE2	1:B:2097:LYS:HB2	1.62	0.49
1:A:865:ILE:HG22	1:A:869:LYS:HD2	1.94	0.48
1:A:2180:ILE:HG23	1:C:2118:LEU:CD2	2.38	0.48
1:B:1338:PHE:CD1	1:B:1339:HIS:CA	2.95	0.48
1:B:1342:ILE:H	1:B:1342:ILE:CD1	2.08	0.48
1:B:2005:LEU:HD11	1:C:2188:TRP:NE1	2.28	0.48
1:B:2193:PHE:CD1	1:B:2194:MET:HA	2.47	0.48
1:B:989:PHE:HB3	1:B:992:TYR:HB3	1.93	0.48
1:B:2065:LEU:O	1:B:2068:PHE:N	2.45	0.48
2:B:2601:L9Q:H25	2:B:2601:L9Q:C32	2.35	0.48
1:A:991:PHE:CE1	1:A:998:ILE:CG2	2.93	0.48
1:A:993:LYS:HB3	1:A:993:LYS:HE3	1.40	0.48
1:A:2193:PHE:CE1	1:A:2194:MET:CA	2.96	0.48
1:C:633:VAL:HG12	1:C:634:VAL:N	2.29	0.48
1:C:1656:ILE:CG2	1:C:1657:PRO:N	2.76	0.48
1:C:1690:LEU:O	1:C:1691:CYS:C	2.55	0.48
1:C:2511:GLU:HA	1:C:2514:ILE:HG13	1.95	0.48
1:B:1656:ILE:CG2	1:B:1657:PRO:N	2.76	0.48
1:A:2012:PHE:HE2	1:B:2184:ILE:CD1	2.27	0.48
2:A:2601:L9Q:H16A	2:A:2601:L9Q:H13A	1.55	0.48
1:B:1338:PHE:HE1	1:B:1339:HIS:CG	2.27	0.48
1:A:2121:VAL:CG1	1:B:2176:GLY:HA2	2.44	0.48
1:A:2188:TRP:NE1	1:C:2005:LEU:HD11	2.28	0.48
1:B:2012:PHE:HE2	1:C:2184:ILE:CD1	2.27	0.48
1:A:2511:GLU:HA	1:A:2514:ILE:HG13	1.96	0.48
2:C:2601:L9Q:H21	2:C:2601:L9Q:H24	1.42	0.48
1:A:1196:LEU:CD1	1:A:1218:LEU:HD22	2.43	0.48
1:A:1338:PHE:HD1	1:A:1339:HIS:H	1.55	0.48
1:A:1690:LEU:O	1:A:1691:CYS:C	2.55	0.48
1:A:2176:GLY:HA2	1:C:2121:VAL:CG1	2.44	0.48
1:C:2504:ILE:HD12	1:C:2504:ILE:HA	1.66	0.48
1:A:1656:ILE:CG2	1:A:1657:PRO:N	2.76	0.48
1:A:2005:LEU:HD11	1:B:2188:TRP:NE1	2.28	0.48
1:C:1744:LYS:HE2	1:C:1744:LYS:HB2	1.37	0.48
1:A:1338:PHE:HE1	1:A:1339:HIS:CG	2.27	0.47
1:A:2097:LYS:HB2	1:A:2097:LYS:HE2	1.62	0.47
1:B:578:LYS:HD2	1:B:708:LEU:HG	1.94	0.47
1:C:708:LEU:HD13	1:C:708:LEU:HA	1.64	0.47
1:A:1103:PHE:C	1:A:1105:LEU:N	2.70	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2193:PHE:CE1	1:B:2194:MET:CA	2.96	0.47
1:C:991:PHE:CE1	1:C:998:ILE:HG21	2.49	0.47
1:C:993:LYS:H	1:C:993:LYS:HG2	1.39	0.47
1:C:2193:PHE:CE1	1:C:2194:MET:CA	2.96	0.47
1:B:2121:VAL:CG1	1:C:2176:GLY:HA2	2.44	0.47
1:A:1228:SER:C	1:A:1230:ASN:N	2.71	0.47
1:A:1710:LEU:HD23	1:A:1710:LEU:HA	1.80	0.47
1:B:865:ILE:HG22	1:B:869:LYS:HD2	1.94	0.47
1:C:2506:LEU:HD12	1:C:2512:THR:HG23	1.97	0.47
1:A:1053:TYR:O	1:A:1053:TYR:CG	2.62	0.47
1:A:1342:ILE:H	1:A:1342:ILE:CD1	2.09	0.47
1:A:2193:PHE:CD1	1:A:2194:MET:HA	2.47	0.47
2:C:2601:L9Q:O31	2:C:2601:L9Q:H39	2.14	0.47
1:B:1347:LEU:HD23	1:B:1347:LEU:HA	1.60	0.47
1:C:993:LYS:HB3	1:C:993:LYS:HE3	1.40	0.47
1:A:627:LYS:HA	1:A:630:TRP:HD1	1.79	0.47
1:A:2119:ARG:HE	1:A:2119:ARG:HB3	1.59	0.47
1:A:2126:TRP:HZ3	1:B:2173:TYR:CZ	2.23	0.47
1:A:2184:ILE:CD1	1:C:2012:PHE:HE2	2.27	0.47
1:A:2312:ALA:HB2	1:B:2366:PRO:HG2	1.97	0.47
2:A:2601:L9Q:C40	2:A:2601:L9Q:C14	2.63	0.47
1:B:980:LEU:HD12	1:B:980:LEU:HA	1.68	0.47
1:B:1231:MET:HB2	1:B:1231:MET:HE2	1.73	0.47
1:B:2166:LYS:HE2	1:B:2166:LYS:HB2	1.39	0.47
1:C:926:LEU:HD13	1:C:926:LEU:HA	1.70	0.47
1:C:1053:TYR:O	1:C:1053:TYR:CG	2.62	0.47
1:C:1232:LEU:O	1:C:1233:SER:CB	2.63	0.47
1:C:2229:GLN:H	1:C:2229:GLN:HG2	1.47	0.47
1:A:604:TYR:OH	1:A:637:THR:CA	2.57	0.47
1:A:2173:TYR:CZ	1:C:2126:TRP:HZ3	2.23	0.47
1:B:790:GLU:H	1:B:790:GLU:HG2	1.49	0.47
1:B:991:PHE:CE1	1:B:998:ILE:HG21	2.49	0.47
1:B:2312:ALA:HB2	1:C:2366:PRO:HG2	1.97	0.47
1:C:604:TYR:OH	1:C:637:THR:CA	2.57	0.47
1:A:1232:LEU:O	1:A:1233:SER:CB	2.63	0.47
2:A:2601:L9Q:O31	2:A:2601:L9Q:H39	2.14	0.47
1:B:991:PHE:CE1	1:B:998:ILE:CG2	2.93	0.47
1:B:2121:VAL:HG11	1:C:2176:GLY:HA2	1.97	0.47
1:B:2317:VAL:CG1	1:B:2366:PRO:HG3	2.45	0.47
1:C:2166:LYS:HB2	1:C:2166:LYS:HE2	1.39	0.47
1:C:2186:ILE:HD12	1:C:2186:ILE:HA	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2601:L9Q:H13A	2:C:2601:L9Q:H16A	1.55	0.47
1:A:2166:LYS:HB2	1:A:2166:LYS:HE2	1.38	0.47
1:A:2180:ILE:HG12	1:C:2118:LEU:HD23	1.97	0.47
1:B:1338:PHE:O	1:B:1342:ILE:CG1	2.63	0.47
1:B:2511:GLU:HA	1:B:2514:ILE:HG13	1.96	0.47
2:B:2601:L9Q:O31	2:B:2601:L9Q:H39	2.14	0.47
1:C:1562:ARG:HD3	1:C:1562:ARG:HA	1.35	0.47
1:A:604:TYR:HH	1:A:637:THR:HA	1.80	0.46
1:A:2118:LEU:HD23	1:B:2180:ILE:HG12	1.98	0.46
1:B:708:LEU:HD13	1:B:708:LEU:HA	1.64	0.46
1:B:1232:LEU:O	1:B:1233:SER:CB	2.63	0.46
1:B:2502:LYS:HE3	1:B:2502:LYS:HB3	1.72	0.46
1:C:1103:PHE:C	1:C:1105:LEU:N	2.70	0.46
1:B:1103:PHE:C	1:B:1105:LEU:N	2.70	0.46
1:C:921:LYS:HE3	1:C:921:LYS:HB2	1.42	0.46
1:A:1007:ILE:HG23	1:A:1015:VAL:HG13	1.98	0.46
1:B:1226:ILE:HA	1:B:1285:ILE:HD11	1.96	0.46
1:C:1226:ILE:HA	1:C:1285:ILE:HD11	1.97	0.46
1:C:1338:PHE:O	1:C:1342:ILE:CG1	2.63	0.46
1:C:1722:ILE:HD11	1:C:1949:ILE:HA	1.96	0.46
1:C:2175:MET:HE2	1:C:2175:MET:HB2	1.73	0.46
1:A:1210:ALA:O	1:A:1212:LEU:N	2.48	0.46
1:A:1647:GLU:H	1:A:1647:GLU:HG3	1.40	0.46
1:B:1744:LYS:HB2	1:B:1744:LYS:HE2	1.37	0.46
1:B:2506:LEU:HD12	1:B:2512:THR:HG23	1.97	0.46
2:B:2601:L9Q:H24	2:B:2601:L9Q:H21	1.42	0.46
1:C:680:LEU:H	1:C:680:LEU:HG	1.38	0.46
1:C:849:ARG:H	1:C:849:ARG:HG2	1.53	0.46
2:C:2601:L9Q:H24A	2:C:2601:L9Q:H27A	1.53	0.46
1:A:1412:VAL:HG21	1:B:2163:LYS:HG2	1.98	0.46
1:A:1722:ILE:HD11	1:A:1949:ILE:HA	1.96	0.46
1:A:1722:ILE:HD13	1:A:2082:ARG:HG2	1.98	0.46
1:A:2504:ILE:HD12	1:A:2504:ILE:HA	1.66	0.46
1:B:627:LYS:HA	1:B:630:TRP:CD1	2.51	0.46
1:B:1053:TYR:C	1:B:1053:TYR:HD1	2.16	0.46
1:B:1228:SER:C	1:B:1230:ASN:N	2.71	0.46
1:C:980:LEU:HD12	1:C:980:LEU:HA	1.68	0.46
1:A:993:LYS:H	1:A:993:LYS:HG2	1.39	0.46
1:B:805:PHE:O	1:B:805:PHE:HD1	1.99	0.46
1:A:2121:VAL:HG11	1:B:2176:GLY:HA2	1.97	0.46
1:A:2126:TRP:CH2	1:B:2173:TYR:CE1	3.04	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:816:LYS:H	1:C:816:LYS:HG2	1.52	0.46
1:C:1676:LEU:HD13	1:C:1676:LEU:HA	1.66	0.46
1:A:2502:LYS:HE3	1:A:2502:LYS:HB3	1.72	0.46
2:A:2601:L9Q:H24A	2:A:2601:L9Q:H27A	1.53	0.46
1:B:2118:LEU:HD23	1:C:2180:ILE:HG12	1.97	0.46
1:C:1228:SER:C	1:C:1230:ASN:N	2.72	0.46
1:A:581:ILE:CA	1:A:697:GLN:HE22	2.29	0.46
1:A:685:LEU:HD12	1:A:685:LEU:HA	1.81	0.46
1:B:2312:ALA:HB2	1:C:2366:PRO:CG	2.46	0.46
1:C:1053:TYR:O	1:C:1053:TYR:HD1	1.88	0.46
1:A:2176:GLY:HA2	1:C:2121:VAL:HG11	1.97	0.46
1:A:2506:LEU:HD12	1:A:2512:THR:HG23	1.96	0.46
1:B:1179:ALA:HB2	1:B:1190:LEU:HD21	1.98	0.46
1:C:2167:LYS:HE2	1:C:2167:LYS:HB2	1.42	0.46
1:C:2317:VAL:CG1	1:C:2366:PRO:HG3	2.46	0.46
1:B:2119:ARG:HE	1:B:2119:ARG:HB3	1.59	0.45
1:B:2193:PHE:HE1	1:B:2194:MET:CG	1.95	0.45
1:B:2317:VAL:HG11	1:B:2366:PRO:HG3	1.97	0.45
1:C:1647:GLU:H	1:C:1647:GLU:HG3	1.40	0.45
1:A:1179:ALA:HB2	1:A:1190:LEU:HD21	1.98	0.45
1:A:2312:ALA:HB2	1:B:2366:PRO:CG	2.46	0.45
1:B:581:ILE:CB	1:B:697:GLN:NE2	2.79	0.45
1:A:991:PHE:CE1	1:A:998:ILE:HG21	2.50	0.45
1:B:874:LEU:HB2	1:B:877:VAL:HG22	1.97	0.45
1:B:2504:ILE:HA	1:B:2504:ILE:HD12	1.66	0.45
1:C:604:TYR:HH	1:C:637:THR:HA	1.77	0.45
1:C:2317:VAL:HG11	1:C:2366:PRO:HG3	1.98	0.45
1:A:1226:ILE:HA	1:A:1285:ILE:HD11	1.99	0.45
1:A:2193:PHE:CE1	1:A:2194:MET:HA	2.52	0.45
1:B:581:ILE:CA	1:B:697:GLN:HE22	2.29	0.45
1:B:2185:ALA:C	1:B:2186:ILE:HD13	2.42	0.45
1:B:2193:PHE:CE1	1:B:2194:MET:HA	2.52	0.45
1:C:581:ILE:CA	1:C:697:GLN:HE22	2.29	0.45
1:C:1215:TRP:NE1	1:C:1298:GLN:HB3	2.31	0.45
1:A:633:VAL:HG13	1:A:690:PHE:CE2	2.52	0.45
1:A:1799:GLN:C	1:A:1801:LEU:H	2.25	0.45
1:B:2154:GLU:O	1:B:2158:LYS:HG3	2.17	0.45
1:C:630:TRP:HB2	1:C:698:LEU:CD1	2.47	0.45
1:C:1104:LEU:HD23	1:C:1104:LEU:HA	1.86	0.45
1:A:1210:ALA:C	1:A:1212:LEU:N	2.75	0.45
1:A:2163:LYS:HG2	1:C:1412:VAL:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2173:TYR:CE1	1:C:2126:TRP:CH2	3.04	0.45
1:A:2293:TYR:CE2	1:A:2339:ALA:HB1	2.51	0.45
1:B:1338:PHE:CE1	1:B:1339:HIS:CG	3.03	0.45
1:B:1412:VAL:HG21	1:C:2163:LYS:HG2	1.98	0.45
1:C:805:PHE:O	1:C:805:PHE:HD1	1.99	0.45
1:C:1799:GLN:C	1:C:1801:LEU:H	2.25	0.45
1:C:2168:LYS:H	1:C:2168:LYS:HG2	1.34	0.45
1:C:2193:PHE:CE1	1:C:2194:MET:HA	2.52	0.45
1:A:1338:PHE:O	1:A:1342:ILE:CG1	2.63	0.45
1:B:630:TRP:HB2	1:B:698:LEU:HD13	1.99	0.45
1:B:1334:LYS:CG	1:B:1335:SER:N	2.80	0.45
2:C:2601:L9Q:C40	2:C:2601:L9Q:C16	2.69	0.45
1:A:588:PHE:CZ	1:A:633:VAL:HG22	2.51	0.45
1:A:2116:VAL:HG12	1:A:2117:GLU:N	2.31	0.45
1:B:1656:ILE:CG2	1:B:1657:PRO:HD2	2.35	0.45
1:A:2478:LEU:HD12	1:A:2478:LEU:HA	1.80	0.45
1:B:1007:ILE:HG23	1:B:1015:VAL:HG13	1.98	0.45
1:B:2126:TRP:CH2	1:C:2173:TYR:CE1	3.04	0.45
2:B:2601:L9Q:H45A	2:B:2601:L9Q:H42A	1.70	0.45
1:C:1007:ILE:HG23	1:C:1015:VAL:HG13	1.98	0.45
1:C:2116:VAL:HG12	1:C:2117:GLU:N	2.31	0.45
1:A:581:ILE:CB	1:A:697:GLN:NE2	2.79	0.45
1:A:2185:ALA:C	1:A:2186:ILE:HD13	2.42	0.45
1:A:2505:PHE:O	1:A:2505:PHE:CG	2.60	0.45
2:A:2601:L9Q:H45A	2:A:2601:L9Q:H42A	1.70	0.45
1:B:1700:MET:HE3	1:B:1700:MET:HB3	1.75	0.45
1:B:2293:TYR:CE2	1:B:2339:ALA:HB1	2.51	0.45
2:B:2601:L9Q:H19A	2:B:2601:L9Q:H16A	1.35	0.45
2:A:2601:L9Q:H16A	2:A:2601:L9Q:H19A	1.35	0.44
1:B:2478:LEU:HD12	1:B:2478:LEU:HA	1.80	0.44
1:B:2505:PHE:O	1:B:2505:PHE:CG	2.60	0.44
1:C:2185:ALA:C	1:C:2186:ILE:HD13	2.42	0.44
1:C:2292:LEU:HB3	1:C:2339:ALA:HB2	1.99	0.44
1:C:2293:TYR:CE2	1:C:2339:ALA:HB1	2.51	0.44
1:A:805:PHE:O	1:A:805:PHE:HD1	1.99	0.44
1:A:1014:LEU:HD23	1:A:1014:LEU:HA	1.79	0.44
1:A:1334:LYS:CG	1:A:1335:SER:N	2.80	0.44
1:A:2456:ARG:HA	1:A:2456:ARG:HD3	1.58	0.44
1:B:2070:LYS:HD2	1:B:2070:LYS:HA	1.81	0.44
2:B:2601:L9Q:H27A	2:B:2601:L9Q:H24A	1.53	0.44
1:A:869:LYS:CB	1:A:929:ILE:HD11	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2154:GLU:O	1:A:2158:LYS:HG3	2.17	0.44
1:B:2167:LYS:HB2	1:B:2167:LYS:HE2	1.42	0.44
1:C:633:VAL:HG13	1:C:690:PHE:CE2	2.51	0.44
1:C:1179:ALA:HB2	1:C:1190:LEU:HD21	1.98	0.44
1:A:597:LEU:H	1:A:597:LEU:HG	1.51	0.44
1:A:1334:LYS:HE3	1:A:1334:LYS:HB2	1.77	0.44
1:A:2292:LEU:HB3	1:A:2339:ALA:HB2	2.00	0.44
1:B:1799:GLN:C	1:B:1801:LEU:H	2.25	0.44
1:C:2154:GLU:O	1:C:2158:LYS:HG3	2.17	0.44
1:A:1215:TRP:NE1	1:A:1298:GLN:HB3	2.31	0.44
1:B:576:TYR:HA	1:B:580:TRP:HB3	1.99	0.44
1:C:991:PHE:CE1	1:C:998:ILE:CG2	2.93	0.44
1:C:874:LEU:HB2	1:C:877:VAL:HG22	1.97	0.44
1:C:972:ARG:HA	1:C:972:ARG:HD2	1.68	0.44
1:C:1231:MET:HB2	1:C:1231:MET:HE2	1.73	0.44
1:A:849:ARG:H	1:A:849:ARG:HG2	1.53	0.44
1:A:876:VAL:O	1:A:876:VAL:HG23	2.18	0.44
1:A:1286:ILE:H	1:A:1286:ILE:HG13	1.52	0.44
1:B:869:LYS:CB	1:B:929:ILE:HD11	2.48	0.44
1:B:2292:LEU:HB3	1:B:2339:ALA:HB2	2.00	0.44
1:C:581:ILE:CB	1:C:697:GLN:NE2	2.79	0.44
1:C:790:GLU:H	1:C:790:GLU:HG2	1.49	0.44
1:A:1327:LEU:N	1:A:1327:LEU:HD23	2.33	0.44
1:A:1354:MET:HE3	1:A:1354:MET:HB2	1.84	0.44
1:A:2045:MET:HB3	1:A:2045:MET:HE3	1.59	0.44
1:B:849:ARG:H	1:B:849:ARG:HG2	1.53	0.44
1:B:1209:ARG:HA	1:B:1209:ARG:HD3	1.81	0.44
1:B:1562:ARG:HD3	1:B:1562:ARG:HA	1.35	0.44
1:C:2178:LEU:HD23	1:C:2182:PHE:CZ	2.53	0.44
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.86	0.44
1:B:1159:LYS:HE2	1:B:1306:TYR:CE2	2.53	0.44
1:B:1220:LEU:HD13	1:B:1220:LEU:HA	1.66	0.44
1:B:1949:ILE:H	1:B:1949:ILE:HG13	1.51	0.44
1:B:2118:LEU:HG	1:C:2183:LEU:CD1	2.48	0.44
1:C:588:PHE:CZ	1:C:633:VAL:HG22	2.53	0.44
1:A:874:LEU:HB2	1:A:877:VAL:HG22	1.97	0.43
1:A:1159:LYS:HE2	1:A:1306:TYR:CE2	2.53	0.43
1:A:2367:GLU:HB3	1:A:2369:ASN:ND2	2.32	0.43
1:C:1100:ILE:H	1:C:1100:ILE:HG13	1.48	0.43
1:C:1159:LYS:HE2	1:C:1306:TYR:CE2	2.53	0.43
1:C:1219:ILE:O	1:C:1223:VAL:HG23	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2167:LYS:HB2	1:A:2167:LYS:HE2	1.42	0.43
1:B:870:MET:C	1:B:872:TYR:N	2.76	0.43
1:B:937:LEU:HD22	1:B:937:LEU:HA	1.75	0.43
1:B:1791:MET:HE2	1:B:1791:MET:HB2	1.86	0.43
1:B:2504:ILE:HD11	1:C:2466:ILE:HD13	2.00	0.43
1:C:876:VAL:O	1:C:876:VAL:HG23	2.18	0.43
1:A:2178:LEU:HD23	1:A:2182:PHE:CZ	2.53	0.43
2:A:2601:L9Q:H21	2:A:2601:L9Q:H24	1.42	0.43
1:B:1214:LEU:HD12	1:B:1214:LEU:HA	1.84	0.43
1:C:1334:LYS:CG	1:C:1335:SER:N	2.80	0.43
1:A:2183:LEU:CD1	1:C:2118:LEU:HG	2.48	0.43
1:A:2320:ALA:HA	1:A:2366:PRO:HA	2.00	0.43
1:B:1656:ILE:HG22	1:B:1657:PRO:N	2.34	0.43
1:C:869:LYS:CB	1:C:929:ILE:HD11	2.48	0.43
1:B:1327:LEU:N	1:B:1327:LEU:HD23	2.33	0.43
1:C:576:TYR:HA	1:C:580:TRP:HB3	1.99	0.43
1:C:810:LEU:HD23	1:C:810:LEU:HA	1.81	0.43
1:C:2189:PHE:C	1:C:2189:PHE:HD1	2.25	0.43
1:A:810:LEU:HD23	1:A:810:LEU:HA	1.81	0.43
1:A:1333:LEU:HD23	1:A:1333:LEU:HA	1.74	0.43
1:A:1656:ILE:HG22	1:A:1657:PRO:N	2.34	0.43
1:A:2118:LEU:HG	1:B:2183:LEU:CD1	2.48	0.43
1:B:2317:VAL:HG21	1:B:2366:PRO:HD3	2.01	0.43
1:A:573:LYS:HB2	1:A:573:LYS:HE2	1.79	0.43
1:B:1100:ILE:H	1:B:1100:ILE:HG13	1.48	0.43
1:B:1722:ILE:HD11	1:B:1949:ILE:HA	2.00	0.43
1:C:581:ILE:CB	1:C:697:GLN:HE22	2.32	0.43
1:A:680:LEU:H	1:A:680:LEU:HG	1.38	0.43
1:B:633:VAL:O	1:B:634:VAL:C	2.59	0.43
1:B:2168:LYS:H	1:B:2168:LYS:HG2	1.33	0.43
1:C:1719:MET:HE2	1:C:1719:MET:HB3	1.89	0.43
1:C:2520:LYS:H	1:C:2520:LYS:HG3	1.53	0.43
1:A:1347:LEU:HD23	1:A:1347:LEU:HA	1.60	0.43
1:A:1791:MET:HE2	1:A:1791:MET:HB2	1.86	0.43
1:B:979:LEU:HD13	1:B:979:LEU:HA	1.85	0.43
1:B:2045:MET:HE3	1:B:2045:MET:HB3	1.59	0.43
1:C:626:LEU:HD12	1:C:626:LEU:HA	1.74	0.43
1:C:2168:LYS:HG2	1:C:2168:LYS:HZ2	1.76	0.43
1:A:581:ILE:CB	1:A:697:GLN:HE22	2.32	0.43
1:A:790:GLU:H	1:A:790:GLU:HG2	1.49	0.43
1:A:1949:ILE:H	1:A:1949:ILE:HG13	1.68	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2118:LEU:CD2	1:B:2180:ILE:HG23	2.38	0.43
1:B:639:LEU:HD13	1:B:639:LEU:HA	1.76	0.43
1:B:2118:LEU:CD2	1:C:2180:ILE:HG23	2.38	0.43
1:B:2186:ILE:HD12	1:B:2186:ILE:HA	1.78	0.43
1:B:876:VAL:O	1:B:876:VAL:HG23	2.18	0.42
1:B:1228:SER:O	1:B:1229:LYS:C	2.62	0.42
1:B:1334:LYS:HE3	1:B:1334:LYS:HB2	1.77	0.42
1:B:2456:ARG:HA	1:B:2456:ARG:HD3	1.55	0.42
1:B:589:ILE:H	1:B:589:ILE:HG13	1.71	0.42
1:B:2116:VAL:HG12	1:B:2117:GLU:N	2.31	0.42
1:B:2228:GLN:HE21	1:B:2228:GLN:HB3	1.60	0.42
1:C:1327:LEU:HD23	1:C:1327:LEU:N	2.33	0.42
1:C:2119:ARG:HE	1:C:2119:ARG:HB3	1.59	0.42
1:A:576:TYR:HA	1:A:580:TRP:HB3	1.99	0.42
1:A:816:LYS:H	1:A:816:LYS:HG2	1.52	0.42
1:B:2195:SER:HA	1:B:2198:ARG:HD2	2.01	0.42
1:C:2317:VAL:HG21	1:C:2366:PRO:HD3	2.01	0.42
1:C:1656:ILE:HG22	1:C:1657:PRO:N	2.34	0.42
1:C:1700:MET:HE3	1:C:1700:MET:HB3	1.75	0.42
1:A:612:LEU:HD23	1:A:612:LEU:HA	1.80	0.42
1:A:1232:LEU:O	1:A:1233:SER:HB3	2.19	0.42
1:A:2195:SER:HA	1:A:2198:ARG:HD2	2.01	0.42
1:B:2462:ILE:H	1:B:2462:ILE:HG13	1.59	0.42
1:A:873:GLN:HE22	1:A:921:LYS:HA	1.84	0.42
1:A:1338:PHE:CE1	1:A:1339:HIS:CG	3.03	0.42
1:A:2070:LYS:HD2	1:A:2070:LYS:HA	1.81	0.42
1:B:581:ILE:CB	1:B:697:GLN:HE22	2.32	0.42
1:B:2253:ALA:HB1	1:B:2374:LEU:HD23	2.02	0.42
1:C:589:ILE:H	1:C:589:ILE:HG13	1.71	0.42
1:C:2045:MET:HE3	1:C:2045:MET:HB3	1.59	0.42
2:C:2601:L9Q:H42A	2:C:2601:L9Q:H45A	1.70	0.42
1:A:639:LEU:HD13	1:A:639:LEU:HA	1.76	0.42
1:A:870:MET:C	1:A:872:TYR:N	2.76	0.42
1:A:1676:LEU:HD13	1:A:1676:LEU:HA	1.66	0.42
1:A:2466:ILE:HD13	1:C:2504:ILE:HD11	2.00	0.42
1:B:680:LEU:H	1:B:680:LEU:HG	1.38	0.42
1:C:2471:LEU:HA	1:C:2472:PRO:HD3	1.93	0.42
1:A:1360:LYS:HE2	1:A:1360:LYS:HB2	1.90	0.42
1:A:2504:ILE:HD11	1:B:2466:ILE:HD13	2.00	0.42
1:B:2178:LEU:HD23	1:B:2182:PHE:CZ	2.53	0.42
2:B:2601:L9Q:H16A	2:B:2601:L9Q:H13A	1.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1228:SER:O	1:C:1229:LYS:C	2.63	0.42
1:C:2097:LYS:HE2	1:C:2097:LYS:HB2	1.63	0.42
1:A:874:LEU:HD23	1:A:874:LEU:HA	1.88	0.42
1:B:581:ILE:HB	1:B:697:GLN:HE22	1.85	0.42
1:C:685:LEU:HD12	1:C:685:LEU:HA	1.81	0.42
1:C:1220:LEU:HA	1:C:1220:LEU:HD13	1.69	0.42
1:C:1232:LEU:O	1:C:1233:SER:HB3	2.19	0.42
1:C:2460:SER:HB3	1:C:2461:GLU:H	1.75	0.42
1:A:1568:LEU:HD12	1:A:1568:LEU:HA	1.93	0.42
1:C:1286:ILE:H	1:C:1286:ILE:HG13	1.52	0.42
1:C:2453:LYS:HZ2	1:C:2453:LYS:HG2	1.76	0.42
1:B:1676:LEU:HD13	1:B:1676:LEU:HA	1.66	0.41
1:A:1549:LEU:H	1:A:1549:LEU:HG	1.72	0.41
1:B:817:LEU:HD22	1:B:817:LEU:HA	1.72	0.41
1:B:1422:GLU:HB3	1:B:1423:SER:H	1.43	0.41
1:B:1963:LEU:O	1:B:1964:MET:C	2.62	0.41
1:C:580:TRP:CD1	1:C:580:TRP:C	2.98	0.41
1:C:1159:LYS:HE2	1:C:1306:TYR:HE2	1.85	0.41
1:C:2253:ALA:HB1	1:C:2374:LEU:HD23	2.02	0.41
1:A:1104:LEU:HD23	1:A:1104:LEU:HA	1.86	0.41
1:A:1219:ILE:O	1:A:1223:VAL:HG23	2.20	0.41
1:A:1228:SER:O	1:A:1229:LYS:C	2.62	0.41
1:B:597:LEU:H	1:B:597:LEU:HG	1.51	0.41
1:B:633:VAL:HG12	1:B:634:VAL:N	2.35	0.41
1:B:1363:LYS:HB3	1:B:1363:LYS:HE2	1.62	0.41
1:C:1363:LYS:HB3	1:C:1363:LYS:HE2	1.62	0.41
1:A:580:TRP:CD1	1:A:580:TRP:C	2.98	0.41
1:B:937:LEU:O	1:B:938:LEU:C	2.63	0.41
1:A:1028:ARG:H	1:A:1028:ARG:HG3	1.58	0.41
1:A:1159:LYS:HE2	1:A:1306:TYR:HE2	1.85	0.41
1:A:2467:MET:HE2	1:A:2467:MET:HB2	1.90	0.41
1:B:580:TRP:CD1	1:B:580:TRP:C	2.98	0.41
1:B:1159:LYS:HE2	1:B:1306:TYR:HE2	1.85	0.41
1:B:2471:LEU:HA	1:B:2472:PRO:HD3	1.93	0.41
1:C:1333:LEU:HD23	1:C:1333:LEU:HA	1.74	0.41
1:C:2070:LYS:HD2	1:C:2070:LYS:HA	1.81	0.41
1:A:937:LEU:HD22	1:A:937:LEU:HA	1.75	0.41
1:B:2520:LYS:H	1:B:2520:LYS:HG3	1.53	0.41
1:B:1286:ILE:H	1:B:1286:ILE:HG13	1.52	0.41
1:C:623:ARG:HA	1:C:626:LEU:HD22	2.03	0.41
1:C:1338:PHE:CE1	1:C:1339:HIS:CG	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2195:SER:HA	1:C:2198:ARG:HD2	2.01	0.41
1:A:2253:ALA:HB1	1:A:2374:LEU:HD23	2.02	0.41
1:B:705:PHE:C	1:B:707:GLN:N	2.78	0.41
1:C:1212:LEU:HD23	1:C:1212:LEU:HA	1.72	0.41
1:A:633:VAL:O	1:A:634:VAL:C	2.62	0.41
1:A:638:MET:HB2	1:A:638:MET:HE2	1.83	0.41
1:A:942:GLU:CG	1:A:943:ALA:N	2.84	0.41
1:A:1209:ARG:HD3	1:A:1209:ARG:HA	1.81	0.41
1:A:1562:ARG:HD3	1:A:1562:ARG:HA	1.35	0.41
1:A:2317:VAL:HG11	1:A:2366:PRO:CG	2.51	0.41
1:B:942:GLU:CG	1:B:943:ALA:N	2.84	0.41
1:B:2124:TRP:HZ2	1:C:2167:LYS:HD2	1.86	0.41
1:B:2367:GLU:HB3	1:B:2369:ASN:ND2	2.36	0.41
1:C:573:LYS:HB2	1:C:573:LYS:HE2	1.79	0.41
1:C:705:PHE:C	1:C:707:GLN:N	2.78	0.41
1:C:870:MET:C	1:C:872:TYR:N	2.76	0.41
1:C:953:ARG:HE	1:C:953:ARG:HB2	1.57	0.41
1:C:1791:MET:HE2	1:C:1791:MET:HB2	1.86	0.41
1:C:2215:LYS:HE2	1:C:2219:TYR:O	2.21	0.41
1:C:2264:ASP:OD2	1:C:2426:LYS:HE3	2.21	0.41
1:C:2285:ARG:HH22	1:C:2391:ARG:HH21	1.69	0.41
1:A:1043:LEU:HD12	1:A:1043:LEU:HA	1.89	0.40
1:A:1196:LEU:HD11	1:A:1218:LEU:HD22	2.03	0.40
1:A:2513:MET:HE2	1:A:2513:MET:HB2	1.93	0.40
1:B:972:ARG:HA	1:B:972:ARG:HD2	1.68	0.40
1:B:2264:ASP:OD2	1:B:2426:LYS:HE3	2.21	0.40
1:C:2367:GLU:HB3	1:C:2369:ASN:ND2	2.36	0.40
1:A:1022:LEU:HD12	1:A:1022:LEU:HA	1.95	0.40
1:A:1112:GLN:HE21	1:A:1112:GLN:HB3	1.70	0.40
1:A:2163:LYS:HG3	1:C:1408:ASP:N	2.37	0.40
1:B:1232:LEU:O	1:B:1233:SER:HB3	2.19	0.40
1:B:1338:PHE:HD1	1:B:1339:HIS:H	1.55	0.40
1:B:2215:LYS:HE2	1:B:2219:TYR:O	2.21	0.40
1:A:1100:ILE:H	1:A:1100:ILE:HG13	1.48	0.40
1:A:2215:LYS:HE2	1:A:2219:TYR:O	2.21	0.40
1:A:2264:ASP:OD2	1:A:2426:LYS:HE3	2.21	0.40
1:A:2285:ARG:HH22	1:A:2391:ARG:HH21	1.69	0.40
1:B:1007:ILE:H	1:B:1007:ILE:HG13	1.61	0.40
1:A:953:ARG:HE	1:A:953:ARG:HB2	1.58	0.40
1:A:1722:ILE:H	1:A:1722:ILE:HG12	1.69	0.40
1:B:812:LEU:H	1:B:812:LEU:HG	1.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1710:LEU:HD23	1:B:1710:LEU:HA	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1249/1952 (64%)	1128 (90%)	109 (9%)	12 (1%)	12	45
1	B	1249/1952 (64%)	1126 (90%)	110 (9%)	13 (1%)	12	45
1	C	1249/1952 (64%)	1127 (90%)	110 (9%)	12 (1%)	12	45
All	All	3747/5856 (64%)	3381 (90%)	329 (9%)	37 (1%)	15	45

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1657	PRO
1	A	2429	PRO
1	B	1657	PRO
1	B	2429	PRO
1	C	1657	PRO
1	C	2429	PRO
1	A	1422	GLU
1	B	1422	GLU
1	C	1422	GLU
1	A	698	LEU
1	A	1008	GLY
1	A	1209	ARG
1	A	2114	PHE
1	B	578	LYS
1	B	698	LEU
1	B	1008	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1209	ARG
1	B	1724	ARG
1	B	2114	PHE
1	C	578	LYS
1	C	698	LEU
1	C	1008	GLY
1	C	1209	ARG
1	C	2114	PHE
1	A	580	TRP
1	A	2066	TRP
1	B	580	TRP
1	B	2066	TRP
1	C	580	TRP
1	C	2066	TRP
1	A	2086	PRO
1	B	1007	ILE
1	B	2086	PRO
1	C	2086	PRO
1	A	1007	ILE
1	A	1723	PRO
1	C	1007	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1113/1693 (66%)	819 (74%)	294 (26%)	0	3
1	B	1113/1693 (66%)	819 (74%)	294 (26%)	0	3
1	C	1112/1693 (66%)	823 (74%)	289 (26%)	0	3
All	All	3338/5079 (66%)	2461 (74%)	877 (26%)	2	3

All (877) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	571	LEU
1	A	572	VAL
1	A	573	LYS
1	A	580	TRP
1	A	581	ILE
1	A	588	PHE
1	A	592	SER
1	A	597	LEU
1	A	598	VAL
1	A	599	VAL
1	A	601	LYS
1	A	612	LEU
1	A	614	LEU
1	A	618	TYR
1	A	624	LYS
1	A	625	LEU
1	A	626	LEU
1	A	627	LYS
1	A	631	TRP
1	A	633	VAL
1	A	639	LEU
1	A	644	VAL
1	A	678	SER
1	A	679	GLU
1	A	680	LEU
1	A	683	SER
1	A	685	LEU
1	A	692	LEU
1	A	697	GLN
1	A	698	LEU
1	A	699	HIS
1	A	702	HIS
1	A	703	ARG
1	A	707	GLN
1	A	708	LEU
1	A	710	ASP
1	A	711	MET
1	A	712	GLU
1	A	789	LEU
1	A	790	GLU
1	A	791	LEU
1	A	799	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	809	LEU
1	A	810	LEU
1	A	812	LEU
1	A	816	LYS
1	A	817	LEU
1	A	820	LEU
1	A	822	THR
1	A	827	LEU
1	A	831	SER
1	A	832	VAL
1	A	835	LEU
1	A	836	LEU
1	A	843	PHE
1	A	845	LEU
1	A	849	ARG
1	A	853	MET
1	A	855	SER
1	A	856	CYS
1	A	858	SER
1	A	867	VAL
1	A	876	VAL
1	A	877	VAL
1	A	878	ASN
1	A	919	VAL
1	A	920	ARG
1	A	921	LYS
1	A	929	ILE
1	A	937	LEU
1	A	938	LEU
1	A	942	GLU
1	A	947	ARG
1	A	948	ARG
1	A	953	ARG
1	A	954	ARG
1	A	955	GLN
1	A	972	ARG
1	A	974	GLN
1	A	976	ASP
1	A	979	LEU
1	A	980	LEU
1	A	982	CYS
1	A	983	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	984	LYS
1	A	993	LYS
1	A	997	GLU
1	A	998	ILE
1	A	1001	LEU
1	A	1002	MET
1	A	1005	ASN
1	A	1006	VAL
1	A	1007	ILE
1	A	1011	MET
1	A	1023	VAL
1	A	1025	ILE
1	A	1026	LEU
1	A	1028	ARG
1	A	1048	PHE
1	A	1053	TYR
1	A	1054	LEU
1	A	1057	LEU
1	A	1099	LEU
1	A	1100	ILE
1	A	1105	LEU
1	A	1112	GLN
1	A	1155	LEU
1	A	1156	ASP
1	A	1158	LEU
1	A	1176	VAL
1	A	1180	THR
1	A	1184	ILE
1	A	1198	LEU
1	A	1204	LEU
1	A	1208	THR
1	A	1209	ARG
1	A	1212	LEU
1	A	1214	LEU
1	A	1215	TRP
1	A	1217	CYS
1	A	1219	ILE
1	A	1220	LEU
1	A	1222	ASN
1	A	1227	ILE
1	A	1228	SER
1	A	1231	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1232	LEU
1	A	1233	SER
1	A	1285	ILE
1	A	1286	ILE
1	A	1304	SER
1	A	1317	THR
1	A	1327	LEU
1	A	1334	LYS
1	A	1335	SER
1	A	1336	ILE
1	A	1338	PHE
1	A	1341	ARG
1	A	1342	ILE
1	A	1346	SER
1	A	1350	LEU
1	A	1351	LYS
1	A	1354	MET
1	A	1360	LYS
1	A	1363	LYS
1	A	1365	ARG
1	A	1366	GLN
1	A	1413	ILE
1	A	1417	ASP
1	A	1420	LEU
1	A	1422	GLU
1	A	1423	SER
1	A	1514	LEU
1	A	1516	MET
1	A	1517	LEU
1	A	1523	ASP
1	A	1524	GLU
1	A	1530	GLN
1	A	1532	PHE
1	A	1534	ARG
1	A	1539	MET
1	A	1546	GLU
1	A	1547	ARG
1	A	1549	LEU
1	A	1550	LEU
1	A	1552	GLN
1	A	1560	VAL
1	A	1561	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1562	ARG
1	A	1565	LEU
1	A	1568	LEU
1	A	1646	SER
1	A	1647	GLU
1	A	1650	LEU
1	A	1652	ARG
1	A	1655	ARG
1	A	1669	GLN
1	A	1673	LEU
1	A	1676	LEU
1	A	1677	ARG
1	A	1682	CYS
1	A	1694	ILE
1	A	1696	ILE
1	A	1701	VAL
1	A	1708	LEU
1	A	1722	ILE
1	A	1724	ARG
1	A	1727	LYS
1	A	1728	ARG
1	A	1731	MET
1	A	1744	LYS
1	A	1782	TYR
1	A	1784	LYS
1	A	1791	MET
1	A	1797	ARG
1	A	1798	SER
1	A	1802	CYS
1	A	1942	LEU
1	A	1943	ARG
1	A	1950	LEU
1	A	1952	THR
1	A	1953	LYS
1	A	1955	ARG
1	A	1958	THR
1	A	1960	VAL
1	A	1963	LEU
1	A	1966	LEU
1	A	2002	GLU
1	A	2005	LEU
1	A	2007	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2009	LEU
1	A	2015	MET
1	A	2024	ARG
1	A	2026	THR
1	A	2027	VAL
1	A	2028	LEU
1	A	2037	LEU
1	A	2041	ILE
1	A	2043	LEU
1	A	2044	TRP
1	A	2045	MET
1	A	2049	LEU
1	A	2061	VAL
1	A	2062	VAL
1	A	2064	GLN
1	A	2065	LEU
1	A	2069	VAL
1	A	2077	SER
1	A	2082	ARG
1	A	2089	ILE
1	A	2090	LEU
1	A	2094	LEU
1	A	2097	LYS
1	A	2100	HIS
1	A	2109	PHE
1	A	2116	VAL
1	A	2118	LEU
1	A	2119	ARG
1	A	2122	MET
1	A	2131	LEU
1	A	2134	SER
1	A	2138	CYS
1	A	2157	LYS
1	A	2161	GLN
1	A	2166	LYS
1	A	2167	LYS
1	A	2168	LYS
1	A	2169	LYS
1	A	2170	ILE
1	A	2175	MET
1	A	2178	LEU
1	A	2181	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2186	ILE
1	A	2189	PHE
1	A	2192	LEU
1	A	2193	PHE
1	A	2199	SER
1	A	2200	VAL
1	A	2201	VAL
1	A	2203	VAL
1	A	2213	THR
1	A	2228	GLN
1	A	2229	GLN
1	A	2231	SER
1	A	2250	GLN
1	A	2261	SER
1	A	2367	GLU
1	A	2434	PHE
1	A	2435	LEU
1	A	2438	TYR
1	A	2440	ILE
1	A	2441	MET
1	A	2443	LEU
1	A	2446	SER
1	A	2453	LYS
1	A	2456	ARG
1	A	2460	SER
1	A	2462	ILE
1	A	2467	MET
1	A	2469	GLU
1	A	2474	VAL
1	A	2475	ASP
1	A	2476	ARG
1	A	2477	ILE
1	A	2486	LEU
1	A	2489	GLU
1	A	2491	ARG
1	A	2504	ILE
1	A	2511	GLU
1	A	2514	ILE
1	A	2515	LYS
1	A	2518	ARG
1	A	2520	LYS
1	B	570	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	571	LEU
1	B	572	VAL
1	B	573	LYS
1	B	580	TRP
1	B	581	ILE
1	B	588	PHE
1	B	592	SER
1	B	597	LEU
1	B	598	VAL
1	B	599	VAL
1	B	601	LYS
1	B	612	LEU
1	B	614	LEU
1	B	618	TYR
1	B	624	LYS
1	B	625	LEU
1	B	626	LEU
1	B	627	LYS
1	B	633	VAL
1	B	639	LEU
1	B	644	VAL
1	B	678	SER
1	B	679	GLU
1	B	680	LEU
1	B	683	SER
1	B	685	LEU
1	B	692	LEU
1	B	697	GLN
1	B	698	LEU
1	B	699	HIS
1	B	702	HIS
1	B	703	ARG
1	B	707	GLN
1	B	708	LEU
1	B	710	ASP
1	B	711	MET
1	B	712	GLU
1	B	789	LEU
1	B	790	GLU
1	B	791	LEU
1	B	799	LEU
1	B	809	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	810	LEU
1	B	812	LEU
1	B	816	LYS
1	B	817	LEU
1	B	820	LEU
1	B	822	THR
1	B	827	LEU
1	B	831	SER
1	B	832	VAL
1	B	835	LEU
1	B	836	LEU
1	B	843	PHE
1	B	845	LEU
1	B	849	ARG
1	B	853	MET
1	B	855	SER
1	B	856	CYS
1	B	858	SER
1	B	867	VAL
1	B	876	VAL
1	B	877	VAL
1	B	878	ASN
1	B	919	VAL
1	B	920	ARG
1	B	921	LYS
1	B	926	LEU
1	B	929	ILE
1	B	937	LEU
1	B	938	LEU
1	B	942	GLU
1	B	947	ARG
1	B	948	ARG
1	B	953	ARG
1	B	954	ARG
1	B	955	GLN
1	B	972	ARG
1	B	974	GLN
1	B	976	ASP
1	B	979	LEU
1	B	980	LEU
1	B	982	CYS
1	B	983	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	984	LYS
1	B	993	LYS
1	B	997	GLU
1	B	998	ILE
1	B	1001	LEU
1	B	1002	MET
1	B	1005	ASN
1	B	1006	VAL
1	B	1007	ILE
1	B	1011	MET
1	B	1023	VAL
1	B	1025	ILE
1	B	1026	LEU
1	B	1028	ARG
1	B	1048	PHE
1	B	1053	TYR
1	B	1054	LEU
1	B	1057	LEU
1	B	1099	LEU
1	B	1100	ILE
1	B	1105	LEU
1	B	1112	GLN
1	B	1155	LEU
1	B	1156	ASP
1	B	1158	LEU
1	B	1176	VAL
1	B	1180	THR
1	B	1184	ILE
1	B	1198	LEU
1	B	1204	LEU
1	B	1208	THR
1	B	1209	ARG
1	B	1212	LEU
1	B	1214	LEU
1	B	1215	TRP
1	B	1219	ILE
1	B	1220	LEU
1	B	1227	ILE
1	B	1228	SER
1	B	1231	MET
1	B	1232	LEU
1	B	1233	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1285	ILE
1	B	1286	ILE
1	B	1304	SER
1	B	1317	THR
1	B	1327	LEU
1	B	1334	LYS
1	B	1335	SER
1	B	1336	ILE
1	B	1338	PHE
1	B	1341	ARG
1	B	1342	ILE
1	B	1346	SER
1	B	1350	LEU
1	B	1351	LYS
1	B	1354	MET
1	B	1360	LYS
1	B	1363	LYS
1	B	1365	ARG
1	B	1366	GLN
1	B	1413	ILE
1	B	1417	ASP
1	B	1420	LEU
1	B	1422	GLU
1	B	1423	SER
1	B	1514	LEU
1	B	1516	MET
1	B	1517	LEU
1	B	1523	ASP
1	B	1524	GLU
1	B	1530	GLN
1	B	1532	PHE
1	B	1534	ARG
1	B	1539	MET
1	B	1546	GLU
1	B	1547	ARG
1	B	1549	LEU
1	B	1550	LEU
1	B	1552	GLN
1	B	1560	VAL
1	B	1561	HIS
1	B	1562	ARG
1	B	1565	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1568	LEU
1	B	1646	SER
1	B	1647	GLU
1	B	1650	LEU
1	B	1652	ARG
1	B	1655	ARG
1	B	1669	GLN
1	B	1673	LEU
1	B	1676	LEU
1	B	1677	ARG
1	B	1682	CYS
1	B	1694	ILE
1	B	1696	ILE
1	B	1701	VAL
1	B	1708	LEU
1	B	1722	ILE
1	B	1724	ARG
1	B	1727	LYS
1	B	1728	ARG
1	B	1731	MET
1	B	1744	LYS
1	B	1782	TYR
1	B	1784	LYS
1	B	1791	MET
1	B	1797	ARG
1	B	1798	SER
1	B	1802	CYS
1	B	1942	LEU
1	B	1943	ARG
1	B	1947	HIS
1	B	1949	ILE
1	B	1950	LEU
1	B	1951	HIS
1	B	1952	THR
1	B	1953	LYS
1	B	1954	TYR
1	B	1958	THR
1	B	1960	VAL
1	B	1963	LEU
1	B	1966	LEU
1	B	2002	GLU
1	B	2005	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2007	MET
1	B	2009	LEU
1	B	2015	MET
1	B	2024	ARG
1	B	2026	THR
1	B	2027	VAL
1	B	2028	LEU
1	B	2037	LEU
1	B	2041	ILE
1	B	2043	LEU
1	B	2044	TRP
1	B	2045	MET
1	B	2049	LEU
1	B	2061	VAL
1	B	2062	VAL
1	B	2064	GLN
1	B	2065	LEU
1	B	2069	VAL
1	B	2077	SER
1	B	2082	ARG
1	B	2089	ILE
1	B	2094	LEU
1	B	2097	LYS
1	B	2100	HIS
1	B	2109	PHE
1	B	2116	VAL
1	B	2118	LEU
1	B	2119	ARG
1	B	2122	MET
1	B	2131	LEU
1	B	2134	SER
1	B	2138	CYS
1	B	2157	LYS
1	B	2161	GLN
1	B	2166	LYS
1	B	2167	LYS
1	B	2168	LYS
1	B	2169	LYS
1	B	2170	ILE
1	B	2175	MET
1	B	2178	LEU
1	B	2181	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2186	ILE
1	B	2189	PHE
1	B	2192	LEU
1	B	2193	PHE
1	B	2199	SER
1	B	2200	VAL
1	B	2201	VAL
1	B	2203	VAL
1	B	2213	THR
1	B	2228	GLN
1	B	2229	GLN
1	B	2231	SER
1	B	2250	GLN
1	B	2261	SER
1	B	2367	GLU
1	B	2434	PHE
1	B	2435	LEU
1	B	2438	TYR
1	B	2440	ILE
1	B	2441	MET
1	B	2443	LEU
1	B	2446	SER
1	B	2453	LYS
1	B	2456	ARG
1	B	2460	SER
1	B	2462	ILE
1	B	2467	MET
1	B	2469	GLU
1	B	2474	VAL
1	B	2475	ASP
1	B	2476	ARG
1	B	2477	ILE
1	B	2486	LEU
1	B	2489	GLU
1	B	2491	ARG
1	B	2504	ILE
1	B	2511	GLU
1	B	2514	ILE
1	B	2515	LYS
1	B	2518	ARG
1	B	2520	LYS
1	C	570	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	571	LEU
1	C	572	VAL
1	C	573	LYS
1	C	580	TRP
1	C	581	ILE
1	C	588	PHE
1	C	592	SER
1	C	597	LEU
1	C	598	VAL
1	C	599	VAL
1	C	601	LYS
1	C	612	LEU
1	C	614	LEU
1	C	618	TYR
1	C	624	LYS
1	C	625	LEU
1	C	626	LEU
1	C	632	LEU
1	C	633	VAL
1	C	639	LEU
1	C	644	VAL
1	C	678	SER
1	C	679	GLU
1	C	680	LEU
1	C	683	SER
1	C	685	LEU
1	C	692	LEU
1	C	697	GLN
1	C	698	LEU
1	C	699	HIS
1	C	702	HIS
1	C	703	ARG
1	C	707	GLN
1	C	708	LEU
1	C	710	ASP
1	C	711	MET
1	C	712	GLU
1	C	789	LEU
1	C	790	GLU
1	C	791	LEU
1	C	799	LEU
1	C	809	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	810	LEU
1	C	812	LEU
1	C	816	LYS
1	C	817	LEU
1	C	820	LEU
1	C	822	THR
1	C	827	LEU
1	C	831	SER
1	C	832	VAL
1	C	835	LEU
1	C	836	LEU
1	C	843	PHE
1	C	845	LEU
1	C	849	ARG
1	C	853	MET
1	C	855	SER
1	C	856	CYS
1	C	858	SER
1	C	867	VAL
1	C	876	VAL
1	C	877	VAL
1	C	878	ASN
1	C	919	VAL
1	C	920	ARG
1	C	921	LYS
1	C	926	LEU
1	C	929	ILE
1	C	937	LEU
1	C	938	LEU
1	C	942	GLU
1	C	947	ARG
1	C	948	ARG
1	C	953	ARG
1	C	954	ARG
1	C	955	GLN
1	C	972	ARG
1	C	974	GLN
1	C	976	ASP
1	C	979	LEU
1	C	980	LEU
1	C	982	CYS
1	C	983	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	984	LYS
1	C	993	LYS
1	C	997	GLU
1	C	998	ILE
1	C	1001	LEU
1	C	1002	MET
1	C	1005	ASN
1	C	1006	VAL
1	C	1007	ILE
1	C	1011	MET
1	C	1023	VAL
1	C	1025	ILE
1	C	1026	LEU
1	C	1028	ARG
1	C	1048	PHE
1	C	1053	TYR
1	C	1054	LEU
1	C	1057	LEU
1	C	1099	LEU
1	C	1100	ILE
1	C	1105	LEU
1	C	1112	GLN
1	C	1155	LEU
1	C	1156	ASP
1	C	1158	LEU
1	C	1176	VAL
1	C	1180	THR
1	C	1184	ILE
1	C	1198	LEU
1	C	1204	LEU
1	C	1208	THR
1	C	1209	ARG
1	C	1212	LEU
1	C	1214	LEU
1	C	1219	ILE
1	C	1220	LEU
1	C	1228	SER
1	C	1231	MET
1	C	1232	LEU
1	C	1233	SER
1	C	1285	ILE
1	C	1286	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1304	SER
1	C	1317	THR
1	C	1327	LEU
1	C	1334	LYS
1	C	1335	SER
1	C	1336	ILE
1	C	1338	PHE
1	C	1341	ARG
1	C	1342	ILE
1	C	1346	SER
1	C	1350	LEU
1	C	1351	LYS
1	C	1354	MET
1	C	1360	LYS
1	C	1363	LYS
1	C	1365	ARG
1	C	1366	GLN
1	C	1413	ILE
1	C	1417	ASP
1	C	1420	LEU
1	C	1422	GLU
1	C	1423	SER
1	C	1514	LEU
1	C	1516	MET
1	C	1517	LEU
1	C	1523	ASP
1	C	1524	GLU
1	C	1530	GLN
1	C	1532	PHE
1	C	1534	ARG
1	C	1539	MET
1	C	1546	GLU
1	C	1547	ARG
1	C	1549	LEU
1	C	1550	LEU
1	C	1552	GLN
1	C	1560	VAL
1	C	1561	HIS
1	C	1562	ARG
1	C	1565	LEU
1	C	1568	LEU
1	C	1646	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1647	GLU
1	C	1650	LEU
1	C	1652	ARG
1	C	1655	ARG
1	C	1669	GLN
1	C	1673	LEU
1	C	1676	LEU
1	C	1677	ARG
1	C	1682	CYS
1	C	1694	ILE
1	C	1696	ILE
1	C	1701	VAL
1	C	1708	LEU
1	C	1722	ILE
1	C	1724	ARG
1	C	1727	LYS
1	C	1728	ARG
1	C	1731	MET
1	C	1744	LYS
1	C	1782	TYR
1	C	1784	LYS
1	C	1791	MET
1	C	1797	ARG
1	C	1798	SER
1	C	1802	CYS
1	C	1942	LEU
1	C	1943	ARG
1	C	1950	LEU
1	C	1952	THR
1	C	1953	LYS
1	C	1954	TYR
1	C	1955	ARG
1	C	1958	THR
1	C	1960	VAL
1	C	1963	LEU
1	C	1966	LEU
1	C	2002	GLU
1	C	2005	LEU
1	C	2007	MET
1	C	2009	LEU
1	C	2015	MET
1	C	2024	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2026	THR
1	C	2027	VAL
1	C	2028	LEU
1	C	2037	LEU
1	C	2041	ILE
1	C	2043	LEU
1	C	2044	TRP
1	C	2045	MET
1	C	2049	LEU
1	C	2061	VAL
1	C	2062	VAL
1	C	2064	GLN
1	C	2065	LEU
1	C	2069	VAL
1	C	2077	SER
1	C	2082	ARG
1	C	2089	ILE
1	C	2094	LEU
1	C	2097	LYS
1	C	2100	HIS
1	C	2116	VAL
1	C	2118	LEU
1	C	2119	ARG
1	C	2122	MET
1	C	2131	LEU
1	C	2134	SER
1	C	2138	CYS
1	C	2157	LYS
1	C	2161	GLN
1	C	2166	LYS
1	C	2167	LYS
1	C	2168	LYS
1	C	2169	LYS
1	C	2170	ILE
1	C	2175	MET
1	C	2178	LEU
1	C	2181	LEU
1	C	2186	ILE
1	C	2189	PHE
1	C	2192	LEU
1	C	2193	PHE
1	C	2199	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2200	VAL
1	C	2201	VAL
1	C	2203	VAL
1	C	2213	THR
1	C	2228	GLN
1	C	2229	GLN
1	C	2231	SER
1	C	2250	GLN
1	C	2261	SER
1	C	2367	GLU
1	C	2434	PHE
1	C	2435	LEU
1	C	2438	TYR
1	C	2440	ILE
1	C	2441	MET
1	C	2443	LEU
1	C	2446	SER
1	C	2453	LYS
1	C	2456	ARG
1	C	2460	SER
1	C	2462	ILE
1	C	2467	MET
1	C	2469	GLU
1	C	2474	VAL
1	C	2475	ASP
1	C	2476	ARG
1	C	2477	ILE
1	C	2486	LEU
1	C	2489	GLU
1	C	2491	ARG
1	C	2504	ILE
1	C	2511	GLU
1	C	2514	ILE
1	C	2515	LYS
1	C	2518	ARG
1	C	2520	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	697	GLN
1	A	915	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	925	ASN
1	A	955	GLN
1	A	988	ASN
1	A	1012	ASN
1	A	1230	ASN
1	A	1315	GLN
1	A	1339	HIS
1	A	1353	GLN
1	A	1414	HIS
1	A	1519	GLN
1	A	1535	HIS
1	A	1681	GLN
1	A	1699	HIS
1	A	1947	HIS
1	A	1951	HIS
1	A	2011	GLN
1	A	2064	GLN
1	A	2165	GLN
1	A	2228	GLN
1	A	2250	GLN
1	A	2464	HIS
1	B	697	GLN
1	B	915	ASN
1	B	925	ASN
1	B	955	GLN
1	B	988	ASN
1	B	1012	ASN
1	B	1222	ASN
1	B	1230	ASN
1	B	1315	GLN
1	B	1339	HIS
1	B	1353	GLN
1	B	1519	GLN
1	B	1535	HIS
1	B	1681	GLN
1	B	1699	HIS
1	B	1947	HIS
1	B	1951	HIS
1	B	2064	GLN
1	B	2165	GLN
1	B	2228	GLN
1	B	2250	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2464	HIS
1	C	697	GLN
1	C	873	GLN
1	C	915	ASN
1	C	955	GLN
1	C	988	ASN
1	C	1012	ASN
1	C	1222	ASN
1	C	1230	ASN
1	C	1315	GLN
1	C	1339	HIS
1	C	1353	GLN
1	C	1519	GLN
1	C	1535	HIS
1	C	1681	GLN
1	C	1699	HIS
1	C	1947	HIS
1	C	2064	GLN
1	C	2165	GLN
1	C	2228	GLN
1	C	2250	GLN
1	C	2464	HIS

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	L9Q	C	2601	-	50,50,50	1.08	3 (6%)	53,55,55	1.10	2 (3%)
2	L9Q	A	2601	-	50,50,50	1.08	3 (6%)	53,55,55	1.10	2 (3%)
2	L9Q	B	2601	-	50,50,50	1.08	3 (6%)	53,55,55	1.10	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	L9Q	C	2601	-	-	35/54/54/54	-
2	L9Q	A	2601	-	-	35/54/54/54	-
2	L9Q	B	2601	-	-	35/54/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2601	L9Q	O2-C31	4.44	1.46	1.34
2	C	2601	L9Q	O2-C31	4.44	1.46	1.34
2	B	2601	L9Q	O2-C31	4.43	1.46	1.34
2	C	2601	L9Q	O3-C11	4.19	1.45	1.33
2	A	2601	L9Q	O3-C11	4.19	1.45	1.33
2	B	2601	L9Q	O3-C11	4.19	1.45	1.33
2	B	2601	L9Q	C40-C39	3.73	1.52	1.31
2	C	2601	L9Q	C40-C39	3.72	1.52	1.31
2	A	2601	L9Q	C40-C39	3.72	1.52	1.31

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2601	L9Q	O2-C31-C32	4.68	121.60	111.48
2	A	2601	L9Q	O2-C31-C32	4.67	121.58	111.48
2	B	2601	L9Q	O2-C31-C32	4.67	121.58	111.48
2	A	2601	L9Q	O3-C11-C12	2.73	120.15	111.83
2	C	2601	L9Q	O3-C11-C12	2.72	120.14	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2601	L9Q	O3-C11-C12	2.72	120.13	111.83

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	L9Q	C1-O3P-P-O1P
2	A	2601	L9Q	C1-O3P-P-O2P
2	A	2601	L9Q	C1-O3P-P-O4P
2	A	2601	L9Q	C32-C31-O2-C2
2	B	2601	L9Q	C1-O3P-P-O1P
2	B	2601	L9Q	C1-O3P-P-O2P
2	B	2601	L9Q	C1-O3P-P-O4P
2	B	2601	L9Q	C32-C31-O2-C2
2	C	2601	L9Q	C1-O3P-P-O1P
2	C	2601	L9Q	C1-O3P-P-O2P
2	C	2601	L9Q	C1-O3P-P-O4P
2	C	2601	L9Q	C32-C31-O2-C2
2	A	2601	L9Q	O31-C31-O2-C2
2	B	2601	L9Q	O31-C31-O2-C2
2	C	2601	L9Q	O31-C31-O2-C2
2	A	2601	L9Q	C38-C39-C40-C41
2	B	2601	L9Q	C38-C39-C40-C41
2	C	2601	L9Q	C38-C39-C40-C41
2	A	2601	L9Q	C12-C11-O3-C3
2	B	2601	L9Q	C12-C11-O3-C3
2	C	2601	L9Q	C12-C11-O3-C3
2	A	2601	L9Q	C21-C22-C23-C24
2	B	2601	L9Q	C21-C22-C23-C24
2	C	2601	L9Q	C21-C22-C23-C24
2	A	2601	L9Q	C16-C17-C18-C19
2	B	2601	L9Q	C16-C17-C18-C19
2	C	2601	L9Q	C16-C17-C18-C19
2	A	2601	L9Q	C24-C25-C26-C27
2	B	2601	L9Q	C24-C25-C26-C27
2	C	2601	L9Q	C24-C25-C26-C27
2	A	2601	L9Q	O11-C11-O3-C3
2	B	2601	L9Q	O11-C11-O3-C3
2	C	2601	L9Q	O11-C11-O3-C3
2	A	2601	L9Q	C44-C45-C46-C47
2	B	2601	L9Q	C44-C45-C46-C47
2	C	2601	L9Q	C44-C45-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2601	L9Q	C13-C14-C15-C16
2	B	2601	L9Q	C13-C14-C15-C16
2	C	2601	L9Q	C13-C14-C15-C16
2	A	2601	L9Q	C41-C42-C43-C44
2	B	2601	L9Q	C41-C42-C43-C44
2	C	2601	L9Q	C41-C42-C43-C44
2	A	2601	L9Q	C12-C13-C14-C15
2	B	2601	L9Q	C12-C13-C14-C15
2	C	2601	L9Q	C12-C13-C14-C15
2	A	2601	L9Q	C23-C24-C25-C26
2	B	2601	L9Q	C23-C24-C25-C26
2	C	2601	L9Q	C23-C24-C25-C26
2	B	2601	L9Q	C20-C21-C22-C23
2	C	2601	L9Q	C20-C21-C22-C23
2	A	2601	L9Q	C20-C21-C22-C23
2	A	2601	L9Q	C3-C2-O2-C31
2	B	2601	L9Q	C3-C2-O2-C31
2	C	2601	L9Q	C3-C2-O2-C31
2	A	2601	L9Q	C17-C18-C19-C20
2	B	2601	L9Q	C17-C18-C19-C20
2	C	2601	L9Q	C17-C18-C19-C20
2	A	2601	L9Q	C32-C33-C34-C35
2	A	2601	L9Q	C33-C34-C35-C36
2	B	2601	L9Q	C32-C33-C34-C35
2	B	2601	L9Q	C33-C34-C35-C36
2	C	2601	L9Q	C32-C33-C34-C35
2	C	2601	L9Q	C33-C34-C35-C36
2	A	2601	L9Q	C1-C2-C3-O3
2	B	2601	L9Q	C1-C2-C3-O3
2	C	2601	L9Q	C1-C2-C3-O3
2	A	2601	L9Q	C42-C43-C44-C45
2	B	2601	L9Q	C42-C43-C44-C45
2	C	2601	L9Q	C42-C43-C44-C45
2	A	2601	L9Q	O3P-C1-C2-O2
2	B	2601	L9Q	O3P-C1-C2-O2
2	C	2601	L9Q	O3P-C1-C2-O2
2	A	2601	L9Q	C15-C16-C17-C18
2	C	2601	L9Q	C15-C16-C17-C18
2	B	2601	L9Q	C15-C16-C17-C18
2	A	2601	L9Q	O3P-C1-C2-C3
2	B	2601	L9Q	O3P-C1-C2-C3
2	C	2601	L9Q	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2601	L9Q	C22-C23-C24-C25
2	B	2601	L9Q	C22-C23-C24-C25
2	C	2601	L9Q	C22-C23-C24-C25
2	C	2601	L9Q	C34-C35-C36-C37
2	A	2601	L9Q	C34-C35-C36-C37
2	B	2601	L9Q	C34-C35-C36-C37
2	A	2601	L9Q	O2-C2-C3-O3
2	B	2601	L9Q	O2-C2-C3-O3
2	C	2601	L9Q	O2-C2-C3-O3
2	A	2601	L9Q	C11-C12-C13-C14
2	B	2601	L9Q	C11-C12-C13-C14
2	C	2601	L9Q	C11-C12-C13-C14
2	A	2601	L9Q	C35-C36-C37-C38
2	B	2601	L9Q	C35-C36-C37-C38
2	C	2601	L9Q	C35-C36-C37-C38
2	B	2601	L9Q	C19-C20-C21-C22
2	A	2601	L9Q	C19-C20-C21-C22
2	C	2601	L9Q	C19-C20-C21-C22
2	A	2601	L9Q	C40-C41-C42-C43
2	B	2601	L9Q	C40-C41-C42-C43
2	C	2601	L9Q	C40-C41-C42-C43
2	A	2601	L9Q	O2-C31-C32-C33
2	B	2601	L9Q	O2-C31-C32-C33
2	C	2601	L9Q	O2-C31-C32-C33
2	A	2601	L9Q	C39-C40-C41-C42
2	B	2601	L9Q	C39-C40-C41-C42
2	C	2601	L9Q	C39-C40-C41-C42

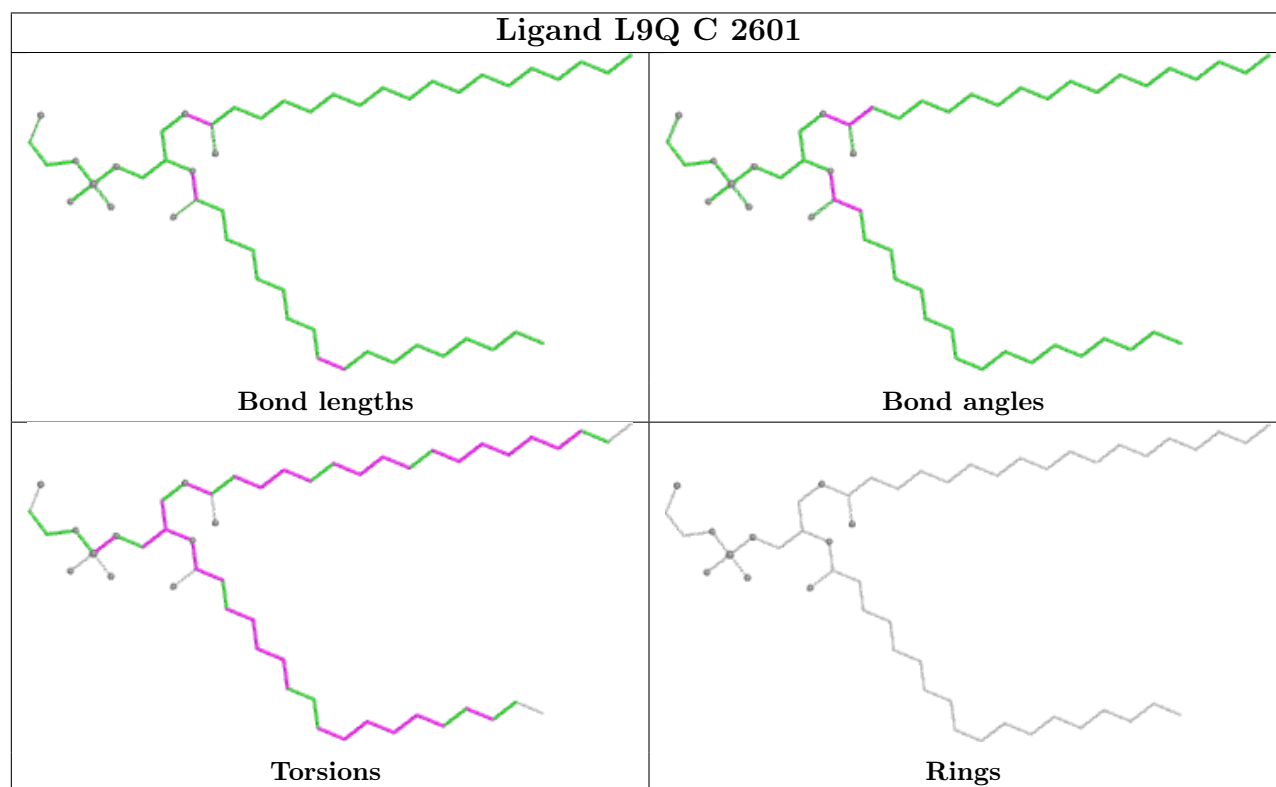
There are no ring outliers.

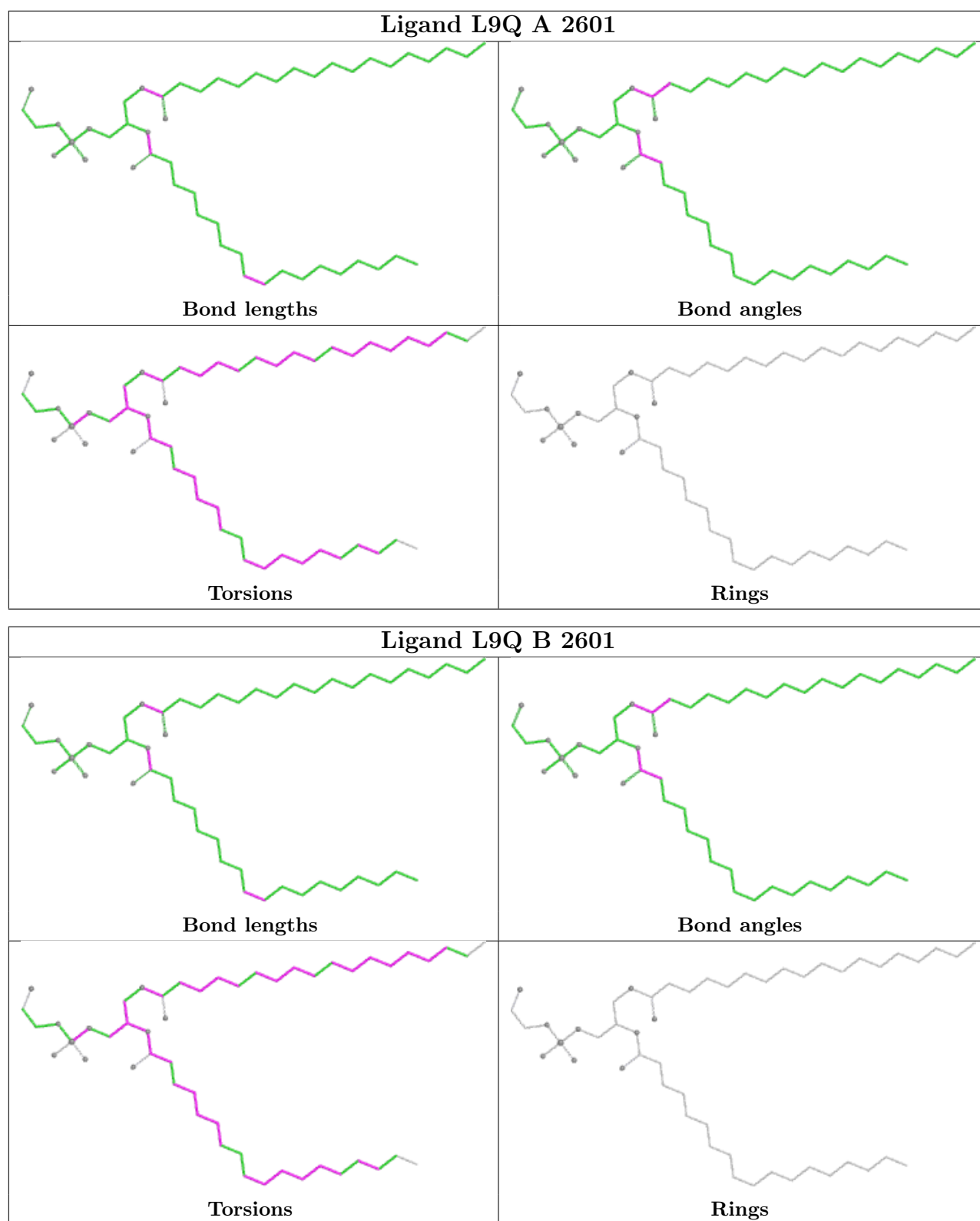
3 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2601	L9Q	19	0
2	A	2601	L9Q	20	0
2	B	2601	L9Q	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

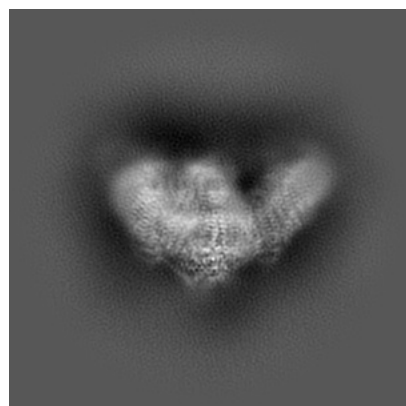
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60481. These allow visual inspection of the internal detail of the map and identification of artifacts.

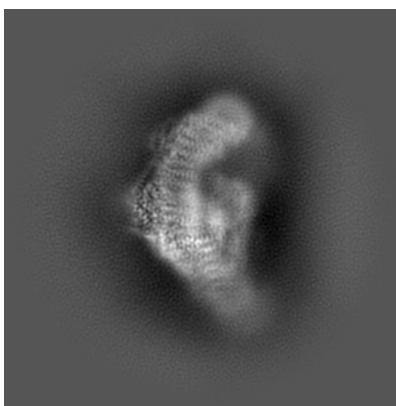
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

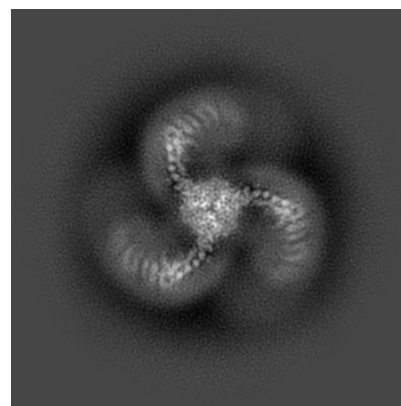
6.1.1 Primary map



X

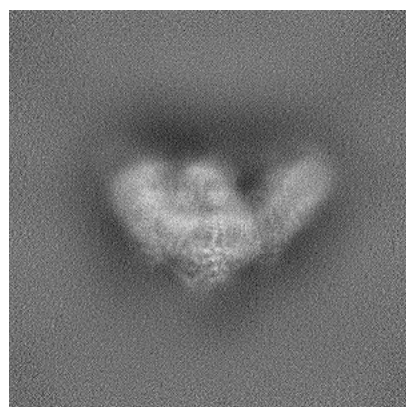


Y

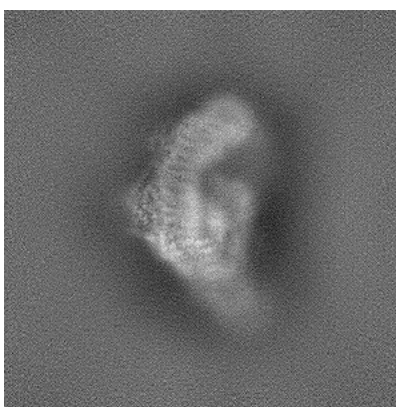


Z

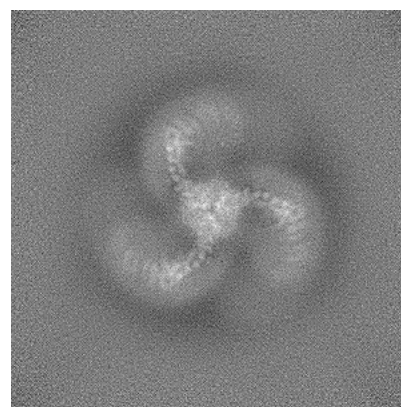
6.1.2 Raw map



X



Y

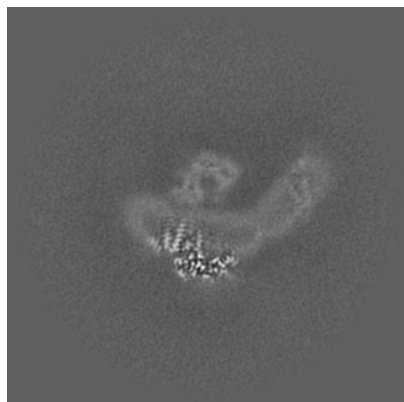


Z

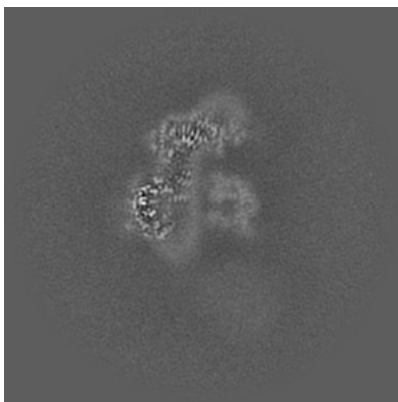
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

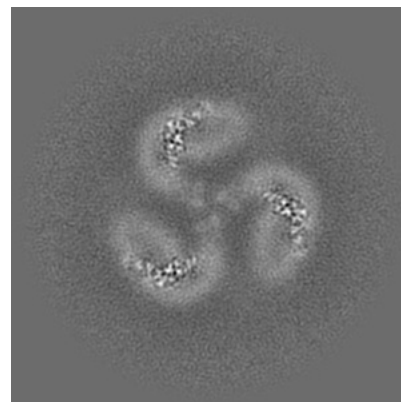
6.2.1 Primary map



X Index: 256



Y Index: 256

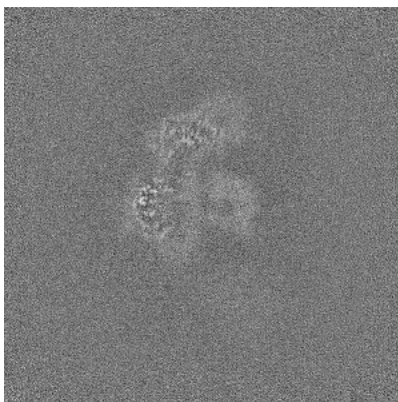


Z Index: 256

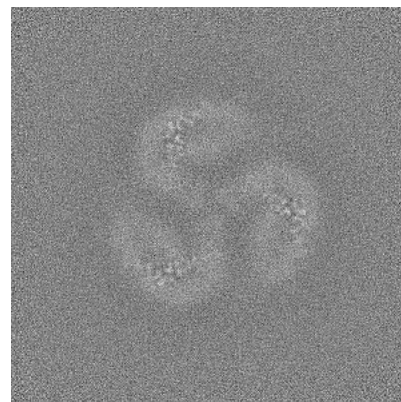
6.2.2 Raw map



X Index: 256



Y Index: 256

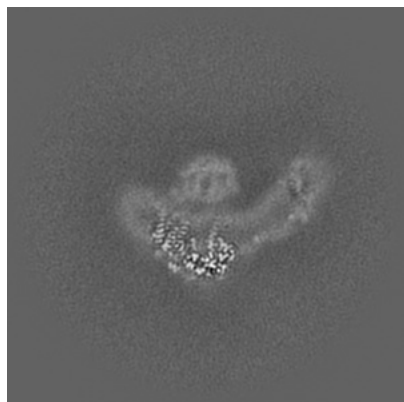


Z Index: 256

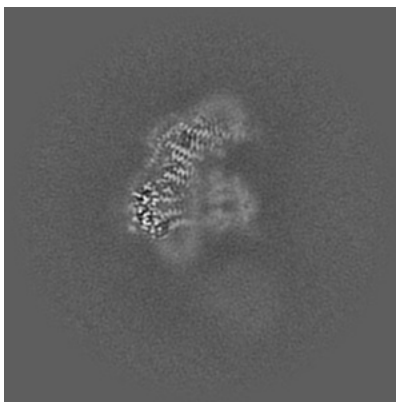
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

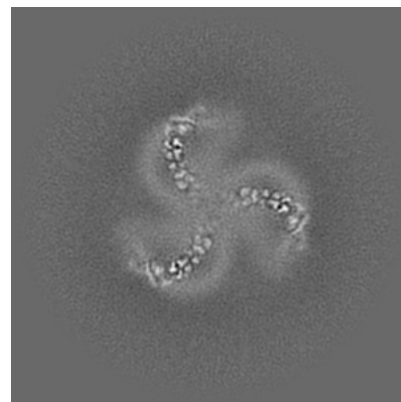
6.3.1 Primary map



X Index: 246

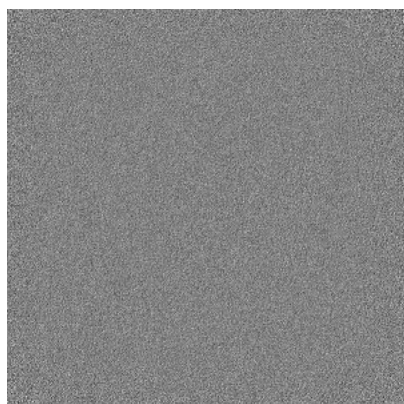


Y Index: 262

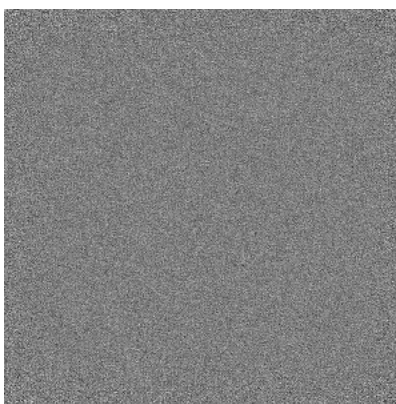


Z Index: 240

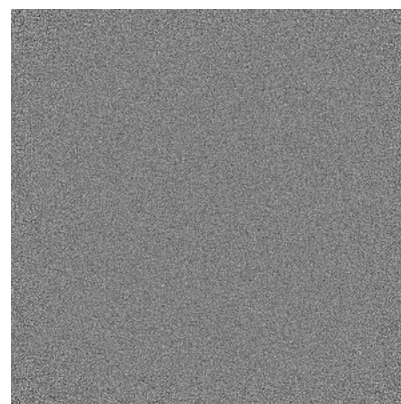
6.3.2 Raw map



X Index: 0



Y Index: 0

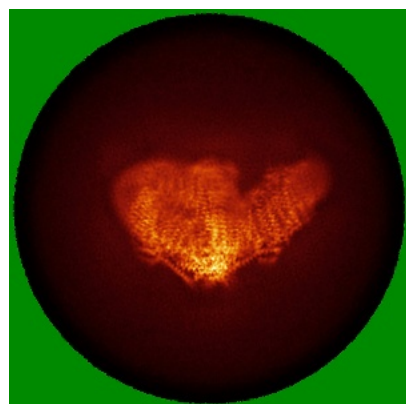


Z Index: 0

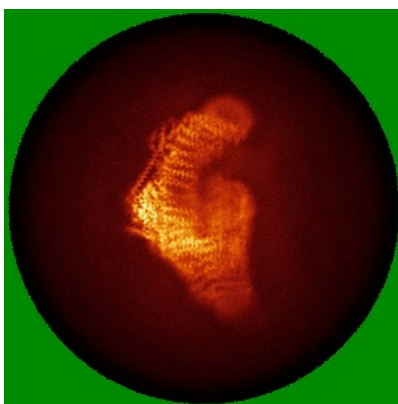
The images above show the largest variance slices of the map in three orthogonal directions.

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

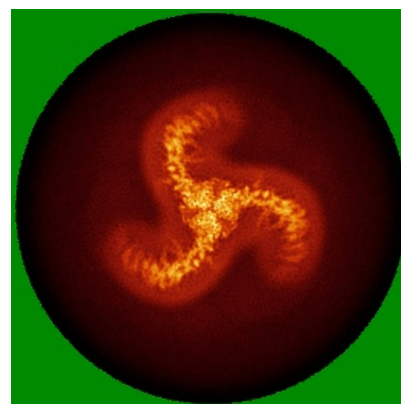
6.4.1 Primary map



X

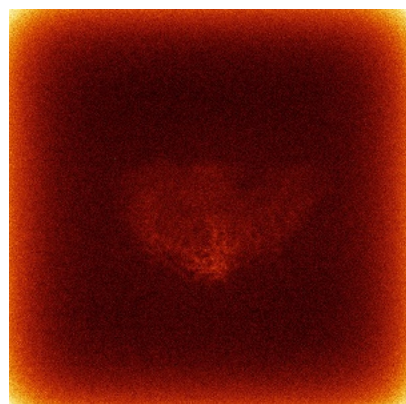


Y

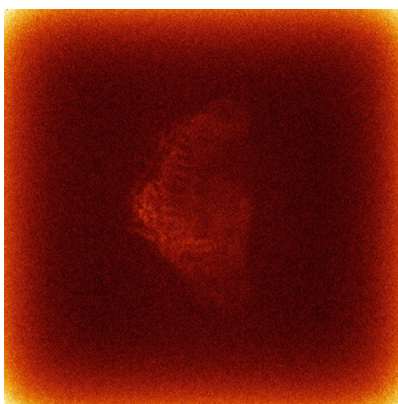


Z

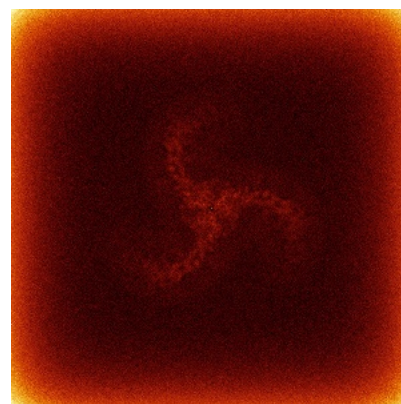
6.4.2 Raw map



X



Y

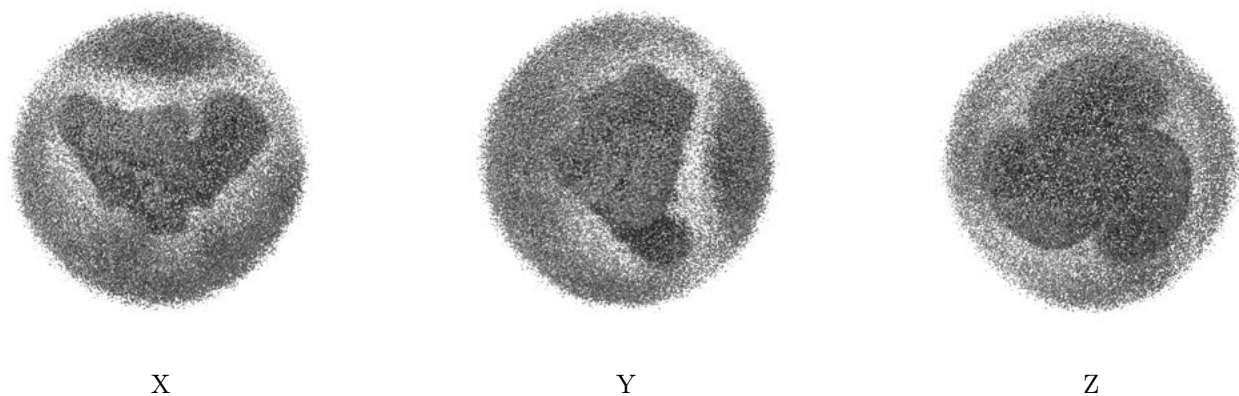


Z

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

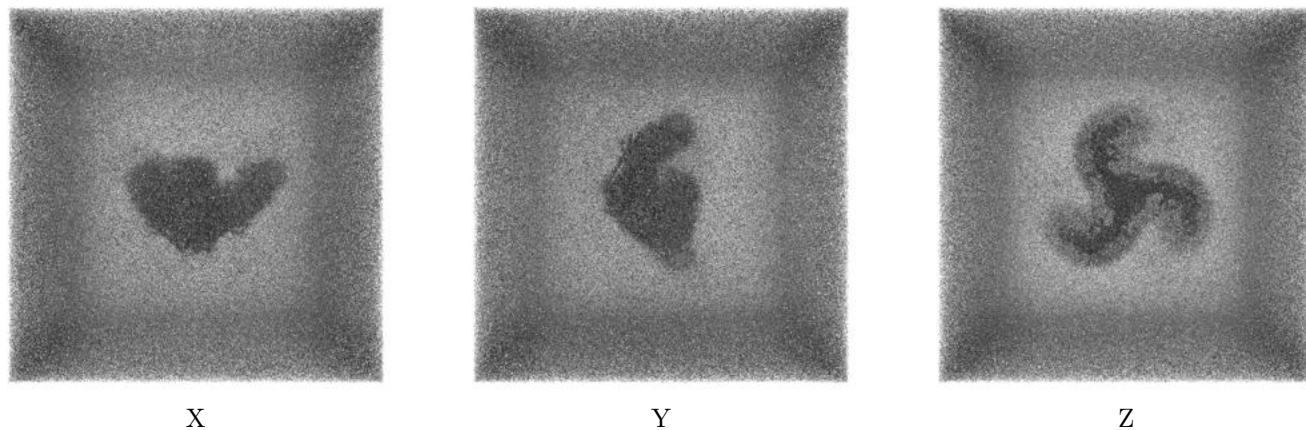
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

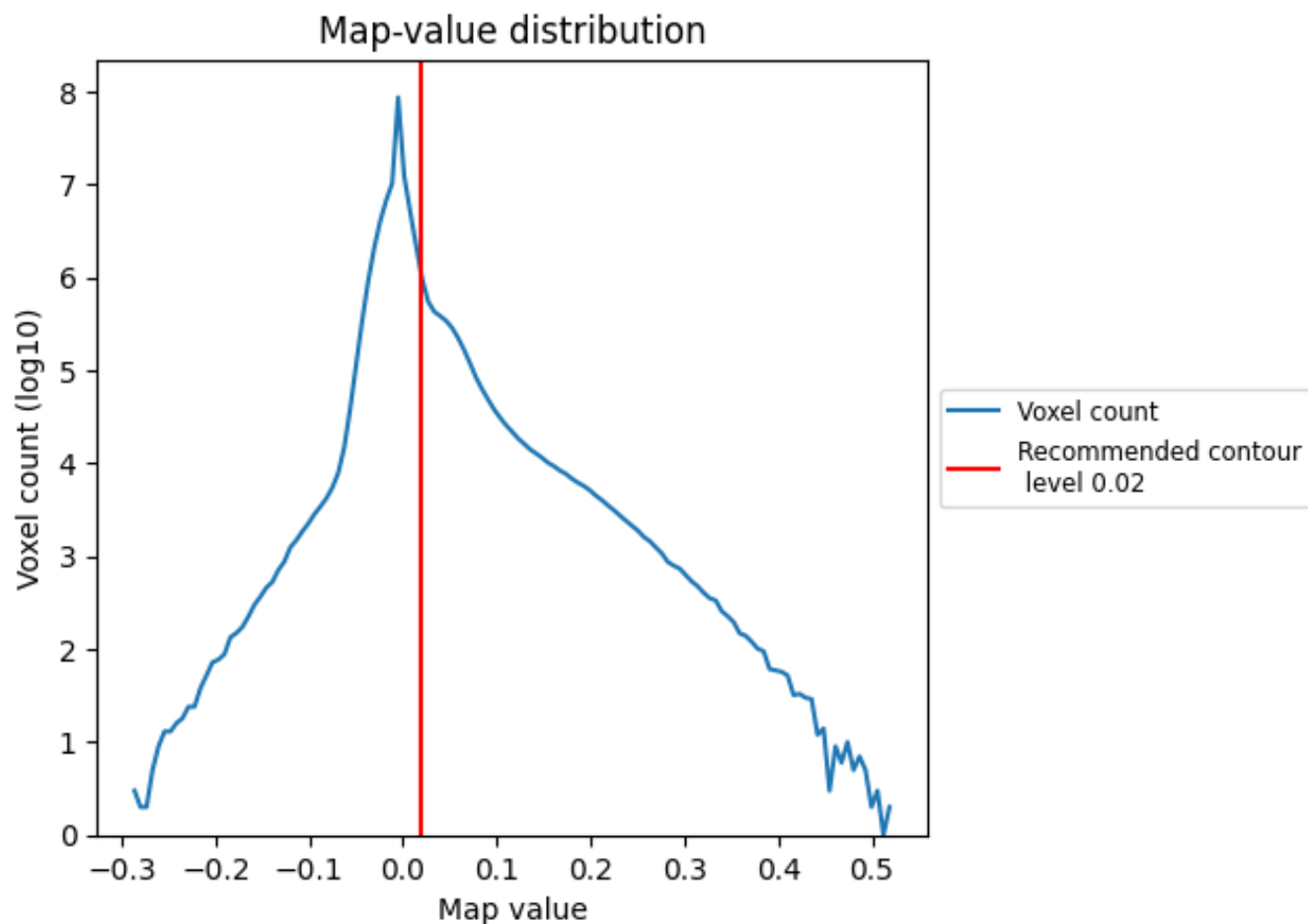
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

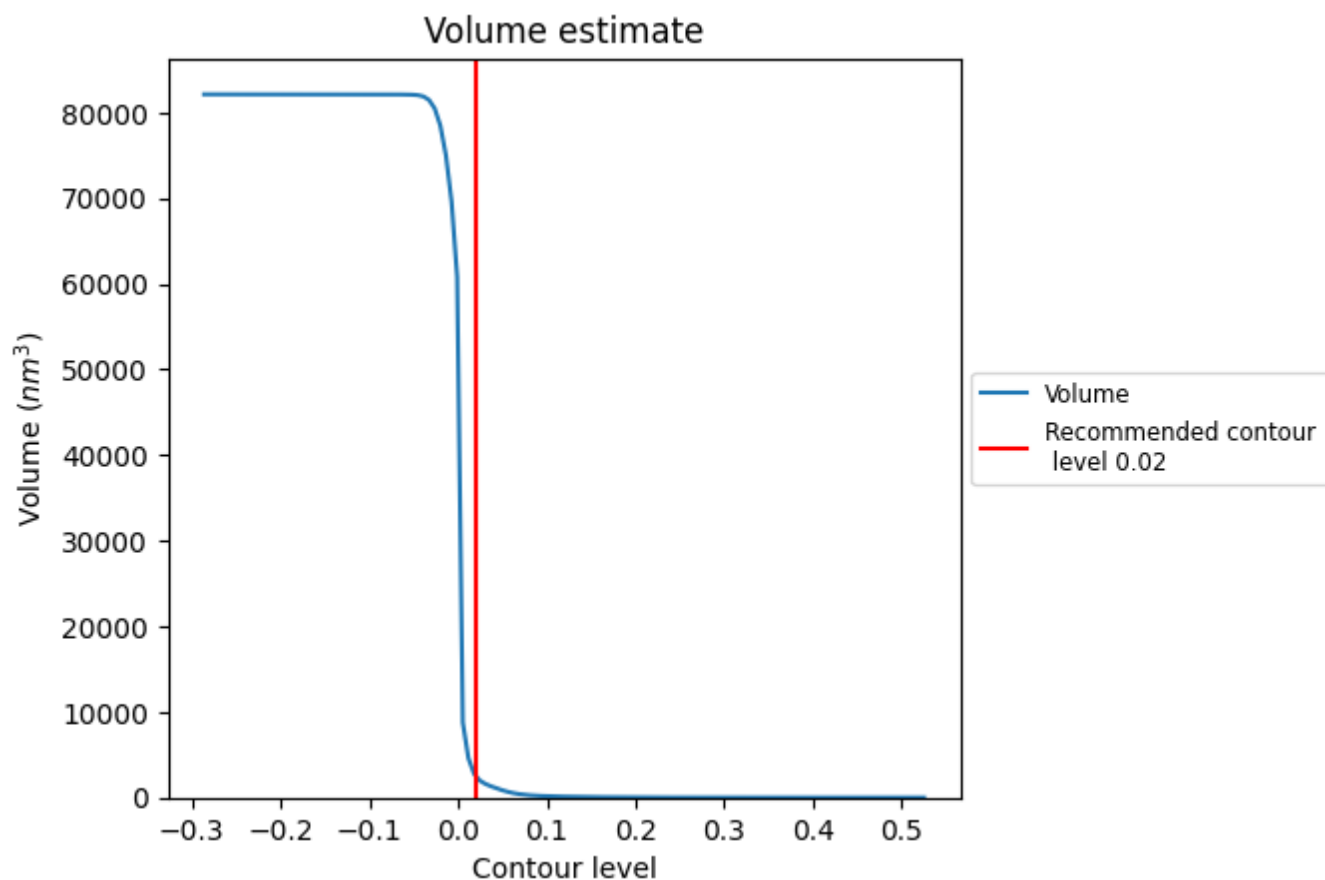
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

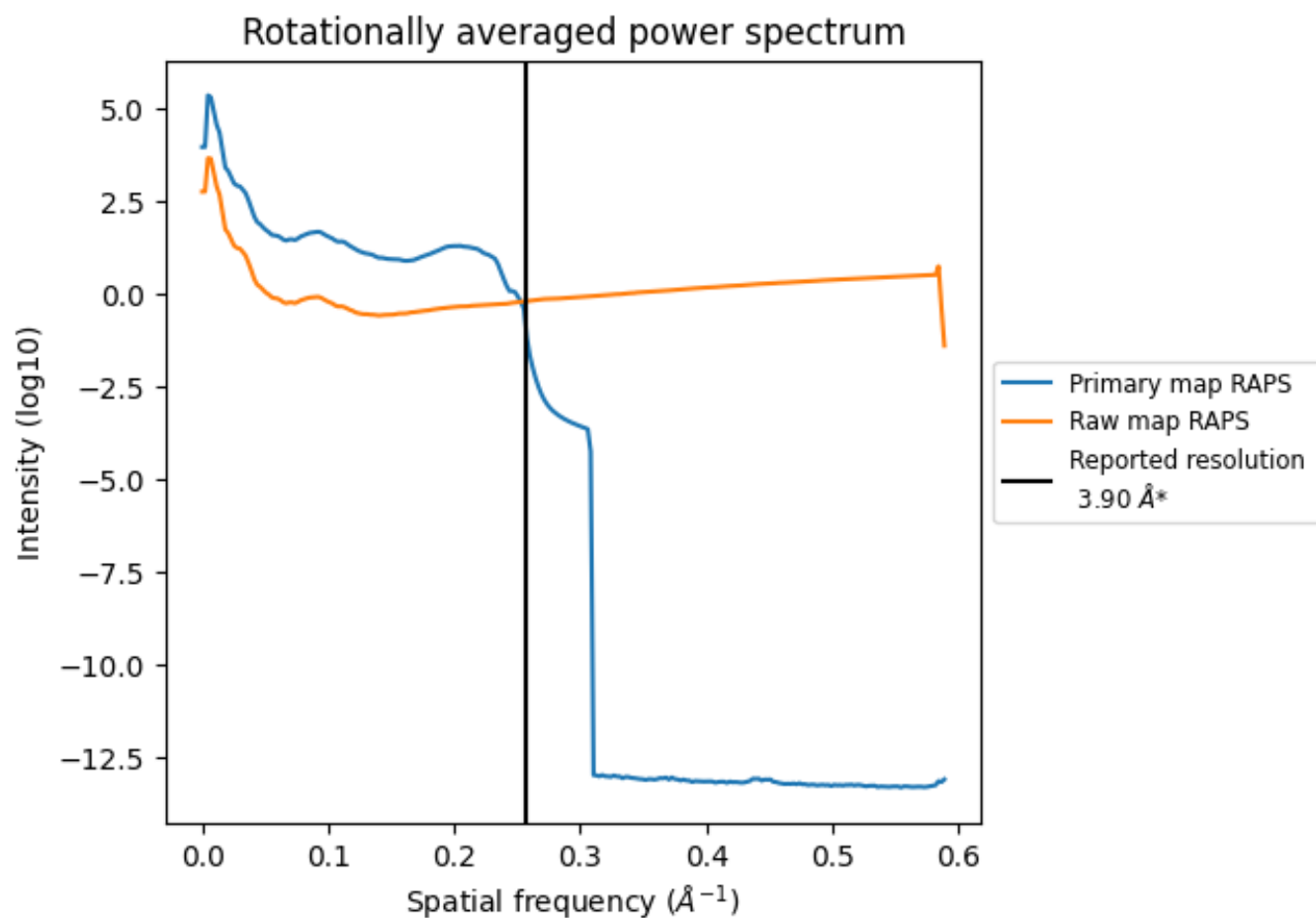
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2526 nm^3 ; this corresponds to an approximate mass of 2282 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 ⓘ

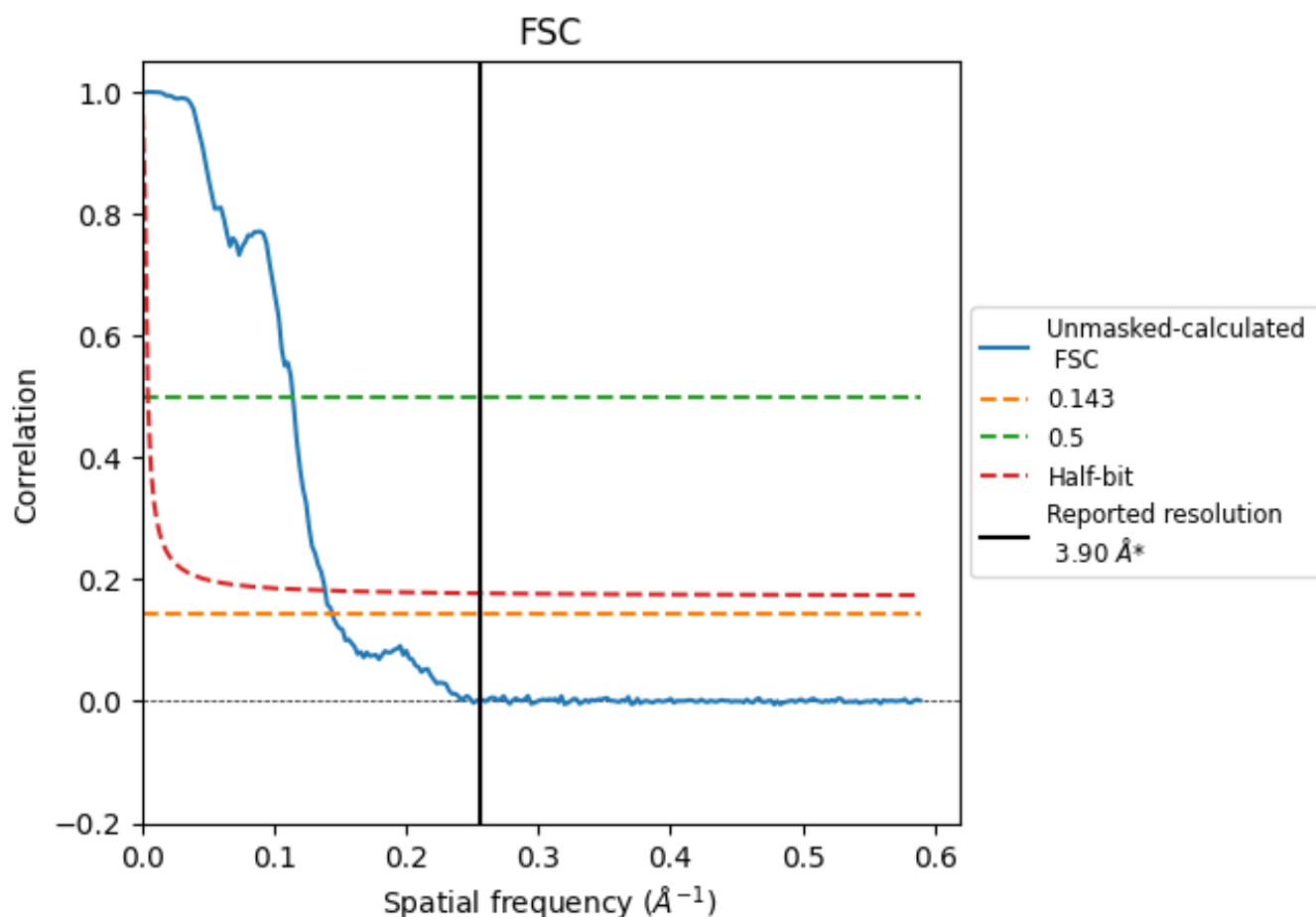


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.94	8.76	7.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.94 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

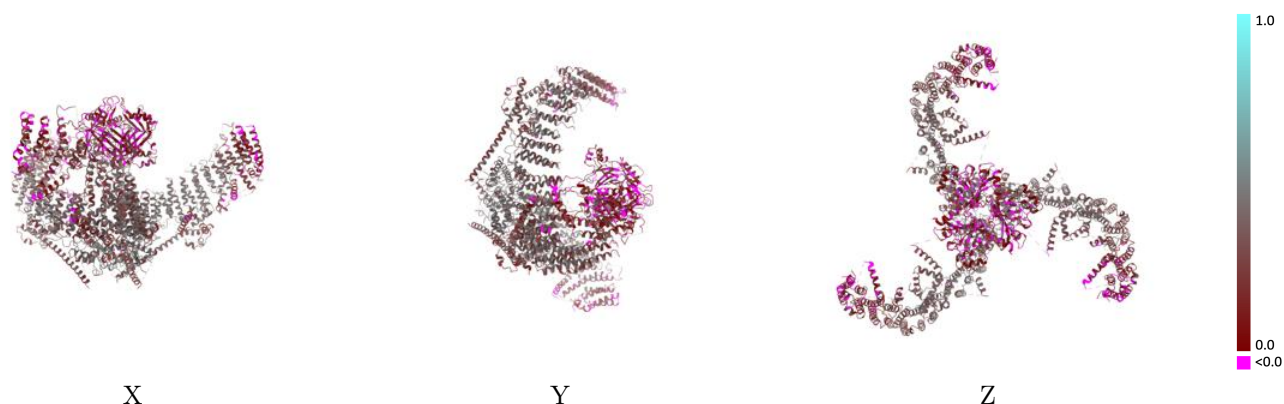
This section contains information regarding the fit between EMDB map EMD-60481 and PDB model 8ZU8. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



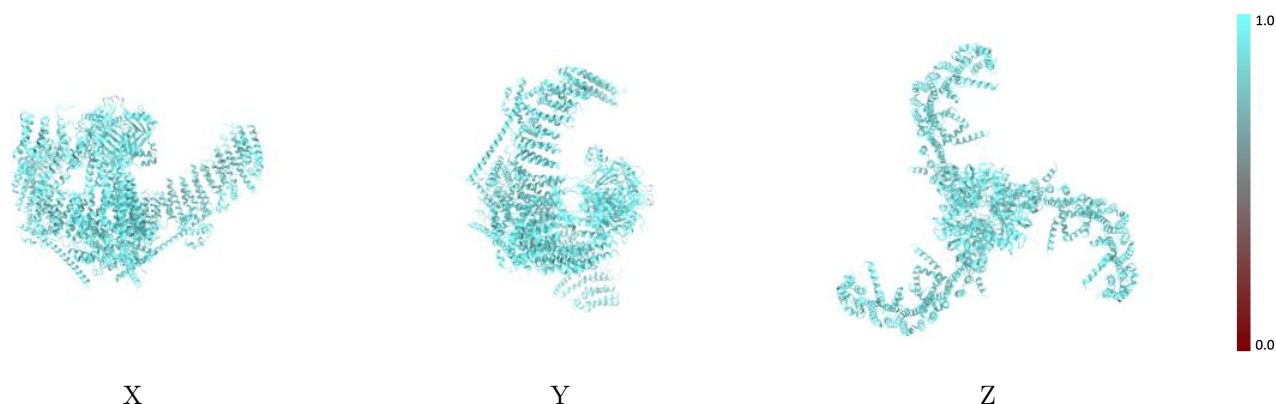
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



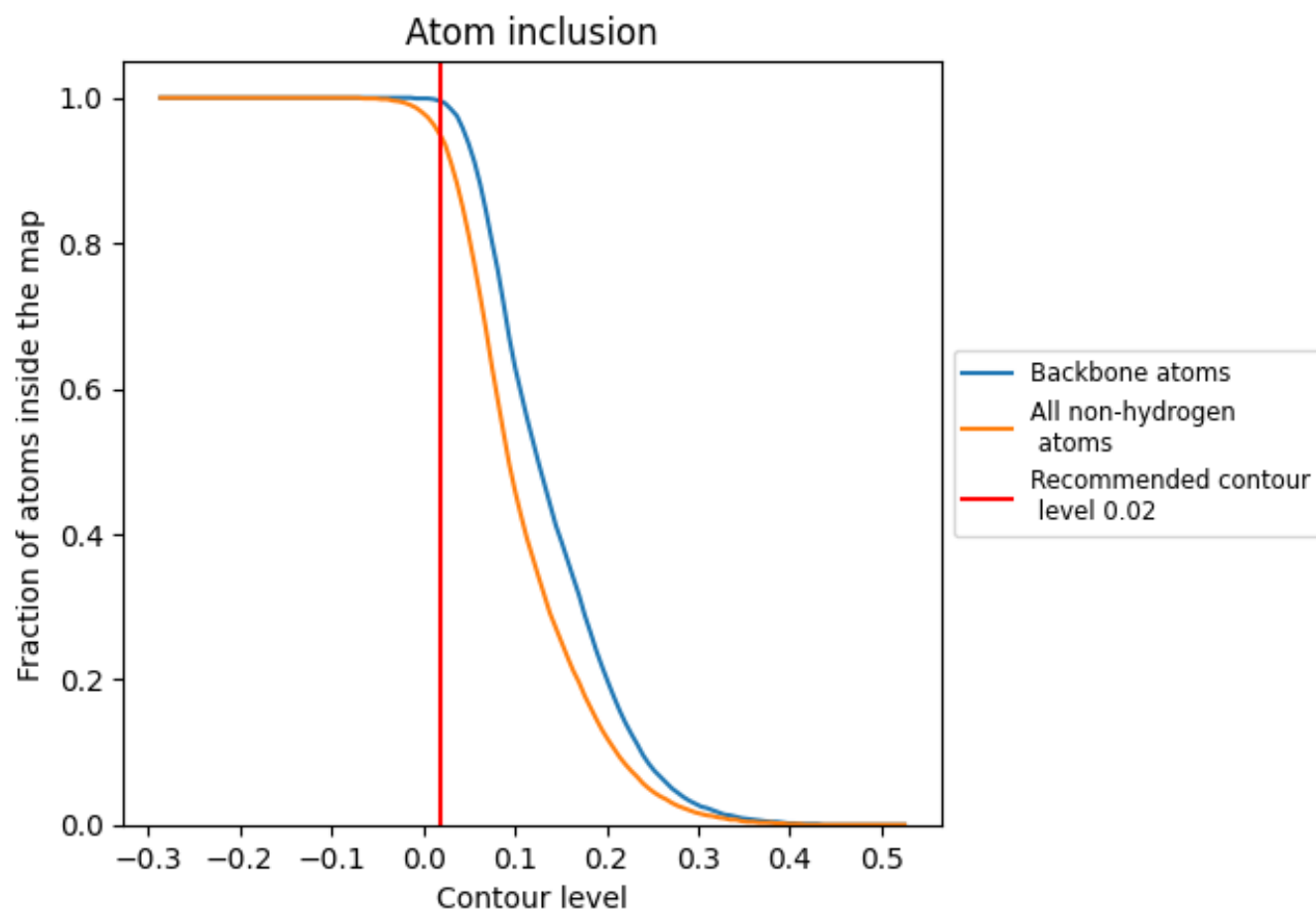
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.2730
A	0.9460	0.2730
B	0.9470	0.2720
C	0.9470	0.2730

