



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:08 PM UTC

PDB ID : 6U5W / pdb_00006u5w
EMDB ID : EMD-20658
Title : Electron cryomicroscopy structure of C. albicans FAS in the KS-stalled state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 3.30 Å(reported)
Based on initial model : 2UV8

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

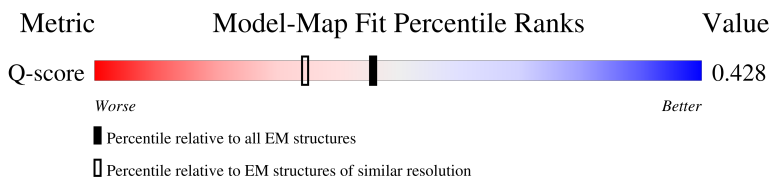
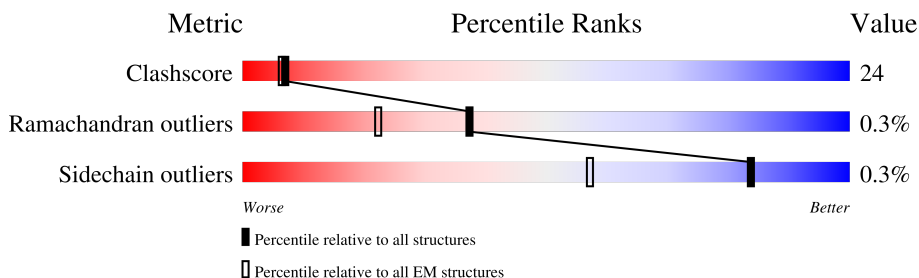
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	1722	21% 50% 33% 17%
2	B	2037	51% 54% 46%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	A	1901	-	-	X	-
3	NAP	B	2102	-	-	X	-
4	FMN	B	2101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27482 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	1435	Total	C	N	O	S	0	0
			11309	7178	1895	2190	46		

There are 173 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	HIS	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	TYR	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
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	356	ALA	LEU	conflict	UNP P43098
A	813	THR	PRO	conflict	UNP P43098
A	1066	LYS	GLN	conflict	UNP P43098
A	1123	VAL	ILE	conflict	UNP P43098
A	1444	GLU	LYS	conflict	UNP P43098
A	1742	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	0	0
			16046	10286	2662	3044	54		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltCon
3	A	1	Total 48	C 21	N 7	O 17	P 3	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0

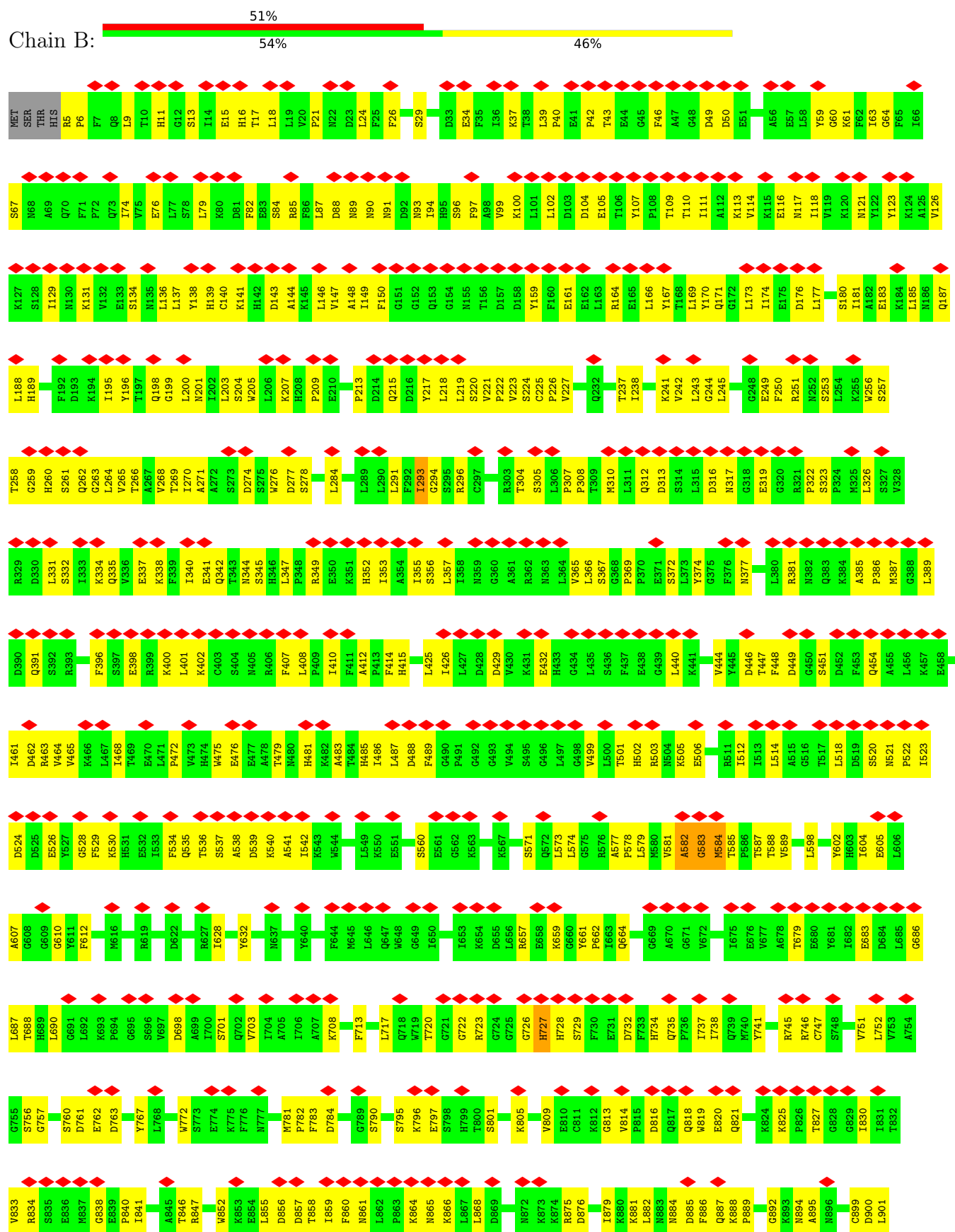
- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



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

SER	Y1709	E1622	T1535	E1462	F1374	T1305	P1208	C1134	F1057	Y976	G906	Y838
ALA	S1710	E1623	I1536	T1463	M1375	E1308	I1209	S1135	N1062	S977	L907	S839
THR	D1711	Y1624	D1537	E1464	E1376	S1309	T1210	K1136	G1063	E978	L908	E840
ARG	E1712	E1625	V1541	L1465	S1380	V1310	Y1212	E1137	N1064	W980	T909	S841
ASP	L1713	E1626	L1542	L1466	T1385	I1312	V1213	K1143	L1065	W981	P910	K842
VAL	E1714	L1628	H1545	Y1467	T1386	I1314	L1214		L1066		L915	S844
ASN	P1715	P1630	G1546	L1468	T1387	G1313	L1215		L1067		C916	L845
GLY		S1631	T1547	E1470	D1388	E1315	V1218		G1068		E919	L848
PRO	R1724	R1632	D1389	E1471	D1389	T1316	E1219		K1068		F849	F849
LYS	V1725	T1636	L1390	E1472	L1390	I1317	P1069		Y1070		N950	N950
ILE	E1726	D1637	M1394	A1473	M1394	L1318	L1222		D1075		D924	E855
LEU	E1727	K1554	G1395	A1474	G1395	S1319	S1223		A1076		L925	D856
HIS	N1728	M1555	V1396	L1474	V1396	G1320	A1224		T1077		N926	W857
GLY	K1729	A1475	P1397	A1475	P1397	K1321	I1226		K1077		L929	L861
ALA	K1730	K1476	H1398	E1476	H1398	K1322	P1229		T1078		Q930	T862
VAL	F1649	E1477	H1399	E1477	H1399	K1323	Y1233		P1081		F931	V863
LYS	K1731	E1478	V1401	E1478	V1401	V1324	V1236		I1082		I932	C964
ALA	V1732	F1479	V1404	F1479	V1404	V1325	V1236		I1083		D933	G865
ALA	F1733	G1480	T1405	G1480	T1405	L1326	V1236		E1084		N934	A866
ALA	F1734	D1481	T1409	D1481	T1409	Y1330	S1245		K1085		F938	V867
LYS	S1735	E1482	D1410	E1482	D1410	D1331	G1246		D1086		I868	G869
ALA	K1736	F1483	K1411	F1483	K1411	F1333	S1247		I1087		W870	T871
GLY	K1737	S1484	I1412	S1484	I1412	G1334	G1248		K1088		R943	R872
VAL	T1738	M1485	G1413	M1485	G1413	E1335	M1249		E1093		T944	G873
ASN	I1739	H1486	R1414	H1486	R1414	E1336	G1250		E1097		D945	T874
ALA	Q1740	E1487	V1416	E1487	V1416	G1337	G1257		K1014		L946	G875
SER	S1741	E1491	P1417	E1491	P1417	T1170	K1260		V1017		L947	L876
ILE	Q1742	R1492	A1418	R1492	A1418	L1171	K1261		V1018		T941	M877
ILE	Y1743	T1493		T1493					V1019		T949	S878
SER	S1744	E1494		E1494					T1020		A950	A879
ASP	Y1745	R1498		R1498					G1021		D951	N880
ALA	V1746	E1499		E1499					F1022		I952	A884
PHE	GLY	K1501		K1501					A1023		I952	E885
THR	GLU	R1502		R1502					V1024		R953	E886
ALA	VAL	Q1503		Q1503					V1025		R954	G886
ALA	ALA	V1504		V1504					G1026		A955	I887
THR	GLN	S1505		S1505					P1027		V956	E888
LYS	LYS	K1509		K1509					V1028		K889	X889
LYS	ALA	Q1510		Q1510					G1029		I958	L890
LEU	SER	W1511		W1511					M1030		L890	G891
SER	THR	G1512		G1512					R1032		E959	V892
LYS	LEU	N1513		N1513					T1033		A961	R893
ALA	ALA	K1517		K1517					M1037		I962	T894
ALA	SER	S1518		S1518					E1038		E963	F895
LEU	LEU	D1519		D1519					F1043		Q964	S896
ILE	GLY	P1520		P1520					S1044		K965	Q897
VAL	VAL	R1521		R1521					V966		V867	X898
VAL	VAL	L1525		L1525					V967		K966	E899
ASP	ASP	L1529		L1529					N968		N968	M900
GLU	GLU	F1532		F1532					G969		G969	A901
LEU	LEU	N1533		N1533					D970		D970	F902
		L1534		L1534					N971		N971	N903
									D973		D973	I904
									A974		A974	L905
									N975		N975	

● Molecule 2: Fatty acid synthase subunit beta



Q1698	L1699	M1702	E1703	L1704	T1705	I1706	H1707	F1708	G1709	K1712	G1713	E1714	A1715	I1716	R1717	D1718	N1719	Y1720	T1721	G1722	M1723	M1724	F1725	E1726	T1727	I1728	G1729	D1730	I1731	G1732	A1733	L1734	K1735	S1736	E1737	K1738	I1739	F1740	K1741	D1742	L1743	D1744	E1745	T1746	T1747	T1748	S1749	Y1750	T1751	F1752	V1753	S1754	P1755	T1756	G1757	L1758	
L1635	P1636	V1637	L1638	I1639	G1640	E1641	A1642	E1643	I1644	E1645	Q1646	T1647	T1648	T1649	T1650	Y1651	V1652	F1653	T1654	G1655	Q1656	G1657	S1658	Q1659	E1660	Q1661	G1662	M1663	G1664	M1665	E1666	L1667	Y1668	N1669	S1670	S1671	E1672	V1673	A1674	R1675	E1676	V1677	W1678	K1680	R1683	L1684	F1685	V1686	N1687	N1688	Y1689	G1690	F1691	L1694	D1695		
S1574	I1575	R1576	A1577	L1578	V1579	E1580	E1581	W1582	A1583	A1584	N1585	N1586	V1587	A1588	A1589	R1590	V1591	R1592	A1593	F1594	K1595	C1596	D1597	F1598	V1599	G1600	M1601	V1602	L1603	P1604	M1605	D1606	T1607	L1608	Q1609	T1610	T1611	M1612	E1613	H1614	M1617	L1618	M1619	G1620	R1621	K1622	L1623	I1624	K1625	V1626	E1627	T1628	R1629	N1630	V1631	E1632	T1633
I1510	E1511	E1512	S1513	E1517	N1518	A1519	I1520	P1521	L1522	S1523	S1524	G1525	E1526	E1527	L1528	T1529	S1530	K1531	A1532	P1533	G1534	T1535	N1536	E1537	P1538	Y1539	A1540	I1541	V1542	S1543	G1544	D1545	N1546	M1547	P1548	I1549	H1550	V1551	S1552	R1553	V1554	F1555	A1556	A1557	K1560	G1563	T1564	I1565	T1566	H1567	G1568	M1569	Y1570	S1571	A1572	A1573	
D1441	V1442	Q1443	F1444	D1445	V1446	L1447	T1448	F1449	R1450	C1451	E1452	S1453	K1456	F1457	K1458	S1459	A1460	V1461	Y1462	T1463	S1464	K1467	T1468	T1469	G1470	Q1471	E1475	L1476	P1477	T1478	K1479	E1480	V1481	L1482	Q1483	V1484	G1485	S1486	V1487	Y1488	E1490	A1491	G1492	H1497	P1498	Y1502	L1503	S1504	H1505	R1506	G1507	K1508	T1509				
V1367	L1368	N1369	Q1370	P1371	K1374	V1375	V1376	E1377	I1382	Y1383	R1384	E1385	G1386	M1390	Q1395	F1396	R1399	G1400	E1401	Y1402	N1403	D1404	Y1405	C1406	N1407	T1408	E1414	T1415	P1416	V1417	Q1418	V1419	A1420	F1421	K1422	G1423	A1424	K1425	D1426	L1427	A1428	V1429	L1430	R1431	S1432	K1433	E1434	W1435	F1436	H1437	L1438	E1439	K1440				
A1304	T1305	L1306	A1307	P1308	M1309	D1310	F1311	A1312	I1313	V1314	I1315	G1316	W1317	K1318	I1321	A1323	I1324	F1325	P1326	K1327	S1328	V1329	D1330	G1331	D1332	L1333	L1334	K1335	L1336	V1337	H1338	L1339	S1340	N1341	G1342	Y1343	K1344	M1345	T1346	T1347	G1348	A1349	A1350	P1351	L1352	K1353	L1354	G1355	V1357	V1358	W1359	T1360	E1363	A1366			
I1235	L1236	E1237	I1238	M1239	E1240	D1241	R1242	R1245	L1246	K1247	E1248	F1249	W1250	W1251	G1256	S1257	S1258	V1259	P1260	Y1261	S1262	N1263	D1264	I1265	N1266	E1268	K1269	A1270	I1271	L1272	G1273	D1274	E1275	L1276	T1277	I1278	S1279	F1286	T1287	H1288	A1289	I1290	G1291	N1292	K1293	C1294	D1295	A1296	F1297	A1299	D1299	R1300	P1301	G1302	K1303		
D1173	K1174	K1175	T1176	K1177	K1178	L1179	T1180	A1181	F1182	E1183	W1184	I1185	K1186	G1187	D1188	L1189	P1191	V1192	V1193	E1194	I1195	E1196	L1197	V1198	K1199	F1200	T1202	I1203	S1206	E1209	H1210	R1211	T1212	A1213	D1214	T1215	M1216	P1217	V1218	A1219	L1220	P1221	F1222	Y1223	Y1224	K1225	Y1226	N1227	T1228	F1229	A1229	D1230	G1231	F1232	A1233	P1234	
Q1111	V1112	E1115	I1116	D1117	S1118	E1119	L1120	P1121	W1122	K1123	Q1124	E1125	W1126	L1127	D1128	L1129	L1130	A1131	G1132	T1133	E1134	L1135	M1136	W1137	L1138	Q1139	A1140	F1141	I1142	S1143	T1144	D1145	R1146	T1147	V1148	Q1149	G1150	S1151	K1152	H1153	M1156	P1157	L1158	H1159	D1160	I1161	L1162	T1163	P1164	A1165	K1166	S1167	L1168	K1169	V1170	T1171	I1172
I1041	L1042	H1043	G1044	P1045	V1046	K1047	S1048	Q1049	Y1050	K1053	V1054	D1055	E1056	P1057	I1058	G1059	D1060	I1061	L1062	N1063	S1064	I1065	H1066	E1067	K1075	E1076	A1079	G1080	D1081	E1082	S1083	K1084	V1087	V1088	E1089	Y1090	G1093	K1094	K1095	P1096	A1097	S1098	V1099	S1100	A1101	T1102	S1103	V1104	N1105	T1106	I1107	D1108	G1109	N1110			
K980	Q981	L982	L983	S984	E985	E986	D987	C988	Y989	F991	L992	H993	L994	R997	P998	G999	D1000	K1001	P1002	V1003	P1004	F1005	V1006	P1007	V1008	L1009	D1010	E1011	R1012	F1013	E1014	F1015	F1016	F1017	K1018	K1019	D1020	S1021	L1022	W1023	Q1024	S1025	E1026	D1027	L1028	E1029	S1030	V1031	V1032	D1033	E1034	D1035	V1036	Q1037	R1038		
Q902	E903	M904	T905	Y906	K907	E908	L916	K920	K921	S922	H923	I926	D927	V928	S929	L930	R931	N932	M933	Y934	R939	R940	E943	R944	F945	S948	A949	G950	T951	L954	L955	Q956	N957	F958	N959	Q960	L961	N962	E963	P964	E965	Q966	F967	T968	A969	D970	F971	F972	E973	K974	Q977						

P2006 F2007 E2008 L2009 T2010 T2011 E2012 Y2013 F2014 Q2015 S2016 T2017 Y2018 D2019 T2021 K2022 S2023 E2024 K2025 L2026 K2027 S2028 L2029 L2030 D2031 N2032 W2033 E2034 Q2035 Y2036 E2037	P1945 I1946 D1947 L1948 E1949 R1950 G1951 F1952 A1953 V1954 I1955 P1956 L1957 K1958 G1959 I1960 V1962 F1963 F1964 H1965 S1966 S1967 L1968 L1969 M1970 V1973 K1974 P1975 F1976 Q1977 R1978 F1979 L1980 C1981 K1982 I1984 P1985 K1986 S1987 S1988 V1989 K1990 P1991 Q1992 L1994 I1995 G1996 K1997 Y1998 P2000 N2001 L2002 T2003 K2004 K2005	Q1885 Y1886 V1887 A1888 A1889 G1890 D1891 L1892 R1893 A1894 L1895 D1896 T1897 L1898 T1899 M1900 V1901 L1902 M1903 V1904 L1905 K1906 I1907 M1908 K1909 D1910 I1911 I1912 V1913 K1914 L1915 Q1916 E1917 Q1918 M1919 S1920 I1921 E1922 K1923 V1924 K1925 E1926 H1927 L1928 Y1929 E1930 I1931 V1932 D1933 E1934 V1935 A1936 A1937 K1938 S1939 L1940 A1941 K1942 P1943 Q1944	T1825 M1826 Q1827 L1828 A1829 V1830 P1831 R1832 D1833 E1834 L1835 G1836 R1837 S1838 M1839 Y1840 G1841 M1842 V1843 A1844 L1845 M1846 P1847 S1848 R1849 V1850 S1851 A1852 T1853 F1854 D1855 D1856 S1857 A1858 L1859 R1860 F1861 V1862 V1863 D1864 E1865 L1866 A1867 M1868 K1869 T1870 K1871 L1872 L1873 L1874 E1875 I1876 V1877 M1878 Y1879 N1880 V1881 E1882 M1883 Q1884	S1760 A1761 T1762 Q1763 F1764 T1765 Q1766 P1767 A1768 L1769 T1770 L1771 M1772 E1773 Y1777 E1778 D1779 I1780 K1783 G1784 L1785 I1786 P1787 S1788 D1789 I1790 M1791 F1792 A1793 G1794 H1795 S1796 L1797 G1798 E1799 Y1800 L1803 S1804 S1805 L1806 A1807 M1808 V1809 M1810 P1811 I1812 E1813 S1814 L1815 D1816 V1817 A1818 V1819 R1822 G1823 M1824
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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	24417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.942	Depositor
Minimum map value	-0.817	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.704	Depositor
Map size ($\text{\AA}$)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	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: FMN, NAP

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	0.51	1/11536 (0.0%)	0.54	0/15595
2	B	0.37	0/16415	0.48	3/22269 (0.0%)
All	All	0.43	1/27951 (0.0%)	0.51	3/37864 (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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	ILE	C-N	-5.44	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	ILE	N-CA-C	-5.44	107.49	111.90
2	B	1386	GLY	CA-C-N	-5.16	111.14	120.94
2	B	1386	GLY	C-N-CA	-5.16	111.14	120.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1301	GLY	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	11309	0	11219	498	0
2	B	16046	0	16024	853	0
3	A	48	0	25	34	0
3	B	48	0	25	49	0
4	B	31	0	17	50	0
All	All	27482	0	27310	1312	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 24.

All (1312) 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:584:MET:HE2	4:B:2101:FMN:C7	1.23	1.64
2:B:584:MET:HB3	4:B:2101:FMN:C5A	1.29	1.61
1:A:712:PHE:CE1	1:A:717:THR:HG22	1.35	1.58
2:B:727:HIS:ND1	3:B:2102:NAP:C4N	1.79	1.45
2:B:727:HIS:ND1	3:B:2102:NAP:C3N	1.73	1.44
2:B:727:HIS:CE1	3:B:2102:NAP:C6N	2.02	1.40
1:A:712:PHE:CE1	1:A:717:THR:CG2	2.08	1.36
2:B:727:HIS:CE1	3:B:2102:NAP:N1N	1.90	1.36
2:B:584:MET:HE3	4:B:2101:FMN:C9A	1.54	1.35
2:B:584:MET:HE2	4:B:2101:FMN:C8	1.58	1.32
1:A:710:SER:OG	3:A:1901:NAP:C4A	1.76	1.30
2:B:584:MET:CE	4:B:2101:FMN:C8	2.10	1.30
2:B:584:MET:CB	4:B:2101:FMN:C5A	2.13	1.27
2:B:612:PHE:CE2	3:B:2102:NAP:N7A	2.02	1.25
2:B:584:MET:CE	4:B:2101:FMN:C9	2.13	1.24
2:B:584:MET:HE2	4:B:2101:FMN:C6	1.68	1.23
2:B:727:HIS:CE1	3:B:2102:NAP:C2N	2.20	1.23
2:B:999:GLY:O	3:B:2102:NAP:H2A	1.40	1.19
2:B:584:MET:CB	4:B:2101:FMN:C6	2.20	1.19
1:A:877:MET:CE	3:A:1901:NAP:O7N	1.90	1.18
2:B:584:MET:HE3	4:B:2101:FMN:C5A	1.74	1.18
2:B:756:SER:HA	4:B:2101:FMN:C5'	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:584:MET:CE	4:B:2101:FMN:C7	2.20	1.17
2:B:727:HIS:CG	3:B:2102:NAP:C2N	2.18	1.15
2:B:756:SER:HA	4:B:2101:FMN:O5'	1.07	1.15
2:B:584:MET:CB	4:B:2101:FMN:N5	2.10	1.13
2:B:584:MET:CE	4:B:2101:FMN:C9A	2.26	1.12
1:A:842:LYS:NZ	3:A:1901:NAP:O2D	1.83	1.11
2:B:999:GLY:C	3:B:2102:NAP:H2A	1.75	1.11
2:B:584:MET:HB3	4:B:2101:FMN:C6	1.82	1.07
2:B:727:HIS:CD2	3:B:2102:NAP:C2N	2.35	1.07
2:B:727:HIS:ND1	3:B:2102:NAP:C2N	2.10	1.07
2:B:584:MET:CE	4:B:2101:FMN:C6	2.35	1.05
2:B:727:HIS:ND1	3:B:2102:NAP:C5N	2.19	1.05
2:B:727:HIS:H	3:B:2102:NAP:H4N	1.14	1.05
2:B:584:MET:HA	4:B:2101:FMN:N5	1.72	1.05
2:B:584:MET:HE1	4:B:2101:FMN:C9	1.83	1.05
2:B:756:SER:CA	4:B:2101:FMN:O5'	2.03	1.04
1:A:773:PHE:O	3:A:1901:NAP:O3D	1.77	1.02
2:B:584:MET:CE	4:B:2101:FMN:C5A	2.37	1.01
2:B:584:MET:CA	4:B:2101:FMN:N5	2.23	1.01
2:B:727:HIS:CE1	3:B:2102:NAP:C5N	2.43	1.01
1:A:877:MET:HE1	3:A:1901:NAP:O7N	1.57	1.00
2:B:584:MET:HB3	4:B:2101:FMN:N5	1.74	1.00
2:B:584:MET:HE1	4:B:2101:FMN:C8	1.92	0.98
1:A:877:MET:HE3	3:A:1901:NAP:C7N	1.93	0.97
2:B:584:MET:HB2	4:B:2101:FMN:C6	1.95	0.97
1:A:712:PHE:CZ	1:A:717:THR:HG22	1.98	0.97
2:B:584:MET:HA	4:B:2101:FMN:C4A	1.95	0.97
2:B:727:HIS:HE1	3:B:2102:NAP:C6N	1.65	0.94
1:A:712:PHE:CZ	1:A:717:THR:CG2	2.51	0.93
2:B:790:SER:HB3	4:B:2101:FMN:C8M	1.99	0.93
2:B:727:HIS:H	3:B:2102:NAP:C4N	1.84	0.91
1:A:877:MET:HE3	3:A:1901:NAP:O7N	1.67	0.91
2:B:584:MET:HB2	4:B:2101:FMN:H6	1.49	0.90
2:B:756:SER:CA	4:B:2101:FMN:C5'	2.50	0.89
1:A:873:GLY:O	1:A:878:SER:HB3	1.73	0.89
2:B:727:HIS:NE2	3:B:2102:NAP:C2N	2.35	0.88
2:B:87:LEU:HB3	2:B:91:ASN:HA	1.54	0.88
2:B:391:GLN:HE22	2:B:400:LYS:H	1.17	0.88
2:B:727:HIS:CE1	3:B:2102:NAP:H2D	2.09	0.88
2:B:582:ALA:O	2:B:605:GLU:HG2	1.74	0.87
2:B:727:HIS:N	3:B:2102:NAP:H4N	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:GLY:O	3:B:2102:NAP:C2A	2.22	0.87
1:A:873:GLY:O	1:A:878:SER:CB	2.22	0.87
1:A:712:PHE:CD2	1:A:738:PRO:HG3	2.11	0.86
1:A:710:SER:OG	3:A:1901:NAP:C5A	2.22	0.86
2:B:612:PHE:CE2	3:B:2102:NAP:C5A	2.58	0.86
2:B:727:HIS:HA	2:B:841:ILE:HD13	1.57	0.86
1:A:1303:CYS:HB2	1:A:1648:GLY:HA2	1.58	0.85
1:A:741:GLN:O	1:A:800:ASN:ND2	2.08	0.85
1:A:877:MET:CE	3:A:1901:NAP:C7N	2.54	0.85
2:B:1720:TYR:O	2:B:1738:LYS:NZ	2.09	0.85
2:B:612:PHE:HE2	3:B:2102:NAP:N7A	1.75	0.85
2:B:727:HIS:HE2	3:B:2102:NAP:C2D	1.89	0.85
2:B:790:SER:CA	4:B:2101:FMN:HM83	2.07	0.84
1:A:1299:PRO:HG3	1:A:1312:ILE:HD12	1.60	0.84
1:A:710:SER:OG	3:A:1901:NAP:N3A	2.08	0.84
2:B:999:GLY:C	3:B:2102:NAP:C2A	2.50	0.83
1:A:878:SER:O	1:A:880:ASN:N	2.10	0.83
2:B:581:VAL:O	2:B:582:ALA:O	1.97	0.83
2:B:727:HIS:NE2	3:B:2102:NAP:C2D	2.42	0.83
1:A:1131:PRO:HG3	1:A:1164:ARG:HE	1.44	0.82
1:A:36:LEU:O	1:A:76:ARG:NH2	2.13	0.82
1:A:686:GLY:HA3	3:A:1901:NAP:O3B	1.78	0.82
2:B:612:PHE:CD2	3:B:2102:NAP:C5A	2.63	0.82
2:B:790:SER:CB	4:B:2101:FMN:C8M	2.58	0.82
2:B:727:HIS:N	3:B:2102:NAP:O7N	1.98	0.82
2:B:347:LEU:O	2:B:349:ARG:NH1	2.13	0.81
1:A:626:ILE:HD12	1:A:626:ILE:O	1.81	0.81
1:A:43:ARG:HB2	2:B:1649:THR:HG22	1.60	0.81
2:B:727:HIS:NE2	3:B:2102:NAP:H2D	1.97	0.80
1:A:26:VAL:HG23	2:B:2001:ASN:HB3	1.64	0.80
1:A:842:LYS:NZ	3:A:1901:NAP:HO2N	1.79	0.79
2:B:894:ASN:ND2	2:B:903:GLU:O	2.15	0.79
2:B:585:THR:N	4:B:2101:FMN:O4	2.16	0.78
2:B:1121:PRO:HG2	2:B:1126:TRP:HB2	1.66	0.77
1:A:795:ARG:HA	1:A:799:THR:HG22	1.66	0.77
1:A:952:ILE:HG22	2:B:1425:LYS:HB3	1.66	0.77
1:A:1032:ARG:NH1	1:A:1050:GLU:OE2	2.18	0.77
2:B:790:SER:CB	4:B:2101:FMN:HM83	2.16	0.76
2:B:984:SER:OG	2:B:986:GLU:OE1	2.02	0.76
2:B:1417:VAL:HA	2:B:1509:THR:HA	1.67	0.76
2:B:582:ALA:O	2:B:605:GLU:CG	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:ASP:O	2:B:861:ASN:ND2	2.20	0.75
2:B:332:SER:H	2:B:335:GLN:HE21	1.34	0.75
1:A:531:GLY:HA2	1:A:534:THR:HA	1.68	0.75
2:B:1020:ASP:N	3:B:2102:NAP:O1A	2.19	0.75
2:B:1024:GLN:N	2:B:1024:GLN:OE1	2.21	0.74
1:A:427:ASP:OD1	1:A:428:ARG:N	2.20	0.74
2:B:756:SER:N	4:B:2101:FMN:O2P	2.20	0.74
2:B:790:SER:HA	4:B:2101:FMN:HM83	1.67	0.74
2:B:251:ARG:NH2	2:B:274:ASP:OD1	2.19	0.74
2:B:727:HIS:NE2	3:B:2102:NAP:N1N	2.31	0.74
2:B:146:LEU:HD22	2:B:487:LEU:HD11	1.70	0.74
2:B:588:THR:HB	2:B:607:ALA:HB2	1.70	0.74
1:A:876:LEU:HD23	3:A:1901:NAP:O2A	1.87	0.74
2:B:475:TRP:HE1	2:B:501:THR:HG22	1.54	0.73
1:A:712:PHE:CZ	1:A:717:THR:HG21	2.23	0.73
2:B:1118:SER:HB2	2:B:1166:LYS:HB2	1.68	0.73
2:B:957:ASN:HD21	2:B:959:ASN:HD22	1.36	0.73
2:B:920:LYS:HE2	2:B:965:GLU:HG2	1.70	0.73
2:B:1108:ASP:HB2	2:B:1133:THR:HG23	1.70	0.72
2:B:847:ARG:NH1	2:B:885:ASP:OD1	2.21	0.72
1:A:527:MET:HE1	1:A:893:ARG:HD2	1.69	0.72
2:B:1199:LYS:O	2:B:1202:THR:OG1	2.08	0.72
2:B:1203:ILE:HD11	2:B:1226:TYR:HB2	1.70	0.72
1:A:712:PHE:HE1	1:A:717:THR:HG22	0.82	0.72
1:A:876:LEU:N	3:A:1901:NAP:O1A	2.21	0.72
2:B:1429:VAL:O	2:B:1432:SER:OG	2.07	0.71
1:A:708:THR:HG21	1:A:739:PHE:HD2	1.55	0.71
1:A:729:ALA:O	1:A:732:SER:OG	2.07	0.71
2:B:1192:VAL:HG23	2:B:1193:VAL:HG23	1.71	0.71
2:B:1876:ILE:HA	2:B:1888:ALA:HA	1.72	0.71
2:B:727:HIS:CD2	3:B:2102:NAP:H2N	2.24	0.71
2:B:225:CYS:O	2:B:262:GLN:NE2	2.24	0.70
2:B:349:ARG:HA	2:B:352:HIS:HB2	1.72	0.70
2:B:801:SER:HB3	2:B:1028:LEU:HD22	1.73	0.70
2:B:1919:MET:HE2	2:B:1923:LYS:HE2	1.71	0.70
1:A:873:GLY:O	1:A:878:SER:HB2	1.92	0.70
2:B:882:LEU:HD13	2:B:1006:VAL:HG11	1.74	0.70
2:B:1093:GLY:O	2:B:1095:LYS:NZ	2.25	0.70
2:B:1596:CYS:HA	2:B:1640:GLY:HA2	1.72	0.70
1:A:983:PRO:HD2	1:A:1085:LYS:HD2	1.73	0.70
1:A:878:SER:C	1:A:880:ASN:H	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:PHE:CD2	3:B:2102:NAP:C6A	2.74	0.70
2:B:657:ARG:HH22	2:B:1153:HIS:HB2	1.56	0.70
2:B:727:HIS:CE1	3:B:2102:NAP:C2D	2.75	0.70
2:B:1158:LEU:HA	2:B:1161:ILE:HG12	1.73	0.70
2:B:1629:ARG:NH2	2:B:1634:GLU:OE1	2.25	0.70
1:A:27:ARG:HH21	2:B:2003:THR:HA	1.56	0.70
1:A:1446:ARG:NH1	1:A:1511:TRP:O	2.24	0.69
1:A:626:ILE:HG23	1:A:627:GLN:N	2.06	0.69
2:B:1799:GLU:OE2	2:B:1998:TYR:OH	2.10	0.69
1:A:984:ARG:HB2	2:B:944:ARG:HA	1.73	0.69
1:A:673:LEU:HD21	1:A:909:THR:HG22	1.75	0.69
1:A:710:SER:N	3:A:1901:NAP:O3X	2.24	0.69
1:A:712:PHE:HD2	1:A:738:PRO:HG3	1.56	0.69
1:A:823:LEU:HD21	1:A:848:LEU:HD12	1.73	0.69
1:A:1476:LYS:NZ	1:A:1482:GLU:O	2.26	0.69
2:B:931:ARG:NH1	2:B:962:ASN:OD1	2.26	0.69
2:B:1766:GLN:HG3	2:B:1819:VAL:HG22	1.74	0.69
1:A:787:ASP:O	1:A:790:SER:OG	2.10	0.69
1:A:874:THR:O	1:A:876:LEU:HD12	1.93	0.69
1:A:1450:LEU:HD13	1:A:1511:TRP:HB2	1.73	0.69
2:B:1003:VAL:HG12	2:B:1005:PHE:H	1.58	0.69
2:B:1110:ASN:OD1	2:B:1175:LYS:N	2.26	0.69
1:A:457:PRO:HB2	1:A:460:LYS:HG3	1.74	0.68
1:A:710:SER:HG	3:A:1901:NAP:C4A	1.94	0.68
1:A:770:ILE:HG22	1:A:772:PRO:HD3	1.75	0.68
2:B:387:MET:HE1	2:B:402:LYS:HB3	1.74	0.68
1:A:338:LYS:NZ	1:A:342:GLU:OE2	2.26	0.68
1:A:511:GLU:OE2	1:A:872:ARG:NH1	2.26	0.68
2:B:612:PHE:HD2	3:B:2102:NAP:C6A	2.06	0.68
2:B:1265:ILE:HB	2:B:1326:PRO:HG3	1.75	0.68
2:B:1878:ASN:HB2	2:B:1887:VAL:HB	1.76	0.68
1:A:533:MET:H	1:A:637:THR:HG23	1.58	0.68
2:B:2017:VAL:HG23	2:B:2026:ILE:HD12	1.75	0.68
2:B:1763:GLN:OE1	2:B:1763:GLN:N	2.25	0.68
1:A:87:GLU:N	1:A:87:GLU:OE1	2.27	0.67
1:A:712:PHE:HE1	1:A:717:THR:CG2	1.70	0.67
1:A:1247:SER:OG	1:A:1248:GLY:N	2.24	0.67
2:B:1854:PHE:HE2	2:B:1859:LEU:HB3	1.59	0.67
1:A:505:GLY:O	1:A:954:ARG:NH1	2.26	0.67
1:A:1260:LYS:NZ	1:A:1336:GLU:OE1	2.26	0.67
2:B:506:GLU:OE2	2:B:746:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:SER:HB3	2:B:1089:GLU:HA	1.76	0.67
2:B:250:PHE:O	2:B:253:SER:OG	2.12	0.67
1:A:1218:VAL:HG11	1:A:1701:PHE:HB2	1.77	0.67
2:B:1131:ALA:HA	2:B:1142:ILE:HG21	1.74	0.67
1:A:41:THR:O	1:A:76:ARG:NH1	2.27	0.67
2:B:703:VAL:HG11	2:B:717:LEU:HD12	1.76	0.67
2:B:723:ARG:NH1	2:B:756:SER:O	2.28	0.67
2:B:148:ALA:O	2:B:257:SER:OG	2.13	0.67
2:B:657:ARG:NH1	2:B:661:TYR:O	2.28	0.67
2:B:331:LEU:HD11	2:B:401:LEU:HD23	1.75	0.67
1:A:1075:ASP:OD2	1:A:1078:THR:N	2.26	0.66
2:B:722:GLY:O	2:B:728:HIS:NE2	2.28	0.66
1:A:657:LEU:HD22	1:A:915:LEU:HD11	1.76	0.66
2:B:847:ARG:NH2	2:B:1035:ASP:OD2	2.28	0.66
2:B:1738:LYS:O	2:B:1741:LYS:NZ	2.22	0.66
1:A:1360:PRO:HA	1:A:1363:MET:HE3	1.76	0.66
2:B:140:CYS:HB2	2:B:143:ASP:HB3	1.77	0.66
2:B:727:HIS:ND1	2:B:841:ILE:CD1	2.59	0.66
2:B:790:SER:CA	4:B:2101:FMN:C8M	2.74	0.66
2:B:1185:ILE:N	2:B:1188:ASP:O	2.24	0.66
1:A:1554:LYS:NZ	1:A:1624:TYR:OH	2.28	0.66
2:B:440:LEU:HB2	2:B:454:GLN:HG2	1.78	0.66
2:B:1124:GLN:CD	2:B:1124:GLN:H	2.04	0.66
2:B:102:LEU:HD11	2:B:111:ILE:HD13	1.76	0.66
2:B:900:ASP:OD1	2:B:901:LEU:N	2.26	0.66
2:B:727:HIS:HE2	3:B:2102:NAP:H2D	1.57	0.65
1:A:1494:GLU:OE1	1:A:1498:ARG:NH2	2.28	0.65
2:B:93:ASN:HD21	2:B:535:GLN:HA	1.60	0.65
2:B:1458:LYS:HB2	2:B:1464:SER:HB3	1.77	0.65
2:B:1866:VAL:HG11	2:B:1898:LEU:HD12	1.78	0.65
1:A:22:PHE:HE1	2:B:1826:MET:HB3	1.60	0.65
1:A:493:ARG:HD3	1:A:513:GLN:HG2	1.78	0.65
2:B:1307:ALA:HB3	2:B:1352:LEU:HB2	1.79	0.65
2:B:1893:ARG:HA	2:B:1946:ILE:HD11	1.78	0.65
2:B:1929:TYR:HA	2:B:1932:VAL:HG12	1.77	0.65
1:A:16:GLU:OE2	2:B:1977:GLN:NE2	2.30	0.65
1:A:1558:ALA:O	1:A:1562:ASN:ND2	2.29	0.65
1:A:59:ARG:NH1	2:B:1884:GLN:OE1	2.28	0.65
1:A:872:ARG:NE	1:A:894:THR:OG1	2.28	0.65
2:B:263:GLY:O	2:B:266:THR:OG1	2.14	0.65
2:B:745:ARG:NH2	2:B:784:ASP:OD1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:HB3	2:B:1877:VAL:HA	1.79	0.65
2:B:123:TYR:HA	2:B:126:VAL:HG12	1.77	0.65
2:B:1022:LEU:HD12	3:B:2102:NAP:O1N	1.96	0.65
2:B:756:SER:CA	4:B:2101:FMN:O2P	2.36	0.65
1:A:40:ASN:HA	1:A:76:ARG:HH22	1.62	0.64
2:B:1843:VAL:HA	2:B:1956:PRO:HA	1.80	0.64
2:B:344:ASN:O	2:B:349:ARG:NH1	2.24	0.64
2:B:1345:MET:HB3	2:B:1592:ARG:HH21	1.61	0.64
1:A:46:GLU:OE1	1:A:54:ALA:N	2.31	0.64
1:A:1117:LYS:NZ	1:A:1335:GLU:OE2	2.29	0.64
2:B:727:HIS:N	3:B:2102:NAP:C4N	2.55	0.64
2:B:1111:GLN:HA	2:B:1173:ASP:HA	1.80	0.64
1:A:1219:GLU:HA	1:A:1222:LEU:HD12	1.80	0.64
1:A:29:ILE:N	2:B:1879:TYR:O	2.31	0.64
2:B:1849:ARG:O	2:B:1906:LYS:NZ	2.27	0.64
2:B:526:GLU:N	2:B:526:GLU:OE2	2.31	0.63
2:B:1019:LYS:HG3	3:B:2102:NAP:O5B	1.99	0.63
1:A:690:ILE:HD11	1:A:871:THR:HG21	1.79	0.63
1:A:32:GLN:HA	1:A:35:PHE:CE1	2.33	0.63
1:A:532:ALA:HB3	1:A:638:ILE:H	1.63	0.63
1:A:647:THR:OG1	1:A:649:ASP:OD1	2.11	0.63
2:B:293:ILE:HG13	2:B:426:ILE:HD13	1.79	0.63
2:B:1458:LYS:HB3	2:B:1462:VAL:HG23	1.79	0.63
1:A:1245:SER:OG	1:A:1246:GLY:N	2.32	0.63
2:B:727:HIS:CE1	3:B:2102:NAP:C1D	2.80	0.63
2:B:1660:GLU:H	2:B:1663:MET:HE2	1.63	0.63
1:A:1207:ASP:O	1:A:1210:THR:OG1	2.17	0.63
1:A:478:CYS:HA	1:A:481:VAL:HG12	1.80	0.63
2:B:1680:LYS:HD2	2:B:1812:ILE:HD12	1.81	0.62
2:B:296:ARG:HH11	2:B:425:LEU:HB3	1.65	0.62
2:B:391:GLN:NE2	2:B:400:LYS:H	1.92	0.62
2:B:939:ARG:NH2	2:B:955:LEU:O	2.28	0.62
1:A:968:ASN:HD21	1:A:972:VAL:HB	1.65	0.62
2:B:1706:ILE:O	2:B:1749:SER:OG	2.13	0.62
2:B:1837:ARG:NH1	2:B:1838:SER:O	2.32	0.62
2:B:26:PHE:O	2:B:29:SER:OG	2.16	0.62
2:B:727:HIS:CE1	2:B:841:ILE:CD1	2.82	0.62
1:A:911:GLU:N	1:A:911:GLU:OE1	2.32	0.62
2:B:1837:ARG:HH11	2:B:1838:SER:H	1.47	0.62
1:A:1030:ASN:ND2	1:A:1050:GLU:OE2	2.33	0.62
2:B:726:GLY:O	2:B:727:HIS:C	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1185:ILE:HD11	2:B:1190:LEU:HD12	1.81	0.62
2:B:1419:VAL:HG12	2:B:1507:GLY:HA3	1.80	0.62
2:B:1830:VAL:O	2:B:1832:ARG:NH1	2.30	0.62
2:B:2024:GLU:HA	2:B:2027:LYS:HE2	1.82	0.62
1:A:684:GLY:HA2	3:A:1901:NAP:H1B	1.81	0.61
1:A:855:GLU:OE1	1:A:857:TRP:NE1	2.32	0.61
1:A:985:ALA:O	2:B:944:ARG:NH1	2.31	0.61
1:A:1365:ARG:NH1	1:A:1370:THR:O	2.28	0.61
2:B:107:TYR:CE2	2:B:109:THR:HA	2.35	0.61
1:A:1494:GLU:OE2	1:A:1498:ARG:NH1	2.33	0.61
2:B:266:THR:O	2:B:269:THR:OG1	2.17	0.61
2:B:801:SER:OG	2:B:1025:SER:O	2.15	0.61
2:B:1766:GLN:NE2	2:B:1819:VAL:O	2.27	0.61
1:A:86:LYS:HB3	1:A:92:PRO:HA	1.82	0.61
2:B:138:TYR:HD1	2:B:144:ALA:HB3	1.64	0.61
1:A:1593:ALA:O	1:A:1597:ASN:ND2	2.33	0.61
2:B:46:PHE:O	2:B:113:LYS:NZ	2.33	0.61
2:B:486:ILE:HB	2:B:512:ILE:HD13	1.82	0.61
2:B:1019:LYS:HA	3:B:2102:NAP:O1A	2.00	0.61
1:A:1018:VAL:HG12	1:A:1401:VAL:HG22	1.81	0.61
1:A:461:GLY:O	1:A:465:LYS:NZ	2.33	0.61
1:A:1143:LYS:NZ	1:A:1150:CYS:O	2.31	0.61
2:B:708:LYS:NZ	2:B:747:CYS:SG	2.73	0.61
1:A:1368:THR:HG22	1:A:1370:THR:H	1.66	0.61
2:B:1439:GLU:HG3	2:B:1485:GLY:HA2	1.83	0.61
2:B:1144:THR:HG22	2:B:1146:ARG:H	1.66	0.60
2:B:1725:PHE:HB3	2:B:1739:ILE:HD11	1.82	0.60
1:A:458:GLU:O	1:A:465:LYS:NZ	2.34	0.60
1:A:686:GLY:CA	3:A:1901:NAP:O3B	2.49	0.60
2:B:400:LYS:O	2:B:402:LYS:NZ	2.32	0.60
2:B:584:MET:CG	4:B:2101:FMN:C6	2.79	0.60
2:B:957:ASN:H	2:B:960:GLN:NE2	2.00	0.60
2:B:331:LEU:HG	2:B:335:GLN:HG3	1.83	0.60
2:B:756:SER:CA	4:B:2101:FMN:H5'2	2.31	0.60
2:B:1581:GLU:HA	2:B:1586:ASN:H	1.66	0.60
2:B:1053:LYS:NZ	2:B:1054:VAL:O	2.33	0.60
2:B:1146:ARG:NH1	2:B:1232:PHE:O	2.29	0.60
2:B:1833:ASP:OD1	2:B:1837:ARG:N	2.30	0.60
1:A:493:ARG:HE	1:A:518:ARG:HG2	1.66	0.60
1:A:643:ILE:N	1:A:658:SER:OG	2.34	0.60
1:A:892:VAL:HG21	1:A:932:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:GLU:OE1	2:B:76:GLU:N	2.31	0.60
2:B:261:SER:HB2	2:B:415:HIS:CE1	2.37	0.60
2:B:584:MET:HG3	2:B:587:THR:HB	1.84	0.60
2:B:1117:ASP:HA	2:B:1167:HIS:H	1.65	0.60
1:A:440:ARG:HA	1:A:730:ALA:HB2	1.83	0.60
1:A:442:ASN:HB2	1:A:445:LEU:HD23	1.83	0.60
1:A:525:TYR:CE1	1:A:629:VAL:HG22	2.37	0.60
1:A:876:LEU:CD2	3:A:1901:NAP:PA	2.77	0.60
2:B:628:ILE:HD12	2:B:632:TYR:HB2	1.83	0.60
1:A:900:MET:HE1	1:A:925:LEU:HD12	1.84	0.59
2:B:726:GLY:C	2:B:727:HIS:O	2.43	0.59
2:B:167:TYR:HA	2:B:174:ILE:HD11	1.84	0.59
2:B:1962:VAL:HG13	2:B:1964:PHE:HD1	1.68	0.59
2:B:1527:GLU:HG2	2:B:1528:LEU:HD22	1.85	0.59
2:B:728:HIS:HB3	2:B:840:PRO:HG2	1.85	0.59
2:B:855:LEU:HB3	2:B:860:PHE:CE2	2.38	0.59
1:A:1330:TYR:HB3	1:A:1380:SER:HB2	1.85	0.59
2:B:391:GLN:HE22	2:B:400:LYS:N	1.96	0.59
1:A:626:ILE:CG2	1:A:627:GLN:N	2.66	0.59
1:A:1525:LEU:HD11	1:A:1657:VAL:HG21	1.85	0.59
2:B:170:TYR:HB3	2:B:173:LEU:HD12	1.84	0.59
2:B:767:TYR:HB3	2:B:783:PHE:HD2	1.67	0.59
2:B:906:TYR:OH	2:B:987:ASP:OD2	2.20	0.59
1:A:1017:VAL:HG21	1:A:1314:ILE:HG12	1.85	0.58
2:B:790:SER:N	4:B:2101:FMN:HM81	2.18	0.58
2:B:1185:ILE:O	2:B:1188:ASP:N	2.36	0.58
2:B:1683:ARG:O	2:B:1687:ASN:ND2	2.36	0.58
2:B:446:ASP:OD1	2:B:447:THR:N	2.36	0.58
2:B:1108:ASP:OD2	2:B:1133:THR:N	2.35	0.58
1:A:679:TYR:O	1:A:768:ASP:N	2.34	0.58
1:A:755:TYR:OH	1:A:812:LYS:NZ	2.36	0.58
2:B:602:TYR:OH	2:B:1063:ASN:OD1	2.15	0.58
2:B:1438:LEU:HA	2:B:1485:GLY:HA3	1.85	0.58
2:B:1899:THR:O	2:B:1903:ASN:ND2	2.36	0.58
2:B:188:LEU:HD23	2:B:291:LEU:HD23	1.84	0.58
2:B:1309:MET:HG2	2:B:1576:ARG:CZ	2.33	0.58
2:B:1363:GLU:N	2:B:1363:GLU:OE1	2.36	0.58
1:A:1413:GLY:O	1:A:1414:ARG:NH1	2.34	0.58
2:B:583:GLY:HA2	2:B:588:THR:HG21	1.86	0.58
1:A:411:VAL:HG11	1:A:449:MET:HG2	1.84	0.58
2:B:136:LEU:HA	2:B:139:HIS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:GLU:OE1	2:B:398:GLU:N	2.37	0.58
1:A:877:MET:HE2	3:A:1901:NAP:H4N	1.86	0.58
2:B:319:GLU:OE2	2:B:381:ARG:NH2	2.35	0.58
2:B:1788:SER:O	2:B:1997:LYS:NZ	2.25	0.58
1:A:1028:TRP:O	1:A:1033:THR:OG1	2.19	0.58
2:B:102:LEU:O	2:B:109:THR:OG1	2.17	0.58
2:B:1181:ALA:HB3	2:B:1193:VAL:HB	1.85	0.58
2:B:1595:LYS:O	2:B:1641:GLU:N	2.36	0.58
2:B:169:LEU:HD22	2:B:170:TYR:CE2	2.39	0.58
2:B:215:GLN:O	2:B:219:LEU:N	2.35	0.58
2:B:727:HIS:CE1	2:B:841:ILE:HD11	2.39	0.58
2:B:809:VAL:HG21	2:B:1054:VAL:HB	1.84	0.58
2:B:1019:LYS:HG3	3:B:2102:NAP:PA	2.44	0.58
2:B:881:LYS:HA	2:B:884:ASN:HB2	1.86	0.57
2:B:889:PRO:HG2	2:B:1032:VAL:HG11	1.84	0.57
2:B:183:GLU:OE2	2:B:187:GLN:NE2	2.37	0.57
2:B:1336:LEU:HD11	2:B:1396:PHE:HB3	1.86	0.57
2:B:181:ILE:HD13	2:B:284:LEU:HD23	1.86	0.57
2:B:535:GLN:O	2:B:541:ALA:HB2	2.03	0.57
2:B:1106:ILE:HG12	2:B:1128:ASP:HB3	1.85	0.57
2:B:385:ALA:HB1	2:B:389:LEU:HD13	1.87	0.57
2:B:1897:THR:O	2:B:1901:VAL:HG13	2.05	0.57
1:A:521:GLU:HG2	1:A:670:ILE:HG22	1.86	0.57
2:B:1827:GLN:O	2:B:1832:ARG:NH2	2.33	0.57
1:A:1005:PRO:O	1:A:1007:LEU:N	2.38	0.57
2:B:1896:ASP:HA	2:B:1899:THR:HG22	1.87	0.57
2:B:876:ASP:N	2:B:876:ASP:OD1	2.37	0.57
2:B:1014:GLU:HA	2:B:1017:PHE:HB3	1.86	0.57
1:A:438:MET:HB2	1:A:481:VAL:HG11	1.87	0.57
1:A:1373:GLY:HA2	1:A:1549:THR:HG22	1.87	0.57
1:A:1404:MET:SD	1:A:1405:THR:N	2.77	0.57
2:B:337:GLU:HA	2:B:340:ILE:HG12	1.87	0.57
2:B:185:LEU:O	2:B:189:HIS:N	2.38	0.57
2:B:218:LEU:O	2:B:224:SER:OG	2.22	0.57
2:B:727:HIS:NE2	3:B:2102:NAP:C1D	2.68	0.57
2:B:790:SER:HB3	4:B:2101:FMN:HM81	1.81	0.57
1:A:1389:ASP:OD1	1:A:1390:LEU:N	2.38	0.56
2:B:139:HIS:HA	2:B:141:LYS:HZ2	1.70	0.56
2:B:1001:LYS:NZ	2:B:1020:ASP:OD2	2.26	0.56
1:A:766:ASP:OD1	1:A:812:LYS:NZ	2.38	0.56
2:B:1712:LYS:HA	2:B:1715:ALA:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:N	1:A:42:GLU:OE1	2.38	0.56
1:A:327:ASP:OD1	1:A:327:ASP:N	2.35	0.56
1:A:766:ASP:HB3	1:A:817:ARG:NH1	2.20	0.56
2:B:446:ASP:N	2:B:451:SER:O	2.34	0.56
2:B:512:ILE:O	2:B:528:GLY:N	2.34	0.56
2:B:1019:LYS:HG3	3:B:2102:NAP:O1A	2.04	0.56
2:B:1116:ILE:HD11	2:B:1164:PRO:HB3	1.86	0.56
2:B:1168:SER:OG	2:B:1169:LYS:N	2.38	0.56
2:B:1702:ASN:ND2	2:B:1755:PRO:O	2.38	0.56
1:A:989:PHE:HE1	1:A:1032:ARG:HH21	1.54	0.56
2:B:161:GLU:OE1	2:B:161:GLU:N	2.39	0.56
1:A:794:HIS:HD2	1:A:841:SER:HB3	1.71	0.56
2:B:79:LEU:HD21	2:B:126:VAL:HG23	1.88	0.56
1:A:796:ILE:CD1	3:A:1901:NAP:N6A	2.68	0.56
1:A:1536:ILE:HD11	1:A:1564:MET:HE1	1.88	0.56
2:B:1536:ASN:ND2	2:B:1550:HIS:O	2.29	0.56
1:A:868:ILE:HG23	1:A:900:MET:HE2	1.88	0.56
2:B:1324:ILE:HG22	2:B:1376:VAL:HG11	1.88	0.56
2:B:1511:GLU:OE2	2:B:1513:SER:N	2.33	0.56
1:A:708:THR:HG23	1:A:739:PHE:HB3	1.87	0.56
2:B:369:PRO:O	2:B:372:SER:OG	2.20	0.56
1:A:710:SER:HB2	3:A:1901:NAP:O3X	2.07	0.56
2:B:138:TYR:CZ	2:B:141:LYS:HA	2.41	0.56
1:A:401:ASP:O	1:A:403:TYR:N	2.38	0.55
2:B:1706:ILE:N	2:B:1750:TYR:O	2.38	0.55
2:B:1757:GLY:O	2:B:1760:SER:OG	2.20	0.55
2:B:1489:TYR:CE1	2:B:1498:PRO:HG2	2.41	0.55
2:B:64:GLY:O	2:B:67:SER:OG	2.24	0.55
1:A:1012:ASP:OD1	1:A:1505:SER:HB3	2.06	0.55
2:B:1160:ASP:O	2:B:1163:THR:OG1	2.22	0.55
2:B:1850:VAL:HG23	2:B:1906:LYS:HB2	1.89	0.55
1:A:839:SER:OG	1:A:840:GLU:N	2.39	0.55
2:B:1767:PRO:HG3	2:B:1819:VAL:HG13	1.87	0.55
1:A:1049:ILE:HG22	1:A:1087:ILE:HG21	1.87	0.55
2:B:584:MET:HG2	2:B:588:THR:OG1	2.06	0.55
2:B:589:VAL:HG21	2:B:610:GLY:HA3	1.87	0.55
2:B:757:GLY:HA2	2:B:1047:ALA:HB2	1.87	0.55
2:B:1342:GLY:HA2	2:B:1595:LYS:HA	1.89	0.55
2:B:1548:PRO:HA	2:B:1551:VAL:HG22	1.89	0.55
2:B:1661:GLN:NE2	2:B:1698:GLN:O	2.40	0.55
2:B:107:TYR:OH	2:B:110:THR:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:ASN:O	2:B:204:SER:OG	2.23	0.55
2:B:860:PHE:CE1	2:B:1014:GLU:HB3	2.41	0.55
2:B:1960:ILE:HG12	2:B:1964:PHE:HE1	1.72	0.55
1:A:69:ASP:O	1:A:73:SER:N	2.40	0.55
1:A:504:LYS:HZ3	1:A:954:ARG:HH21	1.55	0.55
1:A:17:LEU:HD23	2:B:2002:LEU:HD23	1.89	0.55
1:A:69:ASP:OD1	1:A:70:ALA:N	2.40	0.55
1:A:1012:ASP:HB3	1:A:1513:ASN:ND2	2.22	0.55
1:A:1057:PHE:HD1	1:A:1077:LYS:HZ3	1.55	0.55
1:A:1198:ILE:HG12	1:A:1701:PHE:CD2	2.42	0.55
2:B:1668:TYR:CE1	2:B:1675:ARG:HG3	2.42	0.55
2:B:1726:GLU:OE1	2:B:1735:LYS:N	2.39	0.55
1:A:1607:LEU:HD23	1:A:1608:VAL:N	2.22	0.54
2:B:858:THR:OG1	2:B:859:ILE:HD12	2.07	0.54
1:A:1214:LEU:O	1:A:1218:VAL:HG22	2.07	0.54
1:A:1349:ASN:O	1:A:1353:GLU:HG2	2.07	0.54
2:B:13:SER:H	2:B:46:PHE:HZ	1.55	0.54
2:B:60:GLY:O	2:B:63:ILE:HG22	2.06	0.54
2:B:139:HIS:HA	2:B:141:LYS:NZ	2.23	0.54
2:B:1762:THR:HA	2:B:1765:THR:HG22	1.89	0.54
1:A:482:LEU:HG	1:A:483:THR:HG23	1.87	0.54
1:A:1027:PRO:HA	1:A:1188:PRO:HD3	1.87	0.54
2:B:518:LEU:HB2	2:B:530:LYS:HE2	1.88	0.54
2:B:612:PHE:CD2	3:B:2102:NAP:N6A	2.76	0.54
2:B:894:ASN:OD1	2:B:895:ALA:N	2.40	0.54
2:B:1756:THR:OG1	2:B:1760:SER:OG	2.24	0.54
2:B:2010:THR:HG23	2:B:2013:TYR:H	1.72	0.54
2:B:164:ARG:NH1	2:B:205:TRP:O	2.40	0.54
2:B:1531:LYS:NZ	2:B:1605:ASN:O	2.27	0.54
2:B:1582:TRP:HB3	2:B:1612:MET:HE1	1.89	0.54
1:A:1136:LYS:N	1:A:1160:GLU:OE2	2.41	0.54
1:A:1416:VAL:HG13	1:A:1650:GLY:H	1.71	0.54
1:A:1564:MET:HB3	1:A:1569:ARG:HG3	1.87	0.54
2:B:902:GLN:N	2:B:902:GLN:OE1	2.39	0.54
2:B:1425:LYS:O	2:B:1429:VAL:N	2.38	0.54
2:B:584:MET:HA	4:B:2101:FMN:C4	2.37	0.54
2:B:894:ASN:HB3	2:B:899:CYS:SG	2.48	0.54
2:B:1312:ALA:O	2:B:1316:GLY:N	2.39	0.54
2:B:1353:LYS:N	2:B:1356:ASP:OD2	2.26	0.54
2:B:1919:MET:HB2	2:B:1924:VAL:HG13	1.89	0.54
1:A:1247:SER:OG	1:A:1250:GLY:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1678:THR:O	1:A:1681:SER:OG	2.25	0.54
2:B:386:PRO:HD2	2:B:389:LEU:HD12	1.89	0.54
2:B:1452:GLU:OE2	2:B:1469:THR:OG1	2.25	0.54
2:B:1672:GLU:OE1	2:B:1675:ARG:NH1	2.37	0.54
1:A:33:ASP:OD2	1:A:64:LYS:NZ	2.31	0.54
1:A:1044:SER:OG	1:A:1046:GLU:OE1	2.23	0.54
1:A:1269:GLN:NE2	1:A:1271:ASP:OD1	2.41	0.54
1:A:1555:ASN:O	1:A:1559:THR:HG23	2.08	0.54
2:B:888:LYS:NZ	2:B:1019:LYS:O	2.33	0.54
2:B:927:ASP:OD1	2:B:928:VAL:N	2.40	0.54
2:B:1366:ALA:HB3	2:B:1377:GLU:HB2	1.90	0.54
2:B:1898:LEU:HA	2:B:1901:VAL:HG22	1.90	0.54
2:B:905:THR:N	2:B:908:GLU:OE2	2.31	0.54
2:B:1295:ASP:OD1	2:B:1295:ASP:N	2.38	0.54
2:B:2011:LYS:HD2	2:B:2033:TRP:CD1	2.43	0.54
1:A:877:MET:HE2	3:A:1901:NAP:C4N	2.38	0.53
1:A:1545:HIS:O	1:A:1581:LYS:NZ	2.40	0.53
2:B:760:SER:OG	2:B:762:GLU:OE1	2.22	0.53
2:B:196:TYR:HB2	2:B:217:TYR:OH	2.08	0.53
2:B:720:THR:HG21	4:B:2101:FMN:O3'	2.09	0.53
2:B:986:GLU:OE1	2:B:986:GLU:N	2.37	0.53
2:B:1743:ILE:HD11	2:B:1750:TYR:CG	2.43	0.53
2:B:1873:LEU:HD12	2:B:1890:GLY:HA2	1.90	0.53
1:A:35:PHE:HE2	1:A:44:ILE:HG12	1.72	0.53
2:B:215:GLN:HA	2:B:218:LEU:HD12	1.91	0.53
2:B:1674:ALA:O	2:B:1677:VAL:HG22	2.09	0.53
2:B:1123:LYS:NZ	2:B:1163:THR:OG1	2.40	0.53
2:B:1877:VAL:HB	2:B:1965:HIS:HB2	1.91	0.53
1:A:626:ILE:HD12	1:A:626:ILE:C	2.27	0.53
1:A:820:GLN:HA	1:A:862:THR:HG23	1.91	0.53
2:B:855:LEU:HB3	2:B:860:PHE:HE2	1.74	0.53
1:A:1331:ASP:OD2	1:A:1332:ASP:N	2.40	0.53
1:A:1728:ASN:O	1:A:1729:LYS:HG2	2.09	0.53
2:B:1718:ASP:OD1	2:B:1718:ASP:N	2.41	0.53
1:A:1603:LEU:HD13	1:A:1660:HIS:HA	1.90	0.53
1:A:1668:LEU:HD11	1:A:1673:TYR:HB2	1.90	0.53
2:B:146:LEU:HD23	2:B:485:HIS:HB2	1.90	0.53
2:B:929:SER:OG	2:B:1000:GLN:HG3	2.09	0.53
2:B:1436:PHE:CZ	2:B:1438:LEU:HB3	2.44	0.53
2:B:1630:ASN:O	2:B:1634:GLU:N	2.37	0.53
2:B:1872:TRP:CD1	2:B:1893:ARG:HH21	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:PHE:HB3	1:A:1547:THR:O	2.08	0.53
2:B:129:ILE:O	2:B:131:LYS:NZ	2.42	0.53
2:B:659:LYS:O	2:B:1152:LYS:NZ	2.36	0.53
2:B:374:TYR:HA	2:B:377:ASN:HD21	1.73	0.52
2:B:690:LEU:HB2	2:B:713:PHE:HE2	1.72	0.52
2:B:1090:TYR:OH	2:B:1139:GLN:NE2	2.33	0.52
2:B:1666:GLU:OE2	2:B:1666:GLU:N	2.36	0.52
2:B:1708:PHE:CG	2:B:1717:ARG:HB3	2.45	0.52
2:B:1979:PHE:HA	2:B:1982:LYS:HE3	1.91	0.52
1:A:449:MET:HE3	1:A:475:ILE:HG12	1.91	0.52
1:A:1043:PHE:O	1:A:1088:LYS:NZ	2.41	0.52
2:B:797:GLU:CD	2:B:1058:ILE:H	2.17	0.52
2:B:834:ARG:HB3	2:B:838:GLY:HA2	1.91	0.52
2:B:389:LEU:HD22	2:B:391:GLN:HG3	1.90	0.52
2:B:1726:GLU:HB3	2:B:1975:PRO:HD3	1.92	0.52
1:A:871:THR:HB	3:A:1901:NAP:O7N	2.09	0.52
1:A:890:LEU:HD11	1:A:938:PHE:CZ	2.45	0.52
1:A:989:PHE:CZ	1:A:1223:SER:HA	2.44	0.52
2:B:414:PHE:HB3	2:B:415:HIS:ND1	2.24	0.52
2:B:931:ARG:HD3	2:B:961:LEU:HB2	1.91	0.52
2:B:1434:GLU:N	2:B:1434:GLU:OE1	2.42	0.52
1:A:708:THR:HG21	1:A:739:PHE:CD2	2.42	0.52
2:B:846:THR:HB	2:B:1037:GLN:HA	1.91	0.52
2:B:907:LYS:HG3	2:B:972:PHE:CD2	2.45	0.52
1:A:877:MET:C	1:A:879:ALA:H	2.18	0.52
2:B:218:LEU:HA	2:B:223:VAL:HG11	1.90	0.52
2:B:868:LEU:HD12	2:B:868:LEU:H	1.74	0.52
2:B:1591:VAL:HG12	2:B:1644:ILE:HG22	1.92	0.52
1:A:842:LYS:CE	3:A:1901:NAP:O2D	2.58	0.52
1:A:1207:ASP:OD2	1:A:1209:ILE:HG22	2.10	0.52
1:A:1410:ASP:HB2	1:A:1651:GLN:HB3	1.92	0.52
2:B:813:GLY:HA2	2:B:1048:SER:HB2	1.91	0.52
2:B:1401:GLU:OE1	2:B:1402:TYR:N	2.43	0.52
1:A:380:HIS:O	1:A:788:SER:OG	2.15	0.52
1:A:626:ILE:O	1:A:628:PRO:HD3	2.09	0.52
2:B:136:LEU:HD11	2:B:535:GLN:O	2.10	0.52
2:B:818:GLN:OE1	2:B:821:GLN:NE2	2.43	0.52
1:A:1301:GLY:O	1:A:1304:ALA:N	2.43	0.52
2:B:1651:TYR:CG	2:B:1790:ILE:HD11	2.45	0.52
1:A:428:ARG:NH2	1:A:519:LYS:HD3	2.26	0.51
1:A:1117:LYS:HE2	1:A:1339:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:GLY:O	1:A:1683:ARG:NH1	2.43	0.51
1:A:1271:ASP:OD2	1:A:1274:GLN:NE2	2.42	0.51
2:B:9:LEU:O	2:B:17:THR:OG1	2.25	0.51
2:B:1375:LEU:HD11	2:B:1395:GLN:HE21	1.75	0.51
2:B:1530:SER:OG	2:B:1531:LYS:N	2.42	0.51
1:A:734:LEU:HD23	1:A:735:ILE:N	2.26	0.51
2:B:662:PRO:HA	2:B:1153:HIS:HD2	1.75	0.51
2:B:1830:VAL:HG22	2:B:1968:TYR:HE2	1.75	0.51
1:A:1476:LYS:HZ1	1:A:1484:SER:H	1.57	0.51
1:A:1491:GLU:O	1:A:1494:GLU:HG3	2.10	0.51
2:B:861:ASN:OD1	2:B:861:ASN:N	2.43	0.51
2:B:1569:MET:O	2:B:1572:SER:OG	2.23	0.51
1:A:518:ARG:N	1:A:522:GLN:OE1	2.25	0.51
1:A:710:SER:CB	3:A:1901:NAP:O3X	2.59	0.51
1:A:796:ILE:HD13	3:A:1901:NAP:N6A	2.25	0.51
1:A:1404:MET:HE2	1:A:1525:LEU:HD13	1.92	0.51
2:B:221:VAL:HG12	2:B:294:GLY:HA2	1.92	0.51
2:B:1209:GLU:OE2	2:B:1211:ARG:HG2	2.10	0.51
1:A:90:TYR:C	1:A:92:PRO:HD3	2.35	0.51
1:A:625:ILE:O	1:A:625:ILE:HG23	2.10	0.51
1:A:945:ASP:O	1:A:949:THR:HG23	2.11	0.51
2:B:93:ASN:HB3	2:B:96:SER:OG	2.10	0.51
2:B:1332:ASP:OD1	2:B:1335:LYS:N	2.34	0.51
2:B:1480:GLU:HG2	2:B:1482:ILE:HD11	1.92	0.51
2:B:374:TYR:HA	2:B:377:ASN:ND2	2.25	0.51
2:B:927:ASP:OD2	2:B:929:SER:HB3	2.10	0.51
2:B:1266:ASN:ND2	2:B:1269:LYS:H	2.08	0.51
2:B:1416:PRO:HB3	2:B:1450:ARG:HG2	1.92	0.51
2:B:1602:VAL:HG11	2:B:1608:LEU:HD21	1.92	0.51
2:B:1840:TYR:HE2	2:B:1968:TYR:CZ	2.28	0.51
1:A:1409:THR:HA	1:A:1651:GLN:O	2.10	0.51
1:A:979:VAL:N	2:B:956:GLN:OE1	2.29	0.51
2:B:449:ASP:OD2	2:B:463:ARG:NH2	2.43	0.51
1:A:442:ASN:O	1:A:446:ILE:HD12	2.11	0.51
1:A:646:LYS:NZ	1:A:850:ASN:OD1	2.44	0.51
1:A:984:ARG:HG2	2:B:943:GLU:HG2	1.91	0.51
1:A:1535:THR:HG22	1:A:1537:ASP:H	1.76	0.51
2:B:220:SER:OG	2:B:222:PRO:HD2	2.10	0.51
1:A:997:TYR:HB2	1:A:1673:TYR:HD2	1.75	0.51
1:A:1012:ASP:HB3	1:A:1513:ASN:HD21	1.76	0.51
1:A:1305:THR:HG22	1:A:1589:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:SER:OG	2:B:365:VAL:O	2.21	0.51
2:B:741:TYR:OH	2:B:782:PRO:O	2.24	0.51
2:B:1563:GLY:O	2:B:1565:ILE:N	2.44	0.51
2:B:1843:VAL:HG12	2:B:1956:PRO:HB3	1.93	0.51
2:B:265:VAL:O	2:B:269:THR:HG23	2.12	0.50
2:B:761:ASP:HB3	2:B:1065:ILE:HA	1.92	0.50
2:B:1119:GLU:H	2:B:1119:GLU:CD	2.19	0.50
2:B:1368:LEU:HA	2:B:1408:THR:OG1	2.10	0.50
1:A:877:MET:C	1:A:879:ALA:N	2.69	0.50
1:A:1137:GLU:OE1	1:A:1137:GLU:N	2.37	0.50
2:B:1754:SER:HB3	2:B:1758:LEU:HD23	1.93	0.50
2:B:584:MET:HB2	4:B:2101:FMN:N5	2.16	0.50
2:B:833:VAL:HG21	2:B:852:TRP:CD1	2.46	0.50
2:B:834:ARG:HD2	2:B:838:GLY:O	2.11	0.50
2:B:933:MET:HG3	2:B:1000:GLN:HE22	1.77	0.50
2:B:1792:PHE:CZ	2:B:1998:TYR:HB2	2.46	0.50
1:A:903:ASN:HB3	1:A:925:LEU:HD13	1.93	0.50
1:A:1333:PHE:CE1	1:A:1338:SER:HB2	2.47	0.50
2:B:584:MET:HB2	4:B:2101:FMN:C5A	2.26	0.50
2:B:735:GLN:O	2:B:738:ILE:HG22	2.12	0.50
2:B:1791:MET:HE2	2:B:1999:ILE:HD11	1.93	0.50
1:A:675:PHE:HB3	1:A:678:LYS:HD2	1.93	0.50
1:A:982:GLU:OE2	1:A:1085:LYS:HG3	2.11	0.50
2:B:166:LEU:HD23	2:B:174:ILE:HD13	1.94	0.50
2:B:502:HIS:HB2	2:B:512:ILE:HG13	1.92	0.50
2:B:726:GLY:O	2:B:727:HIS:O	2.29	0.50
2:B:790:SER:N	4:B:2101:FMN:C8M	2.75	0.50
2:B:830:ILE:HD12	2:B:1045:PRO:HA	1.94	0.50
2:B:939:ARG:O	2:B:943:GLU:HB2	2.12	0.50
2:B:2019:ASP:O	2:B:2022:LYS:NZ	2.44	0.50
1:A:1075:ASP:OD2	1:A:1077:LYS:N	2.45	0.50
2:B:18:LEU:H	2:B:18:LEU:HD23	1.77	0.50
2:B:1226:TYR:HA	2:B:1235:ILE:HG12	1.94	0.50
1:A:46:GLU:CD	1:A:53:LEU:H	2.20	0.50
1:A:1046:GLU:H	1:A:1046:GLU:CD	2.17	0.50
1:A:1713:LEU:C	1:A:1716:PRO:HD2	2.36	0.50
2:B:1027:ASP:OD2	2:B:1030:SER:N	2.41	0.50
2:B:1156:ASN:HB3	2:B:1159:HIS:HB2	1.92	0.50
2:B:1236:LEU:HD23	2:B:1236:LEU:H	1.75	0.50
2:B:1872:TRP:CZ3	2:B:1893:ARG:HB3	2.47	0.50
1:A:1569:ARG:NH2	1:A:1573:ASN:O	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:GLU:HA	2:B:37:LYS:HE3	1.94	0.50
2:B:261:SER:HB2	2:B:415:HIS:HE1	1.76	0.50
1:A:400:TYR:HB3	1:A:724:TYR:CD2	2.47	0.50
1:A:1236:VAL:N	1:A:1724:ARG:HH12	2.09	0.50
2:B:1534:GLY:HA2	2:B:1605:ASN:OD1	2.12	0.50
2:B:1813:GLU:OE1	2:B:1813:GLU:N	2.41	0.50
1:A:53:LEU:HA	1:A:56:MET:HB3	1.95	0.49
2:B:138:TYR:CE2	2:B:141:LYS:HG3	2.47	0.49
2:B:534:PHE:O	2:B:536:THR:HG23	2.12	0.49
2:B:756:SER:N	4:B:2101:FMN:C5'	2.75	0.49
2:B:1533:PRO:O	2:B:1605:ASN:N	2.43	0.49
1:A:323:SER:C	1:A:325:ALA:H	2.20	0.49
1:A:1376:GLU:OE1	1:A:1376:GLU:N	2.37	0.49
1:A:1713:LEU:HD22	1:A:1739:ILE:HD12	1.92	0.49
1:A:787:ASP:N	1:A:790:SER:OG	2.46	0.49
1:A:1100:GLY:O	1:A:1102:ARG:NH1	2.45	0.49
2:B:323:SER:HB2	2:B:410:ILE:O	2.12	0.49
2:B:944:ARG:NH2	2:B:987:ASP:OD1	2.34	0.49
2:B:1847:PRO:HG3	2:B:1859:LEU:HD13	1.94	0.49
2:B:104:ASP:OD1	2:B:105:GLU:N	2.46	0.49
2:B:342:GLN:O	2:B:345:SER:OG	2.30	0.49
2:B:476:GLU:HA	2:B:479:THR:HG22	1.95	0.49
2:B:945:PHE:CE1	2:B:977:GLN:HG2	2.48	0.49
2:B:1526:GLU:OE2	2:B:1529:THR:OG1	2.30	0.49
2:B:1709:GLY:N	2:B:1713:GLY:HA3	2.27	0.49
1:A:1614:ALA:HB3	1:A:1631:SER:HB2	1.94	0.49
2:B:61:LYS:HA	2:B:121:ASN:ND2	2.26	0.49
2:B:741:TYR:CE1	2:B:781:MET:HB3	2.47	0.49
2:B:977:GLN:H	2:B:977:GLN:CD	2.18	0.49
2:B:1125:GLU:OE1	2:B:1125:GLU:N	2.41	0.49
2:B:1310:ASP:O	2:B:1313:ILE:HG12	2.11	0.49
2:B:1579:VAL:HG12	2:B:1612:MET:SD	2.52	0.49
2:B:1738:LYS:HE3	2:B:1740:PHE:H	1.78	0.49
1:A:35:PHE:CD2	2:B:1650:THR:HG21	2.48	0.49
1:A:878:SER:C	1:A:880:ASN:N	2.62	0.49
2:B:169:LEU:HD22	2:B:170:TYR:CZ	2.47	0.49
2:B:271:ALA:HB1	2:B:440:LEU:HB3	1.95	0.49
2:B:1194:GLU:HB2	2:B:1206:SER:HB2	1.95	0.49
2:B:1877:VAL:HG23	2:B:1878:ASN:OD1	2.13	0.49
2:B:2021:THR:HG23	2:B:2023:SER:H	1.77	0.49
1:A:857:TRP:CE3	1:A:861:LEU:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:ILE:O	2:B:488:ASP:HA	2.13	0.49
2:B:1717:ARG:NH2	2:B:1745:GLU:O	2.43	0.49
1:A:875:GLY:O	1:A:877:MET:N	2.46	0.49
1:A:1008:GLU:HA	1:A:1667:VAL:HA	1.94	0.49
1:A:1222:LEU:HD13	1:A:1691:MET:SD	2.53	0.49
2:B:989:ASP:OD1	2:B:990:TYR:N	2.46	0.49
2:B:1115:GLU:OE1	2:B:1115:GLU:N	2.45	0.49
2:B:1295:ASP:HA	2:B:1298:VAL:HG22	1.94	0.49
2:B:1968:TYR:HD2	2:B:1969:LEU:HD12	1.78	0.49
1:A:416:PHE:HA	1:A:419:ILE:HG12	1.95	0.49
1:A:985:ALA:N	1:A:1084:GLU:OE1	2.22	0.49
1:A:1209:ILE:O	1:A:1213:VAL:HG23	2.13	0.49
2:B:322:PRO:HA	2:B:407:PHE:CG	2.48	0.49
2:B:813:GLY:HA3	2:B:1049:GLN:HB3	1.95	0.49
1:A:469:ARG:HB2	1:A:469:ARG:CZ	2.41	0.48
1:A:477:ASN:ND2	1:A:582:GLU:OE1	2.46	0.48
1:A:824:PRO:HB2	3:A:1901:NAP:H1D	1.95	0.48
1:A:984:ARG:HD2	1:A:1084:GLU:CD	2.38	0.48
1:A:1028:TRP:CE3	1:A:1037:MET:HG2	2.48	0.48
1:A:1236:VAL:HG23	1:A:1323:LYS:HD2	1.95	0.48
2:B:304:THR:OG1	2:B:305:SER:N	2.45	0.48
1:A:32:GLN:HA	1:A:35:PHE:CD1	2.48	0.48
1:A:1709:TYR:HA	1:A:1734:PHE:HB2	1.94	0.48
2:B:129:ILE:O	2:B:131:LYS:N	2.42	0.48
2:B:1512:GLU:HB3	2:B:1618:ILE:HG13	1.96	0.48
1:A:965:LYS:HB3	1:A:970:ASP:OD1	2.13	0.48
1:A:1019:VAL:HG22	1:A:1385:ILE:HG22	1.96	0.48
2:B:584:MET:CB	4:B:2101:FMN:H6	2.12	0.48
2:B:752:LEU:N	2:B:784:ASP:OD2	2.27	0.48
2:B:1539:TYR:O	2:B:1543:SER:OG	2.29	0.48
2:B:1911:ASP:O	2:B:1914:LYS:HG2	2.13	0.48
2:B:1053:LYS:HZ3	2:B:1054:VAL:H	1.61	0.48
1:A:712:PHE:CE1	1:A:717:THR:HG21	2.29	0.48
1:A:1191:TRP:HZ2	1:A:1215:VAL:HG21	1.77	0.48
1:A:1587:PRO:HG3	1:A:1594:TRP:CE3	2.49	0.48
2:B:461:ILE:HA	2:B:464:VAL:HG12	1.95	0.48
2:B:1843:VAL:HG13	2:B:1895:LEU:HD23	1.95	0.48
2:B:1920:SER:OG	2:B:1921:ILE:N	2.43	0.48
2:B:429:ASP:O	2:B:432:GLU:HB2	2.13	0.48
1:A:482:LEU:HD12	1:A:483:THR:H	1.78	0.48
1:A:520:PHE:HA	1:A:523:TYR:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1416:VAL:HG13	1:A:1650:GLY:N	2.29	0.48
2:B:243:LEU:HB3	2:B:245:LEU:HD23	1.95	0.48
2:B:313:ASP:OD1	2:B:317:ASN:ND2	2.46	0.48
2:B:448:PHE:CE1	2:B:472:PRO:HD2	2.48	0.48
2:B:612:PHE:CZ	3:B:2102:NAP:N7A	2.73	0.48
2:B:767:TYR:HB3	2:B:783:PHE:CD2	2.48	0.48
2:B:875:ARG:O	2:B:879:ILE:HG12	2.14	0.48
2:B:1792:PHE:CD1	2:B:1806:LEU:HD22	2.48	0.48
1:A:1233:TYR:OH	1:A:1290:LEU:O	2.26	0.48
2:B:167:TYR:OH	2:B:171:GLN:NE2	2.46	0.48
1:A:768:ASP:OD1	1:A:817:ARG:NE	2.45	0.48
1:A:982:GLU:O	2:B:943:GLU:HG3	2.14	0.48
2:B:313:ASP:OD2	2:B:374:TYR:OH	2.30	0.48
1:A:442:ASN:H	1:A:445:LEU:HB2	1.79	0.48
1:A:1201:ASP:O	1:A:1204:SER:OG	2.26	0.48
1:A:1203:ILE:HD13	1:A:1211:LEU:HD22	1.95	0.48
2:B:1119:GLU:HG2	2:B:1120:LEU:H	1.77	0.48
2:B:1614:HIS:ND1	2:B:1623:ILE:O	2.35	0.48
2:B:2009:LEU:HD23	2:B:2009:LEU:H	1.79	0.48
1:A:22:PHE:CZ	2:B:1969:LEU:HD23	2.49	0.47
1:A:877:MET:O	1:A:879:ALA:N	2.47	0.47
1:A:1358:ARG:NH2	1:A:1615:ASP:OD2	2.33	0.47
2:B:176:ASP:OD2	2:B:241:LYS:NZ	2.47	0.47
2:B:865:ASN:OD1	2:B:866:LYS:NZ	2.47	0.47
2:B:1783:LYS:HB2	2:B:1785:LEU:HD23	1.95	0.47
2:B:1910:ILE:HA	2:B:1914:LYS:HD3	1.95	0.47
1:A:9:LEU:HD21	2:B:2035:GLN:HE22	1.79	0.47
1:A:796:ILE:HD11	3:A:1901:NAP:N6A	2.28	0.47
1:A:864:CYS:SG	1:A:907:LEU:HD13	2.54	0.47
1:A:1013:LEU:O	1:A:1388:ALA:HB3	2.14	0.47
1:A:1365:ARG:NH1	1:A:1370:THR:HG23	2.29	0.47
1:A:326:LEU:O	1:A:329:LEU:HG	2.14	0.47
2:B:140:CYS:SG	2:B:542:ILE:HD13	2.54	0.47
2:B:1230:ASP:OD1	2:B:1232:PHE:N	2.47	0.47
1:A:29:ILE:HG13	2:B:1879:TYR:O	2.14	0.47
1:A:1716:PRO:HB2	1:A:1739:ILE:HD13	1.95	0.47
2:B:698:ASP:O	2:B:701:SER:OG	2.24	0.47
2:B:1227:ASN:N	2:B:1234:PRO:O	2.35	0.47
2:B:1449:PHE:CD2	2:B:1503:LEU:HD21	2.50	0.47
2:B:1456:LYS:O	2:B:1464:SER:N	2.47	0.47
2:B:1857:SER:HA	2:B:1860:ARG:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HE2	2:B:1518:ASN:HB2	1.97	0.47
2:B:147:VAL:HG21	2:B:256:TRP:CE2	2.49	0.47
2:B:1599:VAL:HG21	2:B:1639:ILE:HD13	1.96	0.47
1:A:1063:GLY:O	1:A:1070:TYR:N	2.41	0.47
1:A:1333:PHE:HE1	1:A:1338:SER:HB2	1.78	0.47
1:A:1369:THR:OG1	1:A:1616:ASN:O	2.27	0.47
2:B:539:ASP:N	2:B:539:ASP:OD1	2.47	0.47
2:B:903:GLU:HA	2:B:982:LEU:HD13	1.97	0.47
1:A:533:MET:HE3	1:A:636:GLN:OE1	2.14	0.47
1:A:821:CYS:SG	1:A:861:LEU:HD12	2.55	0.47
1:A:1005:PRO:HB2	1:A:1006:GLU:OE1	2.15	0.47
1:A:1332:ASP:OD1	1:A:1333:PHE:N	2.47	0.47
2:B:5:ARG:HG2	2:B:6:PRO:O	2.14	0.47
2:B:177:LEU:O	2:B:180:SER:OG	2.30	0.47
2:B:237:THR:HG23	2:B:276:TRP:CZ3	2.50	0.47
2:B:679:THR:O	2:B:683:GLU:HG2	2.14	0.47
2:B:738:ILE:HD12	2:B:781:MET:HE1	1.95	0.47
2:B:1156:ASN:ND2	2:B:1159:HIS:HB2	2.30	0.47
2:B:1275:GLU:HG2	2:B:1359:SER:HB2	1.97	0.47
2:B:1728:ILE:HG23	2:B:1732:GLY:HA2	1.96	0.47
2:B:1842:MET:HE2	2:B:1957:LEU:HD12	1.96	0.47
2:B:1856:ASP:N	2:B:1883:ASN:HD21	2.13	0.47
2:B:1893:ARG:HD3	2:B:1944:GLN:OE1	2.14	0.47
1:A:449:MET:O	1:A:453:ILE:HG12	2.15	0.47
1:A:840:GLU:HA	1:A:843:ILE:HG22	1.97	0.47
2:B:21:PRO:HG2	2:B:24:LEU:HD12	1.97	0.47
2:B:111:ILE:HD12	2:B:114:VAL:HB	1.97	0.47
2:B:797:GLU:OE1	2:B:797:GLU:N	2.43	0.47
2:B:907:LYS:HA	2:B:972:PHE:CZ	2.50	0.47
2:B:1672:GLU:O	2:B:1676:GLU:HG2	2.14	0.47
2:B:1878:ASN:HB3	2:B:1880:ASN:OD1	2.15	0.47
2:B:2023:SER:HB3	2:B:2026:ILE:HG12	1.96	0.47
1:A:1156:GLU:H	1:A:1156:GLU:CD	2.21	0.47
2:B:198:GLN:OE1	2:B:213:PRO:HB3	2.15	0.47
2:B:1705:THR:HA	2:B:1751:THR:HA	1.97	0.47
2:B:1769:LEU:O	2:B:1772:MET:HG3	2.15	0.47
2:B:1861:PHE:CD2	2:B:1912:ILE:HG21	2.49	0.47
1:A:1498:ARG:NH1	1:A:1745:TYR:OH	2.47	0.47
1:A:1705:ASP:OD2	1:A:1706:LYS:N	2.48	0.47
2:B:222:PRO:HG3	2:B:294:GLY:O	2.14	0.47
2:B:763:ASP:OD1	2:B:1050:TYR:OH	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:796:LYS:HB2	2:B:1055:ASP:O	2.15	0.47
2:B:852:TRP:CD1	2:B:852:TRP:C	2.93	0.47
2:B:899:CYS:SG	2:B:903:GLU:HG3	2.55	0.47
2:B:1118:SER:N	2:B:1166:LYS:HA	2.30	0.47
2:B:2005:LYS:NZ	2:B:2016:SER:OG	2.48	0.47
1:A:47:ILE:HD12	2:B:1653:PHE:HE1	1.79	0.46
1:A:654:ASN:ND2	1:A:657:LEU:HG	2.30	0.46
1:A:1181:ARG:NH2	1:A:1347:THR:O	2.35	0.46
1:A:1410:ASP:OD1	1:A:1422:GLY:N	2.42	0.46
2:B:332:SER:OG	2:B:334:LYS:HG3	2.15	0.46
2:B:1166:LYS:HE3	2:B:1167:HIS:CE1	2.50	0.46
2:B:1703:GLU:C	2:B:1758:LEU:HD11	2.39	0.46
1:A:984:ARG:HH21	2:B:940:ARG:CZ	2.28	0.46
1:A:997:TYR:O	1:A:1000:ILE:HG22	2.16	0.46
1:A:1628:LEU:HD23	1:A:1629:TYR:N	2.31	0.46
2:B:221:VAL:HG21	2:B:412:ALA:HB2	1.98	0.46
2:B:326:LEU:O	2:B:366:LEU:N	2.33	0.46
2:B:538:ALA:HB3	2:B:540:LYS:NZ	2.29	0.46
2:B:1137:TRP:CE2	2:B:1197:LEU:HG	2.51	0.46
1:A:30:GLU:CD	1:A:30:GLU:H	2.23	0.46
1:A:1193:ALA:O	1:A:1196:TYR:N	2.37	0.46
2:B:1247:LYS:HA	2:B:1333:LEU:HD23	1.97	0.46
1:A:427:ASP:HB3	1:A:430:THR:HG22	1.97	0.46
1:A:693:GLU:HB3	1:A:901:ALA:HB2	1.98	0.46
1:A:1068:LYS:HE2	1:A:1068:LYS:HB2	1.84	0.46
2:B:164:ARG:HH22	2:B:209:PRO:HA	1.80	0.46
2:B:949:ALA:HB1	2:B:951:THR:HG23	1.97	0.46
1:A:743:SER:HB3	1:A:746:ASP:OD1	2.15	0.46
1:A:1226:ILE:HD11	1:A:1394:MET:HE1	1.97	0.46
2:B:9:LEU:HB2	2:B:17:THR:HG23	1.98	0.46
2:B:11:HIS:H	2:B:15:GLU:HG3	1.81	0.46
2:B:136:LEU:HD23	2:B:136:LEU:H	1.81	0.46
2:B:573:LEU:HB3	2:B:574:LEU:HD12	1.98	0.46
2:B:1174:LYS:O	2:B:1175:LYS:HG2	2.15	0.46
1:A:1257:GLY:O	1:A:1261:ASP:HB2	2.15	0.46
1:A:1509:LYS:HA	1:A:1513:ASN:HB2	1.97	0.46
1:A:1744:SER:O	1:A:1744:SER:OG	2.29	0.46
2:B:150:PHE:CE1	2:B:489:PHE:HD2	2.33	0.46
2:B:1211:ARG:HD2	2:B:1551:VAL:HB	1.98	0.46
1:A:500:LYS:NZ	1:A:508:GLU:OE2	2.28	0.46
2:B:136:LEU:HD21	2:B:535:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1919:MET:HE1	2:B:1927:HIS:HB2	1.97	0.46
1:A:86:LYS:HE3	1:A:92:PRO:HA	1.96	0.46
1:A:1000:ILE:HD12	1:A:1003:ILE:HD12	1.96	0.46
2:B:59:TYR:CD2	2:B:82:PHE:HD1	2.34	0.46
2:B:138:TYR:CG	2:B:138:TYR:O	2.69	0.46
2:B:198:GLN:HB2	2:B:217:TYR:CZ	2.51	0.46
1:A:876:LEU:CD2	3:A:1901:NAP:O2A	2.56	0.46
2:B:102:LEU:HD21	2:B:111:ILE:HA	1.97	0.46
2:B:259:GLY:HA3	2:B:264:LEU:HA	1.98	0.46
2:B:797:GLU:OE2	2:B:1058:ILE:HG22	2.16	0.46
1:A:381:GLY:HA3	1:A:788:SER:OG	2.16	0.46
1:A:490:ASP:OD1	1:A:491:VAL:N	2.49	0.46
1:A:989:PHE:HZ	1:A:1223:SER:HA	1.81	0.46
2:B:462:ASP:OD1	2:B:462:ASP:N	2.46	0.46
2:B:1148:VAL:HA	2:B:1152:LYS:O	2.15	0.46
1:A:83:LYS:HG3	1:A:84:ASP:OD1	2.15	0.45
1:A:1151:GLU:HG3	1:A:1166:LEU:HD11	1.98	0.45
1:A:1374:PHE:HA	1:A:1548:SER:OG	2.15	0.45
2:B:521:ASN:CG	2:B:522:PRO:HD2	2.41	0.45
2:B:1649:THR:OG1	2:B:1787:PRO:HG2	2.17	0.45
2:B:1761:ALA:HB3	2:B:1764:PHE:HD2	1.80	0.45
1:A:496:GLY:HA3	1:A:514:LYS:HD3	1.98	0.45
1:A:998:ASP:OD1	1:A:998:ASP:N	2.48	0.45
1:A:1121:GLN:NE2	1:A:1122:GLU:O	2.42	0.45
2:B:396:PHE:CD1	2:B:732:ASP:HB2	2.52	0.45
2:B:461:ILE:O	2:B:465:VAL:HG22	2.15	0.45
2:B:612:PHE:HD2	3:B:2102:NAP:N6A	2.11	0.45
2:B:926:ILE:HD11	2:B:1030:SER:HB2	1.97	0.45
2:B:1328:SER:HB2	2:B:1407:ASN:HB3	1.99	0.45
2:B:1659:GLN:H	2:B:1659:GLN:CD	2.24	0.45
2:B:1990:LYS:HB3	2:B:1992:GLN:HE22	1.82	0.45
1:A:47:ILE:HB	2:B:1653:PHE:CD1	2.51	0.45
1:A:649:ASP:OD1	1:A:650:GLY:N	2.50	0.45
1:A:967:VAL:HG22	2:B:1498:PRO:HG3	1.97	0.45
2:B:94:ILE:HA	2:B:97:PHE:HB3	1.97	0.45
2:B:931:ARG:NH1	2:B:959:ASN:HA	2.31	0.45
2:B:1090:TYR:CE1	2:B:1135:LEU:HB3	2.52	0.45
2:B:1171:THR:HB	2:B:1180:THR:HB	1.98	0.45
2:B:84:SER:HA	2:B:88:ASP:OD1	2.16	0.45
2:B:538:ALA:HB3	2:B:540:LYS:HZ1	1.81	0.45
2:B:687:LEU:HD23	2:B:687:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:940:ARG:HA	2:B:940:ARG:HD3	1.79	0.45
2:B:1311:PHE:O	2:B:1315:ILE:HG13	2.16	0.45
2:B:1517:GLU:OE2	2:B:1517:GLU:N	2.46	0.45
2:B:1547:ASN:HB3	2:B:1550:HIS:CD2	2.52	0.45
2:B:1745:GLU:N	2:B:1745:GLU:OE1	2.50	0.45
2:B:1927:HIS:HA	2:B:1930:GLU:CD	2.41	0.45
1:A:30:GLU:OE1	1:A:30:GLU:N	2.50	0.45
1:A:485:ASP:CG	1:A:674:THR:HG21	2.41	0.45
1:A:1229:PRO:HB3	1:A:1290:LEU:HD23	1.97	0.45
1:A:1317:ILE:HD11	1:A:1325:VAL:HG12	1.97	0.45
2:B:138:TYR:O	2:B:141:LYS:HD2	2.17	0.45
2:B:356:SER:HB3	2:B:367:SER:HB3	1.97	0.45
2:B:816:ASP:O	2:B:819:TRP:HD1	1.99	0.45
2:B:1404:ASP:OD1	2:B:1407:ASN:ND2	2.49	0.45
2:B:1968:TYR:CD2	2:B:1969:LEU:HD12	2.51	0.45
1:A:709:THR:HA	3:A:1901:NAP:O1X	2.16	0.45
1:A:1576:PHE:CD1	1:A:1576:PHE:N	2.83	0.45
2:B:795:SER:O	2:B:805:LYS:NZ	2.32	0.45
2:B:1065:ILE:HG13	2:B:1066:HIS:N	2.31	0.45
2:B:1528:LEU:HD12	2:B:1578:LEU:HD21	1.99	0.45
2:B:2018:TYR:CE1	2:B:2027:LYS:HB3	2.51	0.45
1:A:678:LYS:HE2	1:A:678:LYS:HB2	1.82	0.45
1:A:1587:PRO:HG2	1:A:1591:ALA:HA	1.99	0.45
2:B:257:SER:O	2:B:444:VAL:HA	2.17	0.45
2:B:479:THR:O	2:B:505:LYS:NZ	2.39	0.45
2:B:1230:ASP:OD1	2:B:1231:GLY:N	2.49	0.45
2:B:1475:GLU:OE2	2:B:1479:LYS:HA	2.17	0.45
2:B:1735:LYS:O	2:B:1737:GLU:N	2.50	0.45
2:B:1863:VAL:HG12	2:B:1898:LEU:CD1	2.47	0.45
1:A:14:LEU:HD21	2:B:1803:LEU:HD12	1.99	0.45
2:B:114:VAL:HA	2:B:118:ILE:HD13	1.98	0.45
2:B:277:ASP:OD1	2:B:278:SER:N	2.50	0.45
2:B:323:SER:OG	2:B:407:PHE:HB3	2.17	0.45
2:B:520:SER:HA	2:B:521:ASN:HA	1.72	0.45
2:B:986:GLU:H	2:B:986:GLU:CD	2.15	0.45
1:A:18:LEU:HD22	2:B:1800:TYR:CE1	2.52	0.45
1:A:493:ARG:HH11	1:A:518:ARG:HG2	1.82	0.45
1:A:674:THR:HG22	1:A:676:LYS:H	1.82	0.45
1:A:1006:GLU:O	1:A:1006:GLU:HG2	2.18	0.45
1:A:1104:ILE:HA	1:A:1186:GLN:NE2	2.32	0.45
1:A:1155:ILE:O	1:A:1159:GLY:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:HIS:HE1	2:B:85:ARG:HG2	1.82	0.45
2:B:88:ASP:C	2:B:90:ASN:H	2.24	0.45
2:B:312:GLN:NE2	2:B:316:ASP:OD2	2.49	0.45
2:B:408:LEU:O	2:B:410:ILE:N	2.47	0.45
1:A:864:CYS:HB2	1:A:916:CYS:SG	2.57	0.44
1:A:1446:ARG:NH1	1:A:1512:GLY:HA2	2.32	0.44
2:B:767:TYR:HA	2:B:772:TRP:CD1	2.52	0.44
2:B:1226:TYR:CE2	2:B:1228:PRO:HG3	2.52	0.44
2:B:1602:VAL:HG13	2:B:1637:VAL:HG11	1.99	0.44
2:B:1876:ILE:HG12	2:B:1888:ALA:HB2	1.98	0.44
1:A:57:ALA:O	1:A:61:ILE:HG12	2.17	0.44
1:A:735:ILE:HG22	1:A:737:VAL:HG23	1.99	0.44
1:A:1202:THR:O	1:A:1206:VAL:HG22	2.17	0.44
1:A:1483:PHE:HB3	1:A:1485:MET:HE3	2.00	0.44
2:B:905:THR:HA	2:B:982:LEU:HA	1.98	0.44
2:B:1767:PRO:HA	2:B:1770:THR:HG22	1.98	0.44
2:B:1860:ARG:HA	2:B:1863:VAL:HG22	1.98	0.44
2:B:1874:LEU:HD13	2:B:1895:LEU:HD12	1.98	0.44
1:A:359:PHE:CE2	1:A:363:LYS:HD3	2.53	0.44
2:B:245:LEU:HD12	2:B:249:GLU:HG3	1.98	0.44
2:B:1150:GLY:O	2:B:1151:SER:OG	2.32	0.44
2:B:1263:ASN:HB3	2:B:1327:LYS:HZ1	1.82	0.44
1:A:1446:ARG:HD2	1:A:1511:TRP:O	2.17	0.44
1:A:1676:TYR:CZ	1:A:1680:VAL:HG21	2.51	0.44
1:A:1725:VAL:HG11	1:A:1732:LEU:HB3	2.00	0.44
2:B:215:GLN:HA	2:B:218:LEU:HB2	2.00	0.44
2:B:296:ARG:NH1	2:B:425:LEU:HB3	2.31	0.44
2:B:612:PHE:CD2	3:B:2102:NAP:N7A	2.70	0.44
2:B:856:ASP:HA	2:B:860:PHE:HB2	1.98	0.44
2:B:887:GLN:O	2:B:889:PRO:HD3	2.17	0.44
2:B:934:TYR:OH	2:B:968:THR:HG21	2.18	0.44
2:B:977:GLN:HA	2:B:980:LYS:HG2	1.98	0.44
2:B:1685:PHE:O	2:B:1689:TYR:N	2.32	0.44
2:B:1869:LYS:NZ	2:B:1933:ASP:OD1	2.33	0.44
2:B:1985:PRO:HG2	2:B:1988:SER:OG	2.17	0.44
1:A:763:LEU:HD23	1:A:763:LEU:HA	1.77	0.44
1:A:1151:GLU:HB3	1:A:1153:PHE:CE2	2.51	0.44
1:A:1209:ILE:HD11	1:A:1330:TYR:HD2	1.83	0.44
1:A:1476:LYS:NZ	1:A:1484:SER:H	2.16	0.44
2:B:355:ILE:HA	2:B:366:LEU:HD13	1.99	0.44
2:B:945:PHE:HD1	2:B:977:GLN:HE21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1019:LYS:HD3	3:B:2102:NAP:H4B	1.99	0.44
2:B:1266:ASN:HD21	2:B:1268:GLU:HB3	1.82	0.44
2:B:1382:ILE:HG22	2:B:1390:MET:O	2.18	0.44
2:B:1725:PHE:CD1	2:B:1739:ILE:HG13	2.53	0.44
2:B:1863:VAL:HG11	2:B:1876:ILE:HG13	1.99	0.44
2:B:2029:ILE:HA	2:B:2032:ASN:OD1	2.18	0.44
1:A:387:GLY:O	1:A:740:ASN:ND2	2.48	0.44
1:A:437:ILE:HA	1:A:440:ARG:HH21	1.83	0.44
1:A:681:LEU:HD12	1:A:682:VAL:N	2.32	0.44
1:A:755:TYR:CE1	1:A:766:ASP:HA	2.53	0.44
1:A:820:GLN:NE2	1:A:822:ILE:HD11	2.33	0.44
1:A:991:PHE:CD2	1:A:1397:PRO:HG3	2.52	0.44
1:A:1143:LYS:HA	1:A:1150:CYS:SG	2.58	0.44
2:B:296:ARG:HA	2:B:296:ARG:HD3	1.74	0.44
2:B:1317:TRP:O	2:B:1321:ILE:HG12	2.18	0.44
1:A:1541:VAL:HG12	1:A:1542:ALA:N	2.33	0.44
2:B:400:LYS:HB2	2:B:402:LYS:HZ1	1.83	0.44
2:B:1119:GLU:HG2	2:B:1120:LEU:N	2.33	0.44
2:B:1703:GLU:OE2	2:B:1703:GLU:N	2.50	0.44
2:B:1740:PHE:HB3	2:B:1743:ILE:HD13	2.00	0.44
1:A:403:TYR:HA	1:A:406:TRP:HD1	1.83	0.44
1:A:630:SER:OG	1:A:659:SER:HB2	2.17	0.44
1:A:707:VAL:HG12	1:A:708:THR:N	2.33	0.44
1:A:954:ARG:O	1:A:958:ILE:HG12	2.18	0.44
1:A:1529:LEU:O	1:A:1532:PHE:N	2.40	0.44
2:B:96:SER:HB3	2:B:535:GLN:OE1	2.18	0.44
2:B:189:HIS:CE1	2:B:199:GLY:HA2	2.52	0.44
2:B:265:VAL:HA	2:B:268:VAL:HG12	1.99	0.44
2:B:825:LYS:HB2	2:B:825:LYS:HE3	1.70	0.44
2:B:1985:PRO:O	2:B:1988:SER:OG	2.31	0.44
1:A:680:VAL:HG22	1:A:769:ALA:HB3	2.00	0.44
2:B:266:THR:O	2:B:270:ILE:HG12	2.18	0.44
2:B:756:SER:H	4:B:2101:FMN:C5'	2.30	0.44
2:B:907:LYS:HG3	2:B:972:PHE:CE2	2.53	0.44
2:B:1251:TRP:CE2	2:B:1261:TYR:HA	2.53	0.44
1:A:89:TYR:OH	2:B:1779:ASP:OD2	2.22	0.43
1:A:1065:LEU:HD23	1:A:1081:PRO:HG3	2.00	0.43
1:A:1187:ILE:HG23	1:A:1188:PRO:HD2	2.00	0.43
2:B:42:PRO:HB3	2:B:46:PHE:HE1	1.83	0.43
2:B:577:ALA:HB1	2:B:1066:HIS:CD2	2.53	0.43
2:B:790:SER:HB3	4:B:2101:FMN:HM82	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1094:LYS:HG3	2:B:1095:LYS:N	2.32	0.43
2:B:1764:PHE:C	2:B:1767:PRO:HD2	2.43	0.43
2:B:1840:TYR:HB3	2:B:1963:PRO:HG3	2.00	0.43
1:A:39:HIS:ND1	2:B:1791:MET:SD	2.91	0.43
1:A:485:ASP:OD1	1:A:486:PRO:HD2	2.18	0.43
1:A:979:VAL:O	2:B:956:GLN:NE2	2.46	0.43
1:A:1028:TRP:CZ2	1:A:1100:GLY:HA3	2.53	0.43
2:B:43:THR:O	2:B:46:PHE:N	2.52	0.43
2:B:176:ASP:OD1	2:B:176:ASP:N	2.49	0.43
1:A:401:ASP:H	1:A:1616:ASN:CG	2.25	0.43
1:A:876:LEU:HB2	1:A:877:MET:H	1.72	0.43
1:A:984:ARG:N	2:B:943:GLU:O	2.48	0.43
1:A:1020:THR:HG21	1:A:1386:MET:SD	2.58	0.43
1:A:1115:LYS:HD3	1:A:1182:LEU:HD21	2.00	0.43
1:A:1148:GLU:OE2	1:A:1148:GLU:N	2.47	0.43
1:A:1324:VAL:HG22	1:A:1386:MET:HG3	2.00	0.43
2:B:159:TYR:HE2	2:B:227:VAL:HG23	1.82	0.43
2:B:1453:SER:HA	2:B:1468:THR:HA	1.99	0.43
1:A:1271:ASP:O	1:A:1274:GLN:HG2	2.18	0.43
1:A:1617:VAL:HG11	1:A:1629:TYR:HD2	1.83	0.43
2:B:96:SER:HA	2:B:99:VAL:HG22	2.00	0.43
2:B:238:ILE:O	2:B:242:VAL:HG23	2.18	0.43
2:B:488:ASP:OD1	2:B:514:LEU:HA	2.18	0.43
2:B:537:SER:O	2:B:538:ALA:C	2.62	0.43
2:B:1240:GLU:CD	2:B:1241:ASP:HB2	2.43	0.43
2:B:1338:HIS:CE1	2:B:1569:MET:HE3	2.54	0.43
2:B:1451:CYS:HA	2:B:1470:GLY:HA3	1.99	0.43
2:B:1459:SER:OG	2:B:1462:VAL:HG22	2.18	0.43
2:B:1678:TRP:HB3	2:B:1694:LEU:HD21	1.99	0.43
1:A:40:ASN:HB3	1:A:74:LEU:HD21	2.00	0.43
1:A:832:PHE:HD1	1:A:832:PHE:HA	1.69	0.43
1:A:991:PHE:CE2	1:A:1397:PRO:HG3	2.54	0.43
1:A:1257:GLY:HA2	1:A:1261:ASP:HB2	2.01	0.43
1:A:1395:GLY:O	1:A:1683:ARG:HD2	2.18	0.43
1:A:1603:LEU:HD23	1:A:1603:LEU:HA	1.75	0.43
2:B:93:ASN:HB3	2:B:96:SER:HG	1.83	0.43
2:B:1926:GLU:O	2:B:1930:GLU:HG3	2.19	0.43
1:A:442:ASN:O	1:A:445:LEU:N	2.51	0.43
1:A:933:ASP:OD2	1:A:934:ASN:N	2.51	0.43
1:A:1025:VAL:HG13	1:A:1025:VAL:O	2.19	0.43
2:B:332:SER:N	2:B:335:GLN:HE21	2.10	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:PHE:HD1	2:B:1191:PRO:HA	1.83	0.43
2:B:1613:GLU:O	2:B:1625:LYS:N	2.44	0.43
2:B:1632:GLU:OE1	2:B:1632:GLU:N	2.43	0.43
2:B:1726:GLU:H	2:B:1975:PRO:HG3	1.83	0.43
2:B:1992:GLN:HA	2:B:1995:ILE:HD12	2.00	0.43
1:A:326:LEU:O	1:A:330:THR:HG23	2.19	0.43
1:A:327:ASP:O	1:A:330:THR:OG1	2.29	0.43
1:A:710:SER:OG	3:A:1901:NAP:C2A	2.67	0.43
1:A:1015:ASN:HB2	1:A:1513:ASN:ND2	2.34	0.43
2:B:225:CYS:HB3	2:B:226:PRO:HD3	2.00	0.43
2:B:579:LEU:HD13	2:B:1065:ILE:HD11	2.00	0.43
2:B:585:THR:HA	2:B:607:ALA:HB1	1.99	0.43
2:B:1137:TRP:CZ2	2:B:1197:LEU:HG	2.54	0.43
2:B:1704:LEU:HB2	2:B:1758:LEU:HD13	2.01	0.43
2:B:1990:LYS:HB3	2:B:1992:GLN:NE2	2.34	0.43
1:A:697:GLY:HA3	1:A:905:LEU:HD11	2.01	0.43
1:A:1468:LEU:HD11	1:A:1492:ARG:CG	2.49	0.43
2:B:524:ASP:HB3	2:B:526:GLU:CD	2.44	0.43
2:B:761:ASP:OD1	2:B:761:ASP:N	2.50	0.43
2:B:1547:ASN:HB3	2:B:1550:HIS:HD2	1.83	0.43
2:B:1744:ASP:OD1	2:B:1747:THR:OG1	2.36	0.43
2:B:1860:ARG:O	2:B:1863:VAL:HG22	2.19	0.43
1:A:1477:GLU:HG2	1:A:1483:PHE:CZ	2.53	0.43
1:A:1607:LEU:HD23	1:A:1608:VAL:C	2.43	0.43
1:A:1737:LYS:HA	1:A:1737:LYS:HD2	1.78	0.43
2:B:90:ASN:O	2:B:93:ASN:HB2	2.18	0.43
2:B:136:LEU:C	2:B:139:HIS:H	2.27	0.43
2:B:195:ILE:HG13	2:B:196:TYR:CD1	2.54	0.43
2:B:1126:TRP:CG	2:B:1164:PRO:HG3	2.53	0.43
2:B:1522:LEU:HD22	2:B:1612:MET:HE3	2.01	0.43
2:B:1709:GLY:H	2:B:1713:GLY:HA3	1.84	0.43
2:B:1962:VAL:HA	2:B:1963:PRO:HD3	1.87	0.43
1:A:622:LYS:HZ3	1:A:671:ASN:HB3	1.83	0.43
1:A:710:SER:OG	3:A:1901:NAP:N9A	2.41	0.43
1:A:1226:ILE:HD13	1:A:1226:ILE:HA	1.88	0.43
1:A:1401:VAL:HB	1:A:1659:VAL:HG13	2.01	0.43
1:A:1525:LEU:HD12	1:A:1525:LEU:HA	1.71	0.43
2:B:818:GLN:HB2	2:B:821:GLN:NE2	2.34	0.43
2:B:1338:HIS:CE1	2:B:1396:PHE:HE1	2.36	0.43
2:B:1601:MET:HE3	2:B:1601:MET:HB2	1.96	0.43
2:B:1609:GLN:CD	2:B:1629:ARG:HH12	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1845:VAL:HG23	2:B:1954:VAL:HG22	2.00	0.43
2:B:2011:LYS:HB2	2:B:2033:TRP:CE2	2.53	0.43
1:A:11:His:CG	2:B:1986:LYS:HG3	2.54	0.42
1:A:31:THR:HG23	2:B:1999:ILE:HG21	1.99	0.42
1:A:45:ILE:HD12	2:B:1651:TYR:HE1	1.84	0.42
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.90	0.42
1:A:699:ILE:HG22	1:A:728:GLY:HA2	2.01	0.42
1:A:1135:SER:OG	1:A:1136:LYS:N	2.51	0.42
1:A:1693:ASN:O	1:A:1696:THR:OG1	2.32	0.42
2:B:499:VAL:HG12	2:B:503:ARG:NH1	2.34	0.42
2:B:522:PRO:HD3	2:B:529:PHE:HE2	1.84	0.42
2:B:727:His:CE1	2:B:841:ILE:HD12	2.53	0.42
2:B:1088:VAL:HB	2:B:1135:LEU:HD12	2.00	0.42
2:B:1274:ASP:OD1	2:B:1274:ASP:N	2.51	0.42
2:B:1541:ILE:HA	2:B:1546:TYR:HE1	1.84	0.42
1:A:1501:LYS:HE3	1:A:1501:LYS:HB3	1.91	0.42
2:B:42:PRO:HB3	2:B:46:PHE:CE1	2.53	0.42
2:B:664:GLN:O	2:B:688:THR:OG1	2.37	0.42
2:B:1358:VAL:HG13	2:B:1383:TYR:O	2.18	0.42
2:B:1810:MET:HB2	2:B:1814:SER:OG	2.19	0.42
1:A:699:ILE:CG2	1:A:728:GLY:HA2	2.49	0.42
1:A:1018:VAL:HB	1:A:1398:ILE:HG23	2.01	0.42
1:A:1119:MET:O	1:A:1175:LYS:N	2.47	0.42
1:A:1693:ASN:OD1	1:A:1697:ARG:HD2	2.19	0.42
2:B:396:PHE:N	2:B:820:GLU:OE2	2.49	0.42
2:B:1178:LYS:HD3	2:B:1196:GLU:HB3	2.00	0.42
2:B:1549:ILE:O	2:B:1564:THR:HA	2.19	0.42
2:B:1777:TYR:CD2	2:B:1805:SER:HB2	2.54	0.42
2:B:1963:PRO:O	2:B:1966:SER:OG	2.26	0.42
1:A:428:ARG:HA	1:A:428:ARG:HD3	1.77	0.42
1:A:838:TYR:O	1:A:841:SER:OG	2.34	0.42
1:A:1070:TYR:CZ	1:A:1081:PRO:HB3	2.54	0.42
1:A:1694:ALA:HB1	1:A:1700:MET:HA	2.00	0.42
2:B:523:ILE:HD12	2:B:523:ILE:HA	1.87	0.42
2:B:1248:GLU:HG2	2:B:1261:TYR:CD2	2.54	0.42
2:B:1339:LEU:HD23	2:B:1339:LEU:HA	1.74	0.42
2:B:1878:ASN:CB	2:B:1887:VAL:HB	2.48	0.42
1:A:14:LEU:HD11	2:B:1803:LEU:HD13	2.01	0.42
1:A:665:LEU:HD11	1:A:906:GLY:HA3	2.01	0.42
1:A:766:ASP:O	1:A:817:ARG:NH1	2.52	0.42
2:B:259:GLY:H	2:B:264:LEU:HD13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:728:HIS:CD2	2:B:729:SER:H	2.37	0.42
2:B:885:ASP:O	2:B:1038:ARG:HA	2.20	0.42
2:B:1541:ILE:HA	2:B:1546:TYR:CE1	2.55	0.42
2:B:1594:PHE:HD1	2:B:1642:ALA:HB2	1.85	0.42
1:A:45:ILE:HD12	2:B:1651:TYR:CE1	2.54	0.42
1:A:683:THR:HB	1:A:772:PRO:HA	2.01	0.42
2:B:1638:LEU:HD23	2:B:1638:LEU:HA	1.82	0.42
3:B:2102:NAP:O2N	3:B:2102:NAP:H3D	2.19	0.42
1:A:6:GLU:OE1	2:B:1991:PRO:HG2	2.20	0.42
1:A:816:THR:O	1:A:818:PRO:HD3	2.20	0.42
1:A:857:TRP:HE3	1:A:861:LEU:HB2	1.85	0.42
1:A:971:ASN:OD1	1:A:972:VAL:HG23	2.20	0.42
1:A:1128:ASP:HB3	1:A:1166:LEU:HA	2.01	0.42
2:B:241:LYS:C	2:B:244:GLY:H	2.26	0.42
2:B:957:ASN:HD21	2:B:959:ASN:ND2	2.12	0.42
2:B:1273:GLY:N	2:B:1360:THR:O	2.48	0.42
2:B:1341:ASN:HB2	2:B:1569:MET:HE1	2.01	0.42
2:B:1964:PHE:HD2	2:B:1965:HIS:ND1	2.18	0.42
1:A:2:LYS:HE2	1:A:2:LYS:HB2	1.86	0.42
1:A:624:SER:O	1:A:624:SER:OG	2.37	0.42
1:A:1198:ILE:HA	1:A:1701:PHE:CE2	2.55	0.42
2:B:717:LEU:N	2:B:751:VAL:O	2.38	0.42
2:B:1286:PHE:O	2:B:1290:ILE:HG12	2.20	0.42
2:B:1731:ASP:OD1	2:B:1735:LYS:NZ	2.45	0.42
1:A:20:TYR:CD1	2:B:1973:VAL:HG11	2.55	0.42
2:B:116:GLU:OE2	2:B:117:ASN:ND2	2.52	0.42
2:B:136:LEU:CA	2:B:139:HIS:HB2	2.50	0.42
2:B:887:GLN:HB3	2:B:1038:ARG:O	2.20	0.42
2:B:1726:GLU:OE2	2:B:1728:ILE:HD13	2.19	0.42
1:A:1353:GLU:OE1	1:A:1365:ARG:NH2	2.52	0.42
1:A:1582:TYR:CZ	1:A:1583:LEU:HB2	2.55	0.42
2:B:16:HIS:CE1	2:B:85:ARG:HG2	2.55	0.42
2:B:1099:VAL:O	2:B:1101:ALA:N	2.48	0.42
2:B:1271:ILE:HD13	2:B:1322:LYS:HB3	2.02	0.42
2:B:1576:ARG:NH1	2:B:1580:GLU:OE1	2.53	0.42
1:A:707:VAL:HG12	1:A:708:THR:H	1.84	0.41
1:A:1499:GLU:O	1:A:1503:GLN:HG3	2.20	0.41
2:B:223:VAL:O	2:B:226:PRO:HD2	2.20	0.41
2:B:571:SER:HB3	2:B:578:PRO:HG3	2.02	0.41
2:B:598:LEU:HG	2:B:604:ILE:HD13	2.03	0.41
2:B:886:PHE:CG	2:B:887:GLN:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2000:PRO:HG2	2:B:2013:TYR:OH	2.20	0.41
1:A:1:MET:HE3	1:A:1:MET:HB2	1.95	0.41
1:A:20:TYR:CE2	2:B:2023:SER:HB2	2.55	0.41
1:A:523:TYR:O	1:A:527:MET:HG2	2.20	0.41
1:A:757:GLU:HB2	1:A:760:LYS:HZ3	1.85	0.41
1:A:985:ALA:HB2	1:A:1045:LEU:HD22	2.02	0.41
1:A:1000:ILE:HD11	1:A:1662:ASP:HB3	2.02	0.41
1:A:1310:VAL:HA	1:A:1327:VAL:HG21	2.01	0.41
2:B:93:ASN:ND2	2:B:534:PHE:O	2.53	0.41
2:B:353:ILE:HD11	2:B:372:SER:OG	2.20	0.41
2:B:1174:LYS:C	2:B:1175:LYS:HG2	2.46	0.41
2:B:1190:LEU:HD23	2:B:1190:LEU:HA	1.82	0.41
2:B:1533:PRO:HG3	2:B:1570:TYR:CZ	2.55	0.41
1:A:1023:ALA:HB1	1:A:1219:GLU:HG3	2.02	0.41
1:A:1215:VAL:O	1:A:1219:GLU:HG2	2.20	0.41
1:A:1529:LEU:HB3	1:A:1534:LEU:HB2	2.03	0.41
2:B:261:SER:OG	2:B:262:GLN:N	2.53	0.41
2:B:726:GLY:HA2	2:B:1042:LEU:HD23	2.02	0.41
2:B:882:LEU:HA	2:B:882:LEU:HD23	1.81	0.41
2:B:1014:GLU:H	2:B:1014:GLU:CD	2.27	0.41
1:A:410:ASP:HA	1:A:413:SER:OG	2.20	0.41
1:A:1330:TYR:HA	1:A:1380:SER:HA	2.03	0.41
1:A:1596:LEU:HD12	1:A:1596:LEU:HA	1.77	0.41
1:A:1706:LYS:HD2	1:A:1707:ALA:O	2.21	0.41
2:B:39:LEU:HA	2:B:40:PRO:HD3	1.95	0.41
2:B:200:LEU:HD12	2:B:200:LEU:HA	1.84	0.41
2:B:203:LEU:HB3	2:B:207:LYS:NZ	2.35	0.41
2:B:734:HIS:HE1	2:B:767:TYR:OH	2.04	0.41
2:B:1061:ILE:H	2:B:1061:ILE:HG13	1.67	0.41
2:B:1345:MET:HB3	2:B:1345:MET:HE3	1.94	0.41
2:B:1433:LYS:HB3	2:B:1435:TRP:CE2	2.55	0.41
2:B:1962:VAL:HG13	2:B:1964:PHE:CD1	2.53	0.41
1:A:1192:ASP:OD1	1:A:1193:ALA:N	2.54	0.41
1:A:1280:THR:HG23	1:A:1281:MET:SD	2.60	0.41
1:A:1316:THR:O	1:A:1319:SER:OG	2.29	0.41
1:A:1587:PRO:HB3	1:A:1594:TRP:CH2	2.55	0.41
2:B:137:LEU:H	2:B:137:LEU:HD23	1.86	0.41
2:B:349:ARG:HE	2:B:349:ARG:N	2.19	0.41
2:B:512:ILE:HD13	2:B:512:ILE:HA	1.90	0.41
2:B:814:VAL:HG21	2:B:827:THR:HB	2.01	0.41
2:B:1266:ASN:HD22	2:B:1269:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1563:GLY:O	2:B:1565:ILE:HG23	2.20	0.41
2:B:1844:ALA:HA	2:B:1887:VAL:HA	2.02	0.41
2:B:1863:VAL:HA	2:B:1866:VAL:HG12	2.03	0.41
2:B:2003:THR:HG22	2:B:2005:LYS:HG2	2.02	0.41
2:B:2025:LYS:O	2:B:2028:SER:OG	2.38	0.41
1:A:688:GLY:O	1:A:874:THR:OG1	2.33	0.41
1:A:845:LEU:HA	1:A:845:LEU:HD23	1.88	0.41
1:A:1062:ASN:OD1	1:A:1063:GLY:N	2.51	0.41
1:A:1311:ASP:HB2	1:A:1405:THR:HG22	2.03	0.41
1:A:1442:ASN:OD1	1:A:1444:GLU:HG2	2.20	0.41
2:B:110:THR:O	2:B:114:VAL:HG23	2.20	0.41
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.95	0.41
2:B:892:GLY:HA2	2:B:904:MET:SD	2.61	0.41
2:B:1008:VAL:HG21	2:B:1012:ARG:NH2	2.36	0.41
2:B:1286:PHE:HA	2:B:1542:VAL:HG11	2.01	0.41
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.83	0.41
1:A:871:THR:HG22	1:A:873:GLY:N	2.35	0.41
1:A:1352:GLU:O	1:A:1356:HIS:ND1	2.48	0.41
2:B:260:HIS:CG	2:B:261:SER:H	2.39	0.41
2:B:338:LYS:O	2:B:341:GLU:HG3	2.20	0.41
2:B:1766:GLN:CG	2:B:1767:PRO:HD3	2.50	0.41
1:A:1440:LEU:HD12	1:A:1440:LEU:HA	1.92	0.41
1:A:1446:ARG:HH12	1:A:1512:GLY:HA2	1.84	0.41
2:B:271:ALA:HB3	2:B:440:LEU:HD22	2.03	0.41
2:B:1237:GLU:OE2	2:B:1242:ARG:NE	2.52	0.41
2:B:1855:ASP:OD1	2:B:1858:ALA:N	2.54	0.41
1:A:22:PHE:CE1	2:B:1826:MET:HB3	2.47	0.41
1:A:458:GLU:OE2	1:A:468:LYS:HD2	2.21	0.41
1:A:895:PHE:HB2	1:A:900:MET:HG2	2.03	0.41
1:A:1000:ILE:HD11	1:A:1662:ASP:CG	2.45	0.41
1:A:1082:ILE:HG22	1:A:1083:ASP:O	2.21	0.41
1:A:1131:PRO:HG3	1:A:1164:ARG:NE	2.24	0.41
1:A:1268:VAL:HG11	1:A:1272:ILE:HD13	2.02	0.41
1:A:1289:LEU:HA	1:A:1289:LEU:HD23	1.77	0.41
2:B:24:LEU:HD23	2:B:24:LEU:HA	1.93	0.41
2:B:43:THR:O	2:B:43:THR:OG1	2.37	0.41
2:B:89:ASN:OD1	2:B:89:ASN:C	2.63	0.41
2:B:310:MET:HE2	2:B:310:MET:HB3	1.90	0.41
2:B:475:TRP:O	2:B:479:THR:HG22	2.21	0.41
2:B:968:THR:HA	2:B:971:PHE:HB3	2.03	0.41
2:B:1053:LYS:HA	2:B:1053:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1107:ILE:HD13	2:B:1129:LEU:HD21	2.01	0.41
2:B:1405:TYR:CD2	2:B:1459:SER:HA	2.55	0.41
2:B:1476:LEU:HB3	2:B:1478:THR:HG22	2.03	0.41
1:A:91:LYS:HD2	1:A:91:LYS:HA	1.66	0.41
1:A:1210:THR:HG22	1:A:1281:MET:HG3	2.02	0.41
1:A:1435:LYS:O	1:A:1437:PRO:HD3	2.20	0.41
1:A:1613:ASN:O	1:A:1615:ASP:N	2.53	0.41
1:A:1646:SER:C	1:A:1647:PHE:HD1	2.29	0.41
2:B:727:HIS:CG	2:B:841:ILE:CD1	3.03	0.41
2:B:864:LYS:HD2	2:B:865:ASN:N	2.36	0.41
2:B:1174:LYS:HG3	2:B:1177:LYS:HD2	2.03	0.41
1:A:875:GLY:O	1:A:876:LEU:C	2.64	0.40
1:A:930:GLN:OE1	1:A:930:GLN:N	2.35	0.40
1:A:1022:PHE:HE1	1:A:1399:HIS:ND1	2.19	0.40
1:A:1191:TRP:CZ2	1:A:1215:VAL:HG21	2.55	0.40
1:A:1236:VAL:HG21	1:A:1323:LYS:HB2	2.03	0.40
1:A:1468:LEU:HD21	1:A:1492:ARG:HB3	2.03	0.40
2:B:223:VAL:O	2:B:227:VAL:HG22	2.21	0.40
2:B:258:THR:HA	2:B:444:VAL:HG13	2.03	0.40
2:B:737:ILE:HD11	2:B:772:TRP:CH2	2.56	0.40
2:B:1140:ALA:O	2:B:1144:THR:N	2.49	0.40
2:B:1251:TRP:NE1	2:B:1259:VAL:HG23	2.36	0.40
2:B:1591:VAL:O	2:B:1592:ARG:HD2	2.21	0.40
2:B:1830:VAL:HA	2:B:1968:TYR:OH	2.20	0.40
1:A:16:GLU:HG3	2:B:2026:ILE:HG23	2.03	0.40
1:A:419:ILE:HA	1:A:463:THR:HB	2.03	0.40
1:A:622:LYS:C	1:A:623:THR:O	2.63	0.40
1:A:713:SER:O	1:A:717:THR:HG23	2.21	0.40
2:B:134:SER:OG	2:B:136:LEU:HD22	2.22	0.40
2:B:481:HIS:ND1	2:B:483:ALA:N	2.68	0.40
2:B:727:HIS:ND1	2:B:841:ILE:HD12	2.35	0.40
2:B:1002:PRO:HG2	2:B:1019:LYS:HG2	2.03	0.40
2:B:1112:VAL:N	2:B:1173:ASP:OD1	2.55	0.40
2:B:1512:GLU:OE1	2:B:1512:GLU:N	2.54	0.40
1:A:12:THR:O	1:A:15:THR:OG1	2.36	0.40
1:A:45:ILE:HA	1:A:79:LEU:O	2.21	0.40
1:A:686:GLY:N	3:A:1901:NAP:O3B	2.55	0.40
1:A:726:ARG:HH11	1:A:1632:ARG:NE	2.20	0.40
1:A:1171:LEU:HA	1:A:1171:LEU:HD23	1.69	0.40
1:A:1737:LYS:O	1:A:1741:SER:OG	2.23	0.40
2:B:96:SER:HB2	2:B:100:LYS:NZ	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1359:SER:OG	2:B:1360:THR:N	2.54	0.40
2:B:1874:LEU:HD13	2:B:1895:LEU:CD1	2.51	0.40
1:A:711:ARG:O	1:A:711:ARG:HG2	2.21	0.40
1:A:1288:LEU:HD23	1:A:1288:LEU:HA	1.90	0.40
2:B:147:VAL:O	2:B:486:ILE:HA	2.21	0.40
2:B:322:PRO:HA	2:B:407:PHE:CD2	2.56	0.40
2:B:581:VAL:O	2:B:582:ALA:C	2.62	0.40
2:B:657:ARG:HD3	2:B:686:GLY:O	2.20	0.40
2:B:688:THR:HG21	2:B:1232:PHE:HZ	1.86	0.40
2:B:865:ASN:OD1	2:B:865:ASN:N	2.55	0.40
2:B:1425:LYS:O	2:B:1429:VAL:HG23	2.21	0.40
1:A:926:ASN:OD1	1:A:929:LEU:HB2	2.21	0.40
2:B:49:ASP:OD2	2:B:50:ASP:N	2.55	0.40
2:B:357:LEU:HB2	2:B:365:VAL:HB	2.04	0.40
2:B:464:VAL:O	2:B:468:ILE:HG13	2.21	0.40
2:B:1003:VAL:HA	2:B:1004:PRO:HD3	1.90	0.40
2:B:1435:TRP:HE3	2:B:1487:VAL:HG13	1.86	0.40
2:B:1508:LYS:HE3	2:B:1508:LYS:HB2	1.86	0.40
2:B:1566:THR:HB	2:B:1602:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1427/1722 (83%)	1306 (92%)	115 (8%)	6 (0%)	30	60
2	B	2031/2037 (100%)	1860 (92%)	168 (8%)	3 (0%)	48	75
All	All	3458/3759 (92%)	3166 (92%)	283 (8%)	9 (0%)	37	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	879	ALA
2	B	582	ALA
1	A	623	THR
1	A	876	LEU
2	B	727	HIS
1	A	878	SER
1	A	1006	GLU
1	A	1005	PRO
2	B	583	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1222/1445 (85%)	1215 (99%)	7 (1%)	78	81
2	B	1780/1784 (100%)	1777 (100%)	3 (0%)	87	88
All	All	3002/3229 (93%)	2992 (100%)	10 (0%)	84	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	623	THR
1	A	625	ILE
1	A	626	ILE
1	A	660	LEU
1	A	876	LEU
1	A	877	MET
1	A	1636	THR
2	B	293	ILE
2	B	584	MET
2	B	1667	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	40	ASN
1	A	450	GLN
1	A	473	GLN
1	A	529	GLN
1	A	794	HIS
1	A	968	ASN
1	A	1064	ASN
1	A	1126	GLN
1	A	1127	HIS
1	A	1144	HIS
1	A	1430	HIS
1	A	1562	ASN
1	A	1613	ASN
2	B	16	HIS
2	B	68	ASN
2	B	130	ASN
2	B	171	GLN
2	B	187	GLN
2	B	282	ASN
2	B	317	ASN
2	B	335	GLN
2	B	379	ASN
2	B	572	GLN
2	B	734	HIS
2	B	799	HIS
2	B	872	ASN
2	B	884	ASN
2	B	959	ASN
2	B	960	GLN
2	B	1000	GLN
2	B	1043	HIS
2	B	1066	HIS
2	B	1122	ASN
2	B	1153	HIS
2	B	1338	HIS
2	B	1403	ASN
2	B	1688	ASN
2	B	1702	ASN
2	B	1868	ASN
2	B	1883	ASN
2	B	1965	HIS
2	B	1977	GLN

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Mol	Chain	Res	Type
2	B	2035	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 [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$
3	NAP	A	1901	-	50,52,52	1.17	4 (8%)	71,80,80	1.55	10 (14%)
4	FMN	B	2101	-	33,33,33	6.45	22 (66%)	48,50,50	1.35	6 (12%)
3	NAP	B	2102	-	50,52,52	1.16	4 (8%)	71,80,80	1.55	9 (12%)

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	NAP	A	1901	-	-	11/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	B	2101	-	-	5/18/18/18	0/3/3/3
3	NAP	B	2102	-	-	5/35/67/67	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C6-C7	13.57	1.58	1.39
4	B	2101	FMN	C6-C5A	12.37	1.58	1.40
4	B	2101	FMN	C9-C9A	12.34	1.59	1.39
4	B	2101	FMN	C9-C8	11.96	1.55	1.39
4	B	2101	FMN	O4-C4	9.98	1.42	1.23
4	B	2101	FMN	C4A-N5	9.55	1.51	1.30
4	B	2101	FMN	C9A-C5A	8.75	1.55	1.41
4	B	2101	FMN	O2-C2	8.23	1.40	1.24
4	B	2101	FMN	C2-N1	7.46	1.53	1.36
4	B	2101	FMN	C10-N1	7.13	1.47	1.33
4	B	2101	FMN	C8-C7	7.06	1.58	1.40
4	B	2101	FMN	C10-N10	6.66	1.51	1.37
4	B	2101	FMN	C5A-N5	6.52	1.51	1.39
4	B	2101	FMN	C2-N3	6.15	1.52	1.39
4	B	2101	FMN	C4-N3	6.14	1.50	1.38
4	B	2101	FMN	C9A-N10	5.19	1.50	1.41
3	B	2102	NAP	C5A-C4A	4.70	1.47	1.39
3	A	1901	NAP	C5A-C4A	4.69	1.47	1.39
4	B	2101	FMN	C4A-C10	3.65	1.54	1.44
4	B	2101	FMN	C1'-C2'	3.09	1.56	1.52
4	B	2101	FMN	P-O2P	3.05	1.66	1.54
3	B	2102	NAP	C5A-C6A	2.75	1.48	1.41
3	A	1901	NAP	C5A-C6A	2.74	1.48	1.41
4	B	2101	FMN	P-O3P	2.72	1.64	1.54
4	B	2101	FMN	C4A-C4	2.41	1.53	1.44
3	A	1901	NAP	C8A-N7A	2.37	1.36	1.31
3	B	2102	NAP	C8A-N7A	2.36	1.36	1.31
3	B	2102	NAP	C5A-N7A	-2.26	1.35	1.39
3	A	1901	NAP	C5A-N7A	-2.22	1.35	1.39
4	B	2101	FMN	C7M-C7	2.04	1.54	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	C5A-C4A-N3A	-5.84	118.67	126.72
3	B	2102	NAP	C5A-C4A-N3A	-5.83	118.69	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	N3A-C4A-N9A	4.58	134.96	127.17
3	B	2102	NAP	N3A-C4A-N9A	4.57	134.94	127.17
3	B	2102	NAP	C2A-N3A-C4A	3.71	120.88	111.83
3	A	1901	NAP	C2A-N3A-C4A	3.70	120.87	111.83
4	B	2101	FMN	C4'-C3'-C2'	-3.58	107.61	113.57
3	A	1901	NAP	C4A-C5A-N7A	-3.52	106.56	110.58
3	B	2102	NAP	C4A-C5A-N7A	-3.49	106.60	110.58
3	B	2102	NAP	N3A-C2A-N1A	-3.23	123.69	128.58
3	A	1901	NAP	N3A-C2A-N1A	-3.22	123.71	128.58
4	B	2101	FMN	C4A-C10-N10	3.03	120.83	116.48
4	B	2101	FMN	C10-C4A-N5	-2.77	119.15	124.81
3	A	1901	NAP	C4A-N9A-C8A	2.58	108.44	105.74
3	B	2102	NAP	C5A-N7A-C8A	2.56	107.47	103.45
3	A	1901	NAP	C5A-N7A-C8A	2.55	107.47	103.45
3	B	2102	NAP	C4A-N9A-C8A	2.54	108.40	105.74
3	B	2102	NAP	C2B-C1B-N9A	-2.44	109.73	113.75
4	B	2101	FMN	C4-N3-C2	-2.44	121.31	125.64
3	A	1901	NAP	C2B-C1B-N9A	-2.42	109.77	113.75
3	A	1901	NAP	C6A-C5A-N7A	2.10	136.13	132.09
3	B	2102	NAP	C6A-C5A-N7A	2.08	136.10	132.09
4	B	2101	FMN	O2-C2-N1	-2.03	118.44	121.80
4	B	2101	FMN	C5A-C9A-N10	2.02	119.79	117.97
3	A	1901	NAP	C4D-O4D-C1D	2.00	111.76	109.92

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	NAP	C5B-O5B-PA-O1A
3	A	1901	NAP	C5D-O5D-PN-O3
3	A	1901	NAP	C5D-O5D-PN-O1N
3	A	1901	NAP	C5D-O5D-PN-O2N
3	B	2102	NAP	C5D-O5D-PN-O1N
4	B	2101	FMN	C2'-C3'-C4'-C5'
4	B	2101	FMN	O3'-C3'-C4'-C5'
3	A	1901	NAP	O4B-C4B-C5B-O5B
3	A	1901	NAP	O4D-C4D-C5D-O5D
3	A	1901	NAP	C3D-C4D-C5D-O5D
4	B	2101	FMN	C2'-C3'-C4'-O4'
3	A	1901	NAP	C3B-C4B-C5B-O5B
4	B	2101	FMN	O3'-C3'-C4'-O4'
3	A	1901	NAP	PA-O3-PN-O5D

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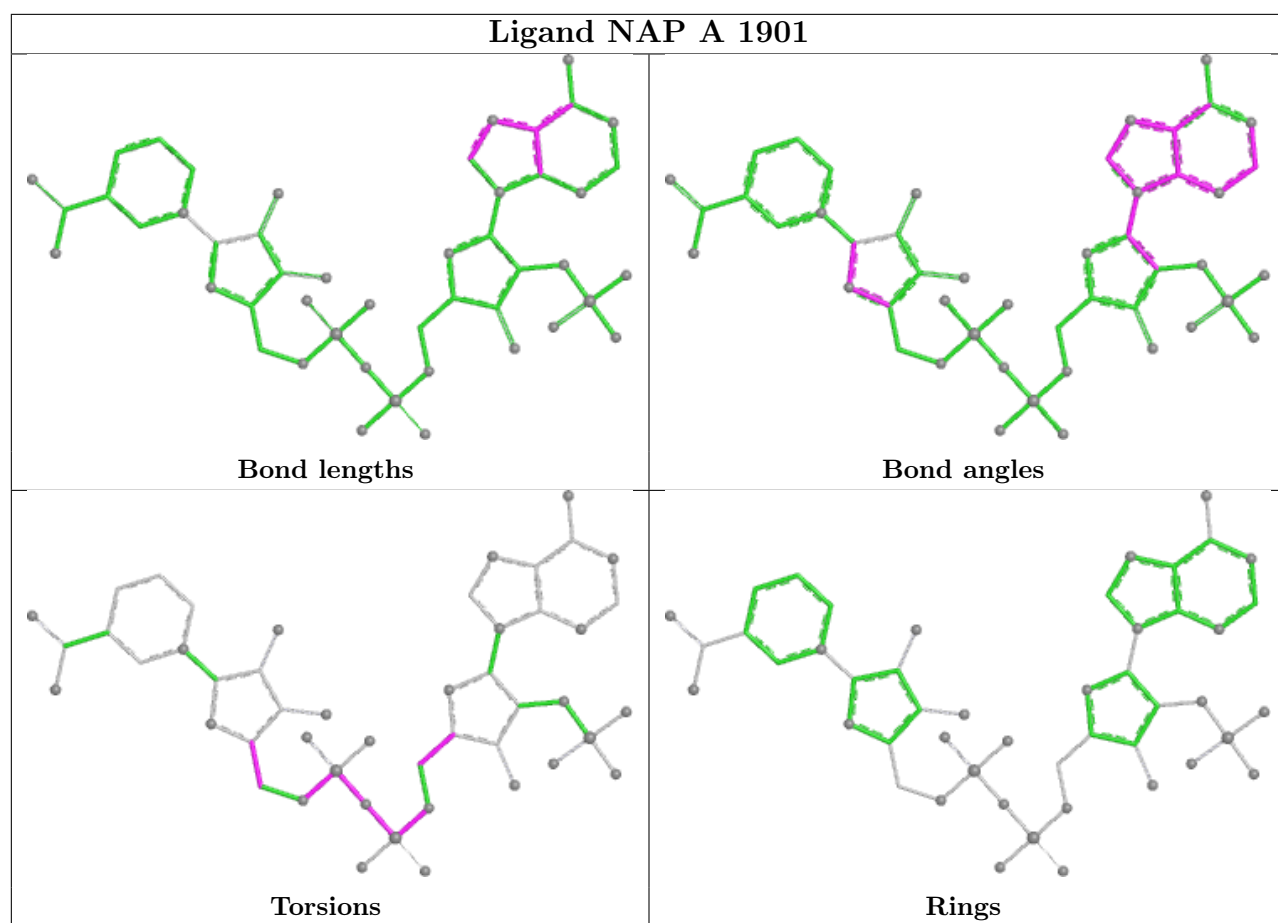
Mol	Chain	Res	Type	Atoms
3	B	2102	NAP	C3B-C4B-C5B-O5B
3	A	1901	NAP	PN-O3-PA-O2A
3	B	2102	NAP	C4D-C5D-O5D-PN
3	B	2102	NAP	PA-O3-PN-O2N
3	A	1901	NAP	PN-O3-PA-O1A
4	B	2101	FMN	C4'-C5'-O5'-P
3	B	2102	NAP	PA-O3-PN-O1N

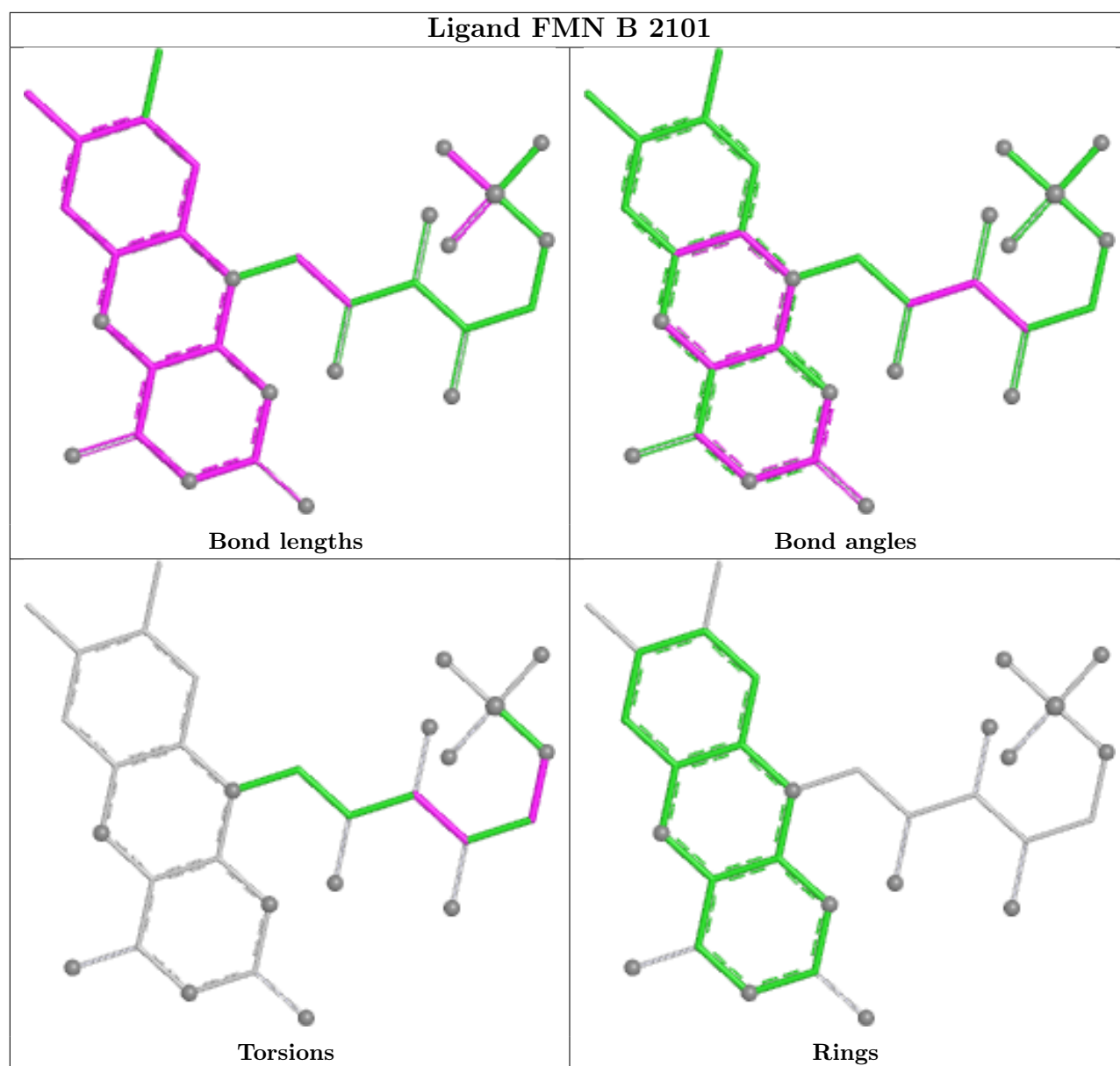
There are no ring outliers.

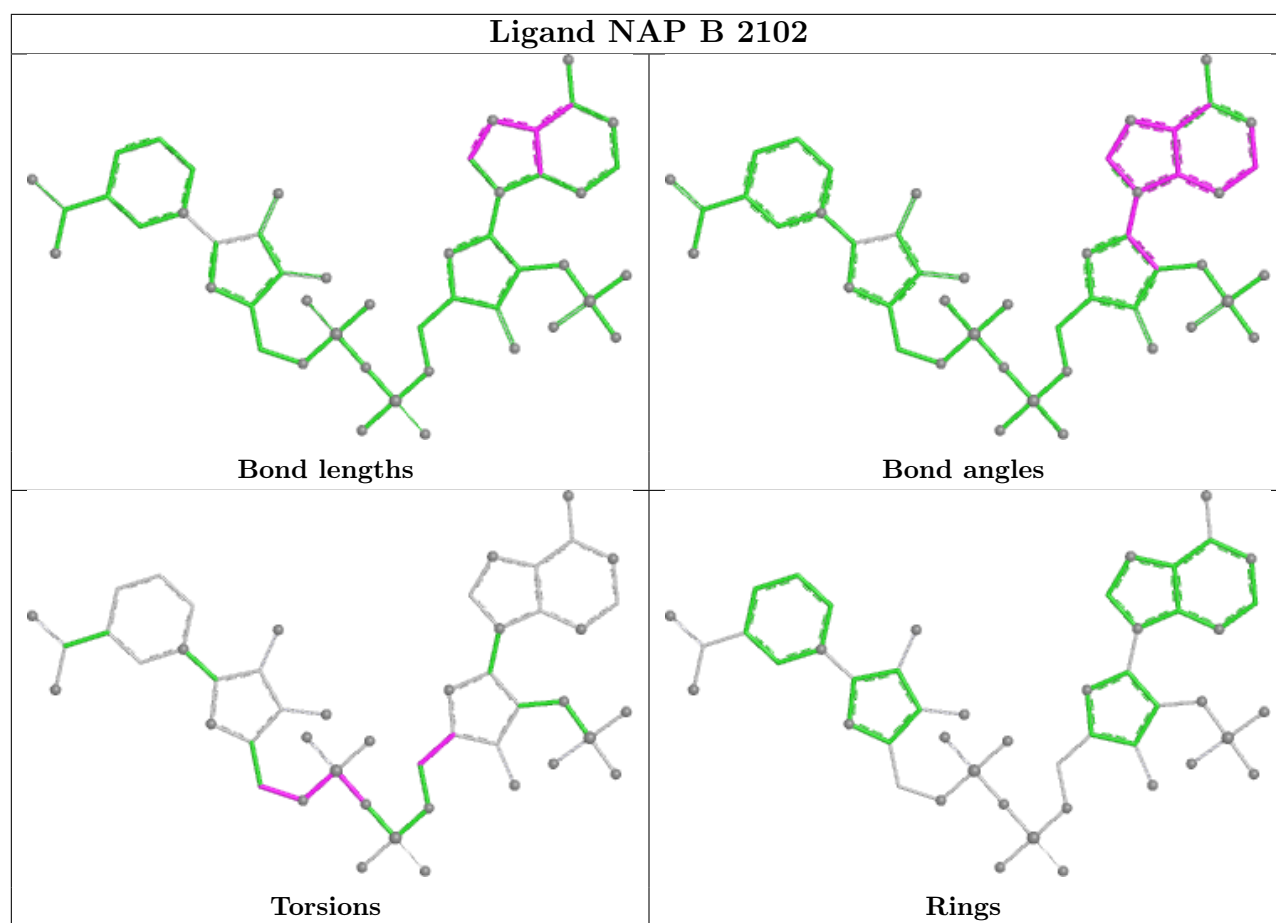
3 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1901	NAP	34	0
4	B	2101	FMN	50	0
3	B	2102	NAP	49	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.

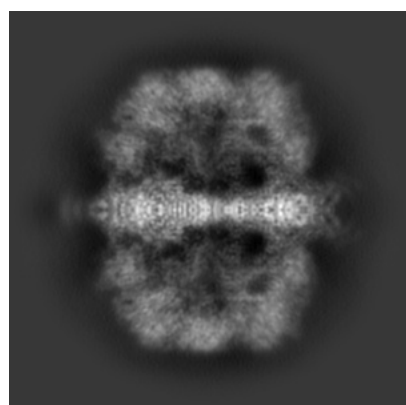
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20658. These allow visual inspection of the internal detail of the map and identification of artifacts.

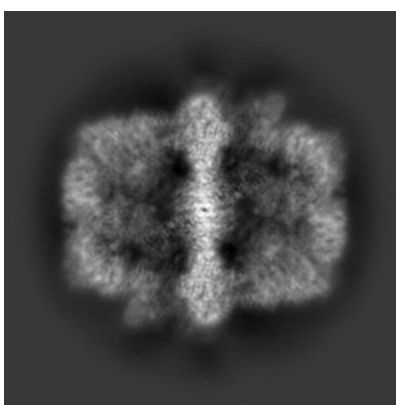
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

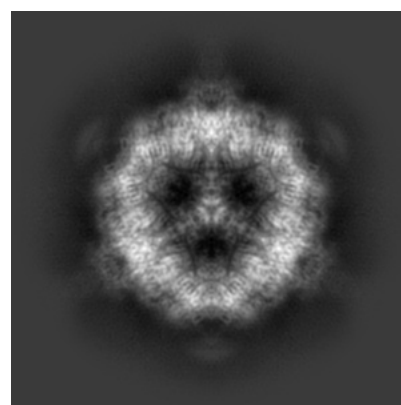
6.1.1 Primary map



X



Y

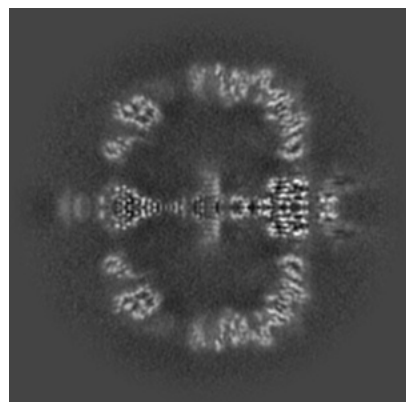


Z

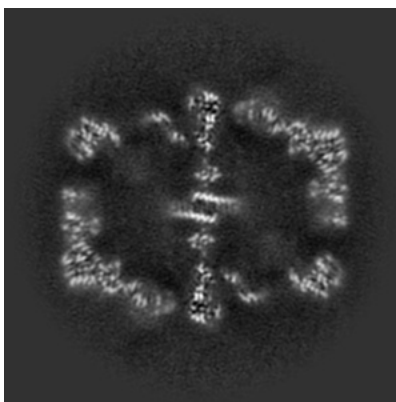
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

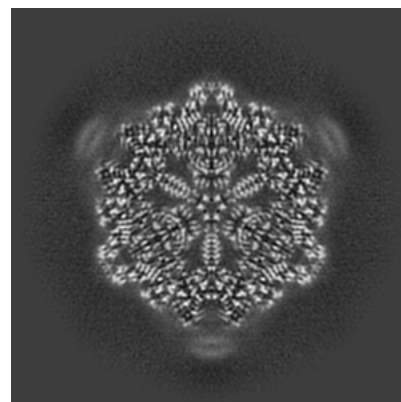
6.2.1 Primary map



X Index: 176



Y Index: 176

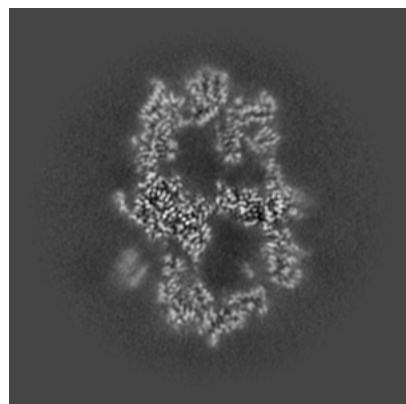


Z Index: 176

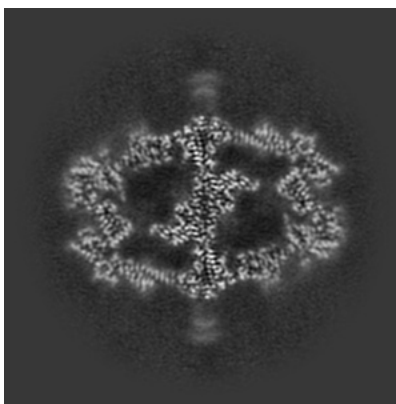
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

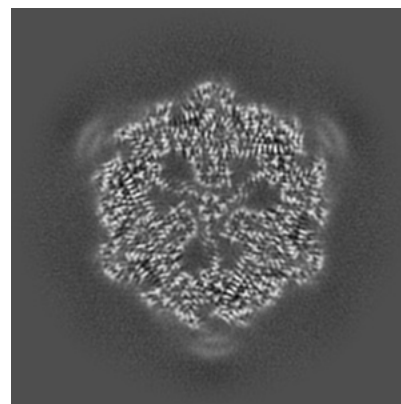
6.3.1 Primary map



X Index: 237



Y Index: 231

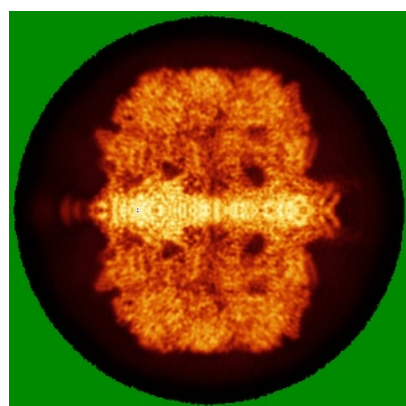


Z Index: 172

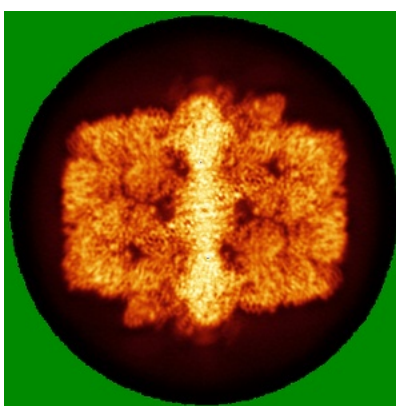
The images above show the largest variance slices of the map in three orthogonal directions.

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

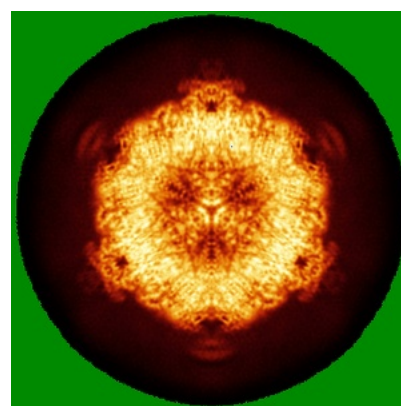
6.4.1 Primary map



X



Y

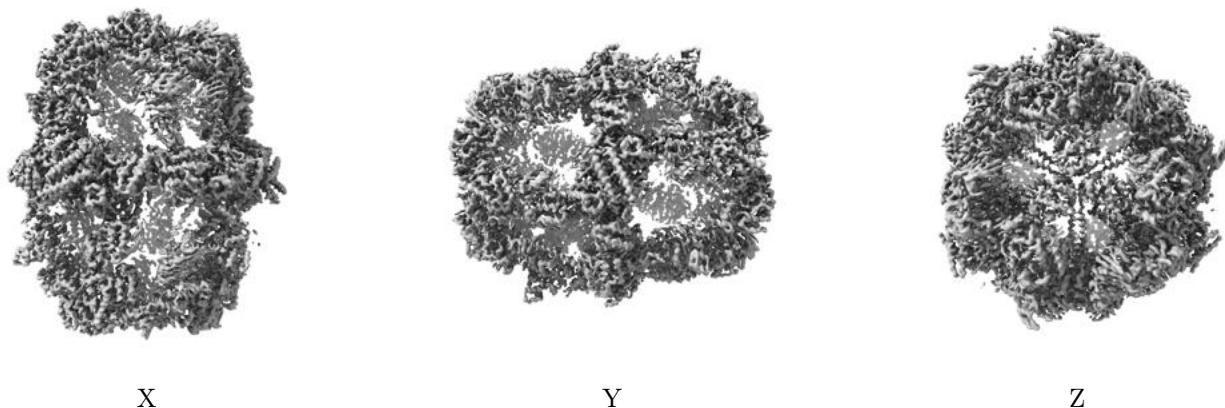


Z

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 0.704. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

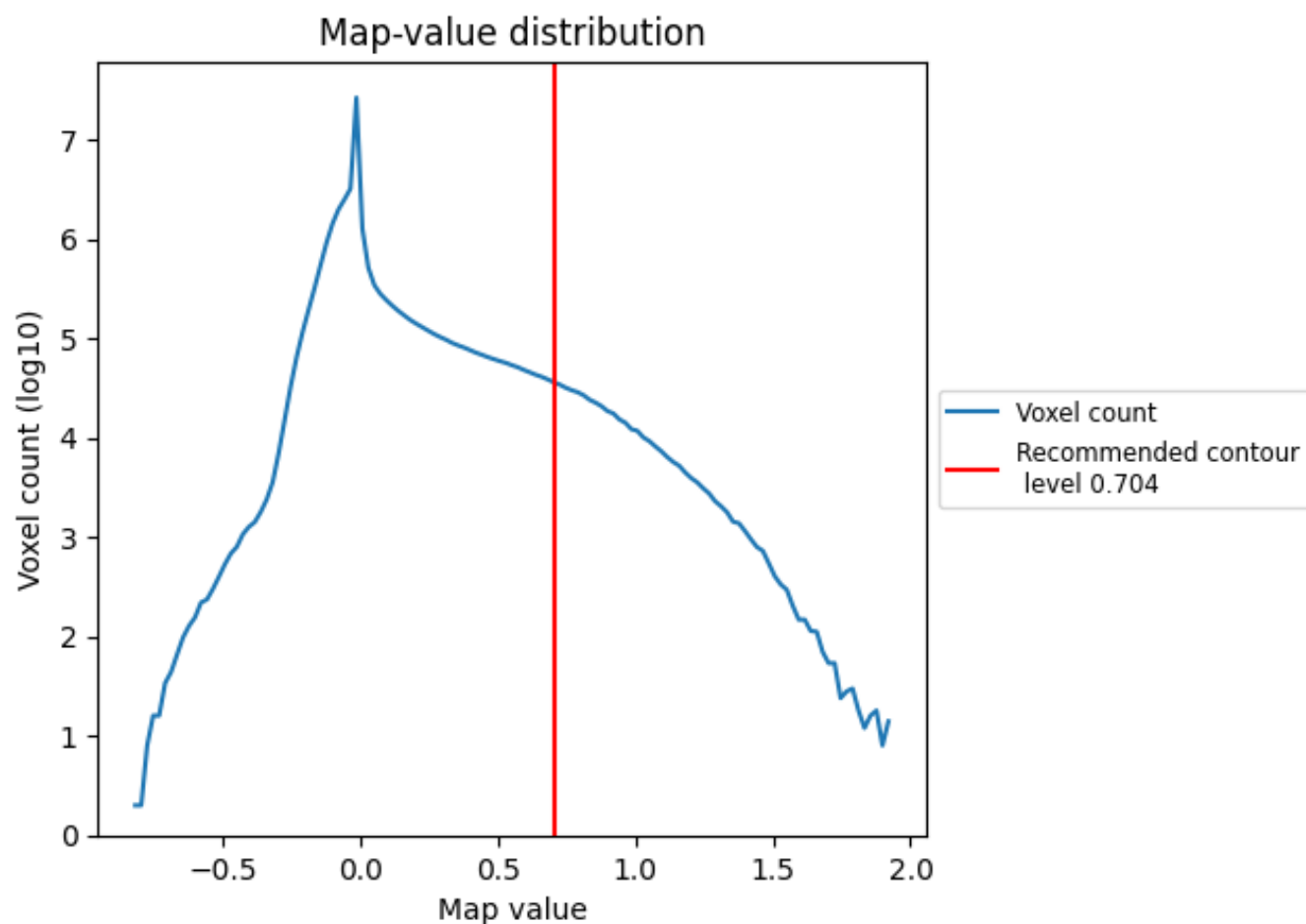
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

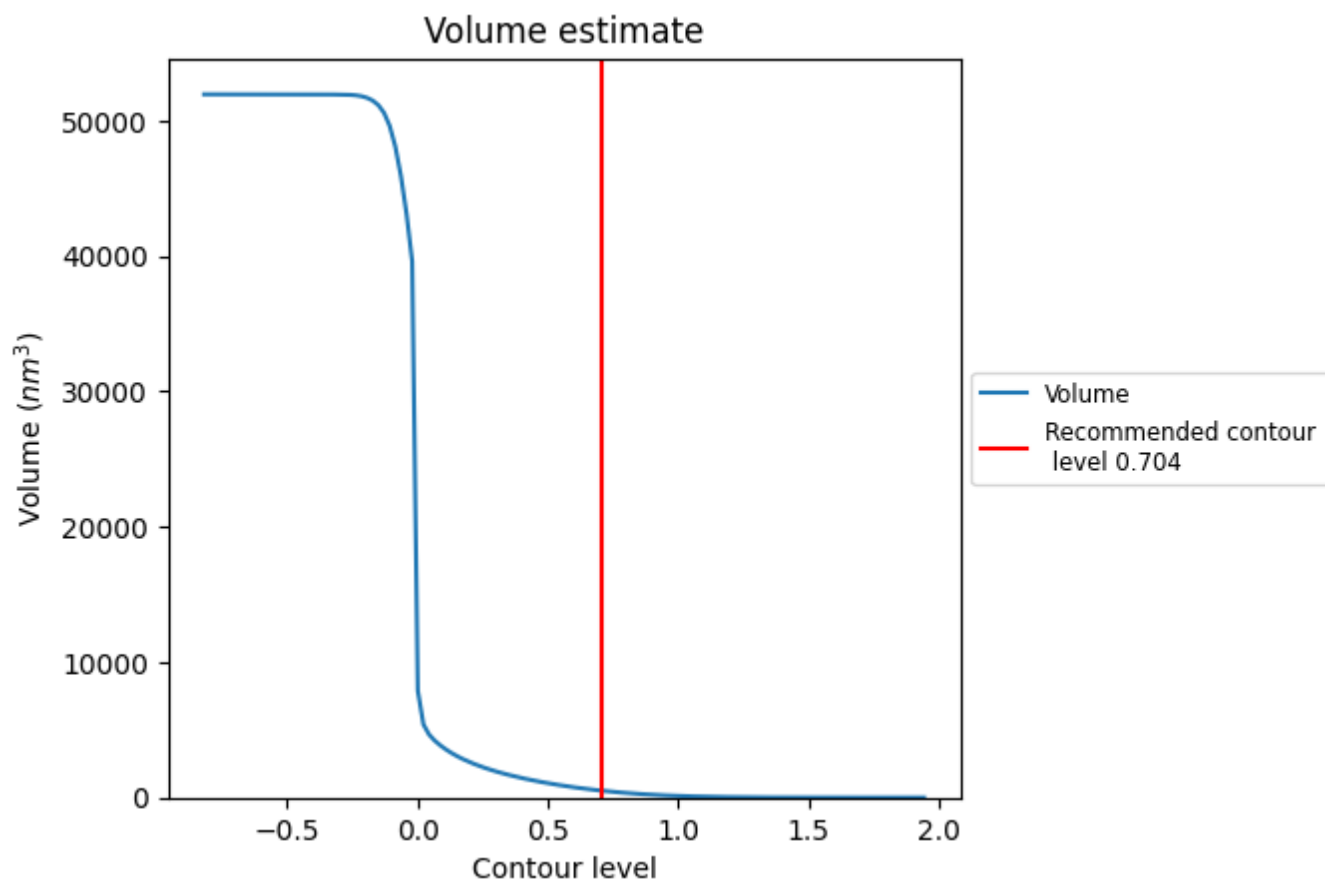
This section contains the results of statistical analysis of the map.

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.

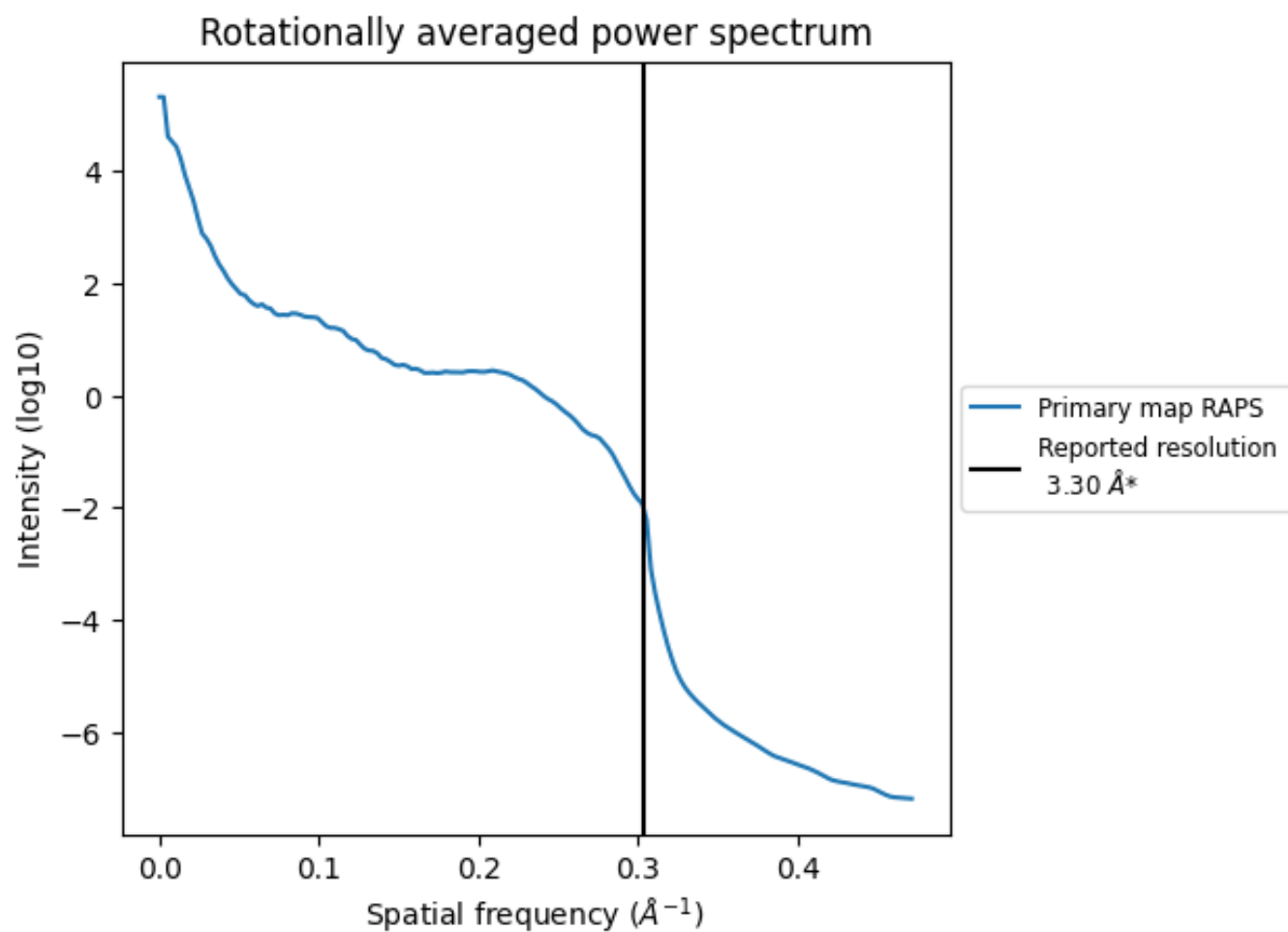
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 513 nm³; this corresponds to an approximate mass of 464 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 0.303 Å⁻¹

8 Fourier-Shell correlation ⓘ

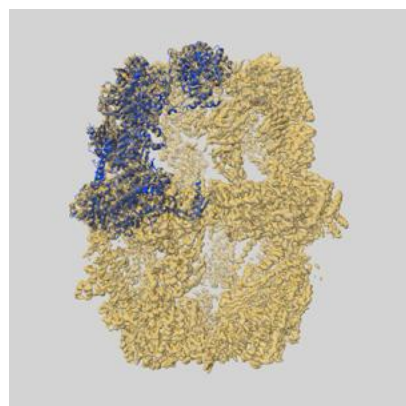
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

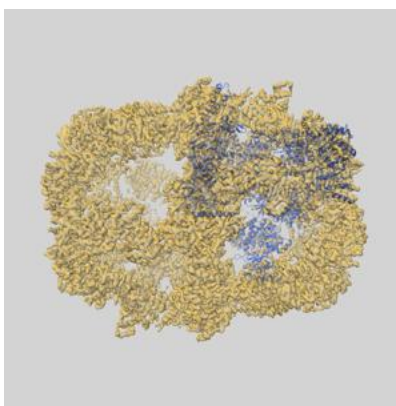
This section contains information regarding the fit between EMDB map EMD-20658 and PDB model 6U5W. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

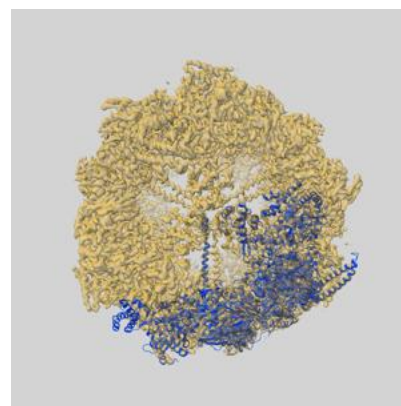
9.1.1 Map-model overlay ⓘ



X



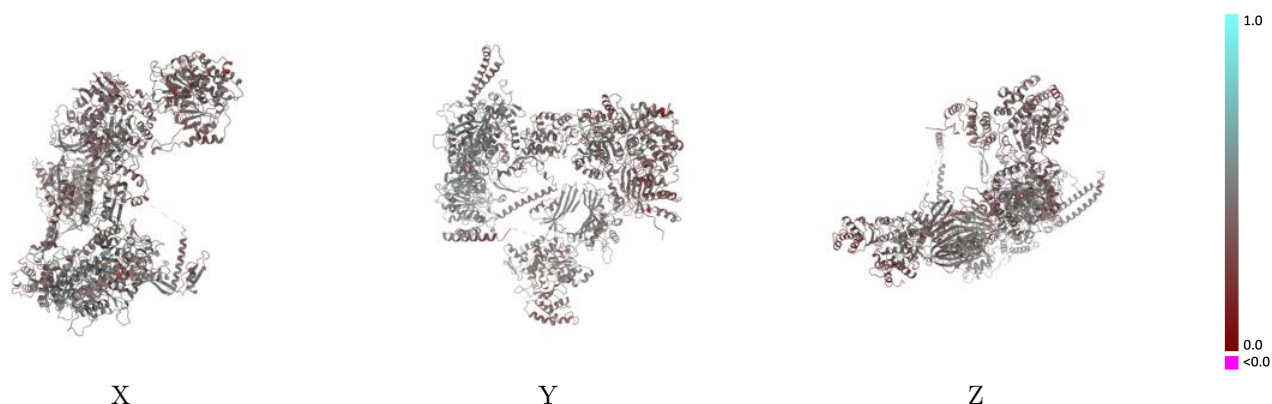
Y



Z

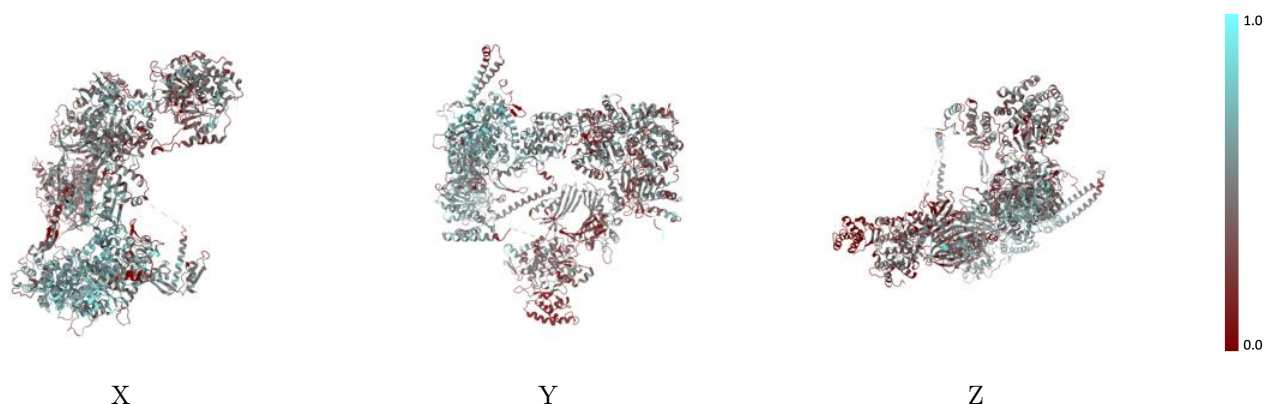
The images above show the 3D surface view of the map at the recommended contour level 0.704 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



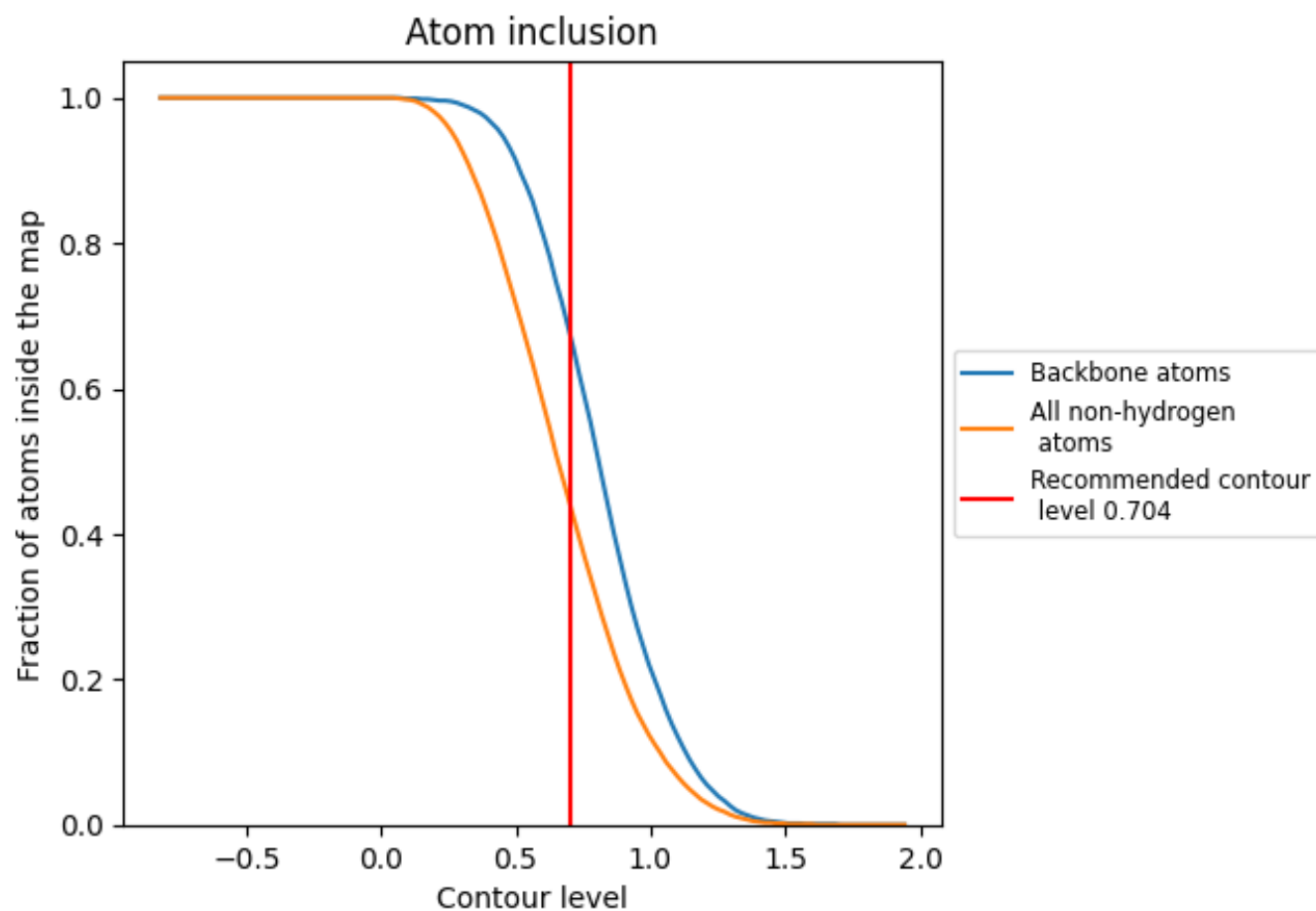
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.704).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 44% 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 (0.704) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4360	0.4280
A	0.5230	0.4560
B	0.3760	0.4080

