



## Full wwPDB EM Validation Report ⓘ

May 28, 2026 – 04:12 PM JST

PDB ID : 9VM4 / pdb\_00009vm4  
EMDB ID : EMD-65176  
Title : Structure of DOCK6-Rac1 complex protomer  
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Yonemochi, M.;  
Hanada, K.; Shirouzu, M.  
Deposited on : 2025-06-27  
Resolution : 4.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

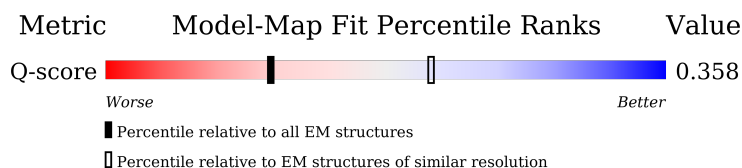
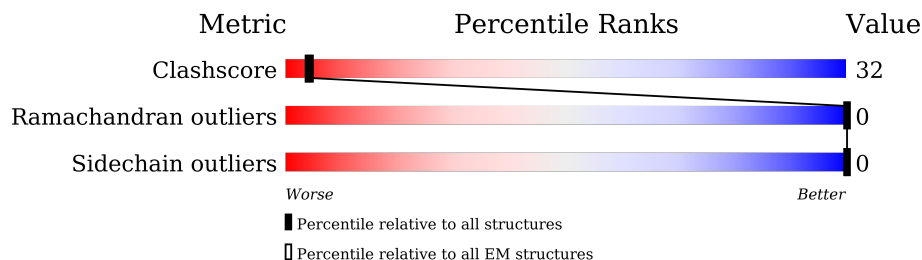
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


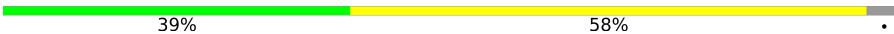
The reported resolution of this entry is 4.20 Å.

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	5410 ( 3.70 - 4.70 )

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  $\geq 3$ , 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	2053	
2	B	184	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14856 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 Deducator of cytokinesis protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1688	Total	C	N	O	S	0	0
			13471	8606	2331	2475	59		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q96HP0
A	-4	GLY	-	expression tag	UNP Q96HP0
A	-3	SER	-	expression tag	UNP Q96HP0
A	-2	GLY	-	expression tag	UNP Q96HP0
A	-1	GLY	-	expression tag	UNP Q96HP0
A	0	SER	-	expression tag	UNP Q96HP0

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 1.

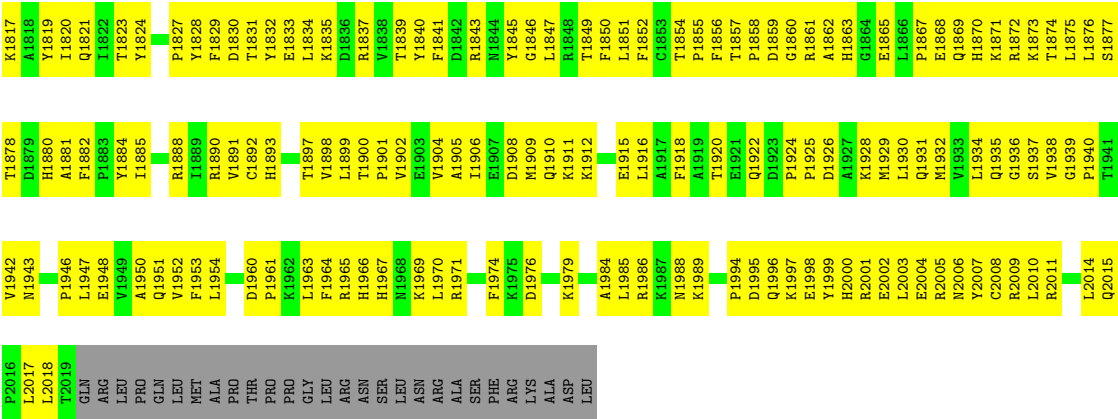
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	expression tag	UNP P63000
B	-5	SER	-	expression tag	UNP P63000
B	-4	SER	-	expression tag	UNP P63000
B	-3	GLY	-	expression tag	UNP P63000
B	-2	SER	-	expression tag	UNP P63000
B	-1	SER	-	expression tag	UNP P63000
B	0	GLY	-	expression tag	UNP P63000
B	15	ALA	GLY	engineered mutation	UNP P63000

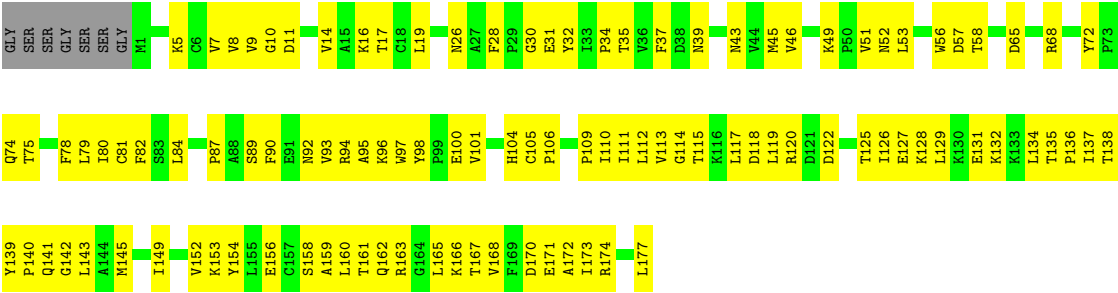


Y1751	E1680	R1587	E1523	L1450	L1168	SER	H1020	L946	LYS	L730
F1752	L1691	Q1590	R1526	E1463	L1169	SER	Y1021	L947	SER	V731
F1753	G1682	E1454	R1527	E1454	S1170	Q1037	Q1022	L948	ILE	H732
G1755	G1685	R1596	S1528	E1457	I1171	DI1090	A1025	R951	SER	V733
F1756	E1688	H1602	L1529	E1457	T1175	PI1091	A1025	R951	SER	L734
Y1757	Q1689	M1603	K1530	D1461	L1176	K1092	T1026	T954	ASN	F741
F1761	A1690	T1531	T1532	L1462	L1179	V1093	R1027	P955	PRO	R742
G1762	F1694	H1607	L1533	C1463	H1180	T1094	L1028	P956	ASP	R743
D1763	F1694	A1608	T1534	L1464	H1180	M1095	Q1029	R957	LEU	K744
L1764	E1698	E1609	Y1535	R1465	E1184	M1096	S1030	L958	ALA	D745
D1765	G1698	L1610	A1586	L1466	GLY	F1097	S1031	R959	VAL	T746
E1766	L1699	G1611	E1537	L1467	PRO	E1098	PI034	F960	ALA	V747
Q1767	E1700	M1612	E1538	R1468	GLY	L1099	A1035	L965	PRO	L748
E1768	E1701	E1615	D1539	E1468	GLY	S1100	A1035	D966	GLY	S749
F1769	A1702	L1616	M1540	R1473	ARG	R1104	A1036	D967	SER	P850
V1770	V1703	G1541	G1541	R1473	ARG	Q1105	L1037	Q831	ASP	Q831
N1771	N1704	A1617	L1542	I1474	SER	Q1106	L1038	L971	VAL	N752
K1772	E1705	Q1618	R1543	T1475	ARG	Q1106	T1039	V972	ASP	V753
E1773	V1706	E1619	F1543	S1475	LEU	L1109	L1040	G973	E898	E754
P1774	Y1707	M1620	T1546	T1476	ALA	A1110	R1041	R973	Y835	Q755
S1775	K1708	V1621	F1547	T1477	SER	G1111	M1042	S974	V836	Q756
T1776	N1709	H1622	F1547	R1478	MET	GLI111	E1043	V975	H837	E756
T1777	L1710	A1623	Q1550	L1479	GLU	L1112	F1044	E978	Y838	L757
K1778	I1711	Q1551	V1551	H1480	ASP	ASP	T1045	V979	F840	R758
L1779	P1712	V1552	V1552	A1408	SER	T1115	R1046	V979	R841	L764
A1780	I1713	D1553	D1553	R1409	ASP	E1116	I1047	T981	L842	A767
E1781	L1714	L1554	L1554	Y1486	THR	E1117	S1050	R982	E910	
I1782	E1715	M1555	M1555	Y1486	GLY	L1121	GLY	R983	E911	
S1783	A1716	F1556	F1556	Y1487	GLY	L1121	H1053	H984	L912	SER
H1784	H1717	R1638	R1557	L1417	GLY	E1124	Y1054	K985	A913	LEU
R1785	H1639	H1639	L1558	L1417	ASP	ASP	PI060	D986	L914	PRO
L1786	L1640	L1640	L1559	Q1491	ILE	ILE	M1059	E988	Q915	GLY
E1787	S1646	S1647	M1560	F1492	ALA	A1128	PI060	V987	V917	ALA
F1788	Q1648	Q1648	I1561	F1493	THR	F1129	PI060	E992	V918	PRO
Y1790	M1649	M1649	L1562	T1495	GLY	L1130	C1061	H992	S919	PRO
T1791	G1728	I1650	T1563	G1496	THR	L1131	C1062	L993	S920	VAL
E1792	L1730	S1651	D1564	H1497	ILE	H1132	C1063	N994	THR	K762
R1793	K1731	S1652	V1565	M1498	ASN	K1133	L1064	F999	R924	L763
F1794	E1732	M1653	K1567	F1499	VAL	A1135	S1065	F999	E925	V784
V1798	E1733	V1654	K1568	V1502	VAL	V1139	PRO	F1000	A926	ALA
F1799	F1734	L1655	K1569	M1503	ALA	L1143	PRO	L1001	I927	ALA
E1800	T1735	E1656	E1570	M1504	ALA	L1143	SER	S1002	L928	THR
I1801	K1736	E1657	H1571	Q1505	ILE	DI149	PRO	D1003	Q929	LEU
I1802	I1737	S1658	T1507	V1506	ALA	DI149	SER	L1004	H930	ALA
K1803	M1738	A1659	T1507	T1507	GLY	Y1152	PRO	L1005	A931	ARG
D1804	H1739	Q1662	S1509	S1509	GLY	A1153	VAL	S1006	W932	GLY
S1805	Q1740	D1662	L1510	L1437	PRO	E1154	SER	D1009	F934	GLY
N1806	S1741	D1663	S1511	L1437	LEU	E1154	SER	G1010	F935	ARG
	G1743	I1664	S1512	Q1440	ALA	V1157	THR	F1012	Q936	PRO
D1809	W1744	I1668	S1516	Q1440	PRO	GLY	THR	F1013	L937	ALA
K1812	V1747	D1668	T1516	A1442	SER	R1160	SER	F1014	M938	SER
L1813	F1748	G1675	T1517	L1443	ARG	E1163	GLN	S1015	W939	LEU
D1814	G1749	K1676	Q1518	F1447	ALA	E1163	SER	S1016	K940	TYR
S1815	H1677	H1677	M1519	P1448	SER	L1166	THR	L1017	S941	LEU
Q1816	T1750	F1678	E1522	E1449	ILE	PI167	THR	R1018	A943	ALA
					THR		PHE	A1019		SER



● Molecule 2: Ras-related C3 botulinum toxin substrate 1

Chain B: 39% 58%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	313646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.044	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	319.2, 319.2, 319.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	0/13787	0.54	0/18706
2	B	0.26	0/1415	0.50	0/1924
All	All	0.39	0/15202	0.53	0/20630

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13471	0	13448	857	0
2	B	1385	0	1407	110	0
All	All	14856	0	14855	943	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 32.

All (943) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1551:VAL:HG12	1:A:1555:MET:HE1	1.43	0.97
1:A:346:LEU:HA	1:A:392:MET:HE1	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:HB3	1:A:296:PHE:HB3	1.53	0.88
1:A:1789:PHE:O	1:A:1793:ARG:NH1	2.06	0.87
1:A:792:ILE:HG22	1:A:797:ILE:HG12	1.57	0.86
1:A:1441:ARG:NH1	1:A:1484:SER:OG	2.09	0.86
1:A:1650:ILE:O	1:A:1845:TYR:OH	1.92	0.86
1:A:1653:ASN:HD21	1:A:1881:ALA:H	1.22	0.84
1:A:571:ALA:HB3	1:A:638:TYR:HB2	1.58	0.84
1:A:1802:ILE:HG21	1:A:1821:GLN:HG3	1.60	0.83
1:A:1869:GLN:NE2	1:A:1870:HIS:O	2.13	0.82
1:A:1421:LEU:O	1:A:1465:ARG:NH2	2.13	0.81
1:A:244:VAL:O	1:A:246:ARG:NH1	2.14	0.81
1:A:1966:HIS:HA	1:A:1969:LYS:HE2	1.63	0.80
1:A:1574:ASP:OD2	1:A:1577:MET:N	2.11	0.79
2:B:8:VAL:HA	2:B:79:LEU:HB2	1.64	0.79
1:A:1512:SER:O	1:A:1516:THR:OG1	2.01	0.78
1:A:1943:ASN:ND2	2:B:35:THR:O	2.16	0.78
1:A:1877:SER:HB2	1:A:1893:HIS:HB3	1.66	0.77
1:A:956:ARG:HD3	1:A:959:ARG:HE	1.50	0.77
1:A:674:LEU:N	1:A:707:PHE:O	2.15	0.77
1:A:1967:HIS:HA	1:A:1970:LEU:HD12	1.68	0.76
1:A:1780:ALA:O	1:A:1784:HIS:ND1	2.18	0.76
1:A:508:HIS:HA	1:A:520:PRO:HD2	1.68	0.75
1:A:1878:THR:HG22	1:A:1891:VAL:HA	1.69	0.75
1:A:1529:LEU:HD22	1:A:1555:MET:HG3	1.67	0.75
1:A:1809:ASP:HB3	1:A:1812:LYS:HE3	1.69	0.74
1:A:291:LYS:NZ	1:A:293:SER:O	2.18	0.74
1:A:837:HIS:O	1:A:940:LYS:NZ	2.20	0.74
1:A:555:PRO:HA	1:A:709:VAL:HG23	1.70	0.74
1:A:246:ARG:O	1:A:826:ARG:NH1	2.20	0.74
1:A:1529:LEU:HA	1:A:1532:ILE:HD12	1.70	0.74
1:A:629:GLU:O	1:A:632:HIS:NE2	2.18	0.74
1:A:487:ARG:HH22	1:A:491:PRO:HD3	1.50	0.73
1:A:1582:MET:HE2	1:A:1603:MET:HG2	1.69	0.73
1:A:1111:GLY:O	1:A:1115:THR:OG1	2.03	0.73
1:A:309:LEU:HD22	1:A:388:GLY:HA2	1.69	0.73
1:A:946:LEU:HD22	1:A:959:ARG:HH11	1.53	0.73
1:A:1403:VAL:HG13	1:A:1409:ARG:HE	1.52	0.73
2:B:158:SER:O	2:B:162:GLN:N	2.22	0.73
1:A:1906:ILE:HA	1:A:1909:MET:HE2	1.69	0.72
1:A:467:LEU:HD11	1:A:475:PHE:HE2	1.54	0.72
1:A:63:ARG:NH1	1:A:1062:CYS:SG	2.63	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:N	1:A:157:ASP:OD2	2.23	0.71
1:A:1916:LEU:O	1:A:1920:THR:OG1	2.04	0.71
1:A:227:ARG:NH2	1:A:1387:GLU:OE1	2.20	0.71
1:A:1012:PHE:O	1:A:1015:SER:OG	2.07	0.71
1:A:1553:ASP:O	1:A:1557:ASN:ND2	2.22	0.71
1:A:1580:ASP:OD2	1:A:1584:ARG:NH2	2.23	0.71
2:B:94:ARG:HB3	2:B:145:MET:HE1	1.73	0.71
2:B:11:ASP:OD1	2:B:97:TRP:NE1	2.23	0.71
1:A:988:GLU:O	1:A:992:HIS:ND1	2.23	0.71
1:A:1412:VAL:O	1:A:1416:VAL:HG23	1.91	0.71
1:A:319:SER:O	1:A:530:LYS:NZ	2.24	0.70
1:A:1837:ARG:NH1	1:A:1845:TYR:O	2.25	0.70
2:B:114:GLY:HA3	2:B:156:GLU:HG2	1.73	0.70
1:A:1540:MET:O	1:A:1543:ARG:NH1	2.24	0.70
1:A:1781:GLU:H	2:B:166:LYS:HZ1	1.39	0.70
1:A:551:LEU:HB3	1:A:621:LEU:HB3	1.73	0.70
1:A:558:LEU:HB2	1:A:615:PHE:HE2	1.55	0.70
1:A:972:VAL:HG21	1:A:1016:LEU:HD23	1.74	0.70
2:B:68:ARG:NE	2:B:100:GLU:OE1	2.22	0.70
1:A:1273:ALA:HA	1:A:1276:LEU:HD13	1.72	0.69
1:A:1857:THR:HG22	1:A:1869:GLN:HA	1.74	0.69
1:A:806:GLU:O	1:A:810:HIS:ND1	2.25	0.69
1:A:1420:VAL:O	1:A:1423:SER:OG	2.08	0.69
1:A:641:SER:HB2	1:A:650:LEU:HA	1.75	0.69
1:A:1637:HIS:HB2	1:A:1640:LEU:HB2	1.75	0.69
1:A:1753:ARG:NE	1:A:1823:THR:OG1	2.26	0.68
2:B:5:LYS:HG2	2:B:75:THR:HG22	1.74	0.68
1:A:1857:THR:N	1:A:1861:ARG:O	2.21	0.68
1:A:1950:ALA:O	1:A:1954:LEU:HB2	1.94	0.68
1:A:462:GLN:NE2	1:A:463:GLU:O	2.27	0.68
1:A:1261:LEU:HD13	1:A:1395:THR:HG21	1.76	0.68
1:A:1935:GLN:NE2	1:A:1939:GLY:O	2.26	0.68
1:A:1260:VAL:O	1:A:1264:THR:OG1	2.11	0.67
1:A:813:SER:O	1:A:817:ARG:HG2	1.95	0.67
1:A:747:VAL:O	1:A:752:ASN:ND2	2.28	0.67
2:B:19:LEU:HD21	2:B:165:LEU:HD11	1.75	0.67
1:A:577:MET:HE3	1:A:579:GLY:H	1.60	0.67
1:A:1771:TYR:OH	1:A:1888:ARG:NH1	2.25	0.67
1:A:1474:ILE:HB	1:A:1477:ILE:HG12	1.77	0.67
1:A:1932:MET:O	2:B:39:ASN:ND2	2.28	0.67
1:A:1265:GLU:OE2	1:A:1268:LEU:N	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1714:LEU:HB3	1:A:1723:LEU:HD11	1.77	0.66
1:A:620:LYS:NZ	1:A:622:HIS:HB2	2.10	0.66
1:A:1984:ALA:O	1:A:1988:ASN:ND2	2.27	0.66
1:A:1716:ALA:O	1:A:1718:ARG:NH1	2.28	0.66
1:A:250:PRO:O	1:A:838:TYR:OH	2.11	0.66
1:A:541:TYR:HB3	1:A:773:VAL:HG11	1.78	0.66
1:A:1755:GLY:N	1:A:1821:GLN:O	2.28	0.66
1:A:1863:HIS:NE2	2:B:32:TYR:O	2.28	0.66
1:A:1998:GLU:HA	1:A:2001:ARG:HD2	1.76	0.66
1:A:2003:LEU:HD23	1:A:2006:ASN:HD22	1.60	0.66
2:B:127:GLU:OE2	2:B:128:LYS:NZ	2.28	0.66
1:A:577:MET:HE1	1:A:581:ASP:O	1.94	0.66
1:A:956:ARG:NH2	1:A:1006:SER:O	2.28	0.66
1:A:1752:PHE:HZ	1:A:1779:LEU:HA	1.61	0.66
1:A:159:SER:C	1:A:1473:ARG:HH12	2.04	0.66
1:A:203:LEU:HB3	1:A:206:LEU:HD23	1.76	0.66
1:A:1064:LEU:HD12	1:A:1096:MET:HE2	1.76	0.66
1:A:400:HIS:HE1	1:A:402:ALA:HB3	1.61	0.66
1:A:573:ARG:HD2	1:A:601:GLU:HB2	1.77	0.66
1:A:755:GLN:OE1	1:A:755:GLN:N	2.29	0.66
1:A:1646:SER:O	1:A:1649:ASN:ND2	2.29	0.66
1:A:1830:ASP:OD1	1:A:1831:THR:N	2.25	0.66
1:A:1960:ASP:HB3	1:A:1963:LEU:HG	1.76	0.66
1:A:285:ASP:OD1	1:A:286:VAL:N	2.29	0.65
1:A:813:SER:O	1:A:817:ARG:NH1	2.30	0.65
1:A:1583:TYR:CD1	1:A:1885:ILE:HD11	2.31	0.65
1:A:400:HIS:CE1	1:A:403:ASN:H	2.15	0.65
1:A:1704:ASN:ND2	1:A:1705:GLU:OE2	2.30	0.65
2:B:139:TYR:O	2:B:143:LEU:N	2.30	0.65
1:A:1971:ARG:NE	1:A:2018:LEU:O	2.30	0.65
1:A:548:ARG:O	1:A:716:SER:N	2.20	0.65
1:A:728:PHE:O	1:A:732:HIS:ND1	2.25	0.65
1:A:1388:ALA:O	1:A:1392:VAL:HG23	1.97	0.65
1:A:79:PRO:HG2	1:A:1053:HIS:CE1	2.32	0.64
1:A:344:LYS:HB3	1:A:394:PHE:HB2	1.79	0.64
1:A:1441:ARG:HH11	1:A:1484:SER:HG	1.43	0.64
1:A:269:LYS:HB2	1:A:495:GLN:HB3	1.80	0.64
1:A:1694:PHE:O	1:A:1698:GLY:N	2.30	0.64
1:A:1999:TYR:O	1:A:2002:GLU:HG3	1.97	0.64
2:B:101:VAL:O	2:B:105:CYS:N	2.17	0.64
2:B:92:ASN:HB3	2:B:96:LYS:NZ	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1426:SER:OG	1:A:1428:GLN:NE2	2.29	0.64
1:A:1486:TYR:HB2	1:A:1532:ILE:HG23	1.78	0.64
1:A:344:LYS:N	1:A:392:MET:O	2.28	0.64
1:A:632:HIS:HB3	1:A:660:PRO:HA	1.79	0.64
1:A:931:ALA:HB1	1:A:935:PHE:HE2	1.63	0.64
1:A:1054:TYR:O	1:A:1058:ASN:ND2	2.30	0.64
1:A:108:GLN:HG2	1:A:732:HIS:NE2	2.13	0.64
1:A:639:HIS:N	1:A:652:THR:O	2.31	0.63
1:A:1918:PHE:O	1:A:1922:GLN:NE2	2.28	0.63
1:A:1851:LEU:HD11	1:A:1873:LYS:HD2	1.79	0.63
2:B:9:VAL:N	2:B:79:LEU:O	2.25	0.63
1:A:207:LEU:O	1:A:209:ARG:NH1	2.26	0.63
1:A:643:GLN:OE1	1:A:645:ARG:NE	2.30	0.63
1:A:347:GLN:NE2	1:A:350:ASP:O	2.31	0.63
1:A:1021:TYR:HH	1:A:1045:THR:HG1	1.46	0.63
1:A:1529:LEU:HD23	1:A:1532:ILE:HD12	1.80	0.63
1:A:454:LEU:HD12	1:A:500:ILE:HD13	1.81	0.63
1:A:326:ILE:HB	1:A:531:GLU:HA	1.81	0.63
1:A:816:HIS:CD2	1:A:823:GLN:HE21	2.17	0.63
1:A:982:ARG:NH2	1:A:986:ASP:OD2	2.32	0.63
1:A:1935:GLN:HB2	1:A:1999:TYR:OH	1.98	0.63
1:A:1176:LEU:HD12	1:A:1179:LEU:HD22	1.79	0.62
1:A:641:SER:N	1:A:650:LEU:O	2.31	0.62
1:A:1449:GLU:OE1	1:A:1449:GLU:N	2.29	0.62
1:A:1750:THR:N	1:A:1773:GLU:O	2.33	0.62
2:B:5:LYS:HA	2:B:56:TRP:CZ3	2.34	0.62
1:A:588:VAL:H	1:A:589:ILE:HD12	1.63	0.62
1:A:1947:LEU:HD11	1:A:2010:LEU:HD13	1.81	0.62
1:A:1560:MET:O	1:A:1563:THR:OG1	2.15	0.62
1:A:1892:CYS:SG	1:A:1893:HIS:N	2.73	0.62
1:A:931:ALA:HB1	1:A:935:PHE:CE2	2.34	0.62
1:A:1763:ASP:O	1:A:1767:GLN:NE2	2.26	0.62
1:A:125:ARG:NH2	1:A:128:GLN:OE1	2.33	0.62
1:A:142:GLN:O	1:A:146:GLN:N	2.32	0.62
1:A:742:ARG:NE	1:A:743:LEU:O	2.29	0.62
1:A:1954:LEU:HA	1:A:1967:HIS:NE2	2.15	0.61
1:A:1948:GLU:N	1:A:1948:GLU:OE1	2.34	0.61
1:A:1752:PHE:O	1:A:1771:TYR:N	2.19	0.61
1:A:1531:THR:HG22	1:A:1535:TYR:HE2	1.64	0.61
1:A:232:LEU:HD23	1:A:1259:TRP:CD1	2.35	0.61
1:A:485:LEU:HD23	1:A:488:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:PRO:O	1:A:668:ARG:NE	2.33	0.61
1:A:1574:ASP:H	1:A:1578:LEU:HD23	1.64	0.61
1:A:1540:MET:HA	1:A:1543:ARG:HH22	1.65	0.61
1:A:484:SER:HA	1:A:487:ARG:HG2	1.83	0.61
1:A:916:TRP:O	1:A:924:ARG:NH1	2.33	0.61
1:A:1408:ALA:O	1:A:1409:ARG:NH1	2.33	0.61
1:A:1522:GLU:OE1	1:A:1522:GLU:N	2.34	0.61
1:A:223:ARG:HG2	1:A:1435:HIS:CD2	2.35	0.61
1:A:663:GLN:O	1:A:666:ARG:N	2.34	0.61
1:A:1063:PRO:O	1:A:1106:GLN:NE2	2.29	0.61
1:A:1121:LEU:HB3	1:A:1175:THR:HG21	1.83	0.61
1:A:1428:GLN:HB3	1:A:1432:PHE:HD2	1.66	0.61
2:B:81:CYS:HA	2:B:113:VAL:HB	1.83	0.61
1:A:816:HIS:HD2	1:A:823:GLN:HE21	1.49	0.60
1:A:1090:ASP:HB2	1:A:1093:VAL:HG22	1.81	0.60
1:A:1566:VAL:HA	1:A:1569:LYS:HE2	1.81	0.60
1:A:1653:ASN:HD21	1:A:1881:ALA:N	1.97	0.60
1:A:223:ARG:NE	1:A:1394:ASP:OD1	2.28	0.60
1:A:254:ARG:HH12	1:A:256:HIS:HA	1.66	0.60
1:A:1417:LEU:O	1:A:1421:LEU:HG	2.01	0.60
1:A:1587:ARG:NH2	1:A:1656:GLU:HB2	2.17	0.60
1:A:444:CYS:SG	1:A:445:SER:N	2.72	0.60
1:A:1827:PRO:HA	1:A:1850:PHE:CD2	2.35	0.60
1:A:1582:MET:HB2	1:A:1603:MET:HE3	1.84	0.60
1:A:1581:LEU:O	1:A:1585:ILE:HD12	2.02	0.60
1:A:1857:THR:OG1	1:A:1859:ASP:OD1	2.10	0.60
1:A:1905:ALA:O	1:A:1909:MET:HG2	2.02	0.60
1:A:743:LEU:HG	1:A:744:LYS:H	1.67	0.60
1:A:1587:ARG:NH1	1:A:1590:GLN:OE1	2.35	0.60
1:A:578:THR:O	1:A:630:ASN:HB3	2.00	0.60
1:A:1865:GLU:O	1:A:1869:GLN:N	2.31	0.59
1:A:344:LYS:O	1:A:392:MET:N	2.29	0.59
1:A:405:VAL:HG11	1:A:446:PHE:HA	1.84	0.59
1:A:820:GLU:OE1	1:A:823:GLN:NE2	2.35	0.59
1:A:1954:LEU:HD23	1:A:1967:HIS:NE2	2.17	0.59
1:A:123:VAL:HG21	1:A:943:ALA:HB1	1.85	0.59
1:A:1768:GLU:N	1:A:1768:GLU:OE1	2.35	0.59
1:A:1812:LYS:HG3	1:A:1813:LEU:HG	1.84	0.59
2:B:159:ALA:O	2:B:162:GLN:NE2	2.35	0.59
1:A:108:GLN:HG2	1:A:732:HIS:CE1	2.38	0.59
1:A:994:ASN:HD22	1:A:1040:LEU:HB3	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1861:ARG:HH11	1:A:1862:ALA:H	1.50	0.59
1:A:292:ILE:O	1:A:535:PHE:N	2.34	0.59
1:A:955:PRO:HB3	1:A:957:LYS:HZ1	1.68	0.59
1:A:312:HIS:HB3	1:A:389:ARG:HG3	1.85	0.58
1:A:1756:PHE:HB3	1:A:1761:PHE:CD2	2.38	0.58
1:A:1780:ALA:N	2:B:166:LYS:HZ1	2.01	0.58
1:A:318:ILE:HG23	1:A:321:LEU:HD12	1.84	0.58
1:A:467:LEU:HD11	1:A:475:PHE:CE2	2.35	0.58
1:A:971:LEU:O	1:A:974:SER:OG	2.20	0.58
1:A:1865:GLU:HB2	1:A:1868:GLU:HB3	1.86	0.58
1:A:1297:TYR:CZ	1:A:1299:GLY:HA2	2.39	0.58
1:A:1430:ALA:O	1:A:1434:GLN:HG3	2.03	0.58
1:A:1437:LEU:O	1:A:1440:GLN:NE2	2.36	0.58
1:A:85:LEU:HB2	1:A:947:LEU:HD21	1.86	0.58
1:A:1160:ARG:NH1	1:A:1163:GLU:OE1	2.31	0.58
1:A:1728:GLY:O	1:A:1732:GLU:HG2	2.03	0.58
1:A:1803:LYS:HE2	2:B:30:GLY:H	1.69	0.58
1:A:1854:THR:OG1	1:A:1872:ARG:NE	2.37	0.58
1:A:112:ALA:HA	1:A:115:MET:SD	2.44	0.58
1:A:1727:HIS:O	1:A:1731:GLN:HG2	2.04	0.58
1:A:568:ARG:O	1:A:610:ASN:N	2.34	0.57
1:A:984:HIS:H	1:A:985:LYS:HZ3	1.50	0.57
1:A:1929:MET:HA	1:A:1932:MET:HG3	1.84	0.57
1:A:281:LEU:N	1:A:296:PHE:O	2.31	0.57
1:A:581:ASP:OD2	1:A:583:SER:OG	2.21	0.57
1:A:676:VAL:HG23	1:A:706:VAL:HG23	1.86	0.57
1:A:1425:GLY:H	1:A:1465:ARG:HH21	1.51	0.57
1:A:220:GLU:OE2	1:A:223:ARG:NH2	2.36	0.57
1:A:742:ARG:NH2	1:A:746:THR:O	2.37	0.57
1:A:344:LYS:HD3	1:A:394:PHE:HD1	1.69	0.57
1:A:607:VAL:HG11	1:A:613:PRO:HB3	1.86	0.57
1:A:956:ARG:HB3	1:A:1009:ASP:HA	1.86	0.57
1:A:1130:LEU:HD13	1:A:1133:LYS:HD3	1.86	0.57
1:A:1523:GLU:N	1:A:1523:GLU:OE2	2.37	0.57
1:A:1780:ALA:HB3	2:B:166:LYS:HE3	1.85	0.57
1:A:638:TYR:CG	1:A:651:GLU:HB3	2.39	0.57
1:A:90:ARG:HH22	1:A:118:GLU:C	2.12	0.57
1:A:466:ARG:CZ	1:A:615:PHE:HA	2.35	0.57
1:A:750:GLU:N	1:A:750:GLU:OE1	2.34	0.57
1:A:1508:MET:O	1:A:1511:SER:OG	2.23	0.57
1:A:553:VAL:HB	1:A:619:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:VAL:HG21	1:A:613:PRO:HB2	1.87	0.57
1:A:1510:LEU:HD23	1:A:1558:LEU:HD22	1.87	0.57
1:A:752:ASN:HA	1:A:755:GLN:HE22	1.69	0.57
2:B:52:ASN:OD1	2:B:53:LEU:N	2.38	0.57
2:B:173:ILE:O	2:B:177:LEU:N	2.30	0.57
1:A:287:ARG:HB2	1:A:335:ASP:OD2	2.05	0.56
1:A:971:LEU:O	1:A:975:VAL:HG23	2.03	0.56
1:A:1954:LEU:HD13	1:A:2017:LEU:HB3	1.87	0.56
1:A:459:PHE:HD2	1:A:494:ALA:HB3	1.70	0.56
2:B:5:LYS:HA	2:B:56:TRP:HZ3	1.69	0.56
1:A:52:GLU:HA	1:A:1018:ARG:HH11	1.68	0.56
1:A:244:VAL:O	1:A:246:ARG:HD3	2.03	0.56
1:A:267:SER:HB3	1:A:269:LYS:HZ1	1.70	0.56
1:A:336:ILE:HG22	1:A:401:LEU:HD12	1.87	0.56
1:A:920:SER:O	1:A:924:ARG:N	2.27	0.56
1:A:975:VAL:O	1:A:979:VAL:HG23	2.05	0.56
1:A:1453:GLU:HG2	1:A:1454:GLU:N	2.21	0.56
1:A:1622:HIS:ND1	1:A:1657:GLU:OE1	2.39	0.56
1:A:1950:ALA:HB1	1:A:1954:LEU:HD12	1.87	0.56
1:A:1997:LYS:O	1:A:2001:ARG:HG3	2.05	0.56
1:A:322:ALA:HA	1:A:527:ARG:HG3	1.88	0.56
1:A:1735:THR:O	1:A:1739:HIS:ND1	2.24	0.56
1:A:572:VAL:HG21	1:A:615:PHE:HZ	1.71	0.56
1:A:663:GLN:HB3	1:A:668:ARG:NH2	2.20	0.56
1:A:835:TYR:HD1	1:A:839:ALA:HB3	1.70	0.56
1:A:1781:GLU:H	2:B:166:LYS:NZ	2.03	0.56
1:A:1805:SER:HB2	1:A:1852:PHE:HE2	1.70	0.56
1:A:1986:ARG:HA	1:A:1989:LYS:HE2	1.87	0.56
1:A:2006:ASN:OD1	1:A:2009:ARG:NH2	2.38	0.56
2:B:97:TRP:O	2:B:101:VAL:HG22	2.05	0.56
2:B:167:THR:HA	2:B:170:ASP:HB3	1.88	0.56
1:A:89:PRO:HA	1:A:119:ASP:CG	2.31	0.56
1:A:321:LEU:O	1:A:527:ARG:NE	2.33	0.56
1:A:342:LEU:HD12	1:A:395:ALA:HB3	1.87	0.56
1:A:466:ARG:HB2	1:A:614:GLU:HB2	1.86	0.56
1:A:569:ASN:OD1	1:A:609:HIS:N	2.39	0.56
1:A:1396:LEU:HA	1:A:1399:ILE:HD12	1.88	0.56
1:A:1534:THR:O	1:A:1537:GLU:HG3	2.06	0.56
1:A:2006:ASN:O	1:A:2010:LEU:HD23	2.06	0.56
1:A:805:PHE:HE1	1:A:912:LEU:HA	1.69	0.56
1:A:1752:PHE:CZ	1:A:1779:LEU:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1911:LYS:HG2	1:A:1915:GLU:OE1	2.05	0.56
1:A:216:ASP:O	1:A:220:GLU:HG2	2.06	0.55
1:A:779:VAL:O	1:A:783:LEU:HD12	2.05	0.55
1:A:1902:VAL:O	1:A:1906:ILE:HG12	2.06	0.55
1:A:1028:LEU:HD11	1:A:1034:PRO:HA	1.87	0.55
1:A:912:LEU:O	1:A:916:TRP:HB2	2.07	0.55
1:A:1856:PHE:N	1:A:1869:GLN:HE22	2.04	0.55
1:A:2005:ARG:HB2	1:A:2009:ARG:HH12	1.70	0.55
1:A:1423:SER:HB2	1:A:1432:PHE:HZ	1.70	0.55
1:A:232:LEU:HD23	1:A:1259:TRP:HD1	1.71	0.55
1:A:334:PRO:HA	1:A:402:ALA:HB2	1.89	0.55
1:A:634:LEU:HA	1:A:658:TRP:HA	1.89	0.55
1:A:1636:ASP:HA	1:A:1640:LEU:HD13	1.86	0.55
1:A:1680:GLU:OE1	1:A:1717:HIS:NE2	2.39	0.55
1:A:1851:LEU:HD11	1:A:1873:LYS:CD	2.36	0.55
1:A:405:VAL:HA	1:A:449:PHE:HB2	1.87	0.55
1:A:710:GLU:OE1	1:A:712:THR:HG23	2.06	0.55
1:A:1416:VAL:O	1:A:1420:VAL:HG23	2.07	0.55
1:A:286:VAL:HG22	1:A:476:LEU:HB3	1.89	0.55
1:A:548:ARG:N	1:A:716:SER:OG	2.39	0.55
1:A:694:LEU:HD22	1:A:697:MET:HG2	1.88	0.55
1:A:1370:THR:C	1:A:1374:MET:HE3	2.32	0.55
1:A:1523:GLU:O	1:A:1527:ARG:HG3	2.06	0.55
1:A:1936:GLY:N	2:B:39:ASN:HD22	2.05	0.55
1:A:1947:LEU:HD21	1:A:2010:LEU:HD11	1.89	0.55
1:A:109:VAL:HG11	1:A:625:ALA:HB1	1.90	0.54
1:A:1713:ILE:HD12	1:A:1713:ILE:H	1.72	0.54
1:A:907:LEU:HB2	1:A:910:GLU:OE1	2.07	0.54
1:A:1849:THR:HA	1:A:1876:LEU:O	2.06	0.54
1:A:1856:PHE:HA	1:A:1862:ALA:HA	1.88	0.54
1:A:76:VAL:HB	1:A:1061:CYS:HB2	1.89	0.54
1:A:1270:GLN:NE2	1:A:1271:ARG:HG2	2.23	0.54
1:A:1803:LYS:HG3	2:B:28:PHE:CD2	2.42	0.54
1:A:1859:ASP:OD1	1:A:1860:GLY:N	2.40	0.54
1:A:1908:ASP:OD2	1:A:1909:MET:N	2.40	0.54
1:A:343:GLU:HA	1:A:394:PHE:H	1.73	0.54
1:A:620:LYS:HZ3	1:A:622:HIS:HB2	1.71	0.54
1:A:1938:VAL:C	1:A:1940:PRO:HD3	2.33	0.54
1:A:334:PRO:HD3	1:A:444:CYS:HB2	1.89	0.54
1:A:1013:VAL:O	1:A:1017:VAL:HG23	2.08	0.54
1:A:978:GLU:O	1:A:982:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2000:HIS:O	1:A:2004:GLU:HG2	2.08	0.54
1:A:1026:THR:O	1:A:1029:GLN:HB2	2.08	0.54
1:A:1403:VAL:HG22	1:A:1409:ARG:HH21	1.72	0.54
1:A:1870:HIS:CD2	1:A:1901:PRO:HD3	2.42	0.54
2:B:14:VAL:HG23	2:B:16:LYS:HG3	1.89	0.54
1:A:719:PRO:HG2	1:A:725:ASP:HA	1.89	0.54
1:A:816:HIS:HB3	1:A:817:ARG:HH12	1.73	0.54
1:A:1583:TYR:OH	1:A:1884:TYR:OH	2.24	0.54
1:A:1749:GLY:HA2	1:A:1775:SER:N	2.23	0.54
1:A:955:PRO:HB3	1:A:957:LYS:NZ	2.23	0.54
1:A:152:GLN:OE1	1:A:1429:SER:OG	2.26	0.54
1:A:551:LEU:HB2	1:A:623:LEU:HD11	1.90	0.54
2:B:80:ILE:HD13	2:B:110:ILE:HG23	1.90	0.54
1:A:495:GLN:HE22	1:A:497:LYS:HG3	1.73	0.53
1:A:1863:HIS:CD2	2:B:34:PRO:HG3	2.43	0.53
2:B:166:LYS:O	2:B:170:ASP:N	2.28	0.53
1:A:317:ALA:O	1:A:320:THR:OG1	2.24	0.53
1:A:554:TYR:HB2	1:A:710:GLU:HG3	1.90	0.53
1:A:1409:ARG:NH2	1:A:1412:VAL:HG21	2.23	0.53
1:A:1516:THR:O	1:A:1518:GLN:NE2	2.41	0.53
1:A:1867:PRO:HA	1:A:1953:PHE:HZ	1.72	0.53
1:A:345:VAL:HG12	1:A:346:LEU:H	1.73	0.53
1:A:955:PRO:HG2	1:A:958:LEU:HD12	1.91	0.53
2:B:90:PHE:CE1	2:B:145:MET:HG3	2.43	0.53
2:B:90:PHE:HE1	2:B:145:MET:HG3	1.73	0.53
1:A:1587:ARG:HH11	1:A:1596:ARG:HH12	1.57	0.53
2:B:122:ASP:O	2:B:125:THR:OG1	2.25	0.53
1:A:232:LEU:HD21	1:A:1259:TRP:HB2	1.90	0.53
1:A:1867:PRO:HG3	1:A:1952:VAL:HG11	1.91	0.53
1:A:1769:PHE:CD2	1:A:1888:ARG:HD2	2.44	0.53
1:A:1769:PHE:HD1	1:A:1890:ARG:HA	1.72	0.53
1:A:1828:TYR:O	1:A:1849:THR:OG1	2.26	0.53
1:A:1558:LEU:O	1:A:1562:LEU:HD23	2.09	0.53
1:A:1846:GLY:N	1:A:1882:PHE:O	2.42	0.53
2:B:65:ASP:OD1	2:B:68:ARG:NH1	2.32	0.53
1:A:46:PRO:O	1:A:1104:ARG:NH2	2.37	0.53
1:A:280:ILE:HG21	1:A:341:LYS:HB2	1.89	0.53
1:A:578:THR:OG1	1:A:584:GLN:O	2.22	0.53
1:A:743:LEU:HD22	1:A:748:LEU:HD21	1.91	0.53
1:A:1160:ARG:O	1:A:1163:GLU:HB3	2.08	0.53
1:A:581:ASP:OD1	1:A:581:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:GLU:HA	1:A:901:ARG:HD2	1.90	0.52
1:A:1547:PHE:HA	1:A:1550:GLN:NE2	2.24	0.52
1:A:1530:LYS:O	1:A:1533:LEU:HB2	2.09	0.52
1:A:466:ARG:NH1	1:A:614:GLU:O	2.42	0.52
1:A:917:VAL:C	1:A:924:ARG:HH12	2.17	0.52
1:A:1829:PHE:HB2	1:A:1834:LEU:HG	1.91	0.52
1:A:919:SER:OG	1:A:920:SER:N	2.43	0.52
1:A:1021:TYR:HA	1:A:1024:VAL:HG12	1.89	0.52
1:A:1028:LEU:HD13	1:A:1037:LEU:HD23	1.92	0.52
1:A:1565:THR:O	1:A:1569:LYS:NZ	2.38	0.52
1:A:1575:PRO:HG2	1:A:1576:GLU:OE1	2.10	0.52
1:A:70:GLY:O	1:A:73:ARG:HG2	2.09	0.52
1:A:258:GLY:HA3	1:A:329:VAL:H	1.74	0.52
1:A:1042:MET:CE	1:A:1134:LYS:HB3	2.40	0.52
1:A:1872:ARG:HA	1:A:1898:VAL:HA	1.92	0.52
2:B:138:THR:N	2:B:141:GLN:OE1	2.30	0.52
1:A:343:GLU:HG2	1:A:393:PRO:HA	1.91	0.52
1:A:558:LEU:HB2	1:A:615:PHE:CE2	2.42	0.52
1:A:567:VAL:HG13	1:A:570:LEU:HD21	1.91	0.52
1:A:1533:LEU:HD23	1:A:1555:MET:CE	2.39	0.52
1:A:1953:PHE:O	1:A:1967:HIS:NE2	2.43	0.52
1:A:734:LEU:HD11	1:A:791:PRO:HB3	1.91	0.52
1:A:777:HIS:NE2	1:A:835:TYR:HB2	2.24	0.52
1:A:1530:LYS:HA	1:A:1533:LEU:HD12	1.91	0.52
1:A:1930:LEU:HG	1:A:1988:ASN:HD21	1.73	0.52
1:A:551:LEU:HD13	1:A:713:ALA:HB2	1.92	0.52
1:A:1578:LEU:O	1:A:1582:MET:HG3	2.08	0.52
1:A:1531:THR:O	1:A:1535:TYR:HD2	1.94	0.51
1:A:1995:ASP:OD1	1:A:1996:GLN:N	2.42	0.51
1:A:90:ARG:NH2	1:A:118:GLU:O	2.33	0.51
1:A:1468:ARG:NH2	1:A:1519:ASN:OD1	2.44	0.51
1:A:1777:THR:O	1:A:1778:LYS:NZ	2.39	0.51
2:B:5:LYS:HG3	2:B:56:TRP:CZ3	2.45	0.51
2:B:8:VAL:O	2:B:58:THR:OG1	2.25	0.51
1:A:125:ARG:HH12	1:A:1003:ASP:HA	1.75	0.51
2:B:10:GLY:HA3	2:B:81:CYS:HB3	1.92	0.51
2:B:110:ILE:O	2:B:152:VAL:HG22	2.11	0.51
1:A:469:ASP:OD1	1:A:470:GLU:N	2.44	0.51
1:A:776:SER:O	1:A:780:LEU:HG	2.10	0.51
2:B:168:VAL:O	2:B:172:ALA:N	2.44	0.51
1:A:263:VAL:HG12	1:A:500:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ARG:O	1:A:806:GLU:HG3	2.11	0.51
1:A:913:ALA:HB1	1:A:967:ASP:HB3	1.92	0.51
1:A:1167:PRO:O	1:A:1171:ILE:HG12	2.10	0.51
1:A:1700:TYR:HB3	1:A:1733:ALA:HB1	1.93	0.51
2:B:129:LEU:HD13	2:B:136:PRO:HD3	1.91	0.51
1:A:281:LEU:HB2	1:A:298:PHE:HE1	1.76	0.51
1:A:573:ARG:O	1:A:636:THR:N	2.44	0.51
1:A:913:ALA:O	1:A:917:VAL:HG23	2.10	0.51
1:A:264:LYS:N	1:A:499:ASP:O	2.44	0.51
2:B:89:SER:O	2:B:93:VAL:HG23	2.11	0.51
1:A:389:ARG:HB2	1:A:390:TYR:CE1	2.46	0.51
1:A:1092:LYS:HG3	1:A:1093:VAL:H	1.76	0.51
1:A:1749:GLY:HA3	1:A:1772:LYS:HE2	1.93	0.51
1:A:1858:PRO:HD3	1:A:1870:HIS:HB2	1.91	0.51
2:B:140:PRO:HA	2:B:143:LEU:HB3	1.93	0.51
1:A:119:ASP:O	1:A:841:ARG:NH1	2.44	0.51
1:A:1154:GLU:HB2	1:A:1157:VAL:HG22	1.92	0.51
1:A:1752:PHE:N	1:A:1771:TYR:O	2.43	0.51
1:A:1546:THR:OG1	1:A:1550:GLN:OE1	2.27	0.50
1:A:1623:ALA:O	1:A:1627:VAL:HG23	2.11	0.50
1:A:1752:PHE:CE1	1:A:1824:TYR:HB2	2.45	0.50
1:A:1767:GLN:HB2	1:A:1890:ARG:HE	1.76	0.50
2:B:122:ASP:O	2:B:126:ILE:HG12	2.11	0.50
1:A:917:VAL:O	1:A:924:ARG:NH1	2.44	0.50
1:A:951:ARG:O	1:A:954:THR:HG22	2.11	0.50
1:A:1109:LEU:HD23	1:A:1112:LEU:HD12	1.92	0.50
1:A:1615:GLU:OE1	1:A:1615:GLU:N	2.38	0.50
1:A:207:LEU:C	1:A:209:ARG:HH12	2.19	0.50
1:A:1676:LYS:HG3	1:A:1677:HIS:ND1	2.27	0.50
1:A:1756:PHE:HB3	1:A:1761:PHE:HD2	1.76	0.50
1:A:1833:GLU:N	1:A:1833:GLU:OE1	2.42	0.50
2:B:117:LEU:HD21	2:B:156:GLU:HB3	1.94	0.50
1:A:392:MET:HG3	1:A:606:VAL:O	2.12	0.50
1:A:573:ARG:HG3	1:A:602:ALA:O	2.11	0.50
1:A:816:HIS:HB3	1:A:817:ARG:NH1	2.26	0.50
1:A:938:MET:O	1:A:942:MET:HG3	2.12	0.50
1:A:984:HIS:HB2	1:A:985:LYS:HD3	1.94	0.50
1:A:1526:ARG:HH12	1:A:1559:HIS:HB3	1.76	0.50
1:A:1528:SER:O	1:A:1532:ILE:HG13	2.11	0.50
1:A:1934:LEU:O	1:A:1938:VAL:HG12	2.11	0.50
2:B:127:GLU:O	2:B:131:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1757:TYR:CE1	1:A:1766:GLU:HA	2.46	0.50
1:A:1803:LYS:HG2	2:B:31:GLU:OE2	2.12	0.50
1:A:1827:PRO:HA	1:A:1850:PHE:HD2	1.77	0.50
1:A:638:TYR:CD2	1:A:651:GLU:HB3	2.47	0.50
1:A:658:TRP:CH2	1:A:690:PRO:HA	2.47	0.50
1:A:1574:ASP:HB3	1:A:1578:LEU:HD23	1.94	0.50
1:A:1447:PHE:HB3	1:A:1450:LEU:HD23	1.93	0.50
1:A:1453:GLU:OE1	1:A:1453:GLU:N	2.44	0.50
1:A:1909:MET:HG3	1:A:1910:GLN:N	2.25	0.50
1:A:743:LEU:HD13	1:A:748:LEU:HD11	1.93	0.50
1:A:1531:THR:HG22	1:A:1535:TYR:CE2	2.44	0.50
1:A:1707:TYR:O	1:A:1711:ILE:HG13	2.11	0.50
2:B:9:VAL:O	2:B:81:CYS:N	2.44	0.50
2:B:117:LEU:CD2	2:B:156:GLU:HB3	2.41	0.50
1:A:1248:GLU:HG2	1:A:1249:SER:N	2.27	0.49
1:A:1556:PHE:HA	1:A:1559:HIS:CD2	2.47	0.49
1:A:1417:LEU:HD13	1:A:1443:LEU:HD23	1.93	0.49
1:A:1900:THR:O	1:A:1904:VAL:N	2.41	0.49
2:B:132:LYS:HZ3	2:B:134:LEU:HB2	1.77	0.49
1:A:297:TYR:CE1	1:A:592:LYS:HA	2.48	0.49
1:A:1938:VAL:HG13	1:A:2003:LEU:HD22	1.93	0.49
1:A:2005:ARG:HD2	1:A:2009:ARG:HH12	1.76	0.49
1:A:2005:ARG:HB2	1:A:2009:ARG:NH1	2.28	0.49
1:A:279:GLY:N	1:A:298:PHE:O	2.45	0.49
1:A:459:PHE:CD2	1:A:494:ALA:HB3	2.46	0.49
1:A:633:LEU:HB2	1:A:659:ILE:CG2	2.42	0.49
1:A:836:VAL:O	1:A:940:LYS:HD3	2.12	0.49
1:A:1534:THR:HG22	1:A:1538:GLU:OE2	2.13	0.49
1:A:1742:SER:HB2	1:A:1744:TRP:HE3	1.78	0.49
1:A:2014:LEU:HA	1:A:2017:LEU:HD12	1.95	0.49
1:A:268:LEU:HG	1:A:300:LEU:HD22	1.94	0.49
1:A:1508:MET:HE2	1:A:1676:LYS:HD2	1.94	0.49
1:A:1653:ASN:OD1	1:A:1880:HIS:HB3	2.13	0.49
1:A:954:THR:CG2	1:A:959:ARG:HG2	2.43	0.49
1:A:1392:VAL:O	1:A:1395:THR:OG1	2.29	0.49
1:A:1504:MET:HE1	1:A:1675:GLY:HA3	1.95	0.49
2:B:100:GLU:O	2:B:104:HIS:ND1	2.44	0.49
1:A:1267:ALA:O	1:A:1270:GLN:HG3	2.12	0.49
1:A:1472:SER:O	1:A:1478:ARG:NH2	2.41	0.49
1:A:1583:TYR:HD1	1:A:1885:ILE:HD11	1.75	0.49
1:A:1805:SER:HB2	1:A:1852:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1928:LYS:NZ	2:B:5:LYS:HB2	2.28	0.49
2:B:84:LEU:HD12	2:B:115:THR:O	2.13	0.49
2:B:98:TYR:CG	2:B:149:ILE:HG23	2.48	0.49
2:B:126:ILE:O	2:B:129:LEU:HG	2.12	0.49
1:A:578:THR:OG1	1:A:584:GLN:HB3	2.13	0.49
1:A:1533:LEU:HD23	1:A:1555:MET:HE3	1.95	0.49
1:A:487:ARG:CZ	1:A:487:ARG:HA	2.43	0.49
1:A:1607:HIS:HA	1:A:1610:LEU:HD12	1.94	0.49
1:A:247:CYS:HA	1:A:826:ARG:HH12	1.76	0.48
1:A:723:TYR:HD2	1:A:767:ALA:HA	1.77	0.48
1:A:1019:ALA:O	1:A:1023:GLN:HG3	2.13	0.48
1:A:1036:ALA:O	1:A:1040:LEU:HG	2.13	0.48
1:A:1128:ALA:O	1:A:1132:HIS:N	2.35	0.48
1:A:1742:SER:HB2	1:A:1744:TRP:CE3	2.48	0.48
1:A:1782:ILE:HD11	1:A:1785:ARG:HE	1.76	0.48
1:A:1831:THR:O	1:A:1835:LYS:HD3	2.11	0.48
1:A:84:GLU:OE2	1:A:124:HIS:ND1	2.46	0.48
1:A:286:VAL:HB	1:A:335:ASP:HB3	1.94	0.48
1:A:807:ALA:O	1:A:811:VAL:HG23	2.12	0.48
1:A:1701:GLU:HG3	1:A:1841:PHE:CD2	2.48	0.48
1:A:1900:THR:O	1:A:1904:VAL:HG23	2.13	0.48
1:A:94:THR:HB	1:A:516:LEU:HB3	1.96	0.48
1:A:650:LEU:HG	1:A:651:GLU:HG3	1.94	0.48
1:A:726:LYS:O	1:A:730:LEU:HD13	2.13	0.48
1:A:754:GLU:HB3	1:A:758:ARG:NH1	2.29	0.48
1:A:1095:SER:O	1:A:1098:GLU:N	2.30	0.48
1:A:1149:ASP:OD2	1:A:1152:TYR:N	2.46	0.48
1:A:677:SER:OG	1:A:697:MET:HE3	2.13	0.48
1:A:721:ASP:OD2	1:A:724:LEU:HG	2.13	0.48
1:A:1857:THR:HG23	1:A:1869:GLN:OE1	2.13	0.48
2:B:129:LEU:HD13	2:B:135:THR:HA	1.95	0.48
1:A:254:ARG:NH1	1:A:255:GLU:O	2.45	0.48
1:A:679:ASP:OD2	1:A:698:ARG:N	2.41	0.48
1:A:120:TRP:CH2	1:A:253:PRO:HG2	2.48	0.48
1:A:1554:LEU:HA	1:A:1557:ASN:HD22	1.79	0.48
1:A:1679:THR:OG1	1:A:1682:GLY:N	2.41	0.48
1:A:1937:SER:HA	2:B:37:PHE:CD1	2.48	0.48
2:B:109:PRO:HB3	2:B:152:VAL:HG11	1.96	0.48
1:A:59:VAL:HG11	1:A:1059:LEU:HD21	1.94	0.48
1:A:553:VAL:N	1:A:619:PHE:O	2.32	0.48
1:A:1522:GLU:CD	1:A:1522:GLU:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASP:OD1	1:A:218:ARG:NH2	2.47	0.48
1:A:334:PRO:HA	1:A:446:PHE:HZ	1.79	0.48
1:A:753:VAL:O	1:A:756:GLU:HG2	2.13	0.48
1:A:1554:LEU:O	1:A:1558:LEU:HG	2.13	0.48
1:A:1931:GLN:HE22	2:B:56:TRP:HE1	1.61	0.48
1:A:2011:ARG:O	1:A:2015:GLN:HG2	2.14	0.48
1:A:1139:VAL:O	1:A:1143:LEU:HD23	2.14	0.48
1:A:1861:ARG:HG3	1:A:1863:HIS:H	1.78	0.48
2:B:11:ASP:O	2:B:16:LYS:NZ	2.47	0.48
1:A:137:VAL:HG13	1:A:137:VAL:O	2.14	0.48
1:A:213:GLU:O	1:A:217:ARG:HG3	2.14	0.48
1:A:656:PHE:O	1:A:677:SER:N	2.39	0.48
1:A:658:TRP:CD1	1:A:686:SER:HA	2.48	0.48
1:A:1426:SER:HG	1:A:1428:GLN:HE22	1.57	0.48
1:A:280:ILE:O	1:A:340:ILE:HG23	2.14	0.47
1:A:342:LEU:HB2	1:A:395:ALA:H	1.79	0.47
1:A:1166:LEU:HB2	1:A:1167:PRO:HD3	1.96	0.47
1:A:1701:GLU:H	1:A:1701:GLU:CD	2.18	0.47
2:B:127:GLU:HG2	2:B:128:LYS:HD2	1.95	0.47
1:A:511:LEU:HD21	1:A:521:TYR:CD2	2.48	0.47
1:A:49:GLU:N	1:A:49:GLU:OE1	2.47	0.47
1:A:589:ILE:O	1:A:598:PHE:HA	2.15	0.47
1:A:590:PHE:CD1	1:A:598:PHE:HE1	2.33	0.47
1:A:645:ARG:HB2	1:A:648:THR:OG1	2.14	0.47
1:A:1248:GLU:HG2	1:A:1249:SER:H	1.79	0.47
1:A:1702:ALA:O	1:A:1706:VAL:HG23	2.14	0.47
1:A:1854:THR:OG1	1:A:1854:THR:O	2.31	0.47
1:A:461:LYS:HE2	1:A:461:LYS:HB3	1.74	0.47
1:A:568:ARG:H	1:A:639:HIS:HE1	1.62	0.47
1:A:743:LEU:HD23	1:A:746:THR:HG22	1.97	0.47
1:A:1406:SER:C	1:A:1409:ARG:HD3	2.39	0.47
1:A:2003:LEU:HD23	1:A:2006:ASN:ND2	2.28	0.47
1:A:2007:TYR:HA	1:A:2010:LEU:HB2	1.95	0.47
2:B:82:PHE:HB3	2:B:93:VAL:HG21	1.96	0.47
1:A:57:GLU:OE2	1:A:1010:ARG:N	2.30	0.47
1:A:138:THR:HG23	1:A:141:THR:H	1.78	0.47
1:A:306:LYS:O	1:A:310:ARG:HD2	2.14	0.47
1:A:674:LEU:O	1:A:706:VAL:N	2.47	0.47
1:A:1395:THR:O	1:A:1399:ILE:HG13	2.15	0.47
1:A:1804:ASP:OD2	1:A:1806:ASN:HB3	2.14	0.47
1:A:1936:GLY:H	2:B:39:ASN:HD22	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1994:PRO:HA	1:A:1997:LYS:HE3	1.96	0.47
1:A:1930:LEU:O	1:A:1934:LEU:HG	2.14	0.47
2:B:31:GLU:N	2:B:31:GLU:OE1	2.47	0.47
1:A:337:PHE:CD1	1:A:400:HIS:HA	2.50	0.47
1:A:396:TRP:N	1:A:460:PHE:O	2.40	0.47
1:A:639:HIS:HB2	1:A:654:VAL:HG13	1.97	0.47
1:A:1090:ASP:HB3	1:A:1092:LYS:HG2	1.95	0.47
1:A:1737:ILE:O	1:A:1741:SER:OG	2.19	0.47
1:A:1771:TYR:CZ	1:A:1888:ARG:HD3	2.50	0.47
1:A:1776:ILE:HG12	2:B:45:MET:HG2	1.95	0.47
1:A:1932:MET:HB3	2:B:56:TRP:NE1	2.29	0.47
2:B:9:VAL:HG22	2:B:79:LEU:O	2.15	0.47
2:B:93:VAL:HA	2:B:97:TRP:CD1	2.50	0.47
1:A:267:SER:HB3	1:A:269:LYS:NZ	2.29	0.47
1:A:244:VAL:HG22	1:A:1047:ILE:HD13	1.97	0.47
1:A:400:HIS:O	1:A:404:ILE:HD12	2.15	0.47
1:A:805:PHE:CZ	1:A:912:LEU:HD22	2.50	0.47
1:A:924:ARG:O	1:A:928:LEU:HG	2.15	0.47
1:A:1708:LYS:HA	1:A:1708:LYS:HD3	1.79	0.47
1:A:1942:VAL:HG21	2:B:17:THR:HG21	1.97	0.47
1:A:158:ALA:HB1	1:A:1473:ARG:CZ	2.45	0.46
1:A:287:ARG:H	1:A:335:ASP:HB3	1.80	0.46
1:A:459:PHE:HB2	1:A:492:VAL:O	2.15	0.46
1:A:1021:TYR:OH	1:A:1045:THR:OG1	2.18	0.46
1:A:1124:GLU:N	1:A:1124:GLU:OE1	2.45	0.46
1:A:1928:LYS:HE3	2:B:56:TRP:HH2	1.80	0.46
2:B:160:LEU:O	2:B:162:GLN:NE2	2.48	0.46
1:A:389:ARG:HB2	1:A:390:TYR:CD1	2.50	0.46
1:A:1012:PHE:CE1	1:A:1016:LEU:HD11	2.50	0.46
1:A:1117:LEU:HD22	1:A:1139:VAL:HG21	1.97	0.46
1:A:1961:PRO:HA	1:A:1964:PHE:CE2	2.51	0.46
1:A:2002:GLU:HA	1:A:2005:ARG:HG2	1.97	0.46
1:A:2008:CYS:HA	1:A:2011:ARG:NE	2.30	0.46
1:A:105:LEU:HD13	1:A:110:ARG:HA	1.97	0.46
1:A:345:VAL:HA	1:A:391:ARG:HA	1.96	0.46
1:A:624:PRO:HD2	1:A:627:VAL:HG22	1.96	0.46
1:A:741:PHE:HB3	1:A:748:LEU:HD12	1.97	0.46
1:A:1491:GLN:HA	1:A:1494:GLU:OE1	2.16	0.46
1:A:343:GLU:HA	1:A:393:PRO:HA	1.98	0.46
1:A:1576:GLU:OE1	1:A:1576:GLU:N	2.44	0.46
2:B:173:ILE:HG13	2:B:177:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:GLN:N	1:A:915:GLN:OE1	2.48	0.46
1:A:1602:ASN:C	1:A:1602:ASN:HD22	2.24	0.46
2:B:159:ALA:HA	2:B:162:GLN:HA	1.98	0.46
1:A:344:LYS:HD3	1:A:394:PHE:CD1	2.50	0.46
1:A:551:LEU:HD12	1:A:712:THR:O	2.16	0.46
1:A:637:PHE:HB2	1:A:655:GLY:H	1.80	0.46
1:A:1408:ALA:C	1:A:1409:ARG:HD2	2.41	0.46
1:A:1620:MET:HB3	1:A:1690:ALA:HB2	1.97	0.46
1:A:1712:PRO:HA	1:A:1715:GLU:HG2	1.97	0.46
1:A:1946:PRO:HG2	1:A:1947:LEU:HD22	1.98	0.46
2:B:5:LYS:HD3	2:B:74:GLN:O	2.15	0.46
2:B:104:HIS:O	2:B:106:PRO:HD3	2.16	0.46
1:A:247:CYS:HA	1:A:826:ARG:NH1	2.30	0.46
1:A:394:PHE:HZ	1:A:492:VAL:HG11	1.80	0.46
1:A:637:PHE:O	1:A:638:TYR:CD1	2.69	0.46
1:A:1782:ILE:O	1:A:1786:LEU:HD23	2.16	0.46
1:A:658:TRP:HZ2	1:A:688:LEU:HD12	1.81	0.46
1:A:1092:LYS:HG3	1:A:1093:VAL:HG13	1.97	0.46
1:A:1424:LEU:HD11	1:A:1440:GLN:HG2	1.97	0.46
2:B:80:ILE:O	2:B:113:VAL:N	2.49	0.46
2:B:112:LEU:HB3	2:B:154:TYR:HD1	1.79	0.46
1:A:1947:LEU:O	1:A:1951:GLN:HG3	2.16	0.46
1:A:576:TYR:HA	1:A:633:LEU:HD23	1.97	0.45
1:A:799:ASN:O	1:A:800:LEU:HD23	2.16	0.45
1:A:1129:PHE:HA	1:A:1132:HIS:ND1	2.31	0.45
1:A:1700:TYR:HA	1:A:1703:VAL:HG22	1.99	0.45
1:A:1726:VAL:O	1:A:1730:LEU:HD23	2.16	0.45
1:A:1831:THR:OG1	1:A:1832:TYR:N	2.50	0.45
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.70	0.45
1:A:106:ASP:OD1	1:A:107:ALA:N	2.48	0.45
1:A:778:HIS:O	1:A:782:LYS:HG2	2.16	0.45
1:A:1751:TYR:HE1	1:A:1772:LYS:HB2	1.79	0.45
1:A:567:VAL:HG12	1:A:570:LEU:HD11	1.98	0.45
1:A:477:ALA:O	1:A:480:ARG:HB3	2.17	0.45
1:A:1050:SER:O	1:A:1050:SER:OG	2.25	0.45
1:A:1985:LEU:HD22	1:A:2004:GLU:OE2	2.17	0.45
1:A:573:ARG:N	1:A:636:THR:O	2.40	0.45
1:A:679:ASP:CG	1:A:698:ARG:H	2.24	0.45
1:A:1246:SER:O	1:A:1250:SER:OG	2.18	0.45
1:A:1873:LYS:HB3	1:A:1897:THR:OG1	2.16	0.45
2:B:7:VAL:HG12	2:B:78:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:TYR:CD1	2:B:104:HIS:HB3	2.51	0.45
1:A:131:SER:OG	1:A:132:ALA:N	2.50	0.45
1:A:254:ARG:NH1	1:A:256:HIS:HA	2.29	0.45
1:A:336:ILE:O	1:A:401:LEU:HB2	2.17	0.45
1:A:348:GLN:HG3	1:A:643:GLN:HG2	1.97	0.45
1:A:399:VAL:HG12	1:A:400:HIS:O	2.17	0.45
1:A:932:TRP:O	1:A:936:GLN:HG3	2.17	0.45
1:A:1043:GLU:O	1:A:1047:ILE:HG12	2.17	0.45
1:A:1447:PHE:HB3	1:A:1450:LEU:HB2	1.97	0.45
2:B:111:ILE:HD13	2:B:153:LYS:HB2	1.98	0.45
1:A:104:LYS:NZ	1:A:626:CYS:SG	2.89	0.45
1:A:213:GLU:HA	1:A:216:ASP:OD2	2.17	0.45
1:A:346:LEU:HB3	1:A:387:LEU:HD13	1.98	0.45
1:A:629:GLU:C	1:A:632:HIS:HE2	2.17	0.45
1:A:788:ILE:HD12	1:A:842:LEU:HD11	1.97	0.45
1:A:1180:HIS:HB2	1:A:1245:LEU:O	2.17	0.45
1:A:1813:LEU:HB3	1:A:1819:TYR:CE1	2.51	0.45
2:B:46:VAL:HG13	2:B:46:VAL:O	2.16	0.45
1:A:764:LEU:HD23	1:A:764:LEU:O	2.17	0.45
1:A:1371:LYS:NZ	1:A:1375:GLU:HB2	2.32	0.45
1:A:1753:ARG:HH22	1:A:1821:GLN:CD	2.25	0.45
1:A:2003:LEU:HA	1:A:2006:ASN:ND2	2.32	0.45
1:A:116:TYR:HE2	1:A:778:HIS:HE2	1.64	0.45
1:A:207:LEU:H	1:A:207:LEU:HD23	1.81	0.45
1:A:1493:PHE:CE2	1:A:1547:PHE:HB2	2.51	0.45
1:A:1700:TYR:O	1:A:1703:VAL:HG22	2.17	0.45
1:A:1771:TYR:CE1	1:A:1888:ARG:HB3	2.51	0.45
1:A:1814:ASP:OD1	1:A:1817:LYS:HB2	2.17	0.45
2:B:158:SER:HB3	2:B:161:THR:HG22	1.98	0.45
1:A:344:LYS:CB	1:A:394:PHE:HB2	2.46	0.44
1:A:590:PHE:CE1	1:A:598:PHE:HE1	2.35	0.44
1:A:632:HIS:HA	1:A:661:LEU:HG	1.99	0.44
1:A:1024:VAL:HG23	1:A:1037:LEU:HD21	1.99	0.44
1:A:1490:ARG:NE	1:A:1494:GLU:OE2	2.42	0.44
1:A:1714:LEU:HB3	1:A:1723:LEU:CD1	2.45	0.44
1:A:1736:LYS:HA	1:A:1739:HIS:HB2	1.99	0.44
1:A:455:THR:OG1	1:A:497:LYS:HG2	2.17	0.44
1:A:511:LEU:O	1:A:530:LYS:HA	2.17	0.44
1:A:2003:LEU:HA	1:A:2006:ASN:HD22	1.83	0.44
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.81	0.44
1:A:1387:GLU:O	1:A:1391:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:THR:O	1:A:1535:TYR:C	2.59	0.44
1:A:1685:GLY:O	1:A:1688:GLU:HG2	2.16	0.44
1:A:1954:LEU:HD11	1:A:1974:PHE:CE1	2.53	0.44
1:A:259:GLN:HB2	1:A:329:VAL:HB	2.00	0.44
1:A:1649:ASN:OD1	1:A:1650:ILE:HG13	2.17	0.44
1:A:1764:LEU:HA	1:A:1767:GLN:NE2	2.32	0.44
1:A:312:HIS:HB2	1:A:388:GLY:HA3	2.00	0.44
1:A:1587:ARG:HH22	1:A:1656:GLU:HB2	1.82	0.44
1:A:1735:THR:C	1:A:1739:HIS:HD1	2.19	0.44
1:A:1747:VAL:HA	1:A:1840:TYR:OH	2.17	0.44
1:A:1816:GLN:HG2	1:A:1817:LYS:HD2	1.99	0.44
1:A:1851:LEU:HA	1:A:1874:THR:O	2.17	0.44
1:A:1976:ASP:O	1:A:1979:LYS:HG2	2.16	0.44
2:B:92:ASN:HA	2:B:95:ALA:HB3	1.99	0.44
1:A:549:ASN:HB3	1:A:717:VAL:HG22	1.99	0.44
1:A:1176:LEU:HD12	1:A:1176:LEU:HA	1.76	0.44
1:A:1676:LYS:HE2	1:A:1677:HIS:CE1	2.51	0.44
2:B:118:ASP:OD2	2:B:119:LEU:N	2.50	0.44
2:B:49:LYS:HG3	2:B:51:VAL:HG13	2.00	0.44
2:B:57:ASP:OD1	2:B:58:THR:N	2.51	0.44
2:B:87:PRO:HA	2:B:137:ILE:HD11	1.99	0.44
1:A:1652:SER:O	1:A:1655:LEU:HG	2.18	0.44
1:A:1830:ASP:HB3	1:A:1833:GLU:OE1	2.17	0.44
1:A:89:PRO:HA	1:A:119:ASP:OD2	2.18	0.44
1:A:105:LEU:HB3	1:A:110:ARG:HB2	1.99	0.44
1:A:927:ILE:O	1:A:930:HIS:N	2.51	0.44
1:A:1005:LEU:HG	1:A:1013:VAL:HG11	2.00	0.44
1:A:1300:LYS:HD3	1:A:1378:ALA:HB2	1.99	0.44
1:A:1399:ILE:O	1:A:1402:THR:HB	2.18	0.44
1:A:1574:ASP:N	1:A:1578:LEU:HD23	2.31	0.44
1:A:1618:GLN:HA	1:A:1621:VAL:HG12	1.99	0.44
1:A:1938:VAL:O	1:A:1940:PRO:HD3	2.16	0.44
1:A:221:THR:O	1:A:225:GLN:HG3	2.18	0.43
1:A:830:PRO:O	1:A:834:ALA:CB	2.66	0.43
1:A:2005:ARG:HA	1:A:2008:CYS:SG	2.58	0.43
1:A:1612:ASN:HB3	1:A:1615:GLU:OE2	2.18	0.43
1:A:268:LEU:O	1:A:269:LYS:NZ	2.50	0.43
1:A:308:LEU:HB3	1:A:384:CYS:SG	2.58	0.43
1:A:331:TYR:CE2	1:A:538:ARG:HB2	2.52	0.43
1:A:1135:ALA:O	1:A:1139:VAL:HG23	2.18	0.43
1:A:1422:TYR:CD1	1:A:1422:TYR:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1431:LEU:HD11	1:A:1435:HIS:HE1	1.82	0.43
1:A:1441:ARG:HD2	1:A:1487:LEU:HD12	2.00	0.43
1:A:1491:GLN:OE1	1:A:1495:ILE:HD12	2.18	0.43
1:A:1574:ASP:OD2	1:A:1576:GLU:N	2.51	0.43
1:A:1965:ARG:NH1	1:A:1966:HIS:CE1	2.86	0.43
1:A:122:ILE:HD11	1:A:838:TYR:CD2	2.53	0.43
1:A:224:ARG:HA	1:A:227:ARG:HG3	2.00	0.43
1:A:1523:GLU:O	1:A:1526:ARG:HB2	2.17	0.43
1:A:1649:ASN:OD1	1:A:1650:ILE:N	2.51	0.43
2:B:43:ASN:HA	2:B:52:ASN:HA	2.01	0.43
1:A:252:PRO:HA	1:A:838:TYR:CE1	2.53	0.43
1:A:280:ILE:HA	1:A:297:TYR:HA	1.99	0.43
1:A:1059:LEU:HG	1:A:1062:CYS:HB3	2.00	0.43
1:A:1924:PRO:HA	1:A:1925:PRO:HD3	1.79	0.43
2:B:5:LYS:HB3	2:B:75:THR:HA	2.01	0.43
1:A:338:LEU:HD12	1:A:339:VAL:H	1.83	0.43
1:A:805:PHE:HZ	1:A:912:LEU:HD22	1.82	0.43
1:A:1499:PHE:HB2	1:A:1502:VAL:HB	2.00	0.43
1:A:2008:CYS:O	1:A:2011:ARG:HG2	2.18	0.43
1:A:588:VAL:N	1:A:589:ILE:HD12	2.30	0.43
1:A:663:GLN:HE22	1:A:667:LEU:C	2.27	0.43
1:A:1098:GLU:O	1:A:1100:SER:N	2.51	0.43
1:A:1550:GLN:HA	1:A:1553:ASP:OD1	2.19	0.43
1:A:1800:GLU:OE2	1:A:1817:LYS:HB3	2.18	0.43
2:B:142:GLY:O	2:B:145:MET:HB2	2.19	0.43
1:A:86:LEU:HB2	1:A:122:ILE:HB	2.00	0.43
1:A:554:TYR:HE1	1:A:618:GLU:HG3	1.84	0.43
1:A:577:MET:HE3	1:A:579:GLY:N	2.29	0.43
1:A:1001:LEU:O	1:A:1004:LEU:HB2	2.19	0.43
1:A:281:LEU:HD21	1:A:327:PHE:CE1	2.54	0.43
1:A:331:TYR:HE2	1:A:538:ARG:H	1.65	0.43
1:A:569:ASN:H	1:A:639:HIS:CE1	2.37	0.43
1:A:585:ALA:O	1:A:600:ARG:HD3	2.19	0.43
1:A:1391:VAL:O	1:A:1395:THR:HG23	2.18	0.43
1:A:1496:GLY:C	1:A:1498:ASN:H	2.27	0.43
1:A:980:ILE:HG23	1:A:1027:ARG:HG2	2.01	0.43
1:A:1781:GLU:OE1	1:A:1782:ILE:N	2.51	0.43
1:A:1856:PHE:C	1:A:1869:GLN:HE22	2.27	0.43
1:A:288:GLU:HB3	1:A:290:LYS:HE3	2.01	0.42
1:A:560:PHE:CD1	1:A:563:ARG:HB2	2.54	0.42
2:B:171:GLU:HA	2:B:174:ARG:HG3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:O	1:A:291:LYS:HG3	2.20	0.42
1:A:285:ASP:N	1:A:290:LYS:O	2.51	0.42
1:A:604:THR:HA	1:A:619:PHE:HZ	1.85	0.42
1:A:633:LEU:HG	1:A:661:LEU:HD21	2.01	0.42
1:A:914:LEU:O	1:A:918:VAL:HG22	2.19	0.42
1:A:1128:ALA:HA	1:A:1131:LEU:HB2	2.01	0.42
1:A:1290:LEU:HD13	1:A:1290:LEU:HA	1.90	0.42
1:A:1457:GLU:HG3	1:A:1461:ASP:OD2	2.19	0.42
1:A:1617:ALA:HB1	1:A:1694:PHE:CE2	2.54	0.42
1:A:1966:HIS:O	1:A:1969:LYS:HG2	2.19	0.42
1:A:400:HIS:CE1	1:A:402:ALA:HB3	2.48	0.42
1:A:1288:LEU:HD22	1:A:1392:VAL:HG13	2.01	0.42
1:A:1493:PHE:HE2	1:A:1542:LEU:HD22	1.83	0.42
1:A:75:LEU:HD11	1:A:1152:TYR:CE1	2.54	0.42
1:A:495:GLN:NE2	1:A:497:LYS:HG3	2.35	0.42
1:A:1036:ALA:O	1:A:1039:THR:OG1	2.33	0.42
1:A:1394:ASP:O	1:A:1398:ILE:HG12	2.20	0.42
1:A:1432:PHE:O	1:A:1435:HIS:N	2.52	0.42
1:A:1509:SER:O	1:A:1512:SER:OG	2.33	0.42
1:A:2008:CYS:HA	1:A:2011:ARG:CZ	2.50	0.42
1:A:1175:THR:O	1:A:1175:THR:HG22	2.19	0.42
1:A:1502:VAL:O	1:A:1506:VAL:HG23	2.19	0.42
1:A:580:GLU:OE1	1:A:685:TYR:N	2.43	0.42
1:A:789:ARG:HG3	1:A:903:LEU:HB3	2.01	0.42
1:A:920:SER:O	1:A:924:ARG:HG3	2.20	0.42
1:A:1028:LEU:HG	1:A:1031:SER:HB3	2.01	0.42
2:B:94:ARG:HB3	2:B:145:MET:CE	2.45	0.42
1:A:127:TYR:HD2	1:A:1053:HIS:NE2	2.17	0.42
1:A:220:GLU:CD	1:A:223:ARG:HH22	2.27	0.42
1:A:283:LEU:HD23	1:A:284:TYR:N	2.34	0.42
1:A:513:PRO:HG3	1:A:531:GLU:O	2.19	0.42
1:A:636:THR:HA	1:A:656:PHE:CE1	2.54	0.42
1:A:999:PHE:O	1:A:1002:SER:OG	2.34	0.42
1:A:1735:THR:HA	1:A:1738:MET:HE2	2.02	0.42
1:A:1787:GLU:O	1:A:1791:THR:OG1	2.30	0.42
1:A:1970:LEU:HB3	1:A:1974:PHE:CE1	2.54	0.42
1:A:345:VAL:HG12	1:A:346:LEU:N	2.34	0.42
1:A:926:ALA:O	1:A:929:GLN:HB3	2.20	0.42
2:B:78:PHE:HE2	2:B:105:CYS:HB3	1.85	0.42
1:A:71:PRO:HB2	1:A:1157:VAL:HG11	2.02	0.42
1:A:397:THR:HB	1:A:459:PHE:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:HIS:CD2	1:A:774:ALA:HB1	2.54	0.42
1:A:933:PHE:HE1	1:A:937:LEU:HD22	1.85	0.42
1:A:957:LYS:HG3	1:A:958:LEU:HG	2.01	0.42
1:A:1425:GLY:HA3	1:A:1465:ARG:NH2	2.35	0.42
1:A:1571:HIS:NE2	1:A:1574:ASP:HB2	2.35	0.42
1:A:1967:HIS:O	1:A:1970:LEU:HB2	2.20	0.42
1:A:262:LEU:N	1:A:503:ALA:HB2	2.35	0.42
1:A:345:VAL:HG22	1:A:391:ARG:NE	2.34	0.42
1:A:711:LEU:HA	1:A:711:LEU:HD23	1.68	0.42
1:A:817:ARG:HG2	1:A:817:ARG:HH11	1.85	0.42
1:A:830:PRO:O	1:A:834:ALA:HB2	2.19	0.42
1:A:1042:MET:HE1	1:A:1135:ALA:N	2.35	0.42
1:A:1639:HIS:CG	1:A:1716:ALA:HB1	2.54	0.42
1:A:1775:SER:O	1:A:1778:LYS:NZ	2.52	0.42
1:A:1847:LEU:O	1:A:1881:ALA:HA	2.20	0.42
1:A:487:ARG:HA	1:A:487:ARG:NH1	2.35	0.41
1:A:957:LYS:H	1:A:957:LYS:HG2	1.59	0.41
1:A:1403:VAL:C	1:A:1405:LEU:H	2.27	0.41
1:A:1565:THR:O	1:A:1568:MET:HB3	2.20	0.41
1:A:1648:GLN:HA	1:A:1651:SER:O	2.20	0.41
1:A:1912:LYS:HA	1:A:1915:GLU:OE2	2.20	0.41
2:B:126:ILE:HD13	2:B:129:LEU:HD21	2.02	0.41
1:A:235:TYR:HE1	1:A:1251:ARG:HG2	1.85	0.41
1:A:336:ILE:C	1:A:337:PHE:CD2	2.98	0.41
1:A:604:THR:HG21	1:A:615:PHE:CE1	2.56	0.41
1:A:782:LYS:O	1:A:786:LEU:HG	2.20	0.41
1:A:1179:LEU:HD23	1:A:1254:LEU:HD21	2.02	0.41
1:A:1253:LEU:O	1:A:1257:VAL:HG23	2.20	0.41
1:A:1574:ASP:H	1:A:1578:LEU:CD2	2.31	0.41
1:A:1813:LEU:HD23	1:A:1813:LEU:HA	1.88	0.41
1:A:1906:ILE:O	1:A:1910:GLN:HG2	2.20	0.41
1:A:1920:THR:HA	1:A:1930:LEU:HD22	2.02	0.41
1:A:265:CYS:HA	1:A:498:ILE:HA	2.02	0.41
1:A:517:HIS:CE1	1:A:521:TYR:HD2	2.39	0.41
1:A:916:TRP:CE2	1:A:927:ILE:HG21	2.55	0.41
1:A:1441:ARG:HD2	1:A:1487:LEU:CD1	2.50	0.41
1:A:1476:THR:O	1:A:1480:HIS:ND1	2.41	0.41
1:A:1557:ASN:O	1:A:1561:ILE:HG13	2.20	0.41
1:A:1562:LEU:O	1:A:1566:VAL:HG23	2.21	0.41
1:A:1583:TYR:HH	1:A:1884:TYR:HH	1.53	0.41
1:A:1794:PHE:O	1:A:1798:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1800:GLU:N	1:A:1800:GLU:OE1	2.53	0.41
1:A:1828:TYR:CG	1:A:1829:PHE:N	2.88	0.41
1:A:54:LEU:HB3	1:A:59:VAL:HG21	2.02	0.41
1:A:558:LEU:HA	1:A:707:PHE:HD1	1.84	0.41
1:A:559:ASN:HB2	1:A:706:VAL:C	2.45	0.41
1:A:569:ASN:O	1:A:640:VAL:N	2.43	0.41
1:A:805:PHE:CE1	1:A:912:LEU:HD13	2.56	0.41
1:A:956:ARG:HD3	1:A:959:ARG:NE	2.26	0.41
1:A:960:PHE:HB2	1:A:965:LEU:HD11	2.02	0.41
1:A:1855:PRO:HA	1:A:1871:LYS:HG3	2.01	0.41
1:A:1946:PRO:HD3	2:B:37:PHE:CE1	2.54	0.41
1:A:283:LEU:HG	1:A:337:PHE:O	2.21	0.41
1:A:338:LEU:HD12	1:A:339:VAL:N	2.34	0.41
1:A:701:ASP:HB3	1:A:704:LYS:HB3	2.03	0.41
1:A:831:GLN:OE1	1:A:831:GLN:N	2.51	0.41
1:A:948:LEU:HD23	1:A:948:LEU:HA	1.79	0.41
1:A:1284:LEU:O	1:A:1287:LEU:HB3	2.21	0.41
1:A:1422:TYR:HA	1:A:1465:ARG:HH22	1.86	0.41
1:A:1448:PRO:HB3	1:A:1491:GLN:HE22	1.85	0.41
1:A:1463:CYS:O	1:A:1467:LEU:HG	2.20	0.41
1:A:1756:PHE:HA	1:A:1820:ILE:HG23	2.03	0.41
1:A:1934:LEU:HD11	1:A:1988:ASN:ND2	2.36	0.41
1:A:1998:GLU:HG3	1:A:2001:ARG:NH1	2.35	0.41
1:A:405:VAL:HG21	1:A:446:PHE:CD1	2.55	0.41
1:A:954:THR:HG21	1:A:959:ARG:HG2	2.03	0.41
1:A:1583:TYR:CE1	1:A:1885:ILE:HD11	2.56	0.41
1:A:1608:ALA:C	1:A:1610:LEU:H	2.28	0.41
1:A:1901:PRO:HA	1:A:1904:VAL:HB	2.02	0.41
1:A:1406:SER:OG	1:A:1407:GLU:N	2.53	0.41
1:A:1607:HIS:CE1	1:A:1615:GLU:HG3	2.56	0.41
1:A:1753:ARG:HE	1:A:1823:THR:HG1	1.67	0.41
2:B:119:LEU:HA	2:B:125:THR:HG21	2.03	0.41
1:A:340:ILE:HB	1:A:397:THR:HG23	2.02	0.41
1:A:631:HIS:C	1:A:632:HIS:CG	2.98	0.41
1:A:658:TRP:NE1	1:A:688:LEU:O	2.47	0.41
1:A:680:GLN:HB3	1:A:681:PRO:HD2	2.02	0.41
1:A:935:PHE:CD1	1:A:1000:PHE:CG	3.08	0.41
1:A:984:HIS:H	1:A:985:LYS:NZ	2.18	0.41
1:A:1551:VAL:HG12	1:A:1555:MET:CE	2.32	0.41
1:A:1779:LEU:H	2:B:26:ASN:HD21	1.69	0.41
1:A:1928:LYS:HE3	2:B:56:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:LEU:HD22	1:A:1974:PHE:HZ	1.85	0.41
2:B:19:LEU:C	2:B:19:LEU:HD23	2.46	0.41
1:A:459:PHE:O	1:A:492:VAL:N	2.45	0.41
1:A:555:PRO:HB2	1:A:615:PHE:HB3	2.03	0.41
1:A:1495:ILE:O	1:A:1497:HIS:ND1	2.53	0.41
1:A:1926:ASP:HB3	1:A:1929:MET:HE1	2.03	0.41
1:A:346:LEU:HD21	1:A:642:CYS:SG	2.61	0.41
1:A:576:TYR:HA	1:A:633:LEU:CD2	2.51	0.41
1:A:724:LEU:O	1:A:727:PHE:N	2.53	0.41
1:A:1009:ASP:OD1	1:A:1009:ASP:N	2.53	0.41
1:A:1285:LEU:HA	1:A:1288:LEU:HD12	2.02	0.41
1:A:109:VAL:HG21	1:A:625:ALA:HB1	2.03	0.40
1:A:1143:LEU:HD13	1:A:1143:LEU:HA	1.75	0.40
1:A:1399:ILE:O	1:A:1403:VAL:HG23	2.21	0.40
1:A:1650:ILE:CD1	1:A:1709:ASN:HD22	2.34	0.40
2:B:120:ARG:HH21	2:B:138:THR:HA	1.85	0.40
2:B:161:THR:HG23	2:B:163:ARG:H	1.85	0.40
1:A:743:LEU:HD12	1:A:743:LEU:HA	1.94	0.40
1:A:785:ARG:HA	1:A:788:ILE:HG22	2.04	0.40
1:A:1676:LYS:HG3	1:A:1677:HIS:CG	2.57	0.40
1:A:1803:LYS:HG3	2:B:28:PHE:HD2	1.86	0.40
1:A:1851:LEU:HD12	1:A:1874:THR:O	2.21	0.40
2:B:11:ASP:OD2	2:B:92:ASN:HB2	2.21	0.40
1:A:259:GLN:H	1:A:329:VAL:HB	1.86	0.40
1:A:775:PHE:O	1:A:779:VAL:HG23	2.22	0.40
1:A:927:ILE:C	1:A:929:GLN:N	2.79	0.40
1:A:1839:THR:O	1:A:1843:ARG:HG3	2.21	0.40
2:B:93:VAL:HA	2:B:97:TRP:HD1	1.86	0.40
1:A:581:ASP:OD1	1:A:584:GLN:HB2	2.22	0.40
1:A:633:LEU:HB2	1:A:659:ILE:HG23	2.02	0.40
1:A:639:HIS:HB2	1:A:654:VAL:CG1	2.52	0.40
1:A:1169:LEU:HD23	1:A:1257:VAL:HG13	2.03	0.40
1:A:1778:LYS:HA	1:A:1778:LYS:HD3	1.94	0.40
1:A:1961:PRO:HA	1:A:1964:PHE:CD2	2.56	0.40
1:A:1997:LYS:O	1:A:2000:HIS:HB3	2.21	0.40
2:B:5:LYS:NZ	2:B:74:GLN:HG2	2.36	0.40
1:A:1296:GLU:OE2	1:A:1298:LYS:NZ	2.35	0.40
1:A:1875:LEU:HD23	1:A:1875:LEU:HA	1.92	0.40
1:A:1898:VAL:C	1:A:1899:LEU:HD23	2.47	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	1672/2053 (81%)	1497 (90%)	175 (10%)	0	100	100
2	B	175/184 (95%)	155 (89%)	20 (11%)	0	100	100
All	All	1847/2237 (83%)	1652 (89%)	195 (11%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1476/1773 (83%)	1476 (100%)	0	100	100
2	B	153/157 (98%)	153 (100%)	0	100	100
All	All	1629/1930 (84%)	1629 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	HIS
1	A	559	ASN
1	A	575	GLN
1	A	823	GLN
1	A	1106	GLN
1	A	1132	HIS

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Mol	Chain	Res	Type
1	A	1557	ASN
1	A	1559	HIS
1	A	1653	ASN
1	A	1704	ASN
1	A	1709	ASN
1	A	1731	GLN
1	A	1844	ASN
1	A	1869	GLN
1	A	1880	HIS
1	A	1910	GLN
1	A	1988	ASN
2	B	39	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

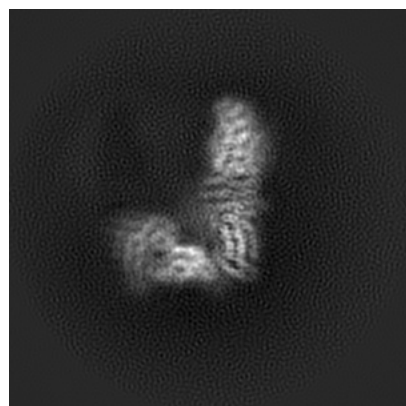
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65176. These allow visual inspection of the internal detail of the map and identification of artifacts.

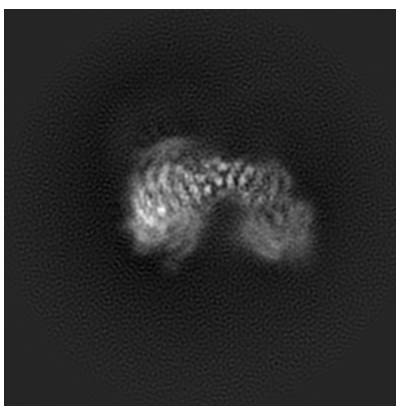
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

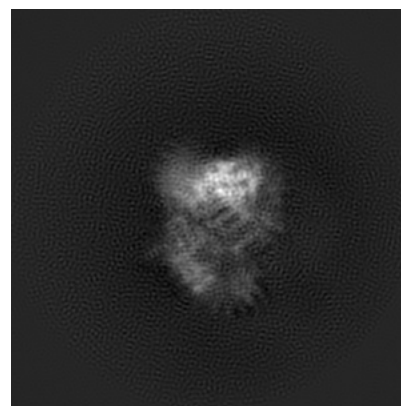
#### 6.1.1 Primary map



X

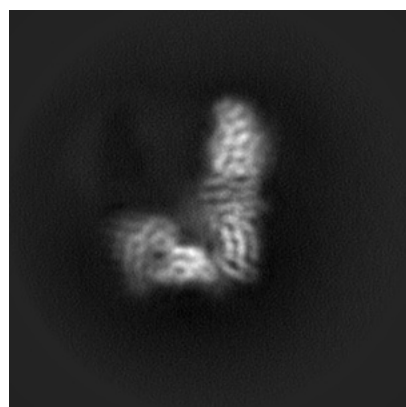


Y

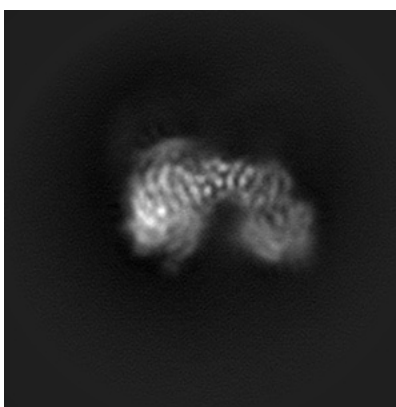


Z

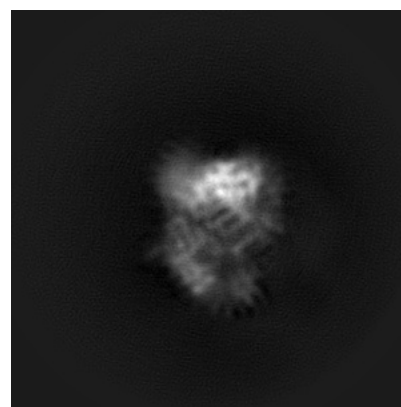
#### 6.1.2 Raw map



X



Y



Z

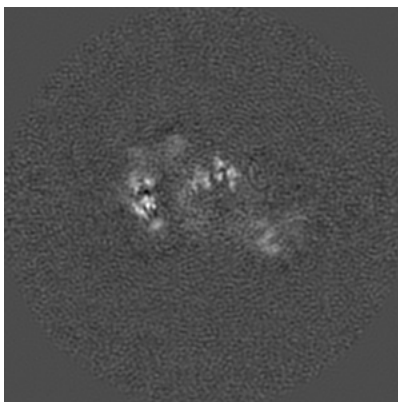
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

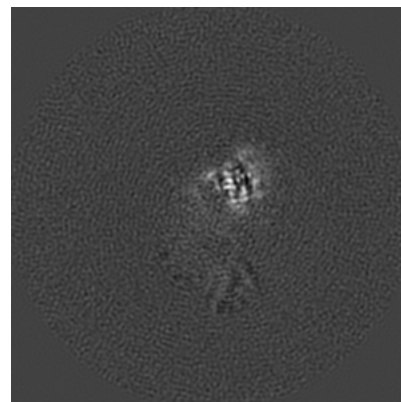
### 6.2.1 Primary map



X Index: 120



Y Index: 120

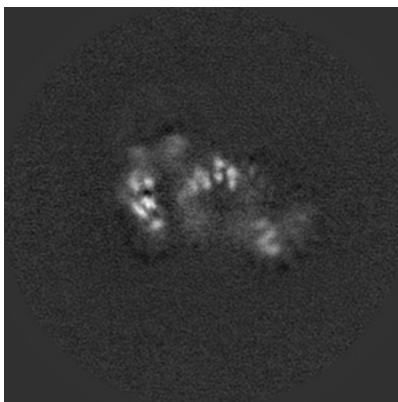


Z Index: 120

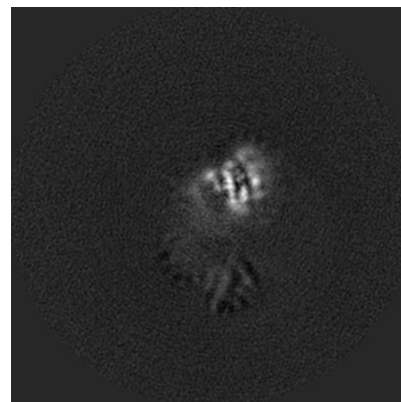
### 6.2.2 Raw map



X Index: 120



Y Index: 120

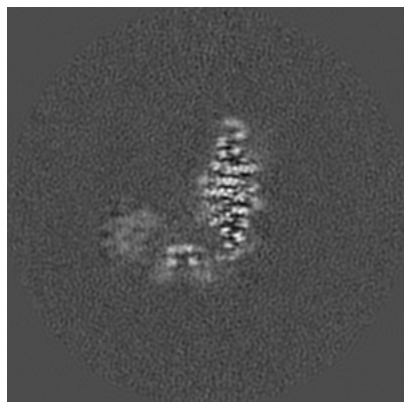


Z Index: 120

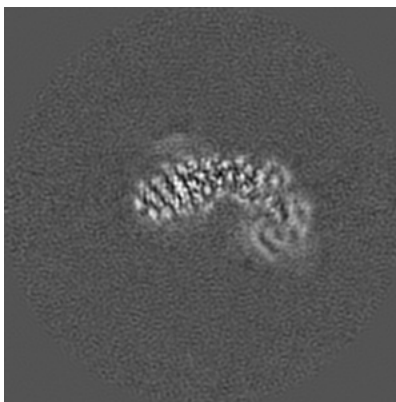
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

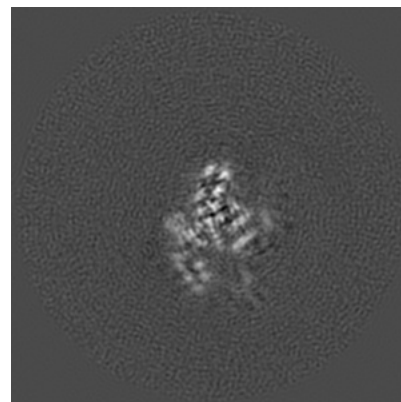
### 6.3.1 Primary map



X Index: 137

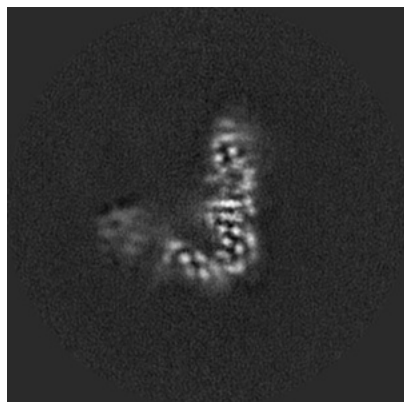


Y Index: 137

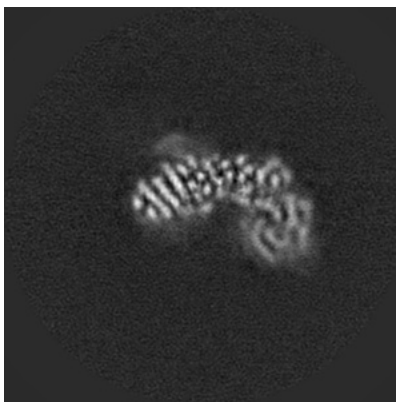


Z Index: 86

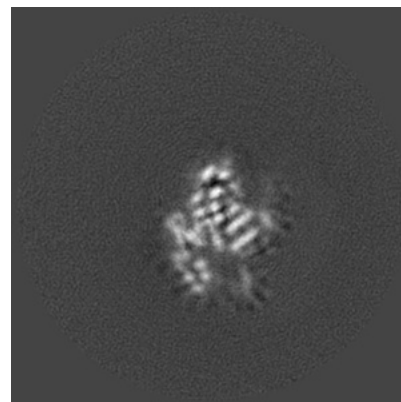
### 6.3.2 Raw map



X Index: 131



Y Index: 138

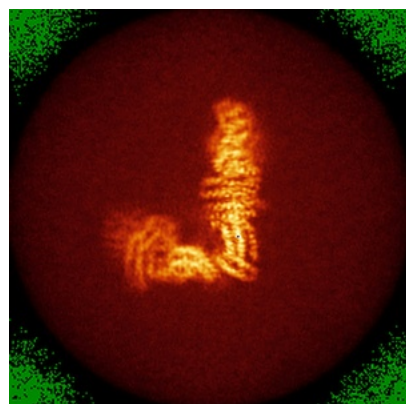


Z Index: 87

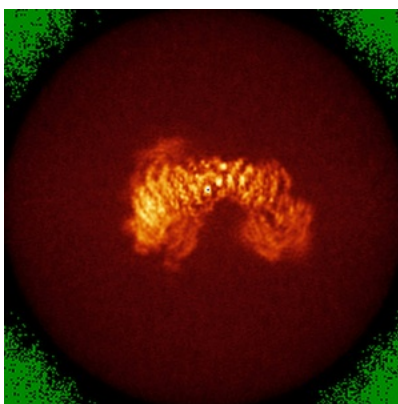
The images above show the largest variance slices of the map in three orthogonal directions.

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

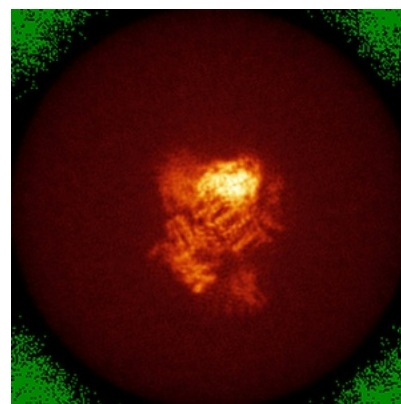
### 6.4.1 Primary map



X



Y

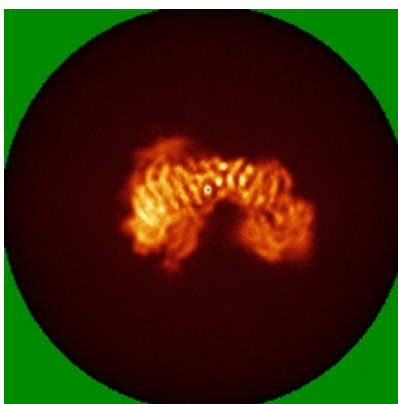


Z

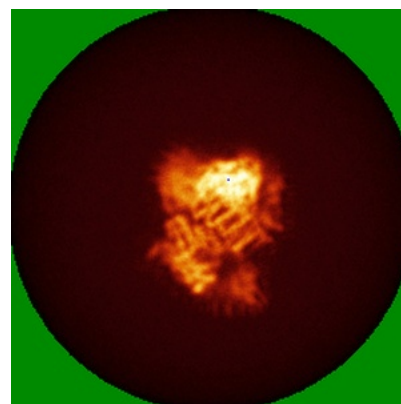
### 6.4.2 Raw map



X



Y



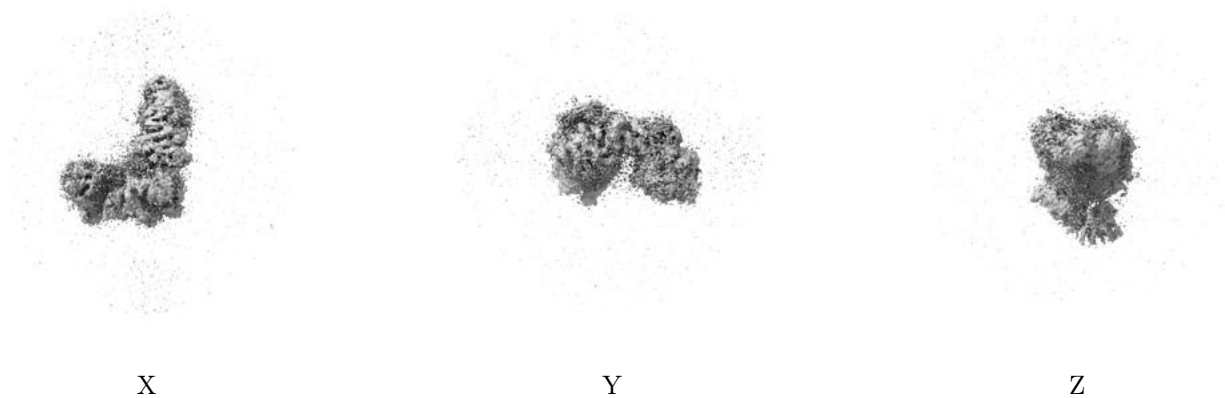
Z

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



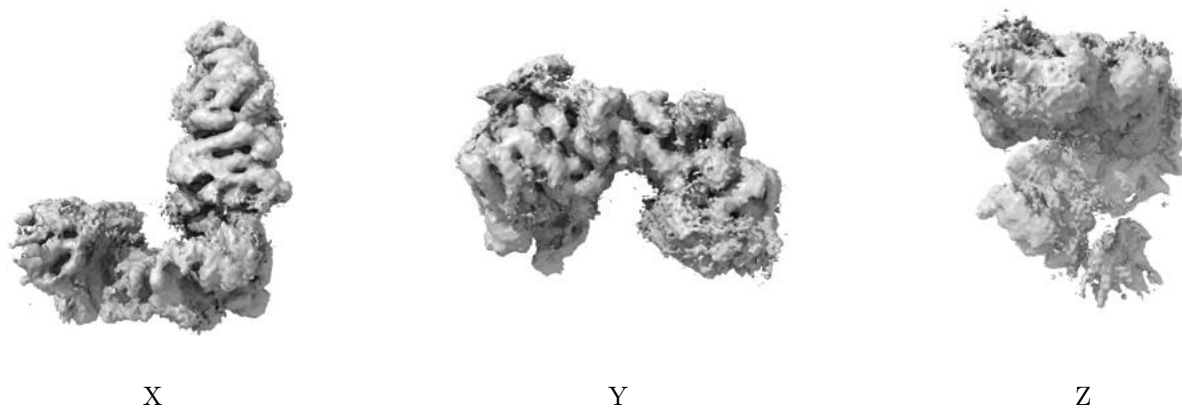
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

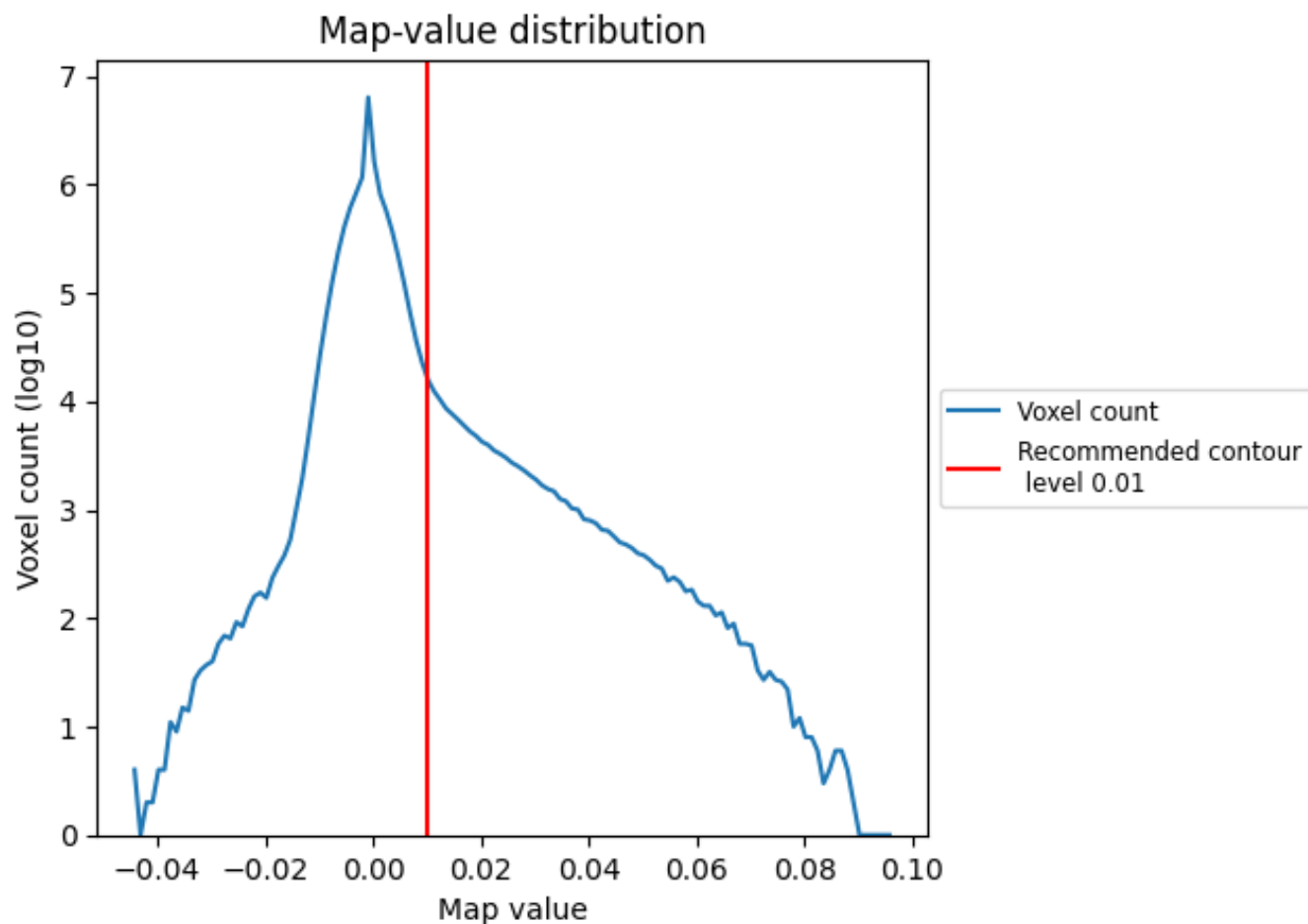
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

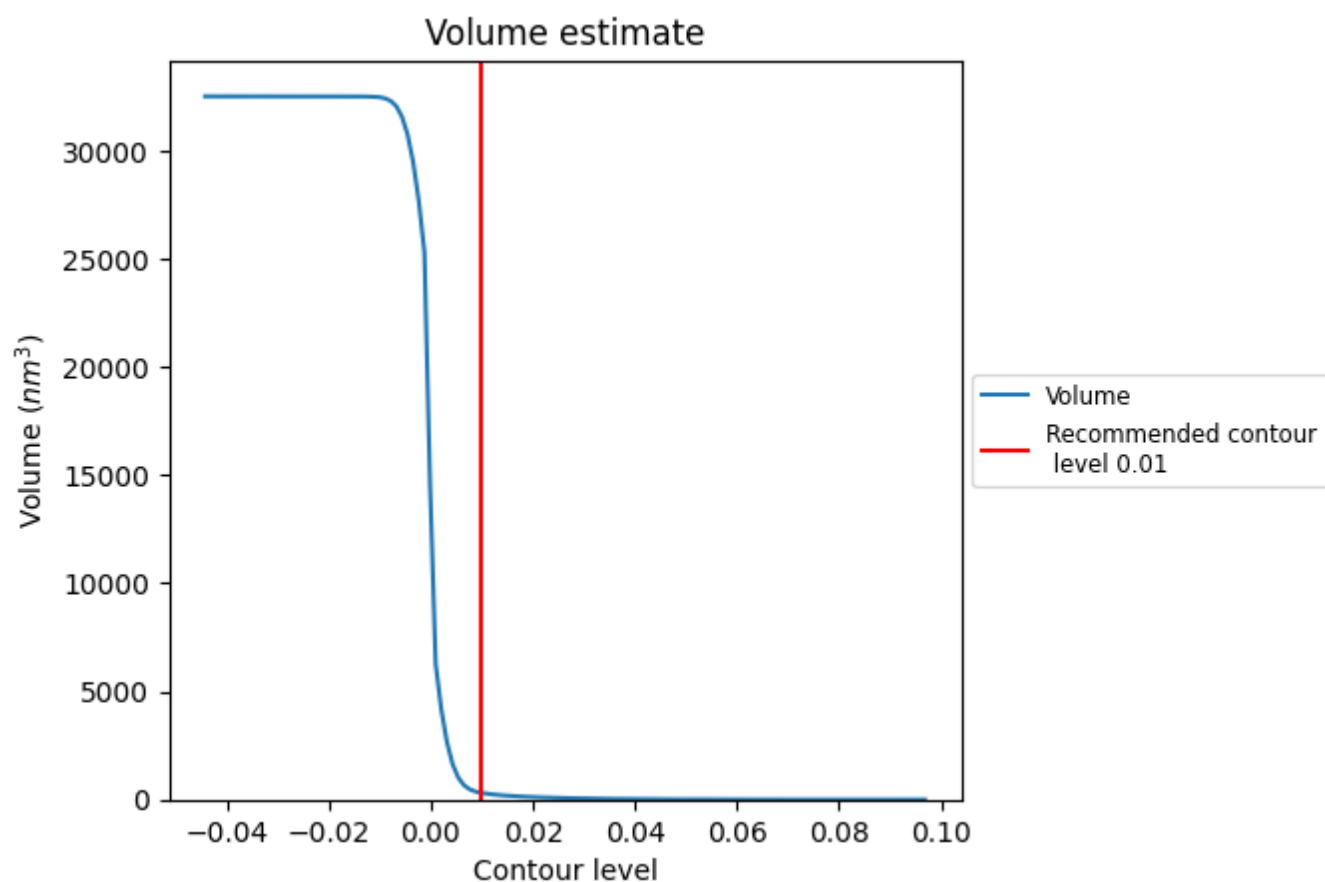
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

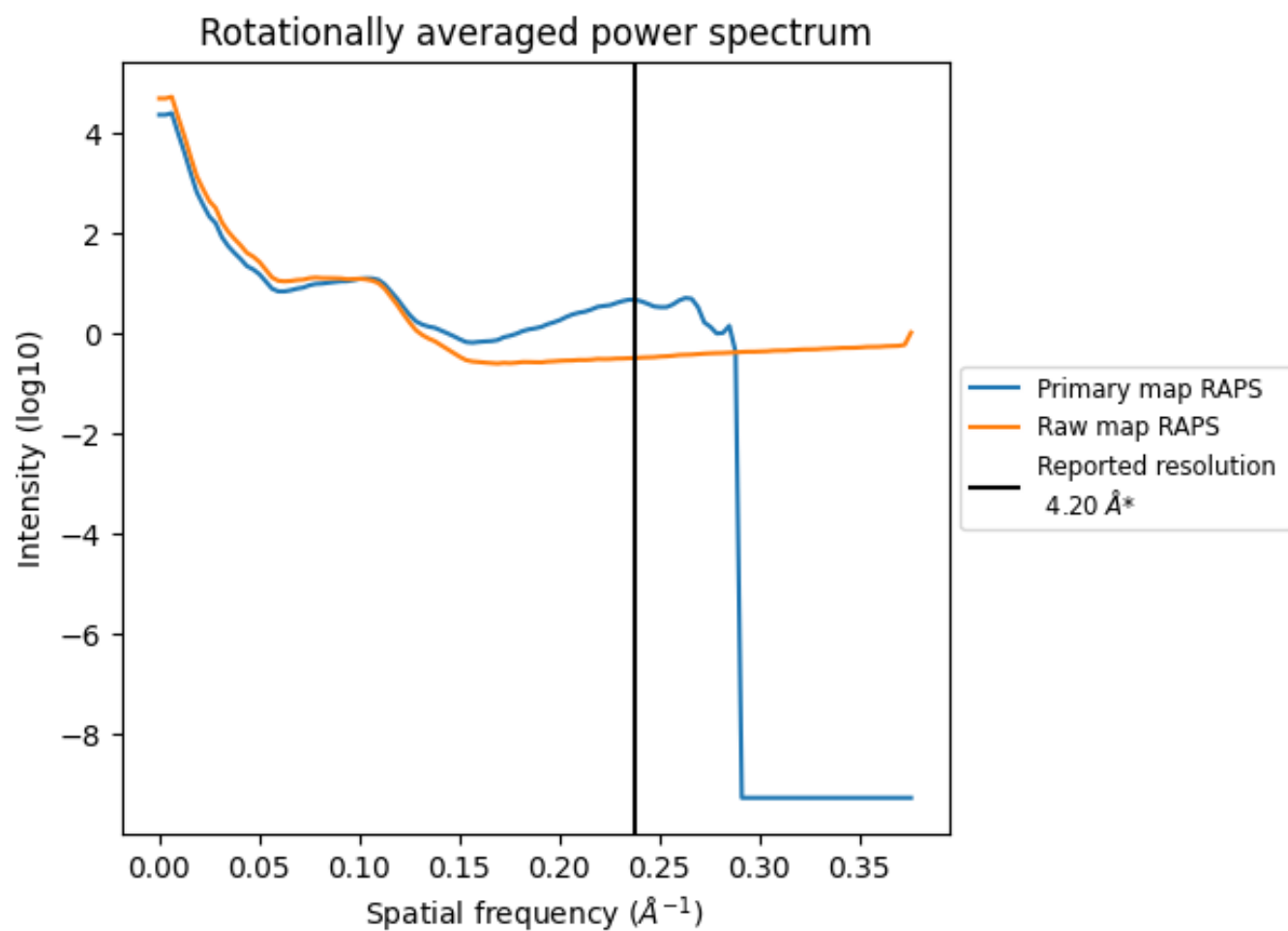


The volume at the recommended contour level is 306  $\text{nm}^3$ ; this corresponds to an approximate mass of 276 kDa.

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 ⓘ

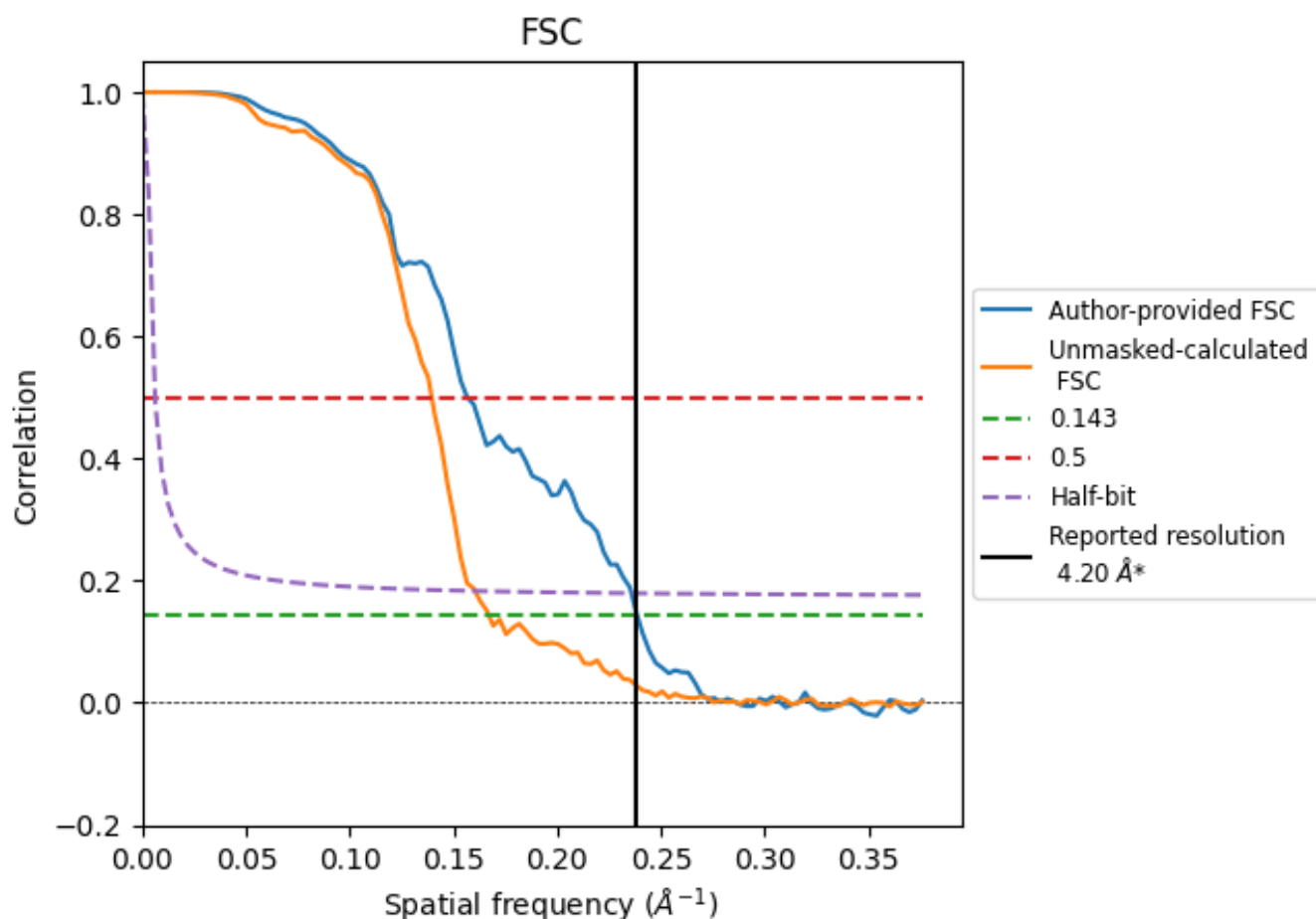


\*Reported resolution corresponds to spatial frequency of 0.238  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

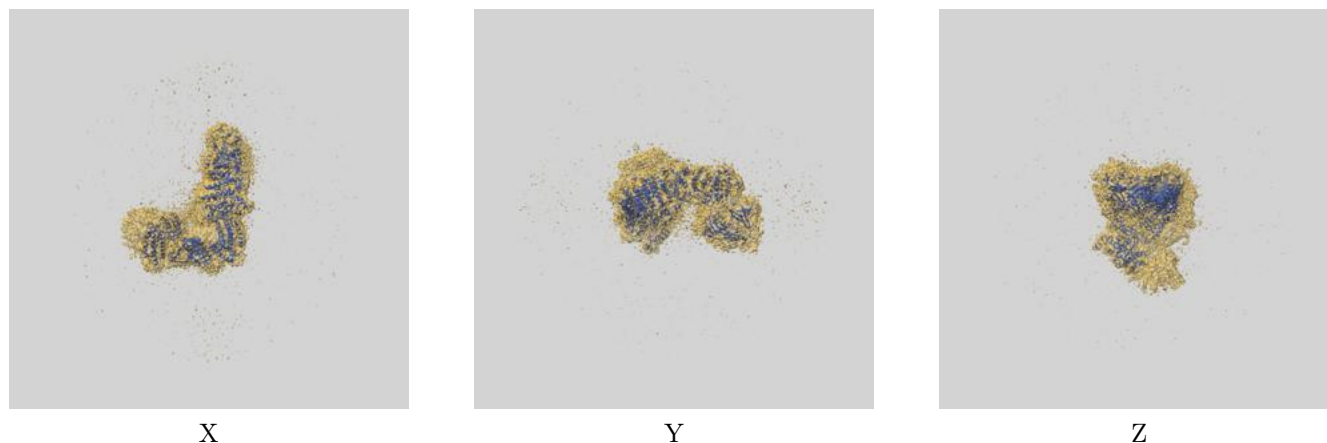
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	6.38	4.24
Unmasked-calculated*	5.98	7.17	6.23

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.98 differs from the reported value 4.2 by more than 10 %

## 9 Map-model fit [i](#)

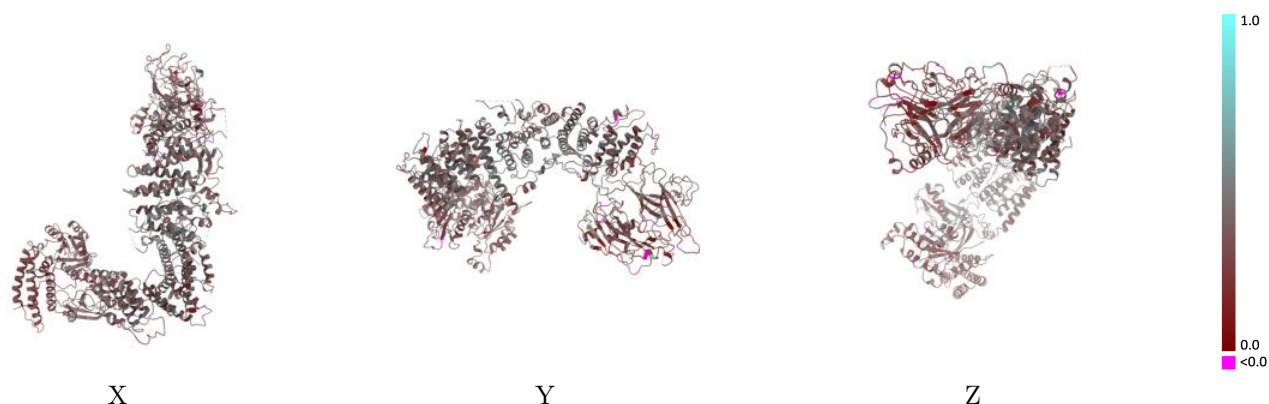
This section contains information regarding the fit between EMDB map EMD-65176 and PDB model 9VM4. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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](#)



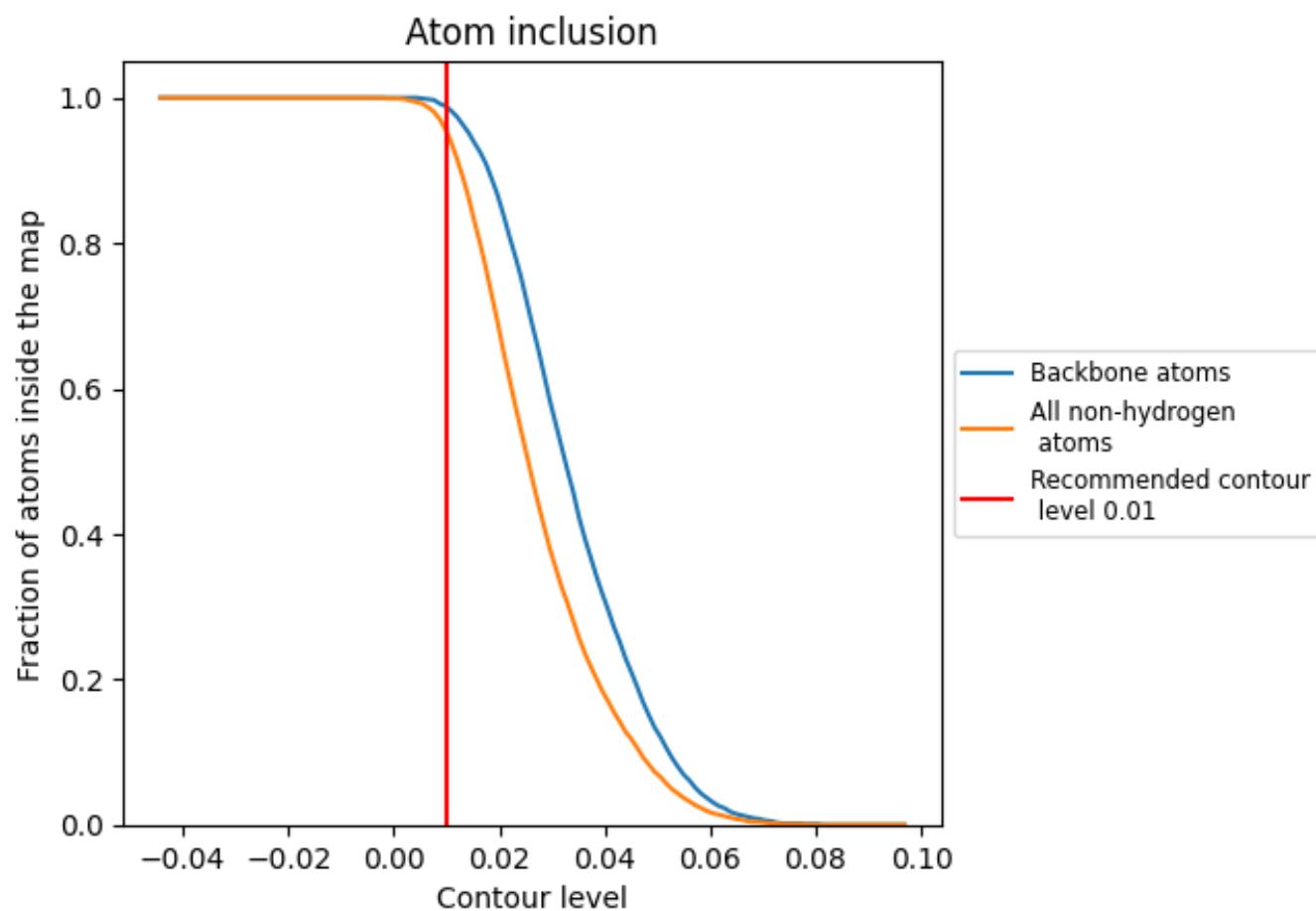
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9540	<div></div> 0.3580
A	<div></div> 0.9570	<div></div> 0.3640
B	<div></div> 0.9280	<div></div> 0.3050

