



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:14 PM UTC

PDB ID : 7TUI / pdb_00007tui
EMDB ID : EMD-26132
Title : Structure of C. albicans FAS in an inhibited state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2022-02-02
Resolution : 2.66 Å(reported)
Based on initial model : 6U5V

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

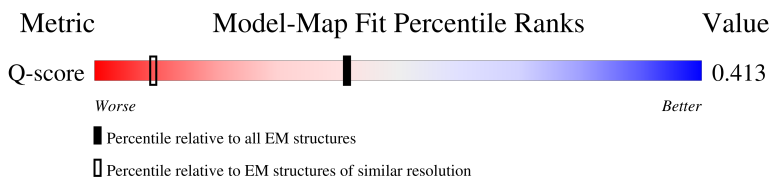
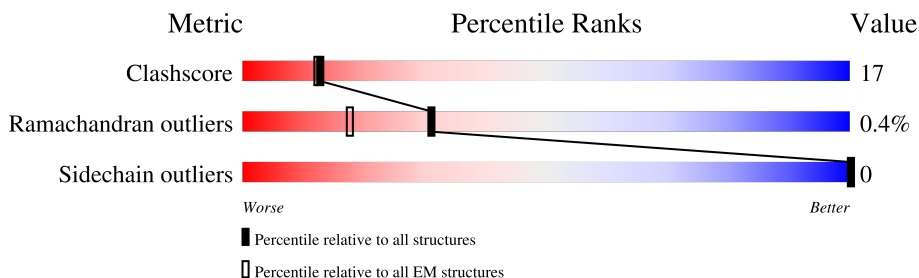
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.66 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	9119 (2.16 - 3.16)

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	1885	11% 54% 22% 24%
2	B	2037	50% 62% 38% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27380 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1433	Total	C	N	O	S	0	0
			11295	7171	1894	2185	45		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	VAL	SER	conflict	UNP P43098
A	351	ASP	ARG	conflict	UNP P43098
A	353	ASN	LYS	conflict	UNP P43098
A	354	LYS	GLN	conflict	UNP P43098
A	357	ALA	LEU	conflict	UNP P43098
A	814	THR	PRO	conflict	UNP P43098
A	1067	LYS	GLN	conflict	UNP P43098
A	1124	VAL	ILE	conflict	UNP P43098
A	1445	GLU	LYS	conflict	UNP P43098
A	1743	SER	ASN	conflict	UNP P43098

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2033	Total	C	N	O	S	1	0
			16054	10290	2665	3045	54		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

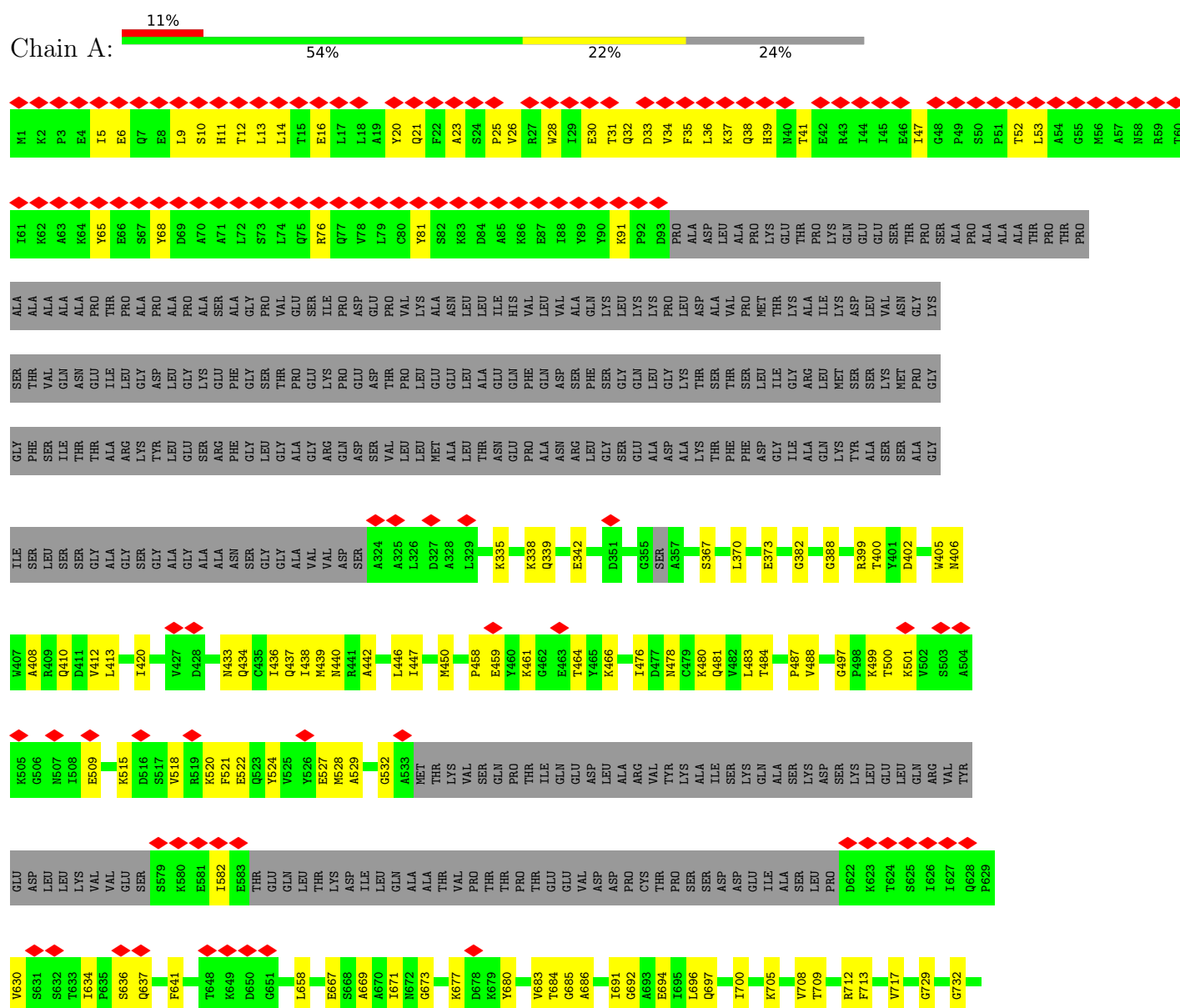


Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

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

- Molecule 1: Fatty acid synthase subunit alpha



S948	K61	N121	A182	V242	P302	V365	L425	I486	P546	M616	D698	Y778	L855	S948	E1026	V1032	D1033	K61	N121	A182	V242	P302	V365	L425	I486	P546	M616	D698	Y778	L855	S948	E1026	V1032	D1033
A949	F62	Y122	E183	L243	R303	L366	I426	L487	D547	D698	A699	Y779	D856	A949	E1027	D1034	E1033	F62	Y122	E183	L243	R303	L366	I426	I487	D547	D698	A699	Y779	D856	A949	E1027	D1034	
L861	I63	Y123	K184	G244	T304	S367	L427	D488	W548	R619	A699	Y780	L857	L861	E1028	L913	E1034	I63	Y123	K184	G244	T304	S367	L427	D488	W548	R619	A699	Y780	L857	L861	E1028	L913	E1034
N962	G64	K124	L185	L245	S305	P369	D428	F489	W549	A620	R620	Y781	T858	N962	E1029	V914	E1035	G64	K124	L185	L245	S305	P369	D428	F489	W549	A620	R620	Y781	T858	N962	E1029	V914	E1035
E963	F65	A125	N186	T246	L306	P370	D429	F490	W551	D622	Y782	Y782	F860	E963	E1030	V915	E1036	F65	A125	N186	T246	L306	P370	D429	F490	W551	D622	Y782	Y782	F860	E1030	V915	E1036	
F967	I66	A126	N187	P247	P307	E371	V430	G492	W552	D623	Y783	Y783	N861	F967	E1031	V916	E1037	I66	A126	N187	P247	P307	E371	V430	G492	W552	D623	Y783	Y783	N861	E1031	V916	E1037	
D970	S67	K127	L188	G248	P308	S372	E432	G493	W553	D624	Y784	Y784	L862	D970	E1032	V917	E1038	S67	K127	L188	G248	P308	S372	E432	G493	W553	D624	Y784	Y784	L862	E1032	V917	E1038	
K974	N68	S128	H189	E249	T309	L373	H433	V494	W554	D625	Y785	Y785	K864	K974	E1033	V918	E1039	N68	S128	H189	E249	T309	L373	H433	V494	W554	D625	Y785	Y785	K864	E1033	V918	E1039	
F975	A69	I129	S191	R251	M310	Y374	G434	S495	W555	D626	Y786	Y786	N865	F975	E1034	V919	E1040	A69	I129	S191	R251	M310	Y374	G434	S495	W555	D626	Y786	Y786	N865	E1034	V919	E1040	
P976	Q70	M130	F192	N252	Q312	F376	L435	G496	W556	D627	Y787	Y787	K866	P976	E1035	V920	E1041	Q70	M130	F192	N252	Q312	F376	L435	G496	W556	D627	Y787	Y787	K866	E1035	V920	E1041	
L982	F71	K131	F192	S253	D313	N377	F437	V499	W557	D628	Y788	Y788	L867	L982	E1036	V921	E1042	F71	K131	F192	S253	D313	N377	F437	V499	W557	D628	Y788	Y788	L867	E1036	V921	E1042	
E985	P72	V132	D193	S254	S314	L378	E438	L500	W558	D629	Y789	Y789	N868	E985	E1037	V922	E1043	P72	V132	D193	S254	S314	L378	E438	L500	W558	D629	Y789	Y789	N868	E1037	V922	E1043	
Y990	Q73	E133	K194	K255	D316	L380	G439	T501	W559	D630	Y790	Y790	D869	Y990	E1038	V923	E1044	Q73	E133	K194	K255	D316	L380	G439	T501	W559	D630	Y790	Y790	D869	E1038	V923	E1044	
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V1006	E76	L137	Q198	T258	E319	Q383	L442	N504	W562	D633	Y793	Y793	K872	V1006	E1041	V926	E1047	E76	L137	Q198	T258	E319	Q383	L442	N504	W562	D633	Y793	Y793	K872	E1041	V926	E1047	
D1010	L77	Y138	G199	G259	E320	L389	T447	F508	W563	D634	Y794	Y794	N873	D1010	E1042	V927	E1048	L77	Y138	G199	G259	E320	L389	T447	F508	W563	D634	Y794	Y794	N873	E1042	V927	E1048	
E1011	S78	H139	Q199	H260	G320	L390	F448	G509	W564	D635	Y795	Y795	K874	E1011	E1043	V928	E1049	S78	H139	Q199	H260	G320	L390	F448	G509	W564	D635	Y795	Y795	K874	E1043	V928	E1049	
F1012	L79	C140	N201	S261	R321	L391	V444	E506	W565	D636	Y796	Y796	N875	F1012	E1044	V929	E1050	L79	C140	N201	S261	R321	L391	V444	E506	W565	D636	Y796	Y796	N875	E1044	V929	E1050	
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D1027	F86	V147	H208	T268	D330	S392	S451	L513	W571	D642	Y802	Y802	N881	D1027	E1050	V935	E1056	F86	V147	H208	T268	D330	S392	S451	L513	W571	D642	Y802	Y802	N881	E1050	V935	E1056	
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V1032	D88	I149	E210	T270	S332	S394	Q454	A515	W573	D644	Y804	Y804	N883	V1032	E1052	V937	E1058	D88	I149	E210	T270	S332	S394	Q454	A515	W573	D644	Y804	Y804	N883	E1052	V937	E1058	
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D1035	D92	G154	D214	Q215	Q335	V336	L457	L518	W576	D647	Y807	Y807	N886	D1035	E1055	V940	E1061	D92	D92	G154	D214	Q215	Q335	V336	L457	L518	W576	D647	Y807	Y807	N886	E1055	V940	E1061
V1036	N93	N155	T156	Q216	E337	E338	L458	S520	W577	D648	Y808	Y808	N887	V1036	E1056	V941	E1062	N93	N155	T156	Q216	E337	E338	L458	S520	W577	D648	Y808	Y808	N887	E1056	V941	E1062	
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P1045	E105	T168	T168	Y168	I229	C230	L463	S525	W582	D653	Y813	Y813	N892	P1045	E1061	V946	E1067	E105	E105	T168	T168	Y168	I229	C230	L463	S525	W582	D653	Y813	Y813	N892	E1061	V946	E1067
A1047	Y107	L169	L169	Y170	Q230	I231	L464	S526	W583	D654	Y814	Y814	N893	A1047	E1062	V947	E1068	Y107	Y107	L169	L169	Y170	Q230	I231	L464	S526	W583	D654	Y814	Y814	N893	E1062	V947	E1068
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	I111	G172	L173	C234	C235	H235	L467	S529	W586	D657	Y817	Y817	N896		E1065	V950	E1071	I111	I111	G172	L173	C234	C235	H235	L467	S529	W586	D657	Y817	Y817	N896	E1065	V950	E1071
	A112	L174	L174	E236	E237	E238	L468	S530	W587	D658	Y818	Y818	N897		E1066	V951	E1072	A112	A112	L174	L174	E236	E237	E238	L468	S530	W587	D658	Y818	Y818	N897	E1066	V951	E1072
	K113	E175	E175	T237	T238	L238	L469	S531	W588	D659	Y819	Y819	N898		E1067	V952	E1073	K113	K113	E175	E175	T237	T238	L238	L469	S531	W588	D659	Y819	Y819	N898	E1067	V952	E1073
	K115	E176	E176	T239	T240	L239	L470	S532	W589	D660	Y820																							

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Y1929	K1869	V1809	A1643	L1578	T1500	D1426	K1354	N1201	E1125	E1056
E1930	K1871	M1810	I1644	V1579	D1501	L1427	V1357	T1202	L1130	D1060
I1931	W1872	P1811	E1645	E1580	Y1502	A1428	K1361	I1203	A1131	
V1932	E1813	E1812	Q1646	E1581	S1503	R1431	A1362	H1210	G1132	N1063
D1933	L1873	T1814	Q1647	W1582	R1505	F1435	E1363	T1212	T1133	S1064
E1934	L1874	L1815	P1647	A1583	G1507	F1436	I1364	A1213	E1134	T1065
E1935	E1875	T1816	T1649	A1584	N1506	K1439	K1365	D1214	L1135	H1066
A1936	V1877	D1817	V1652	A1585	K1508	E1439	A1366	T1215		E1067
A1937	M1878	V1818	V1653	A1586	T1509	K1440	V1367	L1138	L1130	
K1938	Y1879	F1820	F1653	V1587	E1510	D1441	L1368	Q1139	G1132	N1063
S1939	N1880	Y1821	T1654	V1587	E1511	V1442	P1371	I1142	R1211	S1064
L1940	V1881	L1822	Q1655	A1589	E1512	Q1443	S1372		T1212	T1065
A1941	N1883	G1823	G1656	R1590	S1513	F1444	K1373	Y1224	A1213	H1066
K1942	Q1884	T1824	G1657	V1591	V1514	F1445	L1375	M1227	D1214	E1067
P1943	Q1885	Q1826	S1658	R1592	I1515	V1446	V1376		T1215	
Q1944	Q1886	Q1827	Q1659	A1593	F1516	L1447	E1377		Q1139	
P1945	V1887	V1828	M1663	F1594	E1517	L1448	K1384		L1147	
I1946	A1888	V1830	G1664	C1596	N1518	T1448	E1385			
I1947	A1889	A1831	M1665	D1597	A1519	F1449	V1378			
L1948	G1890	R1832	E1672	F1598	E1520	R1450	G1380			
E1949	D1891	T1833	V1677	V1602	P1521	C1451	P1301			
R1950	L1892	E1834	V1677	L1603	S1523	A1452	G1302			
E1951	R1893	L1835	D1682	D1606	S1524	T1454	G1303			
G1951	A1894	G1836	R1683	Q1609	G1525	Y1455	P1308			
F1952	L1895	R1837	F1684	M1612	E1526	F1457	M1309			
A1953	D1896	S1838	F1685	E1613	K1531	K1458	E1391			
V1954	T1897	M1840	N1688	H1614	A1532	S1459	V1392			
I1955	L1898	G1841	I1693	G1616	P1533	A1460	G1316			
P1956	T1899	V1842	I1694	G1617	N1535	N1461	W1317			
L1957	N1900	M1843	V1697	I1618	M1536	Y1462	I1321			
K1958	V1901	A1844	L1699	G1620	N1537	Y1463	I1324			
I1960	N1903	V1845	I1696	R1621	E1537	S1464	P1326			
S1961	V1904	N1846	V1697	I1622	P1538	K1467	F1329			
V1962	L1905	P1847	P1701	I1623	Y1539	T1468	P1326			
P1963	K1906	S1848	G1709	I1624	N1547	T1469	P1326			
F1964	I1907	R1849	G1713	G1625	P1548	Q1471	V1329			
H1965	N1908	V1850	N1719	V1626	I1549	L1472	D1330			
S1966	K1909	S1851	N1719	E1627	H1550	L1474	G1331			
S1967	I1910	A1852	M1723	R1629	V1551	E1475	D1332			
V1968	D1911	T1853	F1724	T1628	S1552	L1476	L1333			
L1969	I1912	F1854	F1725	R1629	F1555	Q1477	L1334			
M1970	V1913	D1855	T1727	N1630	A1556	P1477	H1338			
S1971	K1914	D1856	I1727	V1631	F1557	T1478	M1341			
G1972	L1915	S1857	I1728	E1632	A1557	Y1343	G1342			
V1973	Q1916	A1858	G1729	T1632	E1480	V1416	Y1343			
K1974	E1917	L1859	E1730	F1634	V1481	Q1418	K1344			
P1975	Q1918	R1860	E1731	E1634	L1482	V1419	M1345			
F1976	M1919	F1861	D1731	L1635	Q1483	A1420	I1346			
Q1977	S1920	V1862	G1732	P1636	V1484	F1421	T1347			
R1978	I1921	V1863	S1804	V1637	G1485	K1422	G1348			
F1979	E1922	D1864	S1805	M1569	S1486	A1349	A1350			
L1980	K1923	E1865			V1487					
C1981	V1924									
K1982	K1925									
K1983										
I1984										
P1985										

K1986	S1987	S1988	V1989	K1990	P1991	D1993	L1994	I1995	G1996	K1997	Y1998	I1999	P2000	N2001	L2002	T2003	A2004	K2005	P2006	F2007	E2008	L2009	T2010	Y2011	E2012	Y2013	F2014	Q2015	S2016	Y2017	Y2018	D2019	L2020	T2021	K2022	S2023	E2024	K2025	I2026	K2027	S2028	I2029	L2030	D2031	N2032	K2033	E2034	Q2035	Y2036	E2037
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	252339	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.743	Depositor
Minimum map value	-4.396	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.273	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	333.72, 333.72, 333.72	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/11522	0.49	1/15575 (0.0%)
2	B	0.21	0/16423	0.55	4/22279 (0.0%)
All	All	0.22	0/27945	0.53	5/37854 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1969	LEU	CA-C-N	6.75	134.44	121.54
2	B	1969	LEU	C-N-CA	6.75	134.44	121.54
1	A	1132	PRO	CA-N-CD	-6.30	103.18	112.00
2	B	2034	GLU	CB-CA-C	-5.85	109.28	117.23
2	B	743	LYS	N-CA-C	-5.66	106.05	114.64

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1810	MET	Peptide
2	B	1929	TYR	Peptide
2	B	1982	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11295	0	11214	308	0
2	B	16054	0	16025	625	0
3	B	31	0	19	4	0
All	All	27380	0	27258	905	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 17.

All (905) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1780:ILE:HA	2:B:1783:LYS:HB2	1.54	0.88
2:B:1571:SER:HB3	2:B:1638:LEU:HD11	1.58	0.85
2:B:1620:GLY:HA2	2:B:1786:ILE:HB	1.57	0.85
1:A:709:THR:HG23	1:A:740:PHE:HB3	1.60	0.84
2:B:573:LEU:HB2	2:B:1096:PRO:HG3	1.61	0.83
2:B:1617:MET:HB3	2:B:1784:GLY:H	1.44	0.83
1:A:1300:PRO:HG3	1:A:1313:ILE:HD12	1.60	0.81
1:A:1545:PHE:HD1	1:A:1557:GLU:HG2	1.45	0.81
2:B:1106:ILE:HG22	2:B:1133:THR:HG22	1.62	0.80
1:A:459:GLU:O	1:A:466:LYS:NZ	2.14	0.79
2:B:1345:MET:HB2	2:B:1593:ALA:HB2	1.63	0.79
2:B:1994:LEU:HB3	2:B:2009:LEU:HD13	1.64	0.79
2:B:723:ARG:NH1	2:B:816:ASP:OD2	2.16	0.78
2:B:1773:GLU:HB2	2:B:1801:SER:HB3	1.64	0.78
2:B:1010:ASP:OD1	2:B:1011:GLU:N	2.14	0.78
2:B:1876:ILE:HD12	2:B:1888:ALA:HB2	1.66	0.77
1:A:13:LEU:HD21	2:B:2013:TYR:HB3	1.65	0.77
1:A:487:PRO:HD2	1:A:677:LYS:HD2	1.67	0.77
2:B:1855:ASP:H	2:B:1858:ALA:HB3	1.49	0.77
2:B:1922:GLU:O	2:B:1925:LYS:NZ	2.19	0.76
1:A:53:LEU:HD11	2:B:1795:HIS:HB3	1.66	0.76
1:A:1120:MET:HE2	1:A:1178:LEU:HD23	1.68	0.76
1:A:810:LYS:HG2	1:A:861:LYS:HG2	1.68	0.76
2:B:1869:LYS:NZ	2:B:1933:ASP:OD1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1618:ILE:HG22	2:B:1623:ILE:HG13	1.67	0.76
1:A:1555:LYS:NZ	1:A:1625:TYR:OH	2.17	0.75
2:B:1535:THR:OG1	2:B:1537:GLU:OE1	2.03	0.75
2:B:2000:PRO:HG2	2:B:2004:ALA:H	1.52	0.75
2:B:1772:MET:SD	2:B:1773:GLU:HG3	2.28	0.74
1:A:483:LEU:HD23	1:A:484:THR:HG23	1.70	0.74
2:B:574:LEU:HB3	2:B:576:ARG:HG2	1.68	0.74
1:A:871:TRP:HB2	1:A:930:LEU:HD11	1.69	0.73
2:B:506:GLU:HB3	2:B:779:PRO:HG3	1.70	0.73
1:A:1332:ASP:OD2	1:A:1590:GLY:N	2.20	0.73
1:A:41:THR:HG22	2:B:1648:THR:HG23	1.69	0.72
2:B:1122:ASN:HB3	2:B:1125:GLU:HG2	1.71	0.72
2:B:1977:GLN:HB2	2:B:1980:LEU:HD22	1.71	0.72
2:B:1203:ILE:HB	2:B:1224:TYR:HB2	1.69	0.72
2:B:740:MET:HG3	2:B:743:LYS:HD2	1.72	0.71
1:A:869:ILE:HG23	1:A:901:MET:HE2	1.70	0.71
2:B:1701:PRO:HG2	2:B:1758:LEU:HD12	1.73	0.71
1:A:52:THR:HG23	1:A:53:LEU:HG	1.73	0.70
1:A:524:TYR:O	1:A:528:MET:HG2	1.90	0.70
2:B:1389:VAL:HG12	2:B:1390:MET:HG2	1.72	0.70
2:B:52:PRO:HG3	2:B:61:LYS:HD2	1.72	0.69
2:B:1993:ASP:O	2:B:1997:LYS:HB2	1.92	0.69
1:A:1076:ASP:OD1	1:A:1092:TYR:OH	2.10	0.69
1:A:23:ALA:HB3	2:B:1970:MET:HB2	1.75	0.68
1:A:26:VAL:HG13	2:B:1880:ASN:HB3	1.74	0.68
1:A:446:LEU:HG	1:A:450:MET:HE3	1.75	0.68
2:B:396:PHE:N	2:B:820:GLU:OE2	2.26	0.68
2:B:2008:GLU:HG3	2:B:2012:GLU:HB2	1.75	0.68
2:B:447:THR:HB	2:B:467:LEU:HD21	1.75	0.68
1:A:35:PHE:O	1:A:41:THR:OG1	2.10	0.68
1:A:824:LEU:HD11	1:A:849:LEU:HD12	1.75	0.68
1:A:1137:LYS:HD2	1:A:1162:TYR:HE2	1.56	0.68
1:A:1013:ASP:OD2	1:A:1506:SER:OG	2.10	0.68
2:B:1436:PHE:HA	2:B:1487:VAL:HG23	1.76	0.68
1:A:700:ILE:HG22	1:A:729:GLY:HA2	1.75	0.68
1:A:1116:LYS:HG3	1:A:1183:LEU:HD11	1.76	0.67
2:B:1769:LEU:HD21	2:B:1797:LEU:HD12	1.76	0.67
2:B:1280:SER:HB2	2:B:1354:LYS:HD2	1.75	0.67
1:A:388:GLY:O	1:A:741:ASN:ND2	2.26	0.67
2:B:265:VAL:HG21	2:B:290:LEU:HD11	1.77	0.67
2:B:692:LEU:HD23	2:B:703:VAL:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:TYR:OH	2:B:1063:ASN:OD1	2.12	0.67
2:B:1621:ARG:NH1	2:B:1645:GLU:OE2	2.26	0.67
2:B:222:PRO:HG2	2:B:298:LEU:HD22	1.77	0.67
2:B:1374:LYS:HG3	2:B:1402:TYR:HD2	1.58	0.67
2:B:1774:LYS:NZ	2:B:1810:MET:O	2.28	0.67
2:B:344:ASN:ND2	2:B:353:ILE:O	2.28	0.67
2:B:2002:LEU:O	2:B:2003:THR:OG1	2.10	0.67
2:B:809:VAL:HG21	2:B:1054:VAL:HB	1.76	0.67
1:A:796:ARG:HA	1:A:800:THR:HG22	1.76	0.66
1:A:1166:ILE:HG21	1:A:1172:LEU:HD11	1.77	0.66
2:B:1587:VAL:HB	2:B:1590:ARG:HH21	1.59	0.66
2:B:1617:MET:HB3	2:B:1784:GLY:N	2.09	0.66
2:B:793:MET:HE2	2:B:1043:HIS:HD2	1.61	0.66
2:B:183:GLU:OE2	2:B:187:GLN:NE2	2.28	0.66
1:A:1125:VAL:HG22	1:A:1171:THR:HG22	1.78	0.66
2:B:1602:VAL:HG23	2:B:1637:VAL:HG11	1.77	0.66
2:B:1739:ILE:HG23	2:B:1741:LYS:HG2	1.75	0.66
1:A:1589:LYS:H	1:A:1589:LYS:HD3	1.60	0.66
2:B:847:ARG:NH1	2:B:885:ASP:OD1	2.28	0.66
1:A:1364:MET:HA	1:A:1366:ARG:HE	1.61	0.66
2:B:813:GLY:HA2	2:B:1048:SER:HB2	1.78	0.65
2:B:1044:GLY:O	2:B:1048:SER:OG	2.12	0.65
2:B:1447:LEU:HD22	2:B:1449:PHE:CE1	2.30	0.65
2:B:107:TYR:OH	2:B:110:THR:O	2.13	0.65
2:B:1791:MET:HG2	2:B:1999:ILE:HG23	1.78	0.65
2:B:1995:ILE:HG12	2:B:2009:LEU:H	1.61	0.65
2:B:1180:THR:HG23	2:B:1194:GLU:HG2	1.77	0.65
2:B:1786:ILE:HG23	2:B:1790:ILE:HD13	1.79	0.65
2:B:1843:VAL:HG23	2:B:1956:PRO:HG3	1.79	0.65
1:A:21:GLN:HA	2:B:2002:LEU:HD12	1.76	0.65
1:A:1025:GLU:HG3	1:A:1598:ASN:HD22	1.60	0.65
1:A:1039:GLU:OE2	1:A:1581:GLN:NE2	2.29	0.65
2:B:1456:LYS:O	2:B:1464:SER:N	2.29	0.65
2:B:1146:ARG:NH2	2:B:1232:PHE:O	2.29	0.65
2:B:657:ARG:HH22	2:B:1153:HIS:HB2	1.62	0.65
1:A:1306:THR:HA	1:A:1309:GLU:HG2	1.77	0.65
2:B:1476:LEU:HD22	2:B:1482:ILE:H	1.60	0.65
2:B:1487:VAL:HG22	2:B:1488:ASP:H	1.62	0.65
2:B:887:GLN:HG3	2:B:1039:THR:HA	1.77	0.64
2:B:1663:MET:HE2	2:B:1772:MET:HG2	1.79	0.64
1:A:691:ILE:HD11	1:A:872:THR:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:ILE:H	1:A:1379:GLN:HE21	1.46	0.64
2:B:440:LEU:HD23	2:B:454:GLN:HG3	1.80	0.64
2:B:1854:PHE:HD2	2:B:1859:LEU:HD13	1.61	0.64
2:B:1950:ARG:HG3	2:B:1955:ILE:HA	1.80	0.64
1:A:1105:ILE:HA	1:A:1187:GLN:NE2	2.11	0.64
2:B:446:ASP:HB3	2:B:450:GLY:H	1.63	0.64
1:A:813:LYS:HB2	1:A:861:LYS:HD2	1.80	0.64
1:A:684:THR:HG22	1:A:775:ALA:HB2	1.80	0.64
1:A:1250:MET:HE3	1:A:1253:VAL:HG11	1.79	0.64
2:B:757:GLY:N	3:B:2101:FMN:O1P	2.31	0.64
2:B:268:VAL:HG21	2:B:460:ILE:HG21	1.79	0.64
2:B:1974:LYS:HB2	2:B:1975:PRO:HD3	1.80	0.64
2:B:93:ASN:HD21	2:B:536:THR:HG23	1.62	0.64
2:B:1579:VAL:HG12	2:B:1612:MET:HE3	1.80	0.64
2:B:2007:PHE:HE2	2:B:2009:LEU:HD12	1.62	0.64
2:B:825:LYS:HE3	2:B:827:THR:HG22	1.79	0.64
1:A:16:GLU:HB3	2:B:2017:VAL:HG21	1.80	0.63
2:B:264:LEU:HD23	2:B:464:VAL:HG23	1.81	0.63
2:B:1294:CYS:SG	2:B:1295:ASP:N	2.71	0.63
2:B:1617:MET:HE2	2:B:1783:LYS:HB3	1.79	0.63
2:B:1810:MET:HB3	2:B:1815:LEU:HD22	1.79	0.63
1:A:1420:PRO:HB2	1:A:1556:ASN:HD22	1.64	0.63
2:B:1964:PHE:HB3	2:B:1969:LEU:HD23	1.81	0.63
2:B:593:ILE:HA	2:B:797:GLU:HB3	1.82	0.62
2:B:229:CYS:HB2	2:B:290:LEU:HD22	1.81	0.62
2:B:1621:ARG:HB3	2:B:1643:GLU:HB3	1.81	0.62
2:B:1726:GLU:H	2:B:1975:PRO:HG3	1.64	0.62
2:B:356:SER:OG	2:B:365:VAL:O	2.15	0.62
2:B:1191:PRO:O	2:B:1210:HIS:NE2	2.28	0.62
2:B:1443:GLN:NE2	2:B:1444:PHE:O	2.33	0.62
2:B:1799:GLU:OE2	2:B:1998:TYR:OH	2.18	0.62
2:B:639:ILE:HD11	3:B:2101:FMN:HN3	1.65	0.62
2:B:1108:ASP:OD2	2:B:1133:THR:N	2.27	0.62
2:B:232:GLN:HG2	2:B:490:GLY:HA2	1.82	0.62
2:B:1277:THR:HG23	2:B:1357:VAL:HG22	1.82	0.61
2:B:502:HIS:HB2	2:B:512:ILE:HG13	1.81	0.61
2:B:1590:ARG:HB3	2:B:1645:GLU:H	1.66	0.61
2:B:90:ASN:HB2	2:B:93:ASN:HB2	1.80	0.61
2:B:1848:SER:HB3	2:B:1884:GLN:HA	1.83	0.61
1:A:33:ASP:OD1	1:A:65:TYR:OH	2.18	0.61
2:B:59:TYR:HE2	2:B:82:PHE:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:GLN:HG2	2:B:399:ARG:HE	1.66	0.61
2:B:1416:PRO:HB2	2:B:1510:ILE:HD12	1.82	0.61
2:B:1624:ILE:HB	2:B:1642:ALA:HB3	1.80	0.61
2:B:1763:GLN:OE1	2:B:1827:GLN:NE2	2.33	0.61
2:B:522:PRO:HD3	2:B:529:PHE:HE2	1.66	0.61
2:B:1309:MET:HG3	2:B:1390:MET:HE3	1.83	0.61
1:A:742:GLN:HB3	1:A:797:ILE:HG23	1.83	0.61
2:B:447:THR:HA	2:B:478:ALA:HB2	1.82	0.61
2:B:1905:LEU:HD21	2:B:1931:ILE:HD11	1.83	0.61
2:B:865:ASN:OD1	2:B:866:LYS:N	2.34	0.61
2:B:1253:LEU:HD21	2:B:1548:PRO:HD3	1.82	0.60
2:B:518:LEU:HD13	2:B:530:LYS:HB3	1.82	0.60
2:B:1276:ILE:HD11	2:B:1315:ILE:HG12	1.83	0.60
1:A:442:ALA:HA	1:A:446:LEU:HD23	1.82	0.60
2:B:1740:PHE:CE2	2:B:1743:ILE:HD12	2.37	0.60
2:B:1181:ALA:HB3	2:B:1193:VAL:HB	1.82	0.60
2:B:2008:GLU:HG2	2:B:2013:TYR:HB2	1.82	0.60
2:B:857:ASP:O	2:B:861:ASN:ND2	2.35	0.60
2:B:1762:THR:HA	2:B:1765:THR:HG22	1.82	0.60
1:A:630:VAL:HG23	1:A:667:GLU:OE2	2.02	0.60
1:A:1369:THR:O	1:A:1372:ARG:NH1	2.31	0.60
2:B:1459:SER:HB3	2:B:1462:VAL:HG12	1.84	0.60
2:B:1123:LYS:NZ	2:B:1163:THR:OG1	2.34	0.59
2:B:1419:VAL:HG22	2:B:1447:LEU:H	1.67	0.59
1:A:31:THR:HG23	2:B:1999:ILE:HD12	1.83	0.59
2:B:1094:LYS:HB3	2:B:1099:VAL:HG12	1.82	0.59
2:B:1877:VAL:HG12	2:B:1966:SER:HB3	1.84	0.59
1:A:1210:ILE:O	1:A:1214:VAL:HG23	2.02	0.59
2:B:773:SER:HB3	2:B:778:TYR:HB2	1.83	0.59
2:B:1246:ILE:HD13	2:B:1334:LEU:HD23	1.85	0.59
2:B:1659:GLN:NE2	2:B:1765:THR:OG1	2.36	0.59
2:B:179:VAL:HA	2:B:203:LEU:HD11	1.84	0.59
2:B:1592:ARG:HG2	2:B:1621:ARG:HE	1.68	0.59
2:B:2000:PRO:HD3	2:B:2007:PHE:N	2.18	0.59
1:A:1115:PRO:HB2	1:A:1183:LEU:HD13	1.83	0.59
2:B:195:ILE:HG13	2:B:196:TYR:HD1	1.67	0.59
2:B:847:ARG:NH2	2:B:1035:ASP:OD2	2.36	0.59
2:B:2007:PHE:CE2	2:B:2009:LEU:HD12	2.37	0.59
1:A:1370:THR:HA	1:A:1619:ASP:OD1	2.03	0.59
1:A:1588:PRO:HG3	1:A:1595:TRP:CE3	2.38	0.59
2:B:1811:PRO:HG3	2:B:1985:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:ARG:O	2:B:879:ILE:HG12	2.01	0.59
1:A:21:GLN:HG2	2:B:1799:GLU:HG2	1.84	0.58
1:A:1565:MET:HB3	1:A:1570:ARG:HG3	1.84	0.58
1:A:893:VAL:HG21	1:A:933:ILE:HD11	1.86	0.58
1:A:1588:PRO:O	1:A:1591:ALA:N	2.36	0.58
2:B:1309:MET:HB3	2:B:1576:ARG:NH2	2.19	0.58
2:B:1620:GLY:H	2:B:1784:GLY:HA2	1.69	0.58
2:B:1344:LYS:HE3	2:B:1391:GLU:HB2	1.86	0.58
1:A:406:ASN:HD21	1:A:1630:TYR:HB2	1.68	0.58
2:B:476:GLU:OE2	2:B:504:ASN:ND2	2.36	0.58
2:B:893:LYS:HE3	2:B:912:ARG:HD3	1.85	0.58
2:B:586:PRO:HD2	3:B:2101:FMN:H6	1.86	0.58
1:A:478:ASN:OD1	1:A:582:ILE:HG22	2.04	0.58
2:B:351:LYS:HG2	2:B:369:PRO:HG2	1.86	0.58
2:B:818:GLN:O	2:B:821:GLN:HG3	2.04	0.58
2:B:1880:ASN:OD1	2:B:1881:VAL:N	2.36	0.58
2:B:589:VAL:HG11	2:B:610:GLY:HA3	1.84	0.58
2:B:1842:MET:HE2	2:B:1960:ILE:HG21	1.86	0.58
2:B:251:ARG:NH1	2:B:271:ALA:O	2.36	0.57
2:B:1757:GLY:O	2:B:1760:SER:OG	2.17	0.57
2:B:1982:LYS:O	2:B:1984:ILE:N	2.37	0.57
2:B:716:VAL:HA	2:B:751:VAL:HB	1.86	0.57
2:B:903:GLU:HA	2:B:982:LEU:HD13	1.85	0.57
2:B:1685:PHE:HD2	2:B:1693:ILE:HB	1.68	0.57
2:B:1843:VAL:HG12	2:B:1895:LEU:HD22	1.86	0.57
1:A:887:GLY:O	1:A:890:LYS:HG2	2.04	0.57
2:B:1304:ALA:HA	2:B:1354:LYS:HE2	1.85	0.57
2:B:1897:THR:HA	2:B:1935:VAL:HG11	1.87	0.57
2:B:34:GLU:HA	2:B:37:LYS:HE3	1.85	0.57
2:B:521:ASN:OD1	2:B:522:PRO:HD2	2.05	0.57
2:B:1248:GLU:HG3	2:B:1252:LYS:NZ	2.20	0.57
1:A:1017:VAL:HG11	1:A:1665:LEU:HD13	1.86	0.57
2:B:181:ILE:HD13	2:B:284:LEU:HD23	1.87	0.57
2:B:1792:PHE:HB3	2:B:1806:LEU:HD12	1.86	0.57
1:A:1545:PHE:CD1	1:A:1557:GLU:HG2	2.34	0.57
2:B:855:LEU:HD12	2:B:859:ILE:HD12	1.87	0.57
1:A:1106:GLU:OE1	1:A:1190:THR:OG1	2.23	0.57
1:A:1232:GLU:OE2	1:A:1684:ARG:NH2	2.34	0.57
1:A:1232:GLU:CD	1:A:1684:ARG:HH22	2.12	0.56
2:B:164:ARG:HD3	2:B:206:LEU:HD23	1.86	0.56
2:B:1254:TRP:CE3	2:B:1321:ILE:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1502:TYR:HD1	2:B:1505:ARG:HH21	1.51	0.56
1:A:13:LEU:HD23	2:B:2009:LEU:HA	1.87	0.56
1:A:501:LYS:NZ	1:A:509:GLU:OE2	2.35	0.56
1:A:990:PHE:CD1	1:A:1692:MET:HG3	2.40	0.56
1:A:1099:HIS:HB3	1:A:1190:THR:HB	1.85	0.56
2:B:171:GLN:O	2:B:175:GLU:HB2	2.05	0.56
2:B:486:ILE:HB	2:B:512:ILE:HD13	1.87	0.56
2:B:1185:ILE:HD11	2:B:1190:LEU:HD22	1.87	0.56
2:B:1549:ILE:HD13	2:B:1555:PHE:HB3	1.87	0.56
1:A:25:PRO:HG2	2:B:2020:LEU:HD23	1.87	0.56
1:A:1231:TYR:CZ	1:A:1705:LYS:HD3	2.39	0.56
2:B:831:ILE:HD11	2:B:849:VAL:HG12	1.88	0.56
1:A:440:ASN:ND2	1:A:488:VAL:O	2.38	0.56
2:B:558:LYS:HG2	2:B:564:ILE:HG12	1.86	0.56
2:B:161:GLU:HA	2:B:164:ARG:HB2	1.88	0.56
1:A:1588:PRO:HG3	1:A:1595:TRP:CZ3	2.40	0.56
2:B:556:LEU:HD12	2:B:1074:ILE:HD11	1.88	0.56
2:B:1629:ARG:NH1	2:B:1634:GLU:O	2.39	0.56
1:A:700:ILE:HG13	1:A:735:LEU:HD12	1.88	0.56
2:B:153:GLN:HB2	2:B:262:GLN:HG3	1.88	0.56
2:B:1779:ASP:OD1	2:B:1780:ILE:N	2.39	0.56
2:B:1999:ILE:HG22	2:B:2006:PRO:HD3	1.88	0.56
1:A:1324:LYS:HB3	1:A:1391:LEU:HD22	1.89	0.55
2:B:657:ARG:NH1	2:B:663:ILE:O	2.39	0.55
2:B:1596:CYS:SG	2:B:1638:LEU:HD22	2.46	0.55
2:B:1688:ASN:O	2:B:1719:ASN:ND2	2.39	0.55
1:A:810:LYS:HG3	1:A:858:TRP:HB3	1.89	0.55
1:A:1035:ARG:NH1	1:A:1039:GLU:OE1	2.39	0.55
2:B:638:LEU:HD12	2:B:645:MET:HE2	1.88	0.55
2:B:673:PRO:HD2	2:B:692:LEU:HD11	1.88	0.55
2:B:1723:MET:HB2	2:B:1821:TYR:CE1	2.40	0.55
1:A:1028:PRO:HD3	1:A:1595:TRP:CH2	2.42	0.55
2:B:446:ASP:HB3	2:B:450:GLY:N	2.22	0.55
2:B:446:ASP:OD2	2:B:463:ARG:NH2	2.39	0.55
1:A:10:SER:HA	2:B:2009:LEU:HD23	1.89	0.55
2:B:1366:ALA:H	2:B:1377:GLU:HB3	1.71	0.55
2:B:1877:VAL:HB	2:B:1965:HIS:CG	2.41	0.55
1:A:1248:SER:HB3	1:A:1279:ILE:HG23	1.88	0.55
2:B:703:VAL:HG11	2:B:717:LEU:HD11	1.89	0.55
2:B:1905:LEU:HD22	2:B:1910:ILE:HG12	1.89	0.55
1:A:1026:VAL:HG12	1:A:1188:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PRO:HA	2:B:294:GLY:HA3	1.88	0.55
2:B:1620:GLY:CA	2:B:1786:ILE:HB	2.32	0.55
1:A:520:LYS:HE3	1:A:522:GLU:HB2	1.89	0.55
1:A:1029:TRP:O	1:A:1034:THR:OG1	2.24	0.55
1:A:28:TRP:HB3	2:B:1880:ASN:HB2	1.88	0.54
1:A:528:MET:HE3	1:A:641:PHE:HB2	1.88	0.54
2:B:394:VAL:HB	2:B:399:ARG:HD3	1.87	0.54
2:B:1227:ASN:N	2:B:1234:PRO:O	2.39	0.54
2:B:1877:VAL:HG22	2:B:1887:VAL:C	2.31	0.54
1:A:1105:ILE:HA	1:A:1187:GLN:HE22	1.72	0.54
1:A:1120:MET:HE3	1:A:1176:LYS:HE3	1.87	0.54
2:B:607:ALA:HA	2:B:637:ASN:HB3	1.88	0.54
2:B:656:LEU:HD22	2:B:661:TYR:CD2	2.42	0.54
2:B:721:GLY:N	2:B:756:SER:OG	2.41	0.54
2:B:868:LEU:HD11	2:B:1011:GLU:HB3	1.90	0.54
2:B:1803:LEU:HD13	2:B:1809:VAL:HB	1.89	0.54
1:A:1395:MET:O	1:A:1684:ARG:NE	2.41	0.54
2:B:246:THR:HB	2:B:249:GLU:HG2	1.89	0.54
1:A:1337:GLU:CD	1:A:1337:GLU:H	2.15	0.54
1:A:1372:ARG:NH1	1:A:1619:ASP:OD2	2.35	0.54
2:B:444:VAL:HB	2:B:453:PHE:HD2	1.73	0.54
2:B:1964:PHE:HB3	2:B:1969:LEU:CD2	2.38	0.54
1:A:636:SER:O	1:A:637:GLN:HG3	2.07	0.54
2:B:744:ILE:HG23	2:B:750:ILE:HG12	1.90	0.54
2:B:93:ASN:ND2	2:B:534:PHE:O	2.40	0.54
2:B:2009:LEU:HD23	2:B:2009:LEU:O	2.08	0.54
1:A:1001:ILE:HD11	1:A:1663:ASP:HA	1.89	0.54
1:A:1102:ILE:HG21	1:A:1376:MET:SD	2.48	0.54
1:A:1364:MET:HG2	1:A:1376:MET:HE1	1.90	0.54
1:A:1016:ASN:ND2	1:A:1510:LYS:HG3	2.23	0.53
1:A:1195:ARG:NH1	1:A:1204:ILE:HG21	2.23	0.53
2:B:656:LEU:HD22	2:B:661:TYR:HD2	1.73	0.53
1:A:752:VAL:HG12	1:A:812:LYS:HG3	1.90	0.53
1:A:1270:GLN:NE2	1:A:1272:ASP:OD1	2.41	0.53
2:B:855:LEU:HD21	2:B:1013:PHE:HE2	1.73	0.53
2:B:467:LEU:HD12	2:B:471:LEU:HB2	1.91	0.53
2:B:693:LYS:HA	2:B:717:LEU:O	2.08	0.53
1:A:1025:GLU:OE2	1:A:1035:ARG:NH2	2.38	0.53
2:B:273:SER:HB2	2:B:279:PHE:HB2	1.91	0.53
2:B:1001:LYS:HZ1	2:B:1023:TRP:CD1	2.26	0.53
2:B:1516:PHE:HB2	2:B:1617:MET:SD	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HA	1:A:81:TYR:HB2	1.90	0.53
2:B:1792:PHE:HB2	2:B:1802:ALA:HB1	1.91	0.53
1:A:1199:ILE:HD13	1:A:1702:PHE:CD2	2.44	0.53
2:B:164:ARG:NH2	2:B:212:THR:OG1	2.42	0.53
2:B:290:LEU:HA	2:B:293:ILE:HG22	1.90	0.53
2:B:582:ALA:HB2	2:B:787:LEU:HD13	1.90	0.53
2:B:816:ASP:O	2:B:819:TRP:HD1	1.92	0.53
1:A:1137:LYS:HD2	1:A:1162:TYR:CE2	2.41	0.53
1:A:1258:GLY:HA2	1:A:1262:ASP:HB2	1.91	0.53
2:B:1458:LYS:HB3	2:B:1464:SER:HB2	1.91	0.53
1:A:992:PHE:CD2	1:A:1398:PRO:HG3	2.44	0.52
2:B:585:THR:HG22	2:B:609:GLY:HA3	1.90	0.52
2:B:668:ILE:HD13	2:B:673:PRO:HG2	1.90	0.52
2:B:1287:THR:HA	2:B:1290:ILE:HG22	1.91	0.52
1:A:1076:ASP:HB2	1:A:1083:ILE:HD11	1.90	0.52
1:A:1402:VAL:HG11	1:A:1533:PHE:CZ	2.44	0.52
1:A:1035:ARG:NH2	1:A:1602:GLN:OE1	2.42	0.52
2:B:1984:ILE:HD12	2:B:1984:ILE:H	1.74	0.52
1:A:1278:PHE:HB2	1:A:1281:THR:HB	1.91	0.52
1:A:1374:GLY:HA2	1:A:1550:THR:HG22	1.92	0.52
2:B:475:TRP:CZ2	2:B:497:LEU:HD21	2.45	0.52
2:B:557:VAL:HG21	2:B:1088:VAL:HG22	1.92	0.52
2:B:1377:GLU:OE1	2:B:1395:GLN:HG2	2.10	0.52
2:B:1677:VAL:HG21	2:B:1774:LYS:HG2	1.90	0.52
2:B:1685:PHE:CZ	2:B:1816:VAL:HB	2.45	0.52
2:B:1659:GLN:HB2	2:B:1663:MET:SD	2.49	0.52
1:A:1037:GLU:OE1	1:A:1048:GLY:HA3	2.10	0.52
2:B:576:ARG:NH2	2:B:1230:ASP:OD1	2.42	0.52
2:B:1066:HIS:O	2:B:1070:ILE:HG12	2.09	0.52
2:B:1734:LEU:HD11	2:B:1974:LYS:HG3	1.92	0.52
2:B:1969:LEU:O	2:B:1970:MET:HG2	2.10	0.52
1:A:1588:PRO:HB2	1:A:1591:ALA:HB3	1.92	0.52
2:B:260:HIS:CG	2:B:261:SER:H	2.27	0.52
2:B:448:PHE:HE1	2:B:474:HIS:HE1	1.58	0.52
1:A:986:ALA:HB2	1:A:1050:ILE:HD12	1.91	0.51
1:A:1342:PHE:HE1	1:A:1650:PHE:HE2	1.56	0.51
1:A:20:TYR:CD1	2:B:1970:MET:HB3	2.46	0.51
1:A:1284:ALA:O	1:A:1288:MET:HG3	2.10	0.51
2:B:1548:PRO:HB2	2:B:1555:PHE:CG	2.45	0.51
2:B:1649:THR:HG21	2:B:1787:PRO:HG2	1.91	0.51
1:A:998:TYR:HA	1:A:1001:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:PRO:O	1:A:1008:LEU:N	2.44	0.51
2:B:170:TYR:O	2:B:174:ILE:HG12	2.10	0.51
1:A:1570:ARG:NH2	1:A:1574:ASN:O	2.43	0.51
1:A:23:ALA:HA	2:B:1965:HIS:N	2.25	0.51
1:A:953:ILE:HG22	2:B:1425:LYS:HB3	1.92	0.51
2:B:13:SER:H	2:B:46:PHE:HZ	1.59	0.51
1:A:1361:PRO:HA	1:A:1364:MET:SD	2.50	0.51
1:A:1604:LEU:HD13	1:A:1661:HIS:HA	1.93	0.51
2:B:730:PHE:HD1	2:B:840:PRO:HG3	1.76	0.51
2:B:1812:ILE:HG13	2:B:1813:GLU:N	2.25	0.51
2:B:423:THR:HG21	2:B:466:LYS:HG2	1.91	0.51
2:B:1110:ASN:O	2:B:1174:LYS:N	2.43	0.51
2:B:1612:MET:HA	2:B:1625:LYS:O	2.10	0.51
2:B:1656:GLN:HB2	2:B:1769:LEU:HD22	1.91	0.51
2:B:1954:VAL:HG12	2:B:1956:PRO:HD3	1.93	0.51
1:A:400:THR:HG22	1:A:402:ASP:OD1	2.10	0.51
1:A:709:THR:HG21	1:A:740:PHE:HD2	1.76	0.51
1:A:983:GLU:OE2	1:A:1086:LYS:HE2	2.11	0.51
2:B:423:THR:HA	2:B:426:ILE:HD12	1.93	0.51
2:B:1267:VAL:HG13	2:B:1364:ILE:HG21	1.93	0.51
1:A:436:ILE:HA	1:A:439:MET:HG2	1.93	0.51
1:A:1025:GLU:HG2	1:A:1595:TRP:CD1	2.46	0.51
1:A:1085:GLU:HA	1:A:1088:ILE:HG12	1.92	0.51
1:A:1132:PRO:HB3	1:A:1165:ARG:HB2	1.93	0.51
1:A:1188:ILE:H	1:A:1379:GLN:NE2	2.07	0.51
2:B:1158:LEU:O	2:B:1162:LEU:HB2	2.11	0.50
1:A:410:GLN:NE2	1:A:1633:ARG:HB3	2.27	0.50
1:A:1104:LEU:HD23	1:A:1184:VAL:HG22	1.93	0.50
2:B:566:VAL:HG23	2:B:1066:HIS:CE1	2.47	0.50
2:B:1110:ASN:OD1	2:B:1111:GLN:N	2.43	0.50
1:A:11:HIS:CD2	2:B:1986:LYS:HD2	2.47	0.50
1:A:823:ILE:HD13	1:A:865:CYS:HB3	1.94	0.50
2:B:391:GLN:HG2	2:B:399:ARG:HH21	1.77	0.50
2:B:1317:TRP:O	2:B:1321:ILE:HG12	2.12	0.50
2:B:1547:ASN:HB3	2:B:1550:HIS:HD2	1.76	0.50
2:B:1973:VAL:O	2:B:1975:PRO:HD2	2.12	0.50
2:B:1985:PRO:HB2	2:B:1988:SER:HB3	1.93	0.50
2:B:532:GLU:OE2	2:B:543:LYS:HD2	2.12	0.50
2:B:2028:SER:O	2:B:2032:ASN:N	2.44	0.50
1:A:12:THR:O	1:A:16:GLU:HG2	2.11	0.50
1:A:1019:VAL:HG11	1:A:1665:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:PHE:CE1	2:B:474:HIS:CE1	2.99	0.50
1:A:692:GLY:O	1:A:696:LEU:HG	2.11	0.50
2:B:690:LEU:HB2	2:B:713:PHE:HE2	1.77	0.50
2:B:779:PRO:O	2:B:781:MET:HG3	2.12	0.50
1:A:408:ALA:O	1:A:412:VAL:HG23	2.11	0.50
2:B:595:SER:HB2	2:B:627:ARG:HG3	1.94	0.50
2:B:621:ILE:HD13	2:B:663:ILE:HD11	1.94	0.50
2:B:879:ILE:HD12	2:B:890:TRP:CD2	2.46	0.50
2:B:1735:LYS:NZ	2:B:1737:GLU:OE1	2.42	0.50
1:A:952:ASP:OD1	1:A:953:ILE:N	2.45	0.49
2:B:830:ILE:HG12	2:B:844:ILE:HD13	1.93	0.49
2:B:1824:MET:O	2:B:1828:VAL:HG22	2.12	0.49
1:A:521:PHE:HA	1:A:524:TYR:HB3	1.94	0.49
2:B:173:LEU:HD22	2:B:241:LYS:HB3	1.94	0.49
2:B:1368:LEU:HD21	2:B:1410:GLN:HB2	1.94	0.49
2:B:2002:LEU:O	2:B:2002:LEU:HD23	2.12	0.49
1:A:1223:LEU:HD13	1:A:1692:MET:SD	2.52	0.49
2:B:539:ASP:OD1	2:B:539:ASP:N	2.43	0.49
2:B:566:VAL:HG12	2:B:568:THR:HG23	1.94	0.49
1:A:1076:ASP:O	1:A:1080:GLN:HA	2.12	0.49
1:A:1304:CYS:HA	1:A:1589:LYS:O	2.12	0.49
2:B:340:ILE:HG21	2:B:366:LEU:HD11	1.95	0.49
2:B:1850:VAL:HG23	2:B:1906:LYS:HA	1.93	0.49
2:B:586:PRO:HG2	3:B:2101:FMN:HM71	1.95	0.49
2:B:1199:LYS:HB2	2:B:1200:PRO:HD2	1.95	0.49
2:B:1468:THR:HB	2:B:1489:TYR:HB3	1.94	0.49
2:B:1709:GLY:H	2:B:1713:GLY:HA3	1.77	0.49
2:B:1879:TYR:HB2	2:B:1882:GLU:HB3	1.94	0.49
2:B:1991:PRO:HB3	2:B:1995:ILE:HD12	1.94	0.49
1:A:1714:LEU:HD22	1:A:1740:ILE:HD12	1.94	0.49
2:B:164:ARG:HH22	2:B:209:PRO:HA	1.77	0.49
2:B:1036:VAL:O	2:B:1039:THR:HG22	2.12	0.49
2:B:1384:ARG:HG2	2:B:1385:GLU:OE1	2.13	0.49
2:B:1854:PHE:HB3	2:B:1859:LEU:HD22	1.94	0.49
2:B:1979:PHE:CD1	2:B:1982:LYS:HE3	2.48	0.49
2:B:153:GLN:HG3	2:B:410:ILE:HG12	1.94	0.49
1:A:476:ILE:HG22	1:A:480:LYS:HE2	1.95	0.49
1:A:1234:TYR:HA	1:A:1237:VAL:O	2.13	0.49
1:A:1302:GLY:H	1:A:1306:THR:HB	1.78	0.49
1:A:1710:TYR:HA	1:A:1735:PHE:HB2	1.95	0.49
2:B:448:PHE:CE1	2:B:474:HIS:HE1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1826:MET:O	2:B:1962:VAL:HG11	2.13	0.49
1:A:1132:PRO:HG3	1:A:1165:ARG:CZ	2.43	0.49
2:B:1158:LEU:HD13	2:B:1161:ILE:HD11	1.95	0.49
2:B:1444:PHE:HA	2:B:1474:LEU:HD11	1.95	0.49
2:B:1452:GLU:OE2	2:B:1469:THR:OG1	2.31	0.49
2:B:1624:ILE:O	2:B:1642:ALA:N	2.24	0.49
1:A:338:LYS:O	1:A:342:GLU:HG2	2.13	0.48
1:A:370:LEU:HA	1:A:373:GLU:HG2	1.95	0.48
1:A:888:ILE:HD11	1:A:940:THR:HG22	1.95	0.48
1:A:1016:ASN:HD22	1:A:1510:LYS:HG3	1.77	0.48
2:B:1451:CYS:SG	2:B:1452:GLU:N	2.86	0.48
2:B:1591:VAL:C	2:B:1592:ARG:HD2	2.38	0.48
2:B:1684:HIS:NE2	2:B:1817:ASP:OD1	2.36	0.48
1:A:1181:ASP:HB3	1:A:1350:ASN:OD1	2.13	0.48
1:A:1396:GLY:O	1:A:1684:ARG:HD2	2.13	0.48
2:B:657:ARG:HG2	2:B:686:GLY:H	1.77	0.48
2:B:1174:LYS:O	2:B:1177:LYS:HG2	2.13	0.48
2:B:1449:PHE:CD1	2:B:1472:VAL:HA	2.47	0.48
2:B:1474:LEU:HD23	2:B:1475:GLU:N	2.28	0.48
2:B:1725:PHE:HB3	2:B:1825:THR:HG23	1.95	0.48
1:A:1547:GLY:HA2	1:A:1554:ASP:OD1	2.13	0.48
2:B:243:LEU:HD21	2:B:534:PHE:HA	1.94	0.48
2:B:728:HIS:CD2	2:B:842:HIS:CD2	3.01	0.48
2:B:1272:LEU:HD13	2:B:1361:LYS:HE2	1.94	0.48
2:B:1532:ALA:HB3	2:B:1606:ASP:H	1.79	0.48
1:A:1007:GLU:O	1:A:1448:LYS:NZ	2.25	0.48
1:A:1665:LEU:O	1:A:1668:VAL:HG22	2.13	0.48
1:A:1726:VAL:HG11	1:A:1733:LEU:HB3	1.96	0.48
2:B:1449:PHE:CE1	2:B:1472:VAL:HA	2.48	0.48
2:B:1835:LEU:HD22	2:B:1837:ARG:HH21	1.77	0.48
1:A:458:PRO:HG2	1:A:461:LYS:HD3	1.95	0.48
1:A:1604:LEU:HD11	1:A:1659:VAL:HG12	1.95	0.48
2:B:513:ILE:HG12	2:B:532:GLU:OE1	2.13	0.48
2:B:931:ARG:HD3	2:B:961:LEU:HB2	1.95	0.48
2:B:1840:TYR:HB3	2:B:1963:PRO:HG3	1.94	0.48
1:A:447:ILE:HD13	1:A:483:LEU:HD12	1.95	0.48
1:A:713:PHE:CD2	1:A:739:PRO:HG3	2.49	0.48
2:B:1417:VAL:HA	2:B:1509:THR:HA	1.96	0.48
2:B:330:ASP:HA	2:B:362:ARG:HB2	1.96	0.48
2:B:815:PRO:HB2	2:B:818:GLN:NE2	2.29	0.48
2:B:1271:ILE:HB	2:B:1362:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1368:LEU:O	2:B:1374:LYS:HA	2.14	0.48
1:A:1306:THR:HG22	1:A:1590:GLY:HA2	1.96	0.48
2:B:664:GLN:HE22	2:B:689:HIS:CE1	2.32	0.48
2:B:657:ARG:HD3	2:B:686:GLY:O	2.13	0.48
2:B:1212:THR:HG21	2:B:1218:VAL:HG22	1.95	0.48
2:B:323:SER:HB2	2:B:407:PHE:HB3	1.96	0.47
2:B:855:LEU:HD21	2:B:1013:PHE:CE2	2.49	0.47
1:A:406:ASN:ND2	1:A:1630:TYR:HB2	2.29	0.47
1:A:1304:CYS:HB2	1:A:1649:GLY:HA2	1.95	0.47
1:A:1608:LEU:HD21	1:A:1634:SER:HB3	1.97	0.47
2:B:481:HIS:CE1	2:B:505:LYS:HD3	2.48	0.47
2:B:974:LYS:O	2:B:976:PRO:HD3	2.15	0.47
2:B:1123:LYS:NZ	2:B:1159:HIS:O	2.26	0.47
2:B:136:LEU:HD23	2:B:136:LEU:H	1.79	0.47
2:B:1579:VAL:HG12	2:B:1612:MET:CE	2.45	0.47
1:A:518:VAL:HG21	1:A:527:GLU:HG2	1.95	0.47
1:A:983:GLU:O	2:B:943:GLU:HG2	2.14	0.47
1:A:990:PHE:CE2	1:A:1224:SER:HA	2.49	0.47
2:B:569:LYS:O	2:B:1096:PRO:HB3	2.15	0.47
2:B:572:GLN:HB3	2:B:1096:PRO:HA	1.95	0.47
2:B:741:TYR:OH	2:B:782:PRO:O	2.18	0.47
2:B:805:LYS:O	2:B:809:VAL:HG23	2.14	0.47
1:A:680:TYR:HD2	1:A:766:TRP:CE3	2.32	0.47
2:B:1029:GLU:HA	2:B:1034:GLU:HG3	1.95	0.47
2:B:1840:TYR:HE2	2:B:1873:LEU:HD21	1.80	0.47
1:A:23:ALA:HA	2:B:1965:HIS:CA	2.45	0.47
2:B:1265:ILE:HB	2:B:1326:PRO:HG3	1.95	0.47
2:B:1609:GLN:HB2	2:B:1631:VAL:HG22	1.96	0.47
2:B:1723:MET:HB2	2:B:1821:TYR:HE1	1.80	0.47
1:A:705:LYS:HE3	1:A:732:GLY:O	2.15	0.47
1:A:1562:ASN:OD1	1:A:1627:TYR:HB2	2.15	0.47
1:A:1596:MET:HE2	1:A:1645:VAL:HG13	1.96	0.47
2:B:710:HIS:O	2:B:749:ASN:ND2	2.48	0.47
2:B:1117:ASP:O	2:B:1121:PRO:HD3	2.15	0.47
2:B:1726:GLU:N	2:B:1975:PRO:HG3	2.30	0.47
1:A:28:TRP:CB	2:B:1880:ASN:HB2	2.44	0.47
2:B:583:GLY:CA	2:B:637:ASN:HD22	2.28	0.47
2:B:1103:SER:HA	2:B:1106:ILE:HD12	1.97	0.47
2:B:1198:VAL:HG23	2:B:1199:LYS:H	1.80	0.47
2:B:1422:LYS:O	2:B:1423:SER:OG	2.31	0.47
2:B:1454:THR:HB	2:B:1467:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:THR:HG21	1:A:947:LEU:HD21	1.96	0.47
2:B:1246:ILE:HG22	2:B:1333:LEU:HB2	1.97	0.47
2:B:1623:ILE:O	2:B:1624:ILE:HD13	2.15	0.47
1:A:399:ARG:NH2	1:A:1358:GLY:O	2.47	0.47
1:A:696:LEU:HD11	1:A:708:VAL:HG21	1.96	0.47
2:B:196:TYR:HB2	2:B:217:TYR:HE1	1.79	0.47
2:B:440:LEU:HD22	2:B:453:PHE:HB2	1.97	0.47
2:B:1379:VAL:HA	2:B:1393:THR:HA	1.97	0.47
1:A:742:GLN:OE1	1:A:775:ALA:HB3	2.15	0.46
1:A:801:ASN:HA	1:A:804:ARG:HB2	1.96	0.46
2:B:260:HIS:HA	2:B:475:TRP:CZ3	2.50	0.46
2:B:1685:PHE:CD2	2:B:1693:ILE:HB	2.50	0.46
1:A:1304:CYS:SG	1:A:1587:HIS:NE2	2.78	0.46
2:B:1512:GLU:O	2:B:1618:ILE:HG13	2.14	0.46
2:B:1719:ASN:O	2:B:1723:MET:HG2	2.15	0.46
2:B:1998:TYR:O	2:B:2007:PHE:N	2.48	0.46
2:B:2035:GLN:NE2	2:B:2037:GLU:O	2.48	0.46
1:A:988:MET:O	1:A:1693:HIS:NE2	2.48	0.46
1:A:1118:LYS:HE2	1:A:1340:TYR:CG	2.50	0.46
2:B:1172:ILE:HG22	2:B:1176:THR:HA	1.97	0.46
2:B:1513:SER:HB2	2:B:1618:ILE:HD12	1.96	0.46
2:B:1842:MET:SD	2:B:1889:ALA:HB2	2.55	0.46
1:A:1231:TYR:OH	1:A:1707:LYS:O	2.32	0.46
2:B:9:LEU:O	2:B:15:GLU:HA	2.15	0.46
2:B:606:LEU:HD21	2:B:611:TYR:CE2	2.51	0.46
2:B:938:LEU:HD13	2:B:967:PHE:HE1	1.80	0.46
1:A:1129:ASP:OD1	1:A:1129:ASP:N	2.48	0.46
2:B:700:ILE:HA	2:B:703:VAL:HG12	1.97	0.46
2:B:1120:LEU:HD23	2:B:1120:LEU:O	2.15	0.46
2:B:1427:LEU:HD22	2:B:1444:PHE:HB3	1.98	0.46
2:B:1579:VAL:O	2:B:1580:GLU:HB2	2.14	0.46
2:B:1795:HIS:ND1	2:B:1795:HIS:O	2.48	0.46
1:A:1366:ARG:NH1	1:A:1371:THR:HG23	2.31	0.46
2:B:461:ILE:HA	2:B:464:VAL:HG12	1.97	0.46
2:B:881:LYS:HA	2:B:881:LYS:HD2	1.76	0.46
2:B:1294:CYS:H	2:B:1297:PHE:HB2	1.81	0.46
2:B:1847:PRO:HG3	2:B:1886:TYR:CD2	2.50	0.46
2:B:1849:ARG:HG3	2:B:1952:PHE:O	2.16	0.46
2:B:277:ASP:OD1	2:B:278:SER:N	2.49	0.46
2:B:694:PRO:HG3	2:B:717:LEU:HD11	1.97	0.46
2:B:1578:LEU:HD11	2:B:1582:TRP:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1786:ILE:HG23	2:B:1790:ILE:CD1	2.46	0.46
2:B:555:THR:O	2:B:556:LEU:HD23	2.16	0.46
2:B:1158:LEU:HA	2:B:1161:ILE:HG12	1.98	0.46
1:A:14:LEU:HD12	2:B:2009:LEU:HD11	1.97	0.46
1:A:1193:ASP:OD1	1:A:1194:ALA:N	2.48	0.46
2:B:463:ARG:NH1	2:B:467:LEU:HD22	2.31	0.46
2:B:1855:ASP:O	2:B:1859:LEU:HD23	2.16	0.46
2:B:1991:PRO:O	2:B:1995:ILE:HB	2.16	0.46
1:A:32:GLN:HA	1:A:35:PHE:CE2	2.50	0.46
1:A:1194:ALA:HB1	1:A:1199:ILE:HG13	1.98	0.46
2:B:236:TYR:CG	2:B:270:ILE:HD11	2.51	0.46
2:B:357:LEU:HG	2:B:365:VAL:HB	1.98	0.46
2:B:887:GLN:HE21	2:B:1040:CYS:H	1.64	0.46
2:B:1197:LEU:HD12	2:B:1202:THR:O	2.16	0.46
2:B:1522:LEU:HD22	2:B:1624:ILE:HG13	1.97	0.46
1:A:1231:TYR:CE2	1:A:1705:LYS:HD3	2.51	0.45
2:B:42:PRO:HA	2:B:51:GLU:OE2	2.16	0.45
2:B:64:GLY:HA3	2:B:121:ASN:CG	2.41	0.45
2:B:344:ASN:CG	2:B:353:ILE:H	2.25	0.45
2:B:1974:LYS:HB2	2:B:1975:PRO:CD	2.46	0.45
1:A:694:GLU:OE1	1:A:697:GLN:NE2	2.49	0.45
2:B:716:VAL:HG12	2:B:718:GLN:HG3	1.98	0.45
2:B:1426:ASP:HB3	2:B:1444:PHE:CE2	2.51	0.45
2:B:1840:TYR:HD2	2:B:1963:PRO:HG2	1.81	0.45
1:A:996:LYS:HB3	1:A:1000:GLU:CD	2.41	0.45
1:A:1670:ASP:OD1	1:A:1670:ASP:N	2.50	0.45
1:A:868:VAL:HB	1:A:925:ASP:HA	1.98	0.45
1:A:1354:GLU:HG3	1:A:1364:MET:HG3	1.97	0.45
2:B:914:VAL:HG12	2:B:920:LYS:NZ	2.31	0.45
2:B:1928:LEU:O	2:B:1932:VAL:HG12	2.16	0.45
2:B:115:LYS:HZ3	2:B:169:LEU:HD13	1.82	0.45
2:B:1072:ARG:HA	2:B:1075:LYS:HG2	1.98	0.45
2:B:1324:ILE:O	2:B:1398:TYR:OH	2.32	0.45
2:B:1617:MET:CE	2:B:1785:LEU:HB2	2.47	0.45
1:A:1195:ARG:HH12	1:A:1204:ILE:HG21	1.82	0.45
2:B:336:VAL:O	2:B:340:ILE:HG23	2.17	0.45
1:A:1044:PHE:CE2	1:A:1052:MET:HG3	2.52	0.45
1:A:1318:ILE:HD11	1:A:1326:VAL:HG12	1.99	0.45
2:B:1248:GLU:HG3	2:B:1252:LYS:HZ2	1.78	0.45
2:B:1486:SER:OG	2:B:1487:VAL:N	2.50	0.45
2:B:1509:THR:OG1	2:B:1510:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1539:TYR:HA	2:B:1542:VAL:HG22	1.99	0.45
1:A:433:ASN:O	1:A:437:GLN:HG2	2.17	0.45
2:B:225:CYS:HB2	2:B:226:PRO:HD3	1.97	0.45
2:B:1508:LYS:HD2	2:B:1509:THR:O	2.16	0.45
2:B:1725:PHE:CZ	2:B:1739:ILE:HD13	2.52	0.45
1:A:915:GLN:HA	1:A:918:GLN:NE2	2.32	0.45
1:A:1275:GLN:NE2	1:A:1276:GLU:OE1	2.49	0.45
1:A:1537:ILE:HG13	1:A:1570:ARG:HD3	1.98	0.45
2:B:115:LYS:NZ	2:B:169:LEU:HD13	2.32	0.45
2:B:1590:ARG:HD3	2:B:1645:GLU:O	2.17	0.45
2:B:1862:VAL:HB	2:B:1898:LEU:HG	1.98	0.45
1:A:23:ALA:HA	2:B:1965:HIS:H	1.82	0.45
2:B:1451:CYS:HA	2:B:1470:GLY:HA2	1.98	0.45
2:B:1811:PRO:HG3	2:B:1985:PRO:CD	2.47	0.45
2:B:1812:ILE:HG13	2:B:1813:GLU:H	1.82	0.45
2:B:548:TRP:CD1	2:B:552:LEU:HD13	2.52	0.44
2:B:767:TYR:HA	2:B:772:TRP:CD1	2.51	0.44
2:B:843:LYS:HD3	2:B:1040:CYS:HB2	1.99	0.44
2:B:1198:VAL:HG23	2:B:1199:LYS:N	2.31	0.44
2:B:1305:THR:H	2:B:1354:LYS:HE2	1.81	0.44
1:A:986:ALA:O	2:B:944:ARG:NH1	2.38	0.44
2:B:583:GLY:HA3	2:B:637:ASN:HD22	1.82	0.44
2:B:726:GLY:O	2:B:841:ILE:HA	2.18	0.44
1:A:497:GLY:HA3	1:A:515:LYS:HD3	1.99	0.44
1:A:700:ILE:CG2	1:A:729:GLY:HA2	2.47	0.44
2:B:1131:ALA:HB1	2:B:1139:GLN:HG2	1.99	0.44
2:B:1435:TRP:CD2	2:B:1499:VAL:HG22	2.52	0.44
2:B:1830:VAL:HG22	2:B:1962:VAL:HG12	2.00	0.44
2:B:1844:ALA:HB3	2:B:1955:ILE:H	1.82	0.44
2:B:1882:GLU:HB2	2:B:1886:TYR:HE1	1.82	0.44
2:B:412:ALA:HB3	2:B:414:PHE:CE2	2.53	0.44
2:B:1684:HIS:HB2	2:B:1813:GLU:OE2	2.17	0.44
2:B:2018:TYR:HD1	2:B:2023:SER:HB3	1.82	0.44
2:B:196:TYR:HB2	2:B:217:TYR:CE1	2.53	0.44
2:B:1843:VAL:HG21	2:B:1899:THR:HG21	2.00	0.44
2:B:1928:LEU:H	2:B:1928:LEU:HD23	1.83	0.44
1:A:522:GLU:HG2	1:A:671:ILE:HG13	2.00	0.44
1:A:1144:LYS:HA	1:A:1151:CYS:SG	2.57	0.44
2:B:522:PRO:HG2	2:B:525:ASP:HA	1.98	0.44
2:B:605:GLU:OE1	2:B:667:THR:OG1	2.30	0.44
2:B:832:THR:HA	2:B:841:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1271:ILE:N	2:B:1362:ALA:O	2.45	0.44
2:B:1435:TRP:HB3	2:B:1489:TYR:HD1	1.83	0.44
2:B:1514:VAL:HG22	2:B:1782:SER:C	2.42	0.44
2:B:2005:LYS:O	2:B:2006:PRO:C	2.61	0.44
2:B:149:ILE:HD11	2:B:475:TRP:CZ2	2.53	0.44
2:B:1063:ASN:O	2:B:1066:HIS:N	2.51	0.44
2:B:1444:PHE:HE1	2:B:1447:LEU:CD2	2.30	0.44
2:B:1874:LEU:HD12	2:B:1894:ALA:HB1	2.00	0.44
2:B:1877:VAL:H	2:B:1888:ALA:HA	1.83	0.44
1:A:413:LEU:HD11	1:A:1577:PHE:CZ	2.53	0.44
1:A:684:THR:HA	1:A:709:THR:HB	1.99	0.44
1:A:871:TRP:HB3	1:A:895:THR:HG23	1.99	0.44
2:B:1329:VAL:O	2:B:1329:VAL:HG13	2.18	0.44
2:B:1612:MET:HG2	2:B:1624:ILE:HG21	1.99	0.44
2:B:1665:MET:HE3	2:B:1697:VAL:HG11	1.99	0.44
2:B:1724:MET:HG3	2:B:1725:PHE:N	2.33	0.44
1:A:6:GLU:HA	1:A:9:LEU:HD12	2.00	0.44
1:A:335:LYS:HD3	1:A:339:GLN:NE2	2.33	0.44
1:A:894:ARG:HH22	1:A:900:GLU:CD	2.23	0.44
1:A:1553:ASN:C	1:A:1553:ASN:HD22	2.25	0.44
2:B:1130:LEU:HD12	2:B:1162:LEU:HD13	2.00	0.44
2:B:1312:ALA:HA	2:B:1315:ILE:HD12	2.00	0.44
2:B:1362:ALA:HA	2:B:1380:GLY:CA	2.48	0.44
2:B:2015:GLN:HA	2:B:2018:TYR:HB3	2.00	0.44
1:A:1016:ASN:OD1	1:A:1319:LEU:HD22	2.17	0.43
1:A:1401:ALA:HB1	1:A:1659:VAL:HG13	2.00	0.43
2:B:721:GLY:HA3	2:B:733:PHE:HD1	1.83	0.43
2:B:936:ASP:OD1	2:B:990:TYR:OH	2.25	0.43
2:B:1479:LYS:HD2	2:B:1988:SER:HB2	1.99	0.43
2:B:1800:TYR:OH	2:B:1822:ARG:NH2	2.51	0.43
2:B:1881:VAL:HG12	2:B:1881:VAL:O	2.18	0.43
2:B:2002:LEU:C	2:B:2003:THR:HG1	2.18	0.43
1:A:34:VAL:HG13	1:A:39:HIS:HB2	2.00	0.43
1:A:37:LYS:HG3	1:A:68:TYR:CZ	2.53	0.43
1:A:1106:GLU:H	1:A:1187:GLN:NE2	2.16	0.43
2:B:326:LEU:HD12	2:B:373:LEU:HB3	1.99	0.43
2:B:484:THR:O	2:B:511:ARG:N	2.37	0.43
2:B:580:MET:HE1	2:B:718:GLN:NE2	2.33	0.43
2:B:1787:PRO:HD2	2:B:1790:ILE:HD11	2.00	0.43
2:B:1825:THR:HG21	2:B:1975:PRO:O	2.18	0.43
1:A:1372:ARG:HH12	1:A:1619:ASP:CG	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:LEU:HD23	2:B:174:ILE:HD13	1.98	0.43
2:B:524:ASP:OD1	2:B:746:ARG:HB3	2.19	0.43
2:B:1444:PHE:CE1	2:B:1447:LEU:HG	2.54	0.43
2:B:1621:ARG:HD3	2:B:1645:GLU:OE2	2.18	0.43
1:A:10:SER:OG	1:A:11:HIS:N	2.49	0.43
1:A:1353:GLU:O	1:A:1357:HIS:ND1	2.51	0.43
2:B:620:ALA:O	2:B:624:ILE:HG13	2.18	0.43
2:B:1147:ILE:HG12	2:B:1156:ASN:HA	1.99	0.43
2:B:1416:PRO:HA	2:B:1449:PHE:O	2.19	0.43
2:B:1469:THR:O	2:B:1486:SER:OG	2.35	0.43
2:B:1471:GLN:HA	2:B:1486:SER:HA	2.01	0.43
2:B:1511:GLU:OE2	2:B:1513:SER:HB3	2.18	0.43
2:B:1897:THR:HA	2:B:1935:VAL:CG1	2.49	0.43
1:A:813:LYS:CB	1:A:861:LYS:HD2	2.47	0.43
1:A:1278:PHE:O	1:A:1281:THR:HG22	2.19	0.43
2:B:639:ILE:HD13	2:B:669:GLY:HA3	2.01	0.43
2:B:892:GLY:HA2	2:B:904:MET:SD	2.58	0.43
2:B:1310:ASP:HA	2:B:1343:TYR:HE2	1.83	0.43
1:A:515:LYS:HB2	1:A:518:VAL:O	2.19	0.43
1:A:1417:VAL:HG13	1:A:1651:GLY:HA2	2.01	0.43
2:B:195:ILE:HG13	2:B:196:TYR:CD1	2.51	0.43
2:B:887:GLN:NE2	2:B:1040:CYS:H	2.16	0.43
2:B:935:GLY:O	2:B:939:ARG:HG2	2.19	0.43
2:B:1803:LEU:CD1	2:B:1809:VAL:HB	2.48	0.43
2:B:1869:LYS:HD3	2:B:1929:TYR:CD1	2.53	0.43
1:A:39:HIS:CG	2:B:1648:THR:HG21	2.54	0.43
1:A:1492:GLU:O	1:A:1495:GLU:HG3	2.19	0.43
1:A:1526:LEU:CD1	1:A:1658:VAL:HG21	2.48	0.43
2:B:639:ILE:HB	2:B:645:MET:SD	2.58	0.43
2:B:1313:ILE:O	2:B:1317:TRP:N	2.34	0.43
2:B:1418:GLN:HA	2:B:1447:LEU:O	2.19	0.43
2:B:1763:GLN:CD	2:B:1827:GLN:HE22	2.27	0.43
2:B:1786:ILE:HD12	2:B:1786:ILE:H	1.83	0.43
1:A:927:ASN:HD21	1:A:930:LEU:HB2	1.84	0.43
1:A:1014:LEU:HD13	1:A:1393:LEU:HD12	2.00	0.43
1:A:1031:ASN:HD21	1:A:1051:GLU:HG2	1.84	0.43
1:A:1342:PHE:HB3	1:A:1348:THR:HG23	2.00	0.43
1:A:1607:GLY:O	1:A:1637:THR:OG1	2.33	0.43
2:B:484:THR:HG21	2:B:544:TRP:CZ3	2.53	0.43
2:B:822:THR:HG21	2:B:842:HIS:HE1	1.83	0.43
2:B:1253:LEU:CD2	2:B:1548:PRO:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:O	1:A:76:ARG:NH2	2.41	0.43
1:A:1038:MET:O	1:A:1613:ARG:NH2	2.37	0.43
1:A:1717:PRO:HB2	1:A:1740:ILE:HD13	2.01	0.43
2:B:570:PHE:HD1	2:B:751:VAL:HG11	1.84	0.43
2:B:657:ARG:NH2	2:B:1153:HIS:HB2	2.32	0.43
2:B:1294:CYS:HB3	2:B:1297:PHE:HD2	1.84	0.43
2:B:1317:TRP:CE2	2:B:1321:ILE:HG21	2.54	0.43
2:B:1345:MET:HE1	2:B:1621:ARG:HE	1.84	0.43
1:A:1052:MET:HA	1:A:1055:ILE:HG12	2.00	0.43
2:B:571:SER:O	2:B:575:GLY:N	2.52	0.43
2:B:735:GLN:HA	2:B:738:ILE:HG22	2.01	0.43
2:B:914:VAL:HG12	2:B:920:LYS:HZ2	1.84	0.43
2:B:1616:GLY:C	2:B:1623:ILE:HB	2.44	0.43
1:A:1300:PRO:HG2	1:A:1310:SER:HA	2.00	0.42
2:B:290:LEU:O	2:B:293:ILE:HG22	2.19	0.42
2:B:1459:SER:OG	2:B:1460:ALA:N	2.52	0.42
1:A:1447:ARG:HD2	1:A:1512:TRP:O	2.19	0.42
1:A:1460:SER:O	1:A:1464:THR:HG23	2.19	0.42
1:A:1677:TYR:CZ	1:A:1681:VAL:HG21	2.55	0.42
2:B:514:LEU:HD12	2:B:529:PHE:CE1	2.54	0.42
1:A:33:ASP:O	1:A:38:GLN:N	2.30	0.42
1:A:1477:LYS:HE3	1:A:1489:PHE:HB2	2.01	0.42
1:A:1596:MET:HE1	1:A:1646:THR:O	2.19	0.42
2:B:233:LEU:HD13	2:B:283:SER:HB2	2.01	0.42
2:B:1296:ALA:HB1	2:B:1306:LEU:HD23	2.01	0.42
2:B:1519:ALA:HB2	2:B:1615:VAL:HG22	2.01	0.42
1:A:992:PHE:CE2	1:A:1398:PRO:HG3	2.54	0.42
2:B:1723:MET:O	2:B:1724:MET:HB2	2.18	0.42
1:A:26:VAL:HG23	2:B:2001:ASN:HB3	2.02	0.42
1:A:1400:HIS:HB3	1:A:1601:ILE:HG21	2.02	0.42
2:B:885:ASP:O	2:B:1038:ARG:HA	2.20	0.42
2:B:1063:ASN:O	2:B:1064:SER:C	2.62	0.42
2:B:1313:ILE:HD13	2:B:1569:MET:SD	2.60	0.42
2:B:1971:SER:O	2:B:1973:VAL:N	2.51	0.42
1:A:1588:PRO:O	1:A:1589:LYS:C	2.62	0.42
2:B:129:ILE:O	2:B:129:ILE:HG22	2.20	0.42
2:B:728:HIS:CE1	2:B:840:PRO:HB2	2.53	0.42
2:B:1502:TYR:HD1	2:B:1505:ARG:NH2	2.17	0.42
1:A:1289:LEU:HB3	1:A:1702:PHE:HZ	1.84	0.42
2:B:146:LEU:HD23	2:B:485:HIS:HB2	2.02	0.42
2:B:733:PHE:HE2	2:B:767:TYR:CE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:888:LYS:NZ	2:B:1019:LYS:O	2.46	0.42
1:A:1294:SER:O	1:A:1294:SER:OG	2.36	0.42
1:A:1325:VAL:HG22	1:A:1387:MET:HG3	2.00	0.42
1:A:1367:PRO:O	1:A:1368:THR:HG22	2.20	0.42
2:B:942:GLU:HG3	2:B:975:PHE:CZ	2.55	0.42
2:B:1138:LEU:O	2:B:1142:ILE:HG13	2.20	0.42
2:B:1646:GLN:O	2:B:1788:SER:HB2	2.20	0.42
2:B:1835:LEU:HB2	2:B:1837:ARG:HE	1.84	0.42
1:A:5:ILE:O	1:A:9:LEU:HG	2.19	0.42
2:B:102:LEU:HD23	2:B:107:TYR:HE2	1.85	0.42
2:B:181:ILE:HG21	2:B:230:VAL:HG22	2.02	0.42
2:B:1435:TRP:HE3	2:B:1487:VAL:HG21	1.84	0.42
1:A:499:LYS:HA	1:A:886:GLU:OE2	2.20	0.42
1:A:532:GLY:HA3	1:A:892:GLY:O	2.20	0.42
1:A:796:ARG:HG2	1:A:801:ASN:ND2	2.35	0.42
1:A:990:PHE:CZ	1:A:1224:SER:HA	2.55	0.42
1:A:1589:LYS:HD3	1:A:1589:LYS:N	2.30	0.42
2:B:786:VAL:HG23	2:B:788:PHE:CE1	2.54	0.42
2:B:881:LYS:O	2:B:885:ASP:HB2	2.20	0.42
2:B:1006:VAL:HG11	2:B:1013:PHE:HE1	1.85	0.42
2:B:1548:PRO:O	2:B:1552:SER:N	2.52	0.42
2:B:246:THR:HG22	2:B:248:GLY:H	1.85	0.41
2:B:645:MET:HA	2:B:648:TRP:NE1	2.35	0.41
2:B:765:TYR:OH	2:B:1076:GLU:OE1	2.24	0.41
2:B:846:THR:HB	2:B:1037:GLN:HA	2.02	0.41
2:B:929:SER:OG	2:B:1000:GLN:HG3	2.19	0.41
2:B:1368:LEU:HD12	2:B:1375:LEU:HD23	2.02	0.41
2:B:1488:ASP:OD1	2:B:1489:TYR:N	2.53	0.41
1:A:1180:PHE:CE2	1:A:1182:ARG:HB2	2.56	0.41
1:A:1265:ALA:HB3	1:A:1267:LYS:HG2	2.02	0.41
1:A:1364:MET:HG2	1:A:1376:MET:CE	2.49	0.41
1:A:1598:ASN:O	1:A:1602:GLN:HG3	2.20	0.41
2:B:264:LEU:HD21	2:B:453:PHE:HZ	1.84	0.41
2:B:1321:ILE:O	2:B:1324:ILE:HG12	2.20	0.41
2:B:1815:LEU:O	2:B:1819:VAL:HG23	2.19	0.41
1:A:410:GLN:HE21	1:A:1633:ARG:HB3	1.85	0.41
2:B:488:ASP:OD1	2:B:514:LEU:HA	2.20	0.41
2:B:732:ASP:OD2	2:B:735:GLN:HG2	2.20	0.41
2:B:1341:ASN:HD22	2:B:1569:MET:HE1	1.86	0.41
2:B:1537:GLU:N	2:B:1538:PRO:HD2	2.34	0.41
2:B:1539:TYR:OH	2:B:1569:MET:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1594:PHE:CE2	2:B:1596:CYS:HB2	2.56	0.41
2:B:1627:GLU:HA	2:B:1638:LEU:O	2.20	0.41
1:A:367:SER:HA	1:A:370:LEU:HG	2.02	0.41
1:A:1029:TRP:CZ3	1:A:1038:MET:HE3	2.55	0.41
2:B:107:TYR:CZ	2:B:114:VAL:HG23	2.56	0.41
2:B:448:PHE:HE1	2:B:474:HIS:CE1	2.37	0.41
2:B:644:PHE:HA	2:B:647:GLN:HG2	2.01	0.41
2:B:682:ILE:HG12	2:B:713:PHE:CD2	2.54	0.41
1:A:680:TYR:O	1:A:769:ASP:N	2.47	0.41
1:A:1405:MET:HB2	1:A:1529:ALA:CB	2.51	0.41
2:B:1329:VAL:HG23	2:B:1374:LYS:HD3	2.01	0.41
1:A:712:ARG:O	1:A:717:VAL:HG21	2.20	0.41
1:A:1619:ASP:HB2	1:A:1622:LEU:HG	2.03	0.41
2:B:188:LEU:HD21	2:B:292:PHE:CZ	2.55	0.41
2:B:934:TYR:CZ	2:B:938:LEU:HD11	2.56	0.41
2:B:1295:ASP:OD2	2:B:1586:ASN:ND2	2.53	0.41
2:B:1512:GLU:HB2	2:B:1619:ASN:HB2	2.02	0.41
2:B:1516:PHE:HA	2:B:1783:LYS:NZ	2.35	0.41
2:B:1899:THR:C	2:B:1901:VAL:H	2.28	0.41
1:A:529:ALA:HB1	1:A:634:ILE:HG12	2.01	0.41
1:A:893:VAL:HG11	1:A:930:LEU:HD23	2.03	0.41
1:A:1118:LYS:NZ	1:A:1336:GLU:OE2	2.48	0.41
1:A:1588:PRO:HG2	1:A:1592:ALA:N	2.36	0.41
2:B:1739:ILE:HG13	2:B:1741:LYS:HE3	2.02	0.41
2:B:1766:GLN:O	2:B:1770:THR:HG23	2.20	0.41
2:B:1770:THR:HG21	2:B:1819:VAL:HG21	2.02	0.41
2:B:1846:ASN:HA	2:B:1847:PRO:HD3	1.84	0.41
1:A:400:THR:HG23	1:A:736:ILE:HG13	2.03	0.41
1:A:821:GLN:OE1	1:A:914:VAL:HG22	2.21	0.41
1:A:986:ALA:HB1	1:A:1047:GLU:HG3	2.03	0.41
1:A:1306:THR:CG2	1:A:1590:GLY:HA2	2.51	0.41
1:A:1364:MET:HB2	1:A:1366:ARG:HH21	1.85	0.41
2:B:537:SER:HB2	2:B:541:ALA:N	2.36	0.41
2:B:1499:VAL:O	2:B:1503:LEU:HG	2.20	0.41
2:B:1822:ARG:O	2:B:1826:MET:HG3	2.20	0.41
1:A:420:ILE:HA	1:A:464:THR:HB	2.02	0.41
1:A:447:ILE:HG23	1:A:476:ILE:HG23	2.03	0.41
1:A:683:VAL:HG12	1:A:686:ALA:HB2	2.03	0.41
1:A:1019:VAL:HB	1:A:1399:ILE:HG23	2.03	0.41
1:A:1376:MET:HE3	1:A:1376:MET:HB2	1.87	0.41
1:A:1406:THR:HA	1:A:1656:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:THR:HA	1:A:1652:GLN:O	2.20	0.41
2:B:93:ASN:OD1	2:B:536:THR:OG1	2.31	0.41
2:B:257:SER:O	2:B:444:VAL:HG13	2.20	0.41
2:B:387:MET:HA	2:B:402:LYS:NZ	2.35	0.41
2:B:537:SER:N	2:B:541:ALA:HB2	2.35	0.41
2:B:1362:ALA:HA	2:B:1380:GLY:HA3	2.03	0.41
2:B:1512:GLU:HG2	2:B:1618:ILE:HG13	2.03	0.41
2:B:1878:ASN:HB3	2:B:1887:VAL:H	1.85	0.41
2:B:2033:TRP:HB3	2:B:2036:TYR:CE1	2.56	0.41
1:A:91:LYS:HD3	2:B:1518:ASN:HD21	1.85	0.41
1:A:434:GLN:O	1:A:438:ILE:HG13	2.21	0.41
1:A:478:ASN:HD22	1:A:481:GLN:HE21	1.69	0.41
1:A:865:CYS:HB2	1:A:917:CYS:SG	2.62	0.41
2:B:337:GLU:HA	2:B:340:ILE:HG12	2.03	0.41
2:B:703:VAL:HG11	2:B:717:LEU:CD1	2.51	0.41
2:B:1012:ARG:O	2:B:1012:ARG:HG2	2.21	0.41
2:B:1472:VAL:C	2:B:1473:LEU:HD12	2.47	0.41
2:B:1516:PHE:HB3	2:B:1615:VAL:O	2.21	0.41
2:B:1646:GLN:HB2	2:B:1787:PRO:HB3	2.02	0.41
2:B:1763:GLN:HB2	2:B:1820:PHE:CE1	2.55	0.41
2:B:1835:LEU:HD22	2:B:1837:ARG:NH2	2.35	0.41
2:B:1920:SER:OG	2:B:1923:LYS:HB2	2.21	0.41
2:B:1928:LEU:HA	2:B:1931:ILE:HG22	2.03	0.41
1:A:405:TRP:CD1	1:A:405:TRP:H	2.38	0.40
1:A:658:LEU:HD11	1:A:916:LEU:HD21	2.03	0.40
2:B:858:THR:OG1	2:B:874:LYS:NZ	2.54	0.40
2:B:1307:ALA:HB3	2:B:1352:LEU:HB2	2.03	0.40
2:B:1682:ASP:OD1	2:B:1693:ILE:N	2.54	0.40
1:A:803:LEU:HD22	1:A:849:LEU:HD21	2.03	0.40
1:A:1248:SER:OG	1:A:1332:ASP:OD1	2.35	0.40
1:A:1315:ILE:HD11	1:A:1403:LEU:HB3	2.03	0.40
1:A:1366:ARG:NH1	1:A:1371:THR:O	2.51	0.40
2:B:1338:HIS:O	2:B:1598:PHE:HD2	2.05	0.40
2:B:1379:VAL:HG22	2:B:1393:THR:OG1	2.21	0.40
2:B:1472:VAL:HG22	2:B:1485:GLY:O	2.21	0.40
2:B:1538:PRO:O	2:B:1542:VAL:HG13	2.21	0.40
2:B:1847:PRO:O	2:B:1850:VAL:HG12	2.21	0.40
1:A:10:SER:HA	2:B:2009:LEU:CD2	2.50	0.40
1:A:30:GLU:OE1	2:B:2004:ALA:HB1	2.21	0.40
1:A:1332:ASP:OD2	1:A:1589:LYS:HB2	2.20	0.40
2:B:717:LEU:HA	2:B:717:LEU:HD12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:723:ARG:HB3	2:B:1046:VAL:HG21	2.04	0.40
2:B:1178:LYS:HB3	2:B:1196:GLU:HG2	2.03	0.40
2:B:1311:PHE:CD2	2:B:1314:VAL:HG21	2.57	0.40
2:B:1562:PRO:O	2:B:1603:LEU:HD11	2.21	0.40
2:B:1866:VAL:O	2:B:1870:THR:OG1	2.32	0.40
2:B:1990:LYS:HE2	2:B:1990:LYS:HB3	1.97	0.40
1:A:382:GLY:HA3	1:A:789:SER:HB3	2.03	0.40
1:A:669:ALA:O	1:A:673:GLY:HA2	2.21	0.40
1:A:748:VAL:HG21	1:A:801:ASN:HB3	2.04	0.40
2:B:212:THR:HG22	2:B:218:LEU:HD11	2.03	0.40
2:B:572:GLN:OE1	2:B:1092:GLY:N	2.54	0.40
2:B:1281:GLN:O	2:B:1285:GLU:HG3	2.21	0.40
2:B:1617:MET:HE3	2:B:1785:LEU:HB2	2.04	0.40
2:B:1758:LEU:HD23	2:B:1758:LEU:HA	1.94	0.40
2:B:1840:TYR:HB3	2:B:1963:PRO:CG	2.51	0.40
1:A:685:GLY:HA3	1:A:775:ALA:HA	2.03	0.40
2:B:773:SER:HB3	2:B:778:TYR:CB	2.51	0.40
2:B:1345:MET:HG2	2:B:1345:MET:O	2.22	0.40
2:B:1587:VAL:HB	2:B:1590:ARG:HE	1.86	0.40
2:B:1779:ASP:O	2:B:1783:LYS:N	2.48	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	1425/1885 (76%)	1383 (97%)	42 (3%)	0	100	100
2	B	2032/2037 (100%)	1824 (90%)	194 (10%)	14 (1%)	18	30
All	All	3457/3922 (88%)	3207 (93%)	236 (7%)	14 (0%)	31	45

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1032	VAL
2	B	1477	PRO
2	B	1580	GLU
2	B	1970	MET
2	B	1974	LYS
2	B	2003	THR
2	B	2006	PRO
2	B	1811	PRO
2	B	1937	ALA
2	B	1983	LYS
2	B	2004	ALA
2	B	1778	GLU
2	B	1741	LYS
2	B	1392	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1220/1579 (77%)	1220 (100%)	0	100	100
2	B	1780/1784 (100%)	1780 (100%)	0	100	100
All	All	3000/3363 (89%)	3000 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	339	GLN
1	A	481	GLN
1	A	898	GLN
1	A	904	ASN
1	A	965	GLN
1	A	969	ASN
1	A	1003	GLN

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Mol	Chain	Res	Type
1	A	1270	GLN
1	A	1344	ASN
1	A	1379	GLN
1	A	1432	HIS
1	A	1470	GLN
2	B	93	ASN
2	B	189	HIS
2	B	282	ASN
2	B	317	ASN
2	B	474	HIS
2	B	590	ASN
2	B	637	ASN
2	B	664	GLN
2	B	689	HIS
2	B	710	HIS
2	B	842	HIS
2	B	872	ASN
2	B	887	GLN
2	B	1263	ASN
2	B	1338	HIS
2	B	1403	ASN
2	B	1550	HIS
2	B	1567	HIS
2	B	1707	HIS
2	B	1827	GLN
2	B	1916	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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
3	FMN	B	2101	-	33,33,33	1.08	2 (6%)	48,50,50	1.22	7 (14%)

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
3	FMN	B	2101	-	-	3/18/18/18	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2101	FMN	C4A-N5	3.47	1.38	1.30
3	B	2101	FMN	C10-N1	2.46	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2101	FMN	C4-N3-C2	-3.11	120.12	125.64
3	B	2101	FMN	C4'-C3'-C2'	-2.74	109.02	113.57
3	B	2101	FMN	C4A-C4-N3	2.69	120.10	113.25
3	B	2101	FMN	O4-C4-C4A	-2.51	119.90	126.53
3	B	2101	FMN	C4A-C10-N10	2.46	120.00	116.48
3	B	2101	FMN	C10-C4A-N5	-2.31	120.08	124.81
3	B	2101	FMN	C9A-C5A-N5	-2.24	120.08	122.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

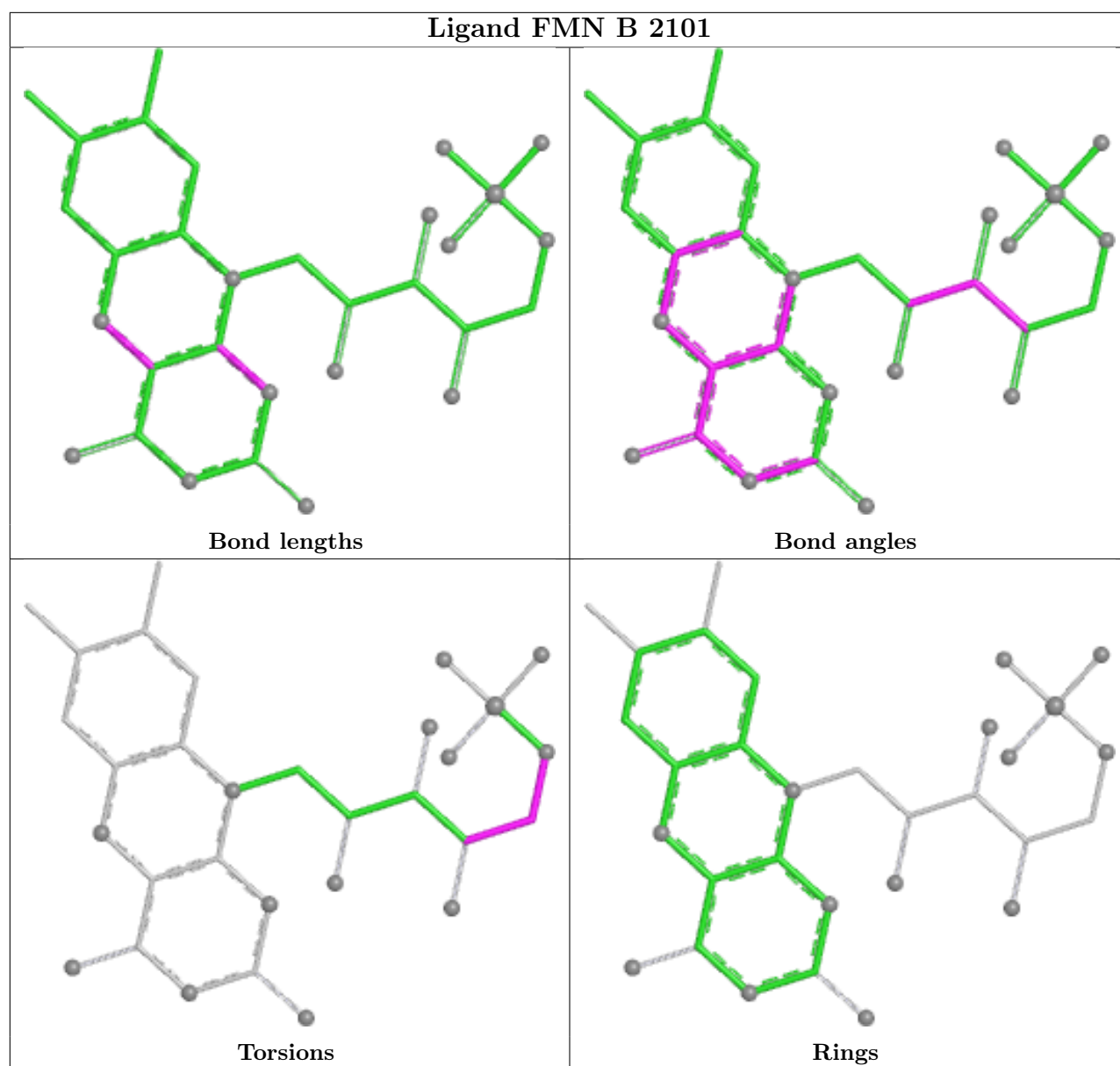
Mol	Chain	Res	Type	Atoms
3	B	2101	FMN	C3'-C4'-C5'-O5'
3	B	2101	FMN	O4'-C4'-C5'-O5'
3	B	2101	FMN	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2101	FMN	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

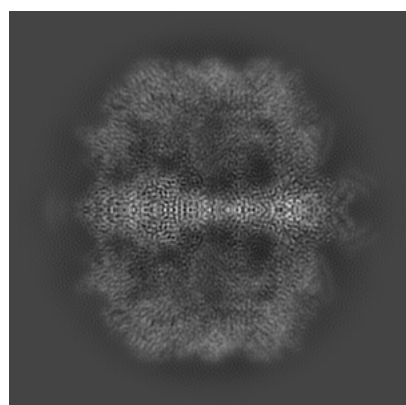
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26132. These allow visual inspection of the internal detail of the map and identification of artifacts.

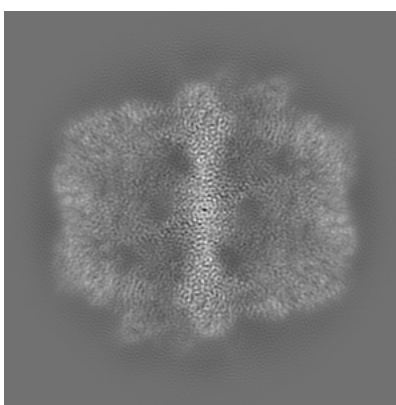
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

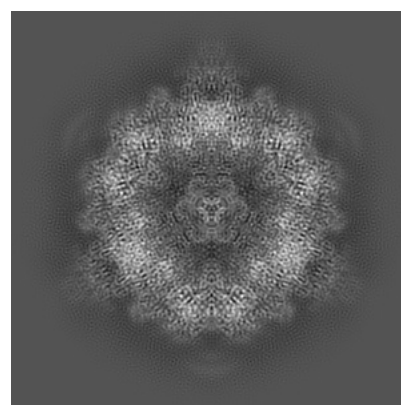
6.1.1 Primary map



X



Y

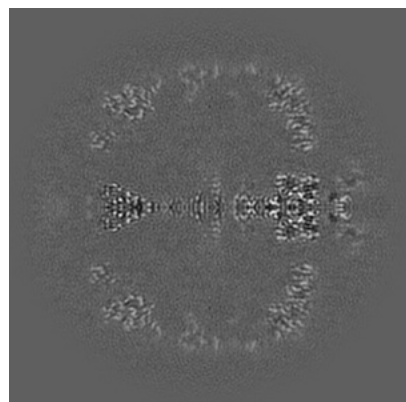


Z

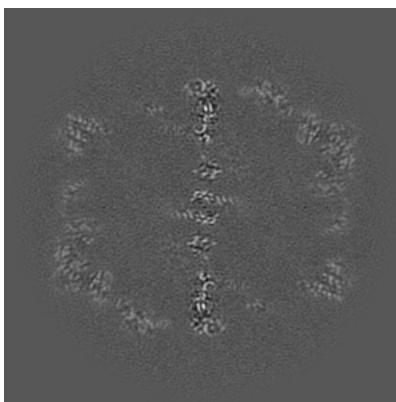
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

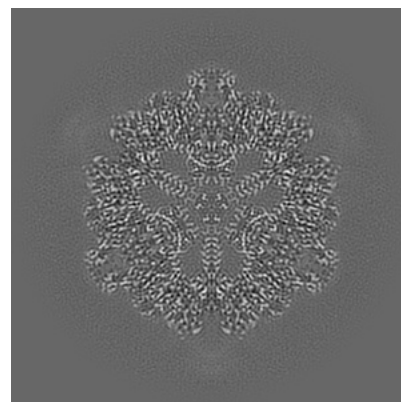
6.2.1 Primary map



X Index: 162



Y Index: 162

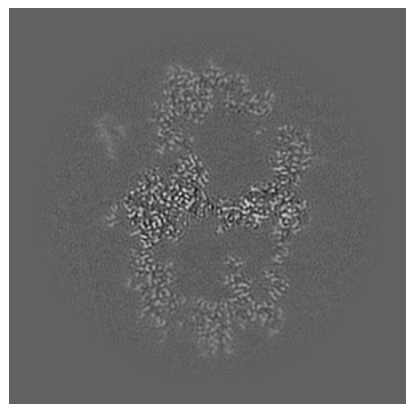


Z Index: 162

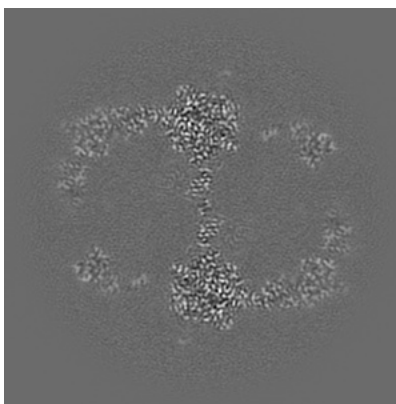
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

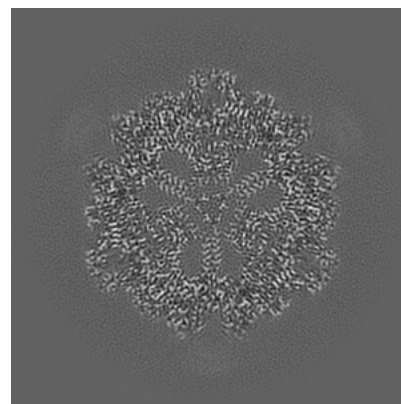
6.3.1 Primary map



X Index: 99



Y Index: 134

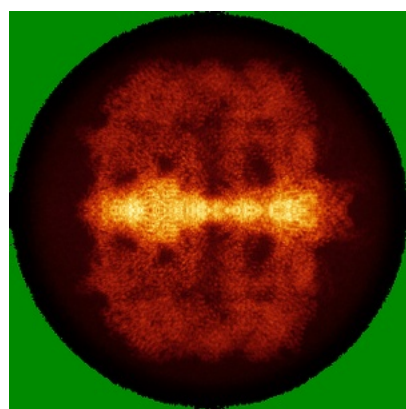


Z Index: 163

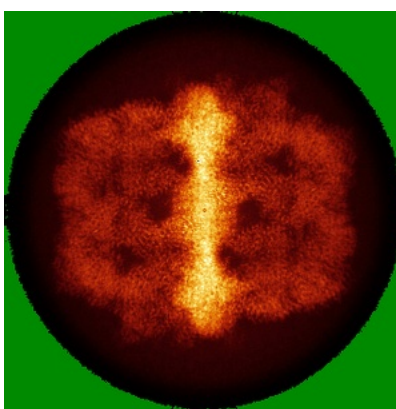
The images above show the largest variance slices of the map in three orthogonal directions.

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

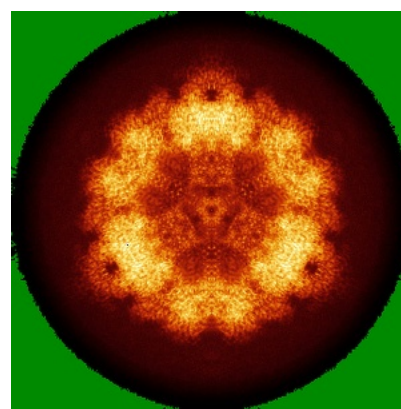
6.4.1 Primary map



X



Y

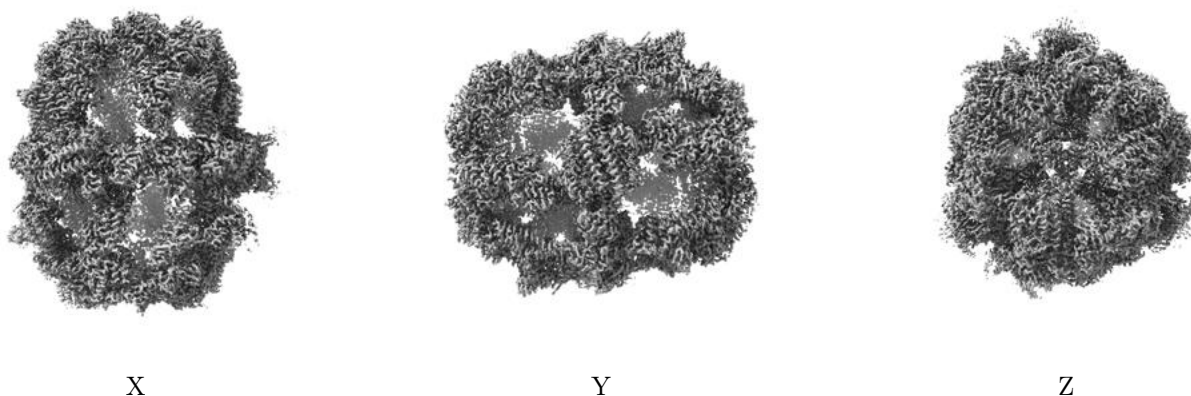


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

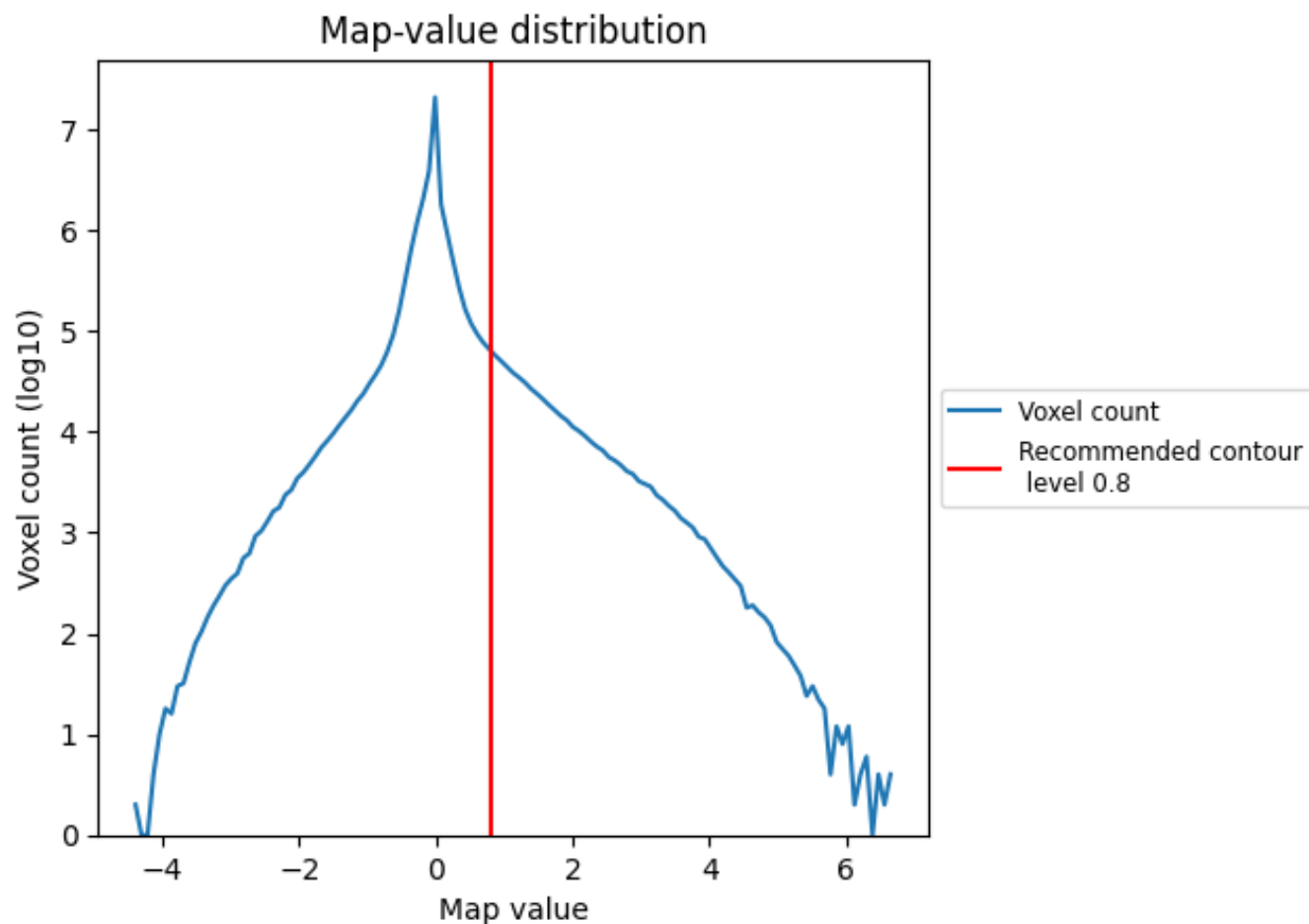
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

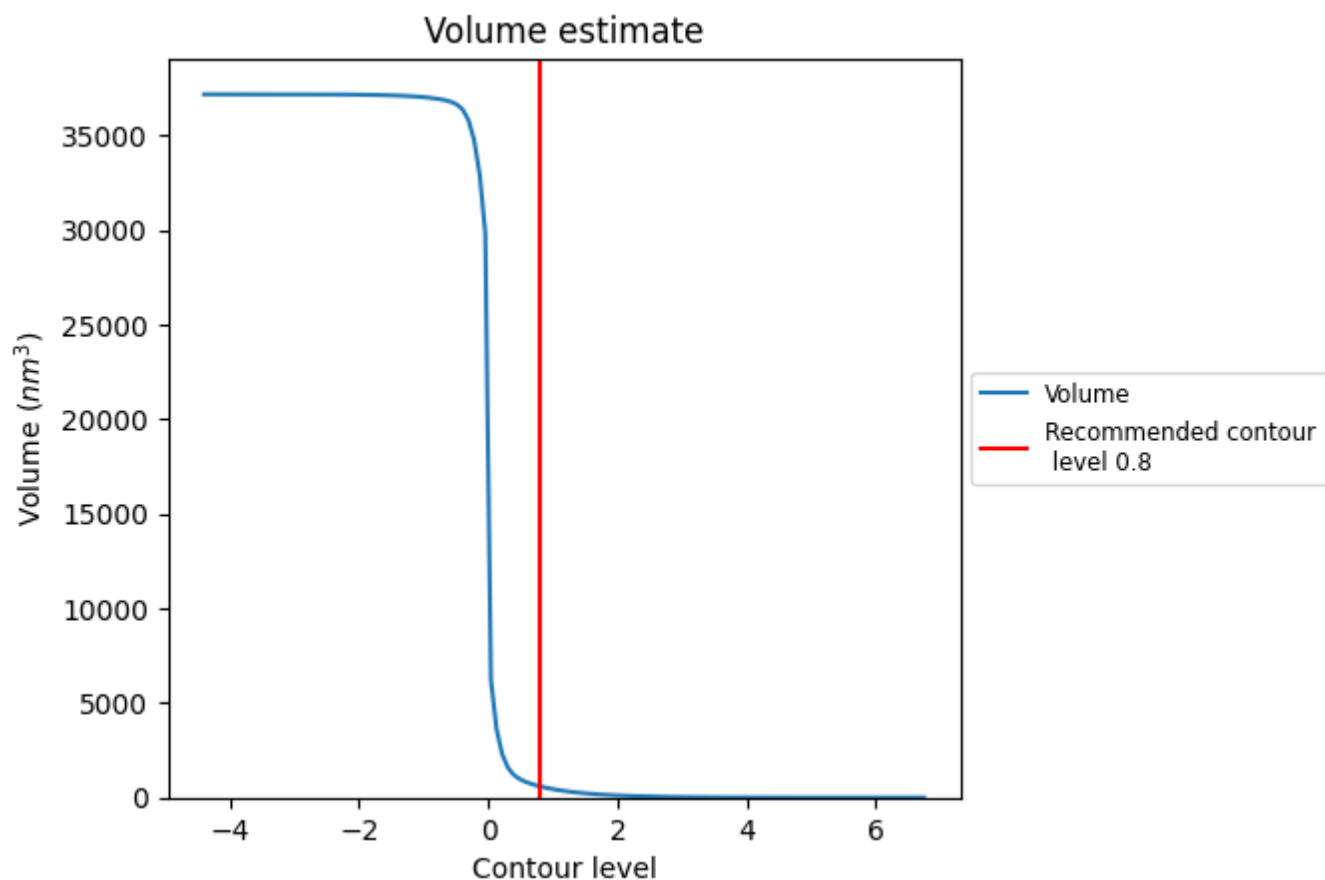
This section contains the results of statistical analysis of the map.

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.

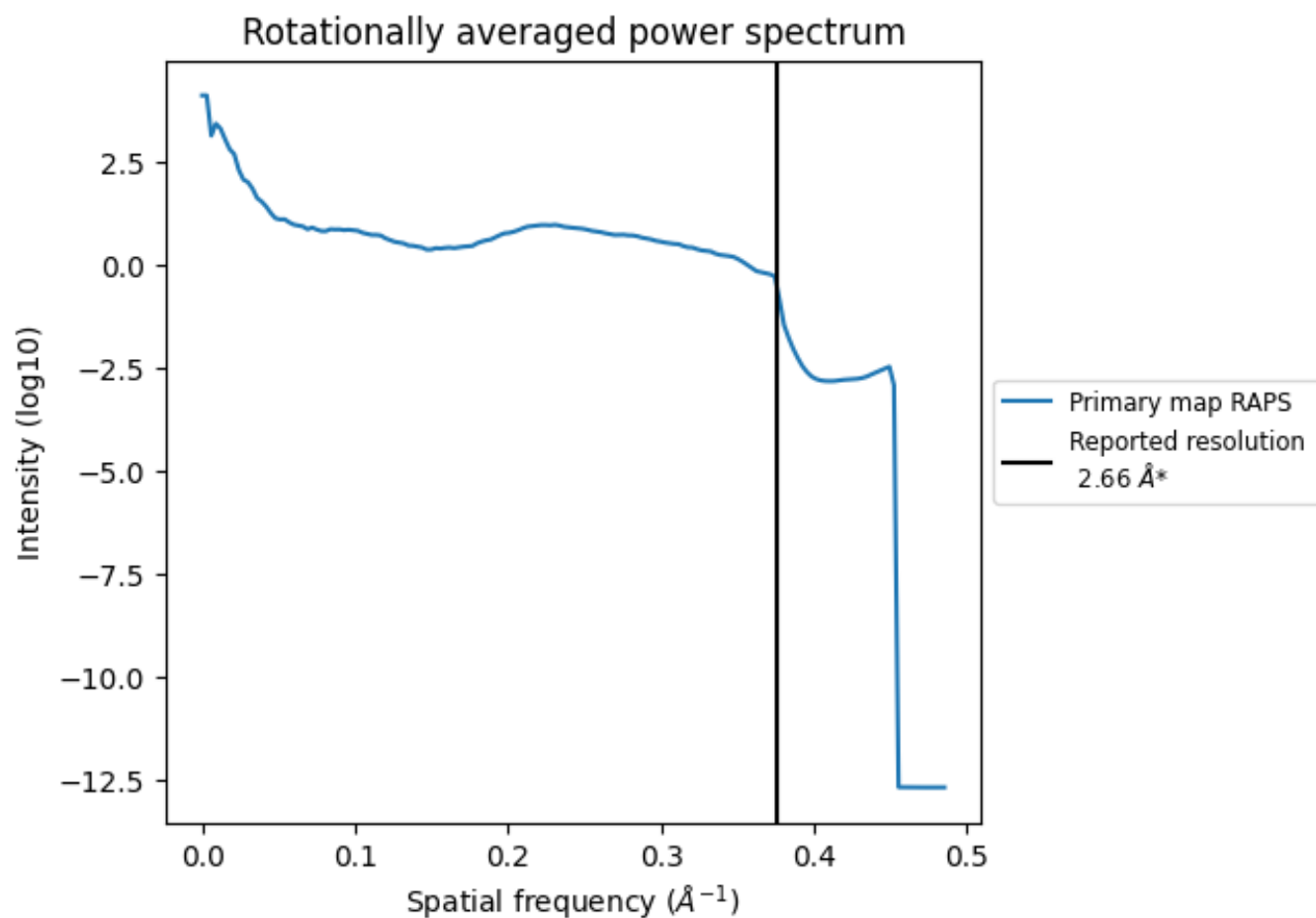
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 593 nm³; this corresponds to an approximate mass of 536 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 0.376 Å⁻¹

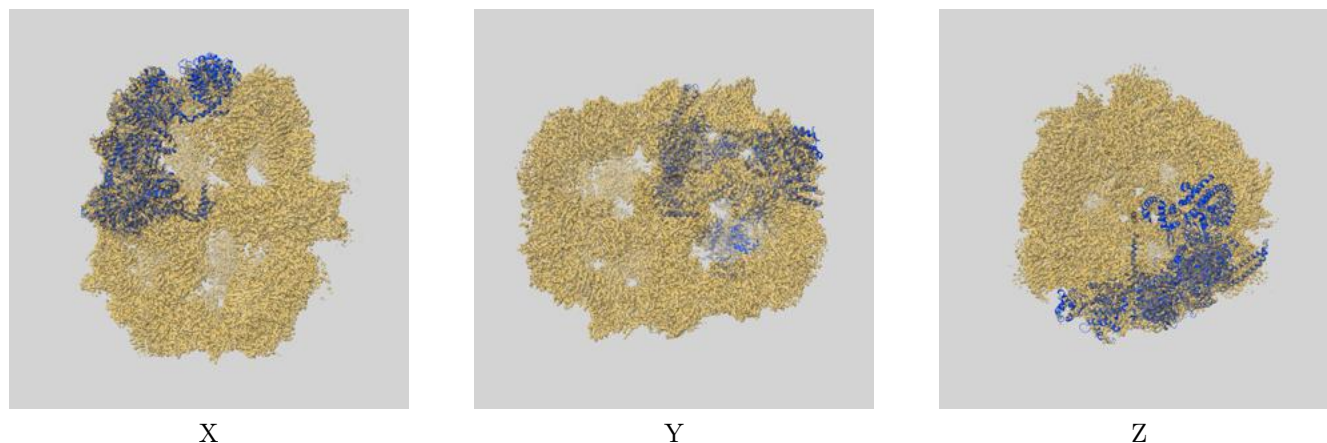
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

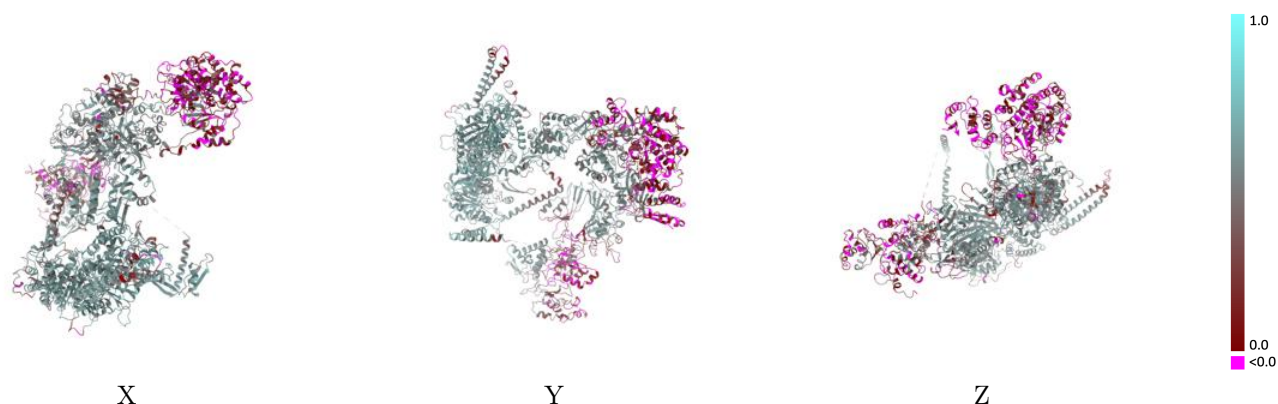
This section contains information regarding the fit between EMDB map EMD-26132 and PDB model 7TUI. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



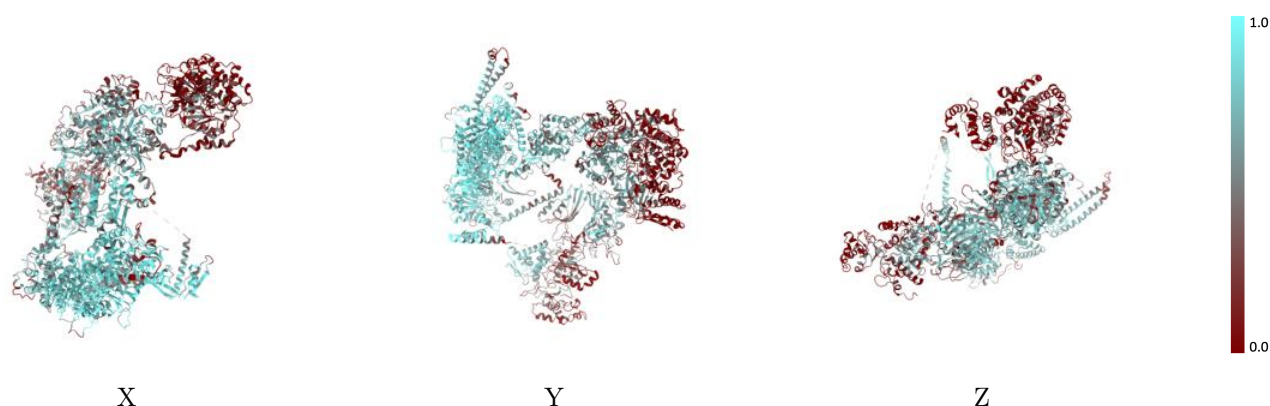
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



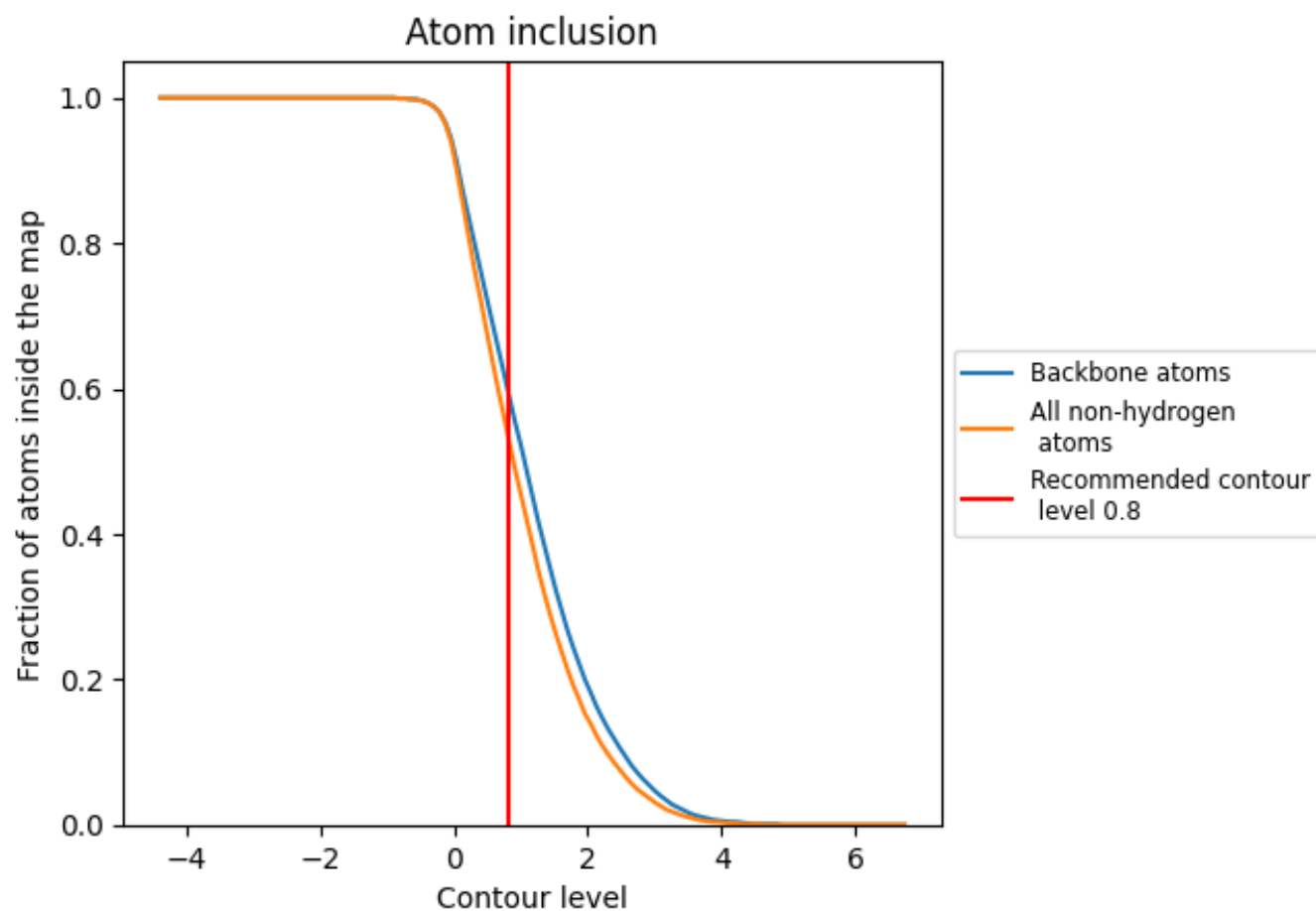
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 54% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5370	0.4130
A	0.7220	0.5220
B	0.4070	0.3370

