



Full wwPDB EM Validation Report ⓘ

Aug 19, 2026 – 04:33 pm BST

PDB ID : 9TUB / pdb_00009tub
EMDB ID : EMD-56255
Title : CryoEM structure of DruE:ATPgammaS:DNA from Druantia type III - dimer
4
Authors : Grass, L.M.; Himpich, S.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on : 2026-01-08
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

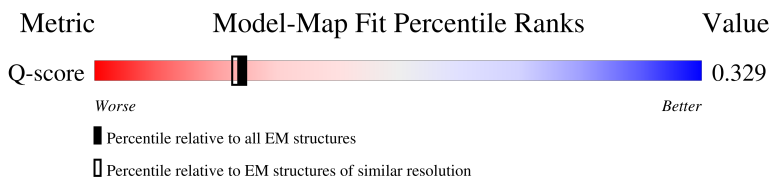
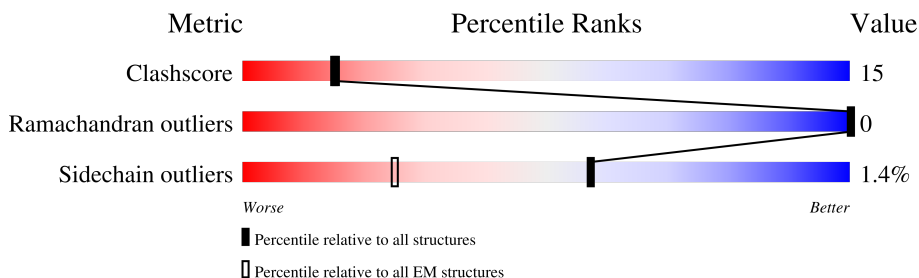
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	G	30	
1	i	30	
2	Y	2108	
2	y	2108	

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Mol	Chain	Length	Quality of chain
3	I	30	17% 47% 30% 23%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31776 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 DNA chain called DNA (5'-D(P*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	5	Total	C	N	O	P	0	0
			102	49	20	28	5		
1	G	12	Total	C	N	O	P	0	0
			249	118	50	69	12		

- Molecule 2 is a protein called DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	y	2048	Total	C	N	O	S	0	0
			16264	10264	2906	3022	72		
2	Y	1843	Total	C	N	O	S	0	0
			14619	9219	2618	2715	67		

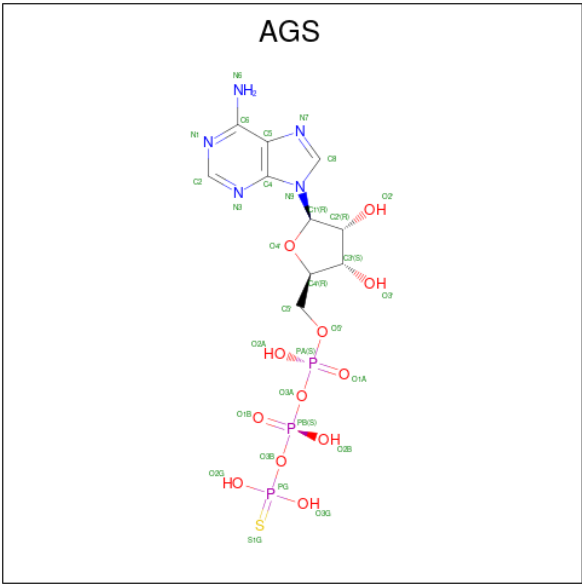
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
y	0	PHE	-	expression tag	UNP A0A4P8BDA5
Y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
Y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
Y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
Y	0	PHE	-	expression tag	UNP A0A4P8BDA5

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*CP*TP*GP*CP*CP*AP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	23	Total	C	N	O	P	0	0
			470	223	86	138	23		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

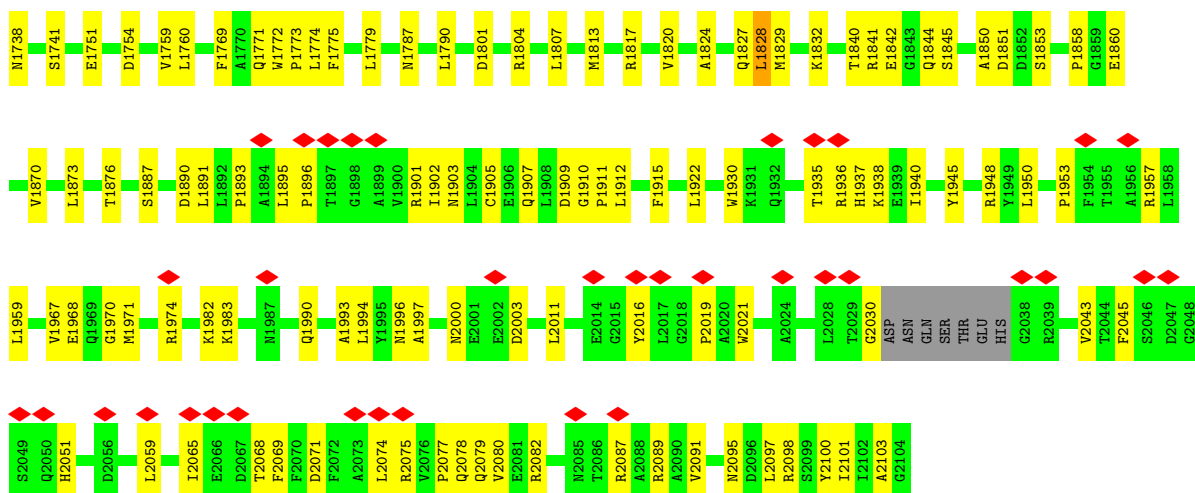


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
4	y	1	31	10	5	12	3	1	0
4	Y	1	31	10	5	12	3	1	0

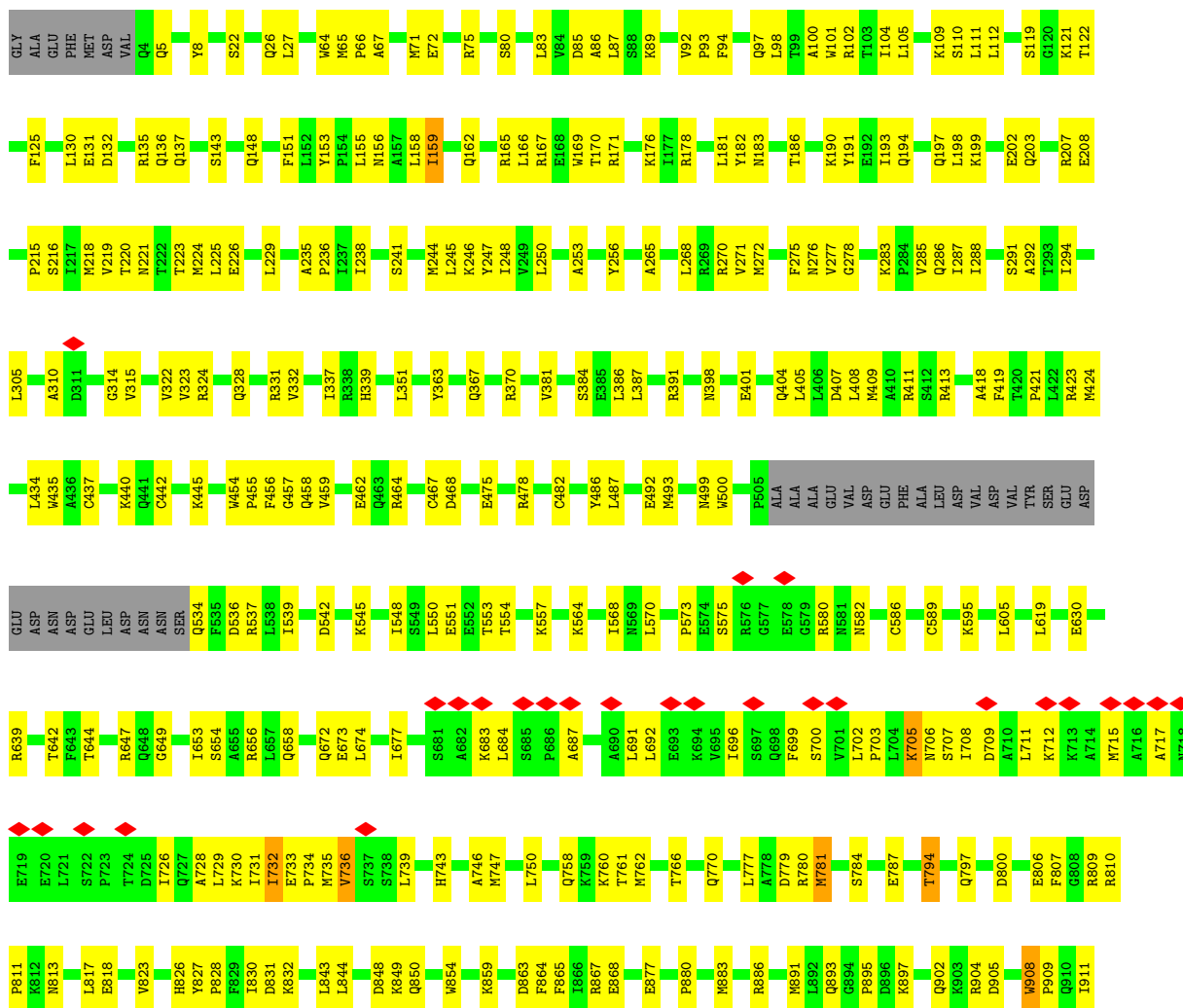
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	y	5	Total	Zn	0
			5	5	
5	Y	5	Total	Zn	0
			5	5	

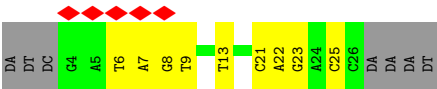
GLU	VAL	ASP	GLU	PHE	ALA	LEU	ASP	VAL	ASP	VAL	TYR	SER	GLU	ASP	GLU	ASP	ASN	ASN	SER	Q534	R537	L538	I539	Y546	I547	I548	S549	L550	E551	E552	T553	T554	K557	I558	D559	E567	I568	N569	L570	L571	R572	P573	E574	S575	R580	N581	S582	S583	F584		
A585	C586	Q593	P586	R594	K595	N596	N597	R604	L605	F609	F610	L611	N612	E613	I614	I615	P616	T617	E620	F621	S622	T627	R628	E629	E630	P634	F635	R638	R639	L640	F643	S646	R647	Q648	G649	T650	I653	L658	Q658	R667	A668	Q672	I677	P680	S681	A682					
K683	L684	S685	P686	A687	H688	C689	E693	K694	V695	I696	F699	S700	V701	L702	P703	L704	K705	N706	S707	I708	L711	K712	K713	A714	M715	A716	A717	N718	E719	E720	L721	S722	P723	T724	D725	I726	Q727	A728	L729	K730	I731	I732	E733	P734	M735	S738	L739	S740	T741		
Q751	A752	N753	S754	G755	N756	M762	S763	W764	Q765	T766	L767	S768	E769	S774	V775	D776	L777	A778	D779	R780	F821	M781	R782	G783	K786	E787	D792	L793	Q796	Q797	L803	N813	T816	L817	E818	S819	L820	G821	L822	V823	F829	K832	V833	C836	P837	Q838	D839	W840	K841		
T842	L843	L844	D848	K849	Q850	R855	N856	L857	L858	K859	I860	T861	L862	D863	F864	F865	I866	R867	E868	N869	S870	A871	V872	F873	N876	E877	Q878	R881	W882	M883	G884	A885	M891	L892	Q893	G894	P895	D896	K900	G901	Q902	K903	R904	D905	Q906	L907	W908	P909	Q910	I911	N917
K921	L922	I930	Q934	A935	H936	W937	K938	N942	M945	E946	I947	V948	W949	R957	E960	Q964	L965	D966	V979	W980	R981	P983	Y984	T985	R986	R987	A988	L994	P998	Y999	L1000	P1001	G1002	S1003	K1004	K1010	I1014	E1015	M1016	G1108	V1109	D1110	I1111	M1114	M1119						
R1037	L1038	E1042	I1047	E1053	G1054	L1055	W1056	S1057	S1060	L1063	A1064	L1065	K1066	W1069	Y1070	R1071	L1072	E1073	Q1078	R1079	Q1083	L1084	Q1085	K1089	Q1090	F1091	K1092	G1094	K1095	V1096	N1097	V1098	L1099	M1100	C1101	T1104	M1105	E1106	G1107	V1109	D1110	I1111	M1114	M1119							
V1122	P1123	Y1129	R1132	R1136	L1141	R1138	S1144	T1148	L1149	C1150	K1151	N1152	M1157	R1177	S1180	I1183	V1184	N1189	A1190	L1191	F1196	L1197	R1198	P1202	D1203	A1204	K1210	W1211	F1212	F1213	E1214	G1215	D1216	E1217	S1218	Q1219	C1220	L1221	R1222	F1223	L1224	L1227	Q1230								
A1231	D1232	Q1233	L1234	A1235	L1238	A1239	R1240	L1241	T1242	Q1243	M1248	S1249	L1250	T1251	L1256	T1257	R1258	T1259	Q1260	A1261	M1262	Q1264	Q1265	R1269	A1270	L1274	A1275	I1276	L1277	M1280	I1281	E1282	K1285	W1291	E1292	E1293	K1298	A1299	I1300	A1301	Y1302	Q1303	L1304	R1308	F1313	S1314					
I1317	S1318	A1320	F1321	L1322	P1323	H1324	G1326	F1327	P1328	V1329	G1330	V1331	L1332	N1333	F1334	N1335	K1344	R1345	R1346	K1349	A1350	T1351	Q1352	A1353	D1354	P1355	ASN	GLU	GLY	GLY	GLU	SER	ARG	ARG	T1366	L1369	R1372	D1373	L1374	F1375	L1376	A1377	R1378	R1379	F1380	Y1381	V1387	V1388	L1389	G1390	
G1391	K1392	V1393	S1396	M1400	L1401	V1404	L1405	A1406	S1407	G1408	Q1409	E1410	G1413	D1414	H1415	I1417	C1439	A1444	L1449	R1453	Y1454	L1455	G1459	F1460	A1461	T1462	Q1467	A1468	H1469	N1470	S1473	A1476	Q1477	L1486	V1487	R1504	H1507	S1508	G1509	E1510	G1517	E1518									
H1521	I1525	C1526	L1527	S1528	C1529	G1530	R1531	A1532	Q1535	L1545	K1546	N1547	P1548	E1549	R1550	T1553	H1554	Y1555	L1556	L1557	R1558	GLY	SER	ASN	ASP	ARG	GLN	GLY	SER	N1568	C1571	D1578	L1579	W1580	L1581	R1586	M1589	V1590	E1591	L1594	R1603	D1604	E1605	V1606	A1607	A1608	E1609				
V1613	G1618	N1627	V1632	T1633	T1634	D1639	Y1643	T1644	F1649	I1650	Y1651	R1652	R1653	N1654	A1655	Y1674	K1677	L1678	L1679	H1689	C1690	L1691	L1692	S1693	Y1694	D1695	S1696	Y1699	R1702	H1707	A1708	L1709	T1710	T1713	R1716	Q1727	Y1728	F1729	G1730	D1731	E1736	T1737									



• Molecule 2: DEAD/DEAH box helicase







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21652	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.350	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1093334, 1.1093334, 1.1093334	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: ZN, AGS

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	G	0.16	0/280	0.30	0/430
1	i	0.17	0/114	0.36	0/173
2	Y	0.11	0/14945	0.30	0/20251
2	y	0.11	0/16630	0.31	0/22543
3	I	0.22	0/526	0.40	0/809
All	All	0.12	0/32495	0.31	0/44206

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	G	249	0	135	4	0
1	i	102	0	57	9	0
2	Y	14619	0	14480	400	0
2	y	16264	0	16076	527	0
3	I	470	0	259	9	0
4	Y	31	0	12	3	0
4	y	31	0	12	1	0
5	Y	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	y	5	0	0	0	0
All	All	31776	0	31031	928	0

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

All (928) 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:Y:863:ASP:O	2:Y:867:ARG:HB2	1.77	0.84
2:y:12:LEU:HD21	2:y:403:LEU:HD21	1.62	0.81
2:y:1317:ILE:HG22	2:y:1322:LEU:HB2	1.64	0.80
2:Y:826:HIS:O	2:Y:972:GLU:HB2	1.83	0.79
2:y:779:ASP:OD1	2:y:780:ARG:N	2.15	0.79
2:Y:736:VAL:HG12	2:Y:743:HIS:HB3	1.65	0.78
2:y:220:THR:HG23	2:y:224:MET:HB3	1.66	0.77
2:y:1210:LYS:HA	2:y:1214:GLU:HB3	1.66	0.76
2:Y:534:GLN:HB3	2:Y:573:PRO:HG2	1.66	0.76
2:Y:151:PHE:HE2	2:Y:153:TYR:HB2	1.51	0.76
2:y:1632:VAL:HG12	2:y:1650:ILE:HG13	1.68	0.75
2:Y:111:LEU:HB3	2:Y:288:ILE:HG22	1.68	0.75
2:y:1741:SER:HB2	2:y:1774:LEU:HD11	1.68	0.74
2:Y:245:LEU:HB3	2:Y:277:VAL:HG11	1.70	0.74
2:y:445:LYS:HA	2:y:458:GLN:HB2	1.69	0.74
2:y:1329:VAL:HG12	2:y:1655:ALA:HB1	1.69	0.73
2:y:1850:ALA:HB2	2:y:1870:VAL:HG23	1.71	0.73
2:Y:487:LEU:HB2	2:Y:539:ILE:HB	1.71	0.73
2:Y:545:LYS:HA	2:Y:568:ILE:O	1.88	0.72
2:Y:1483:PRO:O	2:Y:1635:GLN:NE2	2.22	0.72
2:Y:880:PRO:HA	2:Y:883:MET:HG2	1.71	0.72
2:y:731:ILE:HD13	2:Y:734:PRO:HB3	1.72	0.71
2:y:26:GLN:HG2	2:y:605:LEU:HD11	1.72	0.71
2:y:418:ALA:HB3	2:y:421:PRO:HG3	1.73	0.71
2:Y:1835:TRP:HE1	2:Y:1838:GLN:HB3	1.56	0.71
2:y:1079:ARG:HH21	2:y:1083:GLN:HB3	1.55	0.70
2:y:1937:HIS:HD2	2:y:1970:GLY:HA3	1.56	0.70
2:Y:891:MET:HG3	2:Y:893:GLN:HE21	1.57	0.70
2:y:836:CYS:SG	2:y:841:LYS:NZ	2.65	0.70
2:Y:248:ILE:HB	2:Y:287:ILE:HG22	1.74	0.70
2:Y:580:ARG:HD3	1:G:20:DA:H5'	1.74	0.69
2:y:315:VAL:HB	2:y:319:ASP:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:1227:LEU:HB2	2:y:1256:LEU:HD12	1.76	0.68
2:y:1455:LEU:HB2	2:y:1579:LEU:HD11	1.74	0.68
2:y:2065:ILE:HD11	2:y:2091:VAL:HB	1.76	0.68
2:y:440:LYS:HG2	2:y:456:PHE:HB3	1.75	0.68
2:Y:1373:ASP:OD1	2:Y:1375:PRO:HD2	1.94	0.67
2:y:781:MET:HE1	2:y:1069:TRP:CE2	2.29	0.67
2:Y:125:PHE:HB2	2:Y:288:ILE:HD12	1.75	0.67
2:y:1335:ASN:HB3	2:y:1369:LEU:HD21	1.77	0.67
2:Y:902:GLN:HE22	2:Y:904:ARG:HD3	1.59	0.67
2:Y:696:ILE:HG12	2:Y:708:ILE:HG23	1.76	0.67
2:y:203:GLN:HE21	2:y:205:LEU:HD21	1.60	0.67
2:Y:454:TRP:NE1	2:Y:456:PHE:O	2.28	0.67
2:Y:630:GLU:HG2	2:Y:1094:GLY:HA3	1.76	0.67
2:y:310:ALA:O	2:y:314:GLY:N	2.22	0.67
2:y:1231:ALA:O	2:y:1235:ALA:N	2.26	0.67
2:y:193:ILE:O	2:y:193:ILE:HG13	1.94	0.66
2:y:755:GLY:O	2:y:756:ASN:ND2	2.29	0.66
2:y:900:LYS:HG3	2:y:905:ASP:HB2	1.77	0.66
1:i:3:DA:H2"	1:i:4:DA:C5	2.30	0.66
2:y:726:ILE:HG22	2:y:730:LYS:HE2	1.78	0.66
2:y:163:GLN:HG3	2:y:181:LEU:HD11	1.77	0.66
2:Y:902:GLN:OE1	2:Y:904:ARG:NH1	2.28	0.66
2:Y:250:LEU:HD21	2:Y:256:TYR:HE2	1.61	0.66
2:y:180:ALA:HB2	2:y:215:PRO:HG3	1.78	0.66
2:y:1396:SER:HA	2:y:1462:THR:HG22	1.76	0.66
2:y:101:TRP:HA	2:y:104:ILE:HG22	1.77	0.65
2:y:640:LEU:HG	2:y:1098:VAL:HG12	1.77	0.65
2:y:1405:LEU:HD13	2:y:1527:LEU:HB3	1.78	0.65
2:Y:1728:TYR:HB2	2:Y:1831:GLY:HA3	1.78	0.65
2:y:862:LEU:HD12	2:y:866:ILE:HD13	1.77	0.65
2:y:1277:LEU:O	2:y:1281:ILE:HG12	1.96	0.65
2:y:813:ASN:O	2:y:987:ARG:NH2	2.30	0.65
2:y:1549:GLU:OE2	2:y:1550:ARG:NH1	2.30	0.65
2:Y:86:ALA:O	2:Y:89:LYS:NZ	2.29	0.65
2:Y:66:PRO:HA	2:Y:94:PHE:HA	1.79	0.65
2:Y:229:LEU:HD11	2:Y:271:VAL:HG12	1.78	0.65
2:Y:435:TRP:NE1	2:Y:475:GLU:OE2	2.29	0.65
2:Y:1373:ASP:OD1	2:Y:1374:LEU:N	2.30	0.65
2:Y:777:LEU:HA	2:Y:781:MET:HG3	1.79	0.65
2:y:1828:LEU:C	2:y:1829:MET:HE2	2.23	0.64
2:Y:151:PHE:CE2	2:Y:153:TYR:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:66:PRO:HA	2:y:94:PHE:HA	1.79	0.64
2:y:1609:ARG:NH2	2:y:1634:THR:OG1	2.30	0.64
2:y:857:LEU:O	2:y:861:THR:HG23	1.98	0.64
2:Y:1388:VAL:HG12	2:Y:1393:VAL:HG22	1.79	0.64
2:y:71:MET:SD	2:y:71:MET:N	2.71	0.64
2:y:539:ILE:HG22	2:y:570:LEU:HB3	1.79	0.64
2:y:904:ARG:O	2:y:904:ARG:NH1	2.28	0.63
2:Y:167:ARG:HH22	2:Y:203:GLN:HB2	1.63	0.63
2:y:123:GLU:HA	2:y:126:MET:HG3	1.78	0.63
2:y:647:ARG:HE	2:y:1078:GLN:HB3	1.63	0.63
2:y:1417:ILE:O	2:y:1453:ARG:NH2	2.25	0.63
2:y:2098:ARG:NH1	2:y:2100:TYR:OH	2.31	0.63
2:Y:1107:MET:HE3	2:Y:1107:MET:H	1.64	0.63
2:y:866:ILE:HG23	2:y:871:ALA:HB3	1.81	0.63
2:Y:1690:CYS:SG	2:Y:1691:LEU:N	2.72	0.63
2:Y:1763:PRO:HD2	2:Y:1857:ALA:HB2	1.81	0.63
2:Y:1813:MET:SD	2:Y:1813:MET:N	2.71	0.63
2:y:1180:SER:HG	2:y:1507:HIS:HD1	1.47	0.63
2:y:1807:LEU:HD22	2:y:1891:LEU:HD23	1.80	0.63
2:Y:486:TYR:OH	2:Y:586:CYS:SG	2.56	0.63
2:Y:1122:VAL:HG11	2:Y:1159:VAL:HG11	1.80	0.63
2:Y:1666:ASP:HA	2:Y:1737:THR:HG21	1.81	0.63
2:y:402:LEU:O	2:y:406:LEU:HD12	1.97	0.62
2:Y:156:ASN:ND2	2:Y:183:ASN:OD1	2.32	0.62
2:y:546:TYR:OH	2:y:572:ARG:NH2	2.33	0.62
2:y:1690:CYS:SG	2:y:1691:LEU:N	2.72	0.62
2:y:1807:LEU:HD21	2:y:1820:VAL:HG11	1.80	0.62
2:Y:155:LEU:HG	3:I:21:DC:H5"	1.81	0.62
2:Y:734:PRO:HB2	2:Y:735:MET:HE2	1.80	0.62
2:Y:1602:ILE:HG22	2:Y:1604:ASP:H	1.64	0.62
2:y:1032:ILE:O	2:y:1037:ARG:NH2	2.32	0.62
2:y:727:GLN:O	2:y:731:ILE:HG12	1.99	0.62
2:y:1841:ARG:NH2	2:y:1844:GLN:OE1	2.30	0.62
2:Y:1523:TYR:N	2:Y:1579:LEU:O	2.28	0.62
2:y:74:LEU:HB3	2:y:78:LEU:HB3	1.80	0.62
2:Y:683:LYS:HE3	2:Y:717:ALA:HB2	1.80	0.62
2:y:349:LYS:HA	2:y:411:ARG:HH22	1.64	0.62
2:y:336:LEU:O	2:y:338:ARG:NH1	2.32	0.62
2:y:627:THR:HB	2:y:630:GLU:HB2	1.81	0.62
2:Y:891:MET:O	2:Y:893:GLN:NE2	2.32	0.62
2:y:883:MET:SD	2:y:883:MET:N	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:87:LEU:HD21	2:Y:169:TRP:HE1	1.65	0.62
2:Y:1801:ASP:HA	2:Y:1804:ARG:HD2	1.82	0.61
2:y:75:ARG:NH1	2:y:81:SER:OG	2.32	0.61
2:y:1940:ILE:O	2:y:1974:ARG:NH1	2.33	0.61
2:Y:1238:LEU:HD13	2:Y:1255:LEU:HD11	1.83	0.61
2:Y:1311:TYR:OH	3:I:25:DC:N4	2.30	0.61
2:y:493:MET:HE3	2:y:493:MET:HA	1.82	0.61
2:y:1265:GLN:OE1	2:y:1269:ARG:NH1	2.32	0.61
2:Y:458:GLN:NE2	2:Y:459:VAL:O	2.32	0.61
2:Y:1421:TRP:HB3	2:Y:1436:PRO:HG3	1.81	0.61
2:Y:1587:THR:HA	2:Y:1656:GLY:HA2	1.83	0.61
2:Y:151:PHE:HB3	2:Y:219:VAL:HG12	1.81	0.61
2:y:158:LEU:O	2:y:162:GLN:NE2	2.33	0.61
2:Y:915:HIS:NE2	1:G:23:DC:OP1	2.34	0.61
2:Y:1739:PRO:HG2	2:Y:1742:LEU:HB3	1.82	0.61
2:y:1016:MET:HE2	2:y:1016:MET:HA	1.82	0.61
2:Y:111:LEU:HD12	2:Y:112:LEU:N	2.16	0.61
2:Y:75:ARG:NH1	2:Y:85:ASP:OD1	2.32	0.61
2:y:454:TRP:NE1	2:y:456:PHE:O	2.34	0.60
2:y:1993:ALA:HB1	2:y:2068:THR:HG22	1.83	0.60
2:Y:880:PRO:O	2:Y:886:ARG:NH2	2.34	0.60
2:y:1844:GLN:HA	2:y:1876:THR:HA	1.84	0.60
2:y:1114:MET:SD	2:y:1114:MET:N	2.72	0.60
2:y:1135:ARG:HD2	2:y:1138:ARG:HD2	1.84	0.60
2:y:1379:ARG:HH22	2:y:1477:GLN:HB3	1.66	0.60
2:Y:1725:GLU:HB3	2:Y:1728:TYR:HE2	1.66	0.60
2:y:162:GLN:OE1	2:y:165:ARG:NH2	2.34	0.60
2:y:165:ARG:NH1	4:y:2201:AGS:O2A	2.34	0.60
2:y:730:LYS:HD3	2:y:730:LYS:N	2.15	0.60
2:y:1545:LEU:O	2:y:1554:HIS:ND1	2.31	0.60
2:Y:1536:THR:OG1	2:Y:1540:ARG:NH2	2.34	0.60
2:Y:223:THR:HG21	3:I:22:DA:H1'	1.83	0.60
2:y:1531:ARG:NH1	2:y:1555:TYR:O	2.34	0.60
2:y:1212:PHE:HB2	2:y:1219:GLN:HB2	1.84	0.59
2:y:1521:HIS:O	2:y:1535:GLN:NE2	2.35	0.59
2:y:2071:ASP:HB3	2:y:2074:LEU:HD13	1.83	0.59
2:Y:1340:ASP:N	2:Y:1340:ASP:OD2	2.34	0.59
2:Y:1688:HIS:HA	2:Y:1692:LEU:HB3	1.83	0.59
2:Y:111:LEU:HD11	2:Y:323:VAL:HG22	1.83	0.59
2:y:64:TRP:HA	2:y:327:ARG:HA	1.82	0.59
2:y:356:LEU:O	2:y:360:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:305:LEU:HD11	2:Y:322:VAL:HG23	1.84	0.59
2:Y:644:THR:OG1	2:Y:1120:ASN:OD1	2.20	0.59
2:Y:1177:ARG:NH2	2:Y:1623:LEU:O	2.34	0.59
2:y:2071:ASP:O	2:y:2079:GLN:NE2	2.36	0.59
2:y:747:MET:HA	2:y:750:LEU:HG	1.84	0.59
2:Y:1632:VAL:HG23	2:Y:1650:ILE:HG13	1.85	0.59
2:y:643:PHE:HE2	2:y:1106:GLU:HA	1.66	0.59
2:y:1319:GLU:N	2:y:1319:GLU:OE1	2.35	0.59
2:y:683:LYS:HD2	2:y:689:CYS:HB2	1.84	0.59
2:y:1334:PHE:HA	2:y:1460:PHE:O	2.03	0.59
2:y:1000:LEU:HD12	2:y:1001:PRO:HD2	1.83	0.59
2:Y:692:LEU:HD12	2:Y:715:MET:HE1	1.85	0.59
2:y:549:SER:HB3	2:y:559:ASP:HB3	1.83	0.58
2:Y:1494:SER:HA	2:Y:1502:ARG:HA	1.83	0.58
2:Y:65:MET:HA	2:Y:328:GLN:HB2	1.84	0.58
2:Y:658:GLN:HE22	2:Y:1069:TRP:HE1	1.51	0.58
2:Y:895:PRO:HB3	2:Y:908:TRP:CD1	2.38	0.58
2:Y:1601:LEU:HD23	2:Y:1645:GLY:HA3	1.83	0.58
2:y:861:THR:O	2:y:865:PHE:HB2	2.02	0.58
2:Y:181:LEU:HA	2:Y:219:VAL:HG23	1.85	0.58
2:y:238:ILE:HG23	2:y:275:PHE:HE1	1.69	0.58
2:Y:224:MET:HE1	3:I:23:DG:H5"	1.84	0.58
2:Y:434:LEU:HD21	2:Y:459:VAL:HG13	1.85	0.58
2:Y:777:LEU:HD12	2:Y:781:MET:HG3	1.85	0.58
2:y:1073:GLU:HB2	2:y:1096:VAL:HG21	1.86	0.58
2:y:1216:ASP:OD1	2:y:1217:GLU:N	2.37	0.58
2:y:1401:LEU:HD21	2:y:1405:LEU:H	1.69	0.58
2:Y:672:GLN:NE2	2:Y:1064:ALA:O	2.35	0.58
1:i:4:DA:OP2	2:y:223:THR:OG1	2.20	0.58
2:y:2075:ARG:N	2:y:2078:GLN:HE22	2.01	0.58
2:Y:8:TYR:CD1	2:Y:424:MET:HE1	2.39	0.58
2:Y:1665:ILE:O	2:Y:1668:TRP:NE1	2.37	0.58
2:y:1379:ARG:O	2:y:1379:ARG:NH1	2.33	0.58
2:Y:1764:GLN:HA	2:Y:1767:TRP:HE1	1.69	0.58
2:y:1391:GLY:O	2:y:1470:ASN:ND2	2.37	0.57
2:y:1771:GLN:HE22	2:y:1860:GLU:HB2	1.68	0.57
2:Y:92:VAL:O	4:Y:2206:AGS:N6	2.35	0.57
2:y:844:LEU:O	2:y:850:GLN:NE2	2.32	0.57
2:y:1093:SER:O	2:y:1095:LYS:NZ	2.37	0.57
2:y:1605:GLU:OE1	2:y:1702:ARG:NH1	2.37	0.57
2:y:1824:ALA:HB3	2:y:1827:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:272:MET:O	2:Y:276:ASN:N	2.37	0.57
2:Y:1807:LEU:HD22	2:Y:1891:LEU:HD22	1.85	0.57
2:y:1090:GLN:HG3	2:y:1095:LYS:HB2	1.86	0.57
2:y:13:ASN:HB2	2:y:400:ARG:HH12	1.69	0.57
2:y:1760:LEU:HD22	2:y:1858:PRO:HG3	1.87	0.57
2:Y:1259:THR:HA	2:Y:1262:MET:SD	2.43	0.57
2:y:734:PRO:HB2	2:Y:731:ILE:HG12	1.87	0.57
2:y:1234:LEU:O	2:y:1238:LEU:HG	2.05	0.57
2:Y:736:VAL:HB	2:Y:747:MET:SD	2.45	0.57
2:y:230:ILE:HD11	2:y:270:ARG:HH12	1.70	0.57
2:y:458:GLN:NE2	2:y:459:VAL:O	2.34	0.57
2:y:1151:LYS:HE2	2:y:1152:ASN:H	1.69	0.57
2:Y:1262:MET:HA	2:Y:1265:GLN:HB2	1.87	0.57
2:Y:1829:MET:HE3	2:Y:1830:GLN:H	1.68	0.57
2:y:487:LEU:HB2	2:y:539:ILE:HG13	1.86	0.57
2:y:776:ASP:HA	2:y:780:ARG:HD2	1.87	0.57
2:y:876:ASN:HD21	2:y:878:GLN:HB2	1.68	0.57
2:Y:105:LEU:HD22	2:Y:135:ARG:HH12	1.70	0.57
2:Y:277:VAL:O	2:Y:283:LYS:NZ	2.38	0.57
2:Y:462:GLU:OE2	2:Y:464:ARG:NH2	2.38	0.57
2:Y:630:GLU:OE2	2:Y:639:ARG:NH1	2.36	0.57
2:y:252:GLU:OE1	2:y:254:HIS:NE2	2.35	0.56
2:y:1652:ASP:OD1	2:y:1652:ASP:N	2.35	0.56
2:Y:190:LYS:HG3	2:Y:208:GLU:HB2	1.87	0.56
2:y:1909:ASP:O	2:y:1911:PRO:HD2	2.04	0.56
2:Y:218:MET:HE3	2:Y:219:VAL:N	2.20	0.56
2:Y:917:ASN:HD21	2:Y:919:VAL:HG12	1.70	0.56
2:Y:1487:VAL:HG21	2:Y:1504:ARG:HD3	1.87	0.56
2:y:234:ASP:N	2:y:234:ASP:OD1	2.35	0.56
2:y:437:CYS:HB3	2:y:458:GLN:H	1.71	0.56
2:y:696:ILE:HD12	2:y:711:LEU:HB3	1.86	0.56
2:y:714:ALA:HB1	2:y:750:LEU:HD13	1.86	0.56
2:Y:398:ASN:ND2	2:Y:401:GLU:OE2	2.39	0.56
2:Y:404:GLN:O	2:Y:408:LEU:HD22	2.06	0.56
2:Y:705:LYS:HA	2:Y:708:ILE:HB	1.87	0.56
2:y:1529:CYS:SG	2:y:1530:GLY:N	2.78	0.56
2:y:58:PHE:HD2	2:y:422:LEU:HD13	1.70	0.56
2:Y:548:ILE:HD11	2:Y:568:ILE:HD13	1.87	0.56
2:Y:1753:TYR:HA	2:Y:1841:ARG:HD3	1.87	0.56
2:Y:272:MET:SD	2:Y:278:GLY:N	2.64	0.56
2:y:711:LEU:HD22	2:y:732:ILE:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:750:LEU:HA	2:y:753:ASN:ND2	2.20	0.56
2:y:1243:GLN:NE2	2:y:1751:GLU:OE1	2.39	0.56
2:Y:911:ILE:O	2:Y:914:ARG:NE	2.36	0.56
2:Y:966:ASP:OD2	2:Y:969:GLN:NE2	2.39	0.56
2:y:1983:LYS:NZ	2:y:2030:GLY:O	2.37	0.55
2:y:628:ARG:HH12	3:I:9:DT:H3'	1.72	0.55
2:y:672:GLN:NE2	2:y:1064:ALA:O	2.38	0.55
2:Y:351:LEU:O	2:Y:411:ARG:NH2	2.39	0.55
2:y:150:ILE:HD13	2:y:218:MET:HG2	1.87	0.55
2:Y:800:ASP:OD2	2:Y:968:LYS:NZ	2.40	0.55
2:y:908:TRP:CE2	2:y:945:MET:HE2	2.42	0.55
2:y:1609:ARG:HE	2:y:1634:THR:HG23	1.72	0.55
2:y:1912:LEU:HD13	2:y:1957:ARG:HH22	1.72	0.55
2:Y:109:LYS:O	2:Y:286:GLN:NE2	2.40	0.55
2:Y:677:ILE:HG12	2:Y:1022:ARG:HH21	1.71	0.55
2:Y:1529:CYS:SG	2:Y:1530:GLY:N	2.79	0.55
2:y:1772:TRP:HD1	2:y:1773:PRO:HD2	1.69	0.55
2:Y:542:ASP:N	2:Y:542:ASP:OD1	2.39	0.55
2:Y:1424:ARG:NH2	2:Y:1447:GLN:O	2.39	0.55
2:y:1400:MET:HE1	2:y:1461:ALA:HB2	1.89	0.55
2:Y:696:ILE:HG13	2:Y:711:LEU:HD23	1.88	0.55
2:Y:1296:ALA:O	2:Y:1300:ILE:HG12	2.07	0.55
2:y:1014:ILE:HG12	2:y:1053:GLU:HG3	1.89	0.55
2:y:1525:ILE:HD13	2:y:1532:ALA:HB2	1.87	0.55
2:y:1639:ASP:OD1	2:y:1643:TYR:N	2.40	0.55
2:Y:191:TYR:HA	2:Y:194:GLN:HB2	1.89	0.55
2:Y:699:PHE:HA	2:Y:702:LEU:HD23	1.89	0.55
2:Y:728:ALA:HA	2:Y:731:ILE:HD12	1.87	0.55
2:Y:758:GLN:OE1	2:Y:760:LYS:HD2	2.07	0.55
2:y:266:LEU:HD11	2:y:1184:VAL:HG12	1.88	0.55
2:y:979:VAL:HG11	2:y:988:ALA:HB1	1.87	0.55
2:Y:893:GLN:NE2	2:Y:905:ASP:OD1	2.40	0.55
2:y:1224:LEU:HD22	2:y:1260:GLN:HG3	1.88	0.54
2:Y:1090:GLN:HB3	2:Y:1096:VAL:HG21	1.89	0.54
2:y:551:GLU:OE1	2:y:554:THR:OG1	2.21	0.54
2:y:2069:PHE:HB3	2:y:2082:ARG:HH21	1.72	0.54
2:Y:809:ARG:NH2	2:Y:868:GLU:O	2.40	0.54
2:y:639:ARG:HB2	2:y:1091:PHE:CE1	2.42	0.54
2:Y:649:GLY:O	2:Y:653:ILE:HG23	2.08	0.54
2:y:820:LEU:HB3	2:y:822:LEU:HD23	1.89	0.54
2:y:848:ASP:OD1	2:y:849:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:467:CYS:SG	2:Y:468:ASP:N	2.80	0.54
2:y:210:ILE:HG22	2:y:215:PRO:HD3	1.90	0.54
2:y:1332:VAL:HG13	2:y:1459:GLY:HA2	1.89	0.54
2:Y:1212:PHE:HB2	2:Y:1312:LEU:HD11	1.89	0.54
2:Y:1495:LEU:HD23	2:Y:1503:TYR:HD2	1.72	0.54
2:y:1460:PHE:HZ	2:y:1581:LEU:HD21	1.71	0.54
2:y:18:ARG:NH1	2:y:617:THR:OG1	2.41	0.54
2:Y:726:ILE:HG22	2:Y:730:LYS:HE3	1.90	0.54
2:Y:218:MET:HE3	2:Y:219:VAL:H	1.72	0.54
2:Y:1590:VAL:HG21	2:Y:1664:LEU:HD22	1.88	0.54
3:I:6:DT:H2"	3:I:7:DA:H5"	1.88	0.54
2:y:158:LEU:HD23	2:y:1107:MET:SD	2.48	0.54
2:y:672:GLN:HG3	2:y:1066:LYS:NZ	2.24	0.54
2:Y:696:ILE:O	2:Y:700:SER:OG	2.24	0.54
2:y:440:LYS:NZ	2:y:455:PRO:O	2.37	0.53
2:y:1276:ILE:HG12	2:y:1401:LEU:HD22	1.89	0.53
2:Y:310:ALA:O	2:Y:314:GLY:N	2.41	0.53
2:y:1293:GLU:O	2:y:1298:LYS:NZ	2.41	0.53
2:Y:97:GLN:NE2	2:Y:119:SER:O	2.41	0.53
2:Y:153:TYR:CZ	2:Y:158:LEU:HB3	2.44	0.53
2:Y:536:ASP:O	2:Y:537:ARG:NH1	2.40	0.53
2:Y:1424:ARG:HH21	2:Y:1448:GLN:HA	1.74	0.53
2:y:1550:ARG:O	2:y:1553:THR:OG1	2.22	0.53
2:y:1603:ARG:HH22	2:y:1643:TYR:HB3	1.73	0.53
2:y:829:PHE:HA	2:y:832:LYS:HE2	1.89	0.53
2:y:1841:ARG:NH1	2:y:1842:GLU:OE2	2.41	0.53
2:y:1736:GLU:OE1	2:y:1738:ASN:N	2.42	0.53
2:Y:983:PRO:HD3	2:Y:1011:ALA:HA	1.90	0.53
2:Y:1248:MET:N	2:Y:1248:MET:HE2	2.24	0.53
2:Y:699:PHE:HE2	2:Y:736:VAL:HG22	1.74	0.53
2:y:902:GLN:OE1	2:y:904:ARG:NH1	2.41	0.53
2:Y:554:THR:HB	2:Y:557:LYS:HB3	1.91	0.53
2:y:383:LEU:HD12	2:y:386:LEU:HD11	1.91	0.53
2:y:583:SER:HB2	2:y:593:GLN:HB3	1.90	0.53
2:y:1332:VAL:HG21	2:y:1374:LEU:HD13	1.90	0.53
2:Y:100:ALA:O	2:Y:104:ILE:HG12	2.08	0.53
2:Y:1382:ALA:O	2:Y:1396:SER:OG	2.27	0.53
2:y:233:LYS:HG3	2:y:1204:ALA:HB3	1.90	0.52
2:y:1736:GLU:HB3	2:y:1870:VAL:HG13	1.91	0.52
2:y:892:LEU:HA	2:y:906:GLN:HB3	1.90	0.52
2:y:908:TRP:NE1	2:y:945:MET:HE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:122:THR:OG1	4:Y:2206:AGS:O1A	2.25	0.52
2:Y:1091:PHE:HA	2:Y:1096:VAL:HB	1.90	0.52
2:y:658:GLN:HE22	2:y:1069:TRP:HE1	1.57	0.52
2:y:724:THR:O	2:y:727:GLN:HG3	2.09	0.52
2:y:1840:THR:HG23	2:y:1845:SER:HB2	1.90	0.52
2:Y:186:THR:HG21	2:Y:207:ARG:HG2	1.90	0.52
2:Y:423:ARG:HA	2:Y:1144:SER:O	2.09	0.52
2:y:1801:ASP:HA	2:y:1804:ARG:HD2	1.92	0.52
2:Y:98:LEU:HA	2:Y:101:TRP:CE2	2.43	0.52
2:y:98:LEU:HA	2:y:101:TRP:CE2	2.45	0.52
2:y:896:ASP:N	2:y:896:ASP:OD1	2.43	0.52
2:Y:221:ASN:OD1	2:Y:223:THR:OG1	2.22	0.52
2:Y:235:ALA:HA	2:Y:238:ILE:HD12	1.92	0.52
2:Y:241:SER:HB3	2:Y:275:PHE:HE2	1.73	0.52
2:y:1759:VAL:HG11	2:y:1828:LEU:HD13	1.91	0.52
2:y:150:ILE:HD11	2:y:220:THR:HB	1.91	0.52
2:y:1227:LEU:HD11	2:y:1260:GLN:HB2	1.91	0.52
2:y:1277:LEU:HA	2:y:1280:ASN:HD21	1.75	0.52
2:Y:67:ALA:N	2:Y:93:PRO:O	2.38	0.52
2:y:368:GLN:OE1	2:y:392:ARG:NH1	2.43	0.52
2:y:1230:GLN:HG3	2:y:1233:GLN:HE22	1.75	0.52
2:y:1967:VAL:HG11	2:y:2021:TRP:HD1	1.75	0.52
2:Y:1441:HIS:NE2	2:Y:1488:PRO:O	2.43	0.52
2:Y:1741:SER:HA	2:Y:1774:LEU:HD22	1.91	0.52
2:y:711:LEU:HG	2:y:715:MET:HE2	1.92	0.52
2:y:1467:GLN:OE1	2:y:1468:ALA:N	2.42	0.52
2:Y:761:THR:OG1	2:Y:972:GLU:OE1	2.27	0.52
2:Y:828:PRO:O	2:Y:832:LYS:NZ	2.42	0.52
2:Y:893:GLN:HB3	2:Y:897:LYS:HD2	1.92	0.52
2:Y:1804:ARG:HA	2:Y:1891:LEU:HD23	1.91	0.52
2:y:981:ARG:NH1	2:y:1053:GLU:O	2.43	0.52
2:y:1109:VAL:O	2:y:1135:ARG:NH2	2.41	0.52
2:Y:413:ARG:HA	2:Y:418:ALA:HA	1.92	0.52
2:Y:1305:ARG:HG2	2:Y:1308:ARG:HH21	1.75	0.52
2:Y:1521:HIS:CD2	2:Y:1538:PRO:HD3	2.44	0.52
2:Y:779:ASP:OD1	2:Y:780:ARG:N	2.44	0.51
2:Y:1245:THR:H	2:Y:1248:MET:HE3	1.74	0.51
2:Y:1293:GLU:HA	2:Y:1298:LYS:HE3	1.90	0.51
2:y:97:GLN:HG2	2:y:124:CYS:HB2	1.93	0.51
2:y:193:ILE:HD12	2:y:196:ASP:HB2	1.92	0.51
2:y:1439:CYS:HB3	2:y:1444:ALA:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:2074:LEU:HB3	2:y:2078:GLN:NE2	2.25	0.51
2:Y:331:ARG:NH2	2:Y:332:VAL:O	2.36	0.51
2:Y:747:MET:HE2	2:Y:747:MET:N	2.25	0.51
2:y:817:LEU:HG	2:y:823:VAL:HG12	1.93	0.51
2:y:246:LYS:HA	2:y:285:VAL:HA	1.93	0.51
2:Y:1428:ALA:HB2	2:Y:1489:SER:HB2	1.93	0.51
2:y:193:ILE:HD11	2:y:205:LEU:HB3	1.91	0.51
2:y:262:ALA:HB2	2:y:1177:ARG:H	1.75	0.51
2:Y:1838:GLN:NE2	2:Y:1879:LYS:O	2.43	0.51
2:Y:706:ASN:O	2:Y:709:ASP:HB3	2.11	0.51
2:y:1240:ARG:O	2:y:1240:ARG:NH1	2.40	0.51
2:y:1895:LEU:HD12	2:y:1896:PRO:HD2	1.91	0.51
2:Y:178:ARG:HG3	2:Y:215:PRO:HA	1.92	0.51
2:Y:1075:HIS:HB2	2:Y:1099:LEU:HD11	1.93	0.51
2:Y:1105:MET:HA	2:Y:1105:MET:HE2	1.93	0.51
2:Y:1377:ALA:O	2:Y:1381:TYR:N	2.26	0.51
2:y:766:THR:HA	2:y:769:GLU:HG2	1.93	0.51
2:y:1285:LYS:HA	2:y:1291:TRP:HB3	1.91	0.51
2:Y:294:ILE:O	2:Y:324:ARG:NH2	2.43	0.51
2:Y:104:ILE:HD11	2:Y:111:LEU:HB2	1.91	0.51
2:Y:1760:LEU:HD11	2:Y:1790:LEU:HD13	1.93	0.51
2:y:575:SER:HA	2:y:582:ASN:HA	1.92	0.51
2:y:1454:TYR:HA	2:y:1580:TRP:O	2.10	0.51
2:y:1713:THR:HG23	2:y:1716:ARG:H	1.76	0.51
2:Y:1107:MET:H	2:Y:1107:MET:CE	2.23	0.51
2:y:153:TYR:HD2	2:y:159:ILE:HG13	1.75	0.50
2:y:2095:ASN:HB2	2:y:2097:LEU:HD23	1.93	0.50
2:Y:912:ARG:HA	2:Y:914:ARG:HH21	1.77	0.50
2:Y:979:VAL:HG11	2:Y:988:ALA:HB1	1.91	0.50
2:y:9:ALA:HB3	2:y:10:PRO:HD3	1.93	0.50
2:Y:440:LYS:HA	2:Y:457:GLY:H	1.75	0.50
2:Y:1223:PHE:O	2:Y:1227:LEU:HG	2.11	0.50
2:y:96:HIS:CE1	2:y:119:SER:HB2	2.46	0.50
2:y:1219:GLN:HA	2:y:1222:ARG:HG3	1.93	0.50
2:Y:442:CYS:HB2	2:Y:445:LYS:HB3	1.93	0.50
2:Y:683:LYS:HD2	2:Y:684:LEU:H	1.76	0.50
2:y:125:PHE:HB2	2:y:288:ILE:HD12	1.92	0.50
2:y:1400:MET:SD	2:y:1400:MET:N	2.85	0.50
2:Y:673:GLU:HB3	2:Y:674:LEU:HD23	1.93	0.50
2:Y:1693:SER:N	2:Y:1696:SER:OG	2.43	0.50
2:y:1072:LEU:HD13	2:y:1098:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:1554:HIS:O	2:y:1571:CYS:N	2.39	0.50
2:y:1707:HIS:O	2:y:1710:THR:OG1	2.24	0.50
2:Y:421:PRO:HB3	2:Y:1142:SER:HA	1.92	0.50
2:Y:1263:MET:HE3	2:Y:1263:MET:HA	1.94	0.50
2:y:232:ARG:HD2	2:y:1198:ARG:HD2	1.94	0.50
2:y:777:LEU:HA	2:y:781:MET:CG	2.42	0.50
2:y:1693:SER:OG	2:y:1694:TYR:N	2.44	0.50
2:y:1895:LEU:HD22	2:y:1901:ARG:HG2	1.94	0.50
2:Y:155:LEU:HA	3:I:21:DC:H4'	1.93	0.50
2:y:1002:GLY:O	2:y:1004:LYS:NZ	2.36	0.50
2:y:1579:LEU:HD12	2:y:1580:TRP:N	2.26	0.50
2:Y:978:GLN:HB2	2:Y:1013:LEU:HD11	1.94	0.50
2:y:297:ASP:OD2	2:y:326:TYR:OH	2.30	0.50
2:Y:482:CYS:SG	2:Y:589:CYS:HB3	2.51	0.50
2:y:1591:GLU:HG3	2:y:1649:PHE:CE2	2.47	0.49
2:Y:813:ASN:O	2:Y:987:ARG:NH2	2.41	0.49
2:y:816:THR:HG23	2:y:819:SER:H	1.76	0.49
2:y:922:LEU:HD22	2:y:998:PRO:HA	1.93	0.49
2:y:1787:ASN:HA	2:y:1817:ARG:HB3	1.94	0.49
2:y:1804:ARG:HB2	2:y:1893:PRO:HG3	1.94	0.49
2:Y:1519:PHE:HB3	2:Y:1521:HIS:ND1	2.27	0.49
2:y:1851:ASP:OD2	2:y:1853:SER:OG	2.31	0.49
2:Y:455:PRO:HG2	2:Y:456:PHE:CE2	2.47	0.49
2:Y:500:TRP:CE2	2:Y:557:LYS:HB2	2.47	0.49
2:y:69:GLU:OE2	2:y:73:ASP:HB2	2.12	0.49
2:y:620:GLU:O	2:y:638:ARG:NH1	2.46	0.49
2:y:702:LEU:HB3	2:y:708:ILE:HD11	1.95	0.49
2:y:893:GLN:HB2	2:y:907:LEU:HA	1.95	0.49
2:y:1586:ARG:HB2	2:y:1586:ARG:NH1	2.27	0.49
2:y:115:SER:OG	2:y:119:SER:OG	2.20	0.49
2:y:1940:ILE:HG12	2:y:1971:MET:O	2.12	0.49
2:Y:198:LEU:HD12	2:Y:199:LYS:N	2.28	0.49
2:y:833:VAL:O	2:y:855:ARG:NH2	2.46	0.49
2:y:1277:LEU:HB3	2:y:1304:LEU:HD21	1.93	0.49
2:Y:26:GLN:HG2	2:Y:605:LEU:HD11	1.94	0.49
2:Y:159:ILE:HB	2:Y:181:LEU:HD11	1.94	0.49
2:Y:1474:MET:HE2	2:Y:1474:MET:HA	1.95	0.49
2:y:409:MET:O	2:y:412:SER:OG	2.31	0.49
2:y:482:CYS:SG	2:y:484:SER:OG	2.60	0.49
2:y:1345:ARG:HD2	2:y:1345:ARG:HA	1.58	0.49
2:y:1556:LEU:HA	2:y:1571:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:80:SER:HB3	2:Y:83:LEU:HB2	1.93	0.49
2:y:891:MET:HE2	2:y:891:MET:HA	1.94	0.49
2:y:911:ILE:HG12	2:y:938:LYS:HG2	1.95	0.49
2:y:1304:LEU:HD12	2:y:1308:ARG:HE	1.78	0.49
2:Y:1490:SER:O	2:Y:1504:ARG:NH2	2.45	0.49
2:y:108:LYS:HA	2:y:286:GLN:HE21	1.78	0.49
2:y:108:LYS:HA	2:y:286:GLN:NE2	2.28	0.49
2:y:696:ILE:O	2:y:700:SER:N	2.46	0.49
2:y:1990:GLN:NE2	2:y:1997:ALA:O	2.45	0.49
2:y:423:ARG:HD2	2:y:425:HIS:CE1	2.48	0.49
2:y:1911:PRO:HA	2:y:2087:ARG:HH12	1.77	0.49
2:Y:656:ARG:NH2	2:Y:1473:SER:O	2.45	0.49
2:Y:1777:GLU:O	2:Y:1780:GLN:HG3	2.12	0.49
2:y:653:ILE:HD11	2:y:1100:ASN:HD21	1.77	0.48
2:y:892:LEU:HD12	2:y:893:GLN:N	2.28	0.48
2:Y:1106:GLU:O	2:Y:1131:GLN:NE2	2.40	0.48
3:I:13:DT:H2'	3:I:13:DT:O2	2.11	0.48
2:y:231:ARG:HG3	2:y:1313:PHE:HE2	1.78	0.48
2:y:777:LEU:HA	2:y:781:MET:HG2	1.94	0.48
2:y:1557:LEU:HG	2:y:1558:ARG:HG2	1.95	0.48
2:y:98:LEU:HA	2:y:101:TRP:NE1	2.28	0.48
2:Y:162:GLN:HG3	2:Y:166:LEU:HD21	1.95	0.48
2:Y:707:SER:HB3	2:Y:732:ILE:HD13	1.95	0.48
2:Y:1745:ALA:HA	2:Y:1777:GLU:HG3	1.95	0.48
2:y:1258:ARG:O	2:y:1262:MET:HG3	2.13	0.48
2:Y:194:GLN:HA	2:Y:197:GLN:HB2	1.96	0.48
2:Y:405:LEU:HG	2:Y:409:MET:HE3	1.95	0.48
2:Y:482:CYS:HB3	2:Y:589:CYS:HB3	1.96	0.48
2:y:148:GLN:HG2	2:y:244:MET:HB3	1.96	0.48
2:y:241:SER:HA	2:y:244:MET:HE1	1.95	0.48
2:y:1727:GLN:HB3	2:y:1730:GLY:HA2	1.95	0.48
2:y:190:LYS:HG3	2:y:191:TYR:H	1.78	0.48
2:y:1085:GLN:O	2:y:1089:LYS:HG2	2.12	0.48
2:y:1387:VAL:O	2:y:1393:VAL:HA	2.14	0.48
2:Y:844:LEU:HD23	2:Y:850:GLN:HA	1.96	0.48
2:Y:1590:VAL:HG23	2:Y:1661:ALA:HB1	1.96	0.48
1:i:4:DA:C8	2:y:1327:PHE:HZ	2.32	0.48
2:y:786:LYS:HZ3	2:y:792:ASP:HA	1.79	0.48
2:y:843:LEU:HD11	2:y:930:ILE:HD11	1.95	0.48
2:Y:110:SER:OG	2:Y:111:LEU:N	2.46	0.48
2:Y:817:LEU:HG	2:Y:823:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:945:MET:HA	2:Y:948:VAL:HG22	1.96	0.48
2:y:1107:MET:HG3	2:y:1108:GLY:N	2.28	0.48
2:y:1968:GLU:HG3	2:y:2019:PRO:HG2	1.95	0.48
2:Y:1242:THR:O	2:Y:1248:MET:HE1	2.14	0.48
2:Y:1696:SER:HB2	2:Y:1703:LEU:HD11	1.96	0.48
2:Y:1772:TRP:O	2:Y:1776:LYS:NZ	2.46	0.48
2:y:149:ALA:HB3	2:y:217:ILE:HG22	1.95	0.48
2:y:409:MET:HE2	2:y:419:PHE:CE2	2.48	0.48
2:y:728:ALA:O	2:y:731:ILE:HB	2.14	0.48
2:y:1101:CYS:SG	2:y:1105:MET:HB3	2.53	0.48
2:y:1242:THR:HB	2:y:1248:MET:HE1	1.95	0.48
2:Y:1265:GLN:O	2:Y:1269:ARG:HG2	2.14	0.48
2:Y:1841:ARG:HH21	2:Y:1844:GLN:HG3	1.78	0.48
2:y:282:ASP:N	2:y:282:ASP:OD1	2.44	0.47
2:y:486:TYR:OH	2:y:586:CYS:SG	2.70	0.47
2:y:1760:LEU:HD12	2:y:1790:LEU:HD13	1.96	0.47
2:Y:381:VAL:HG21	2:Y:386:LEU:HD21	1.95	0.47
2:y:750:LEU:HA	2:y:753:ASN:HD21	1.78	0.47
2:y:1439:CYS:HB2	2:y:1449:LEU:HD21	1.95	0.47
2:Y:437:CYS:HB3	2:Y:458:GLN:H	1.80	0.47
2:Y:1245:THR:HG23	2:Y:1247:LEU:H	1.78	0.47
2:Y:1755:SER:OG	2:Y:1840:THR:O	2.29	0.47
2:y:382:ARG:N	2:y:385:GLU:OE2	2.41	0.47
2:y:1106:GLU:HG3	2:y:1132:ARG:HG2	1.96	0.47
2:y:137:GLN:OE1	2:y:141:ARG:NH2	2.47	0.47
2:y:735:MET:SD	2:y:735:MET:N	2.88	0.47
2:y:2075:ARG:HG2	2:y:2077:PRO:HD2	1.97	0.47
1:i:4:DA:H61	2:y:1314:SER:HB3	1.79	0.47
2:y:762:MET:HE1	2:y:767:LEU:HG	1.96	0.47
2:y:1372:ARG:HH12	2:y:1376:THR:HB	1.79	0.47
2:y:1510:GLU:OE2	2:y:1586:ARG:NE	2.45	0.47
2:y:1887:SER:H	2:y:1890:ASP:HB2	1.79	0.47
2:Y:67:ALA:HB3	2:Y:93:PRO:HG2	1.95	0.47
2:Y:137:GLN:HG3	2:Y:176:LYS:HB3	1.96	0.47
2:Y:1076:SER:HA	2:Y:1104:THR:HG21	1.95	0.47
2:Y:1495:LEU:HD12	2:Y:1500:LEU:HB2	1.96	0.47
2:Y:1603:ARG:HH11	2:Y:1645:GLY:H	1.62	0.47
2:Y:1694:TYR:O	2:Y:1697:GLN:NE2	2.48	0.47
2:y:1967:VAL:HG21	2:y:2021:TRP:CD1	2.50	0.47
2:Y:22:SER:HB3	2:Y:1058:THR:HG21	1.95	0.47
1:i:3:DA:H2''	1:i:4:DA:C4	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:423:ARG:HG3	2:y:1144:SER:OG	2.15	0.47
2:y:702:LEU:HA	2:Y:702:LEU:HD21	1.95	0.47
2:y:708:ILE:HG22	2:y:712:LYS:HD2	1.97	0.47
2:y:838:GLN:HA	2:y:841:LYS:HE2	1.97	0.47
2:y:1603:ARG:NH2	2:y:1643:TYR:HB3	2.30	0.47
2:y:2059:LEU:H	2:y:2059:LEU:HD23	1.78	0.47
2:Y:1057:SER:N	2:Y:1060:SER:OG	2.48	0.47
2:Y:1129:TYR:HE1	2:Y:1148:THR:HG21	1.80	0.47
2:Y:1503:TYR:HE1	2:Y:1665:ILE:HD11	1.80	0.47
3:I:8:DG:H2'	3:I:9:DT:H71	1.96	0.47
2:y:248:ILE:HD12	2:y:248:ILE:HA	1.76	0.47
2:y:729:LEU:HD13	2:y:751:GLN:HG2	1.95	0.47
2:y:917:ASN:O	2:y:921:LYS:NZ	2.37	0.47
2:Y:132:ASP:OD2	2:Y:247:TYR:OH	2.33	0.47
2:Y:1526:CYS:HA	2:Y:1575:VAL:HA	1.97	0.47
2:Y:1815:GLY:HA3	2:Y:1817:ARG:HH21	1.79	0.47
2:y:891:MET:O	2:y:906:GLN:N	2.48	0.47
2:Y:8:TYR:CE1	2:Y:424:MET:HE1	2.50	0.47
2:Y:1375:PRO:HB3	2:Y:1513:HIS:CG	2.50	0.47
2:y:750:LEU:O	2:y:754:SER:OG	2.30	0.47
2:y:1157:MET:HG3	2:y:1689:HIS:ND1	2.30	0.47
2:Y:1278:LEU:HA	2:Y:1281:ILE:HG22	1.96	0.47
2:Y:1375:PRO:HB3	2:Y:1513:HIS:CD2	2.50	0.47
2:y:596:ASN:OD1	2:y:597:ASN:N	2.48	0.46
2:Y:992:THR:OG1	2:Y:996:TYR:N	2.47	0.46
2:Y:1528:SER:OG	2:Y:1571:CYS:SG	2.73	0.46
2:y:57:VAL:HG12	2:y:425:HIS:HB2	1.98	0.46
2:y:357:TYR:CD2	2:y:414:GLU:HB2	2.50	0.46
2:y:682:ALA:HB3	2:y:753:ASN:HD22	1.81	0.46
2:y:895:PRO:HA	2:y:908:TRP:HB3	1.97	0.46
2:y:1214:GLU:OE2	2:y:1308:ARG:NH1	2.47	0.46
2:y:1775:PHE:HD2	2:y:1779:LEU:HD23	1.79	0.46
2:Y:148:GLN:HG2	2:Y:244:MET:SD	2.56	0.46
2:Y:1220:CYS:O	2:Y:1224:LEU:HG	2.15	0.46
2:Y:1225:HIS:O	2:Y:1229:HIS:ND1	2.48	0.46
2:Y:1331:VAL:HG22	2:Y:1371:SER:OG	2.15	0.46
2:y:232:ARG:NH2	2:y:1202:PRO:O	2.49	0.46
2:Y:1796:LEU:HD23	2:Y:1796:LEU:H	1.81	0.46
2:y:130:LEU:O	2:y:134:ILE:HG12	2.15	0.46
2:y:836:CYS:HB2	2:y:840:TRP:CD1	2.51	0.46
2:y:957:ARG:HD3	2:y:966:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:1191:LEU:HD22	2:y:1241:LEU:HD13	1.96	0.46
2:y:1729:PHE:HB3	2:y:1873:LEU:HD22	1.96	0.46
2:y:1905:CYS:N	2:y:1907:GLN:OE1	2.48	0.46
2:Y:715:MET:SD	2:Y:715:MET:N	2.88	0.46
2:Y:1041:LEU:HD11	2:Y:1061:ASP:HB2	1.96	0.46
2:Y:1210:LYS:HD3	2:Y:1308:ARG:HB2	1.98	0.46
2:y:693:GLU:HA	2:y:696:ILE:HG22	1.97	0.46
2:y:908:TRP:CZ2	2:y:949:TRP:HB2	2.49	0.46
2:y:1486:LEU:HD12	2:y:1487:VAL:N	2.30	0.46
2:Y:370:ARG:HB2	2:Y:419:PHE:HE1	1.81	0.46
2:y:74:LEU:O	2:y:79:ILE:N	2.36	0.46
2:y:121:LYS:HD2	2:y:290:THR:HG23	1.98	0.46
2:y:249:VAL:HG22	2:y:288:ILE:HD11	1.98	0.46
2:y:368:GLN:OE1	2:y:393:THR:OG1	2.32	0.46
2:y:704:LEU:C	2:y:706:ASN:H	2.24	0.46
2:y:911:ILE:HG21	2:y:938:LYS:HB3	1.98	0.46
2:y:1027:SER:OG	2:y:1028:GLY:N	2.49	0.46
2:y:1907:GLN:HB3	2:y:1922:LEU:HD11	1.98	0.46
2:Y:162:GLN:O	2:Y:166:LEU:HG	2.16	0.46
2:Y:223:THR:O	2:Y:226:GLU:HG3	2.16	0.46
2:Y:1593:GLN:HB3	2:Y:1601:LEU:HD11	1.96	0.46
2:y:432:ALA:HA	2:y:604:ARG:HA	1.98	0.46
2:y:460:TRP:CZ3	2:y:467:CYS:HB2	2.51	0.46
2:y:1066:LYS:HE3	2:Y:960:GLU:CD	2.40	0.46
2:y:1677:LYS:HD3	2:y:1677:LYS:HA	1.71	0.46
2:Y:1227:LEU:HB3	2:Y:1256:LEU:HD22	1.98	0.46
2:y:554:THR:OG1	2:y:554:THR:O	2.33	0.46
2:Y:384:SER:O	2:Y:387:LEU:HG	2.15	0.46
2:Y:990:ASP:OD1	2:Y:991:VAL:HG12	2.14	0.46
2:y:11:LEU:HA	2:y:621:PHE:CE2	2.51	0.46
2:y:65:MET:HE2	2:y:65:MET:HA	1.96	0.46
2:y:133:LEU:HD11	2:y:217:ILE:HG23	1.98	0.46
2:y:248:ILE:HG22	2:y:287:ILE:HA	1.97	0.46
2:y:731:ILE:O	2:Y:735:MET:HE1	2.15	0.46
2:y:844:LEU:HD23	2:y:850:GLN:HA	1.97	0.46
2:y:865:PHE:O	2:y:869:ASN:HB2	2.15	0.46
2:Y:121:LYS:HZ3	2:Y:121:LYS:H	1.64	0.46
2:y:111:LEU:O	2:y:288:ILE:HA	2.16	0.46
2:y:934:GLN:HE22	2:y:936:HIS:HB3	1.80	0.46
2:Y:178:ARG:O	2:Y:216:SER:OG	2.27	0.46
2:Y:225:LEU:HD21	2:Y:271:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1256:LEU:HA	2:Y:1259:THR:HG22	1.98	0.46
2:y:227:TYR:HB3	2:y:231:ARG:HH21	1.81	0.45
2:y:878:GLN:HG2	2:y:881:ARG:HH22	1.80	0.45
2:y:1106:GLU:HB2	2:y:1132:ARG:HE	1.80	0.45
2:Y:218:MET:HE2	2:Y:220:THR:HG1	1.81	0.45
2:y:150:ILE:HG22	2:y:245:LEU:HD11	1.97	0.45
2:y:454:TRP:CE3	2:y:455:PRO:HD2	2.51	0.45
2:y:982:CYS:SG	2:y:985:THR:N	2.88	0.45
2:y:1945:TYR:CE2	2:y:1959:LEU:HD11	2.51	0.45
2:y:427:PHE:HB3	2:y:1150:CYS:SG	2.57	0.45
2:y:1517:GLY:C	2:y:1518:GLU:HG3	2.42	0.45
2:Y:550:LEU:HB2	2:Y:564:LYS:HB3	1.98	0.45
2:Y:595:LYS:HB3	1:G:19:DG:H21	1.81	0.45
2:Y:1264:GLN:O	2:Y:1268:ILE:HG12	2.15	0.45
2:y:605:LEU:HD12	2:y:609:PHE:CD2	2.51	0.45
2:y:1313:PHE:O	2:y:1317:ILE:HG23	2.16	0.45
2:Y:1020:PRO:HD3	2:Y:1040:TRP:CZ2	2.52	0.45
2:y:1936:ARG:HD3	2:y:1938:LYS:HE3	1.98	0.45
2:Y:80:SER:N	2:Y:131:GLU:OE1	2.49	0.45
2:Y:1197:LEU:HD13	2:Y:1201:VAL:HB	1.97	0.45
2:Y:1827:GLN:O	2:Y:1879:LYS:NZ	2.45	0.45
2:y:231:ARG:HG3	2:y:1313:PHE:CE2	2.52	0.45
2:y:266:LEU:HD12	2:y:1183:ILE:HG22	1.98	0.45
2:y:721:LEU:HB3	2:y:725:ASP:HB2	1.99	0.45
2:Y:848:ASP:OD1	2:Y:849:LYS:N	2.49	0.45
4:Y:2206:AGS:O3A	4:Y:2206:AGS:O2G	2.35	0.45
2:y:1212:PHE:HE2	2:y:1220:CYS:HB2	1.81	0.45
2:y:1282:GLU:HA	2:y:1285:LYS:HE3	1.99	0.45
2:Y:8:TYR:H	2:Y:407:ASP:CG	2.24	0.45
2:Y:153:TYR:HD2	2:Y:159:ILE:HG23	1.81	0.45
2:Y:1798:ASN:OD1	2:Y:1798:ASN:N	2.49	0.45
2:Y:687:ALA:O	2:Y:691:LEU:HG	2.17	0.45
2:Y:1266:VAL:HA	2:Y:1269:ARG:NE	2.31	0.45
1:i:4:DA:H2''	1:i:5:DC:C5	2.52	0.45
2:y:126:MET:HE3	2:y:169:TRP:CD2	2.51	0.45
2:y:140:THR:HG23	2:y:142:GLN:H	1.82	0.45
2:y:696:ILE:HD11	2:y:708:ILE:HG23	1.98	0.45
2:y:796:GLN:N	2:Y:877:GLU:OE2	2.31	0.45
2:y:1731:ASP:OD1	2:y:1731:ASP:N	2.48	0.45
2:Y:492:GLU:C	2:Y:493:MET:HE2	2.42	0.45
2:Y:1538:PRO:HB2	2:Y:1539:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:48:GLN:O	2:y:51:SER:OG	2.33	0.45
2:y:248:ILE:HG12	2:y:268:LEU:HD11	1.99	0.45
2:y:1948:ARG:HB2	2:y:1982:LYS:HB2	1.99	0.45
2:Y:310:ALA:HA	2:Y:315:VAL:HB	1.99	0.45
2:y:268:LEU:O	2:y:271:VAL:HG12	2.17	0.44
2:y:934:GLN:NE2	2:y:936:HIS:HB3	2.32	0.44
2:y:934:GLN:OE1	2:y:937:TRP:N	2.42	0.44
2:y:1487:VAL:HG22	2:y:1504:ARG:HH21	1.82	0.44
2:Y:1401:LEU:HA	2:Y:1401:LEU:HD23	1.84	0.44
2:y:1119:MET:HG3	2:y:1148:THR:HA	1.99	0.44
2:y:1323:PRO:O	2:y:1325:HIS:ND1	2.50	0.44
2:y:1829:MET:HE2	2:y:1829:MET:N	2.32	0.44
2:Y:550:LEU:N	2:Y:564:LYS:O	2.47	0.44
2:y:610:PHE:O	2:y:614:ILE:HG23	2.17	0.44
2:y:1377:ALA:O	2:y:1381:TYR:N	2.49	0.44
2:Y:1509:GLY:HA3	2:Y:1589:MET:SD	2.57	0.44
2:Y:1822:SER:H	2:Y:1886:LEU:HG	1.83	0.44
2:y:286:GLN:C	2:y:287:ILE:HD13	2.42	0.44
2:y:1590:VAL:HG13	2:y:1650:ILE:HB	2.00	0.44
2:Y:136:GLN:OE1	2:Y:148:GLN:NE2	2.45	0.44
2:Y:911:ILE:HD13	2:Y:938:LYS:HB3	2.00	0.44
2:Y:1429:GLY:HA3	2:Y:1486:LEU:HD23	1.99	0.44
2:Y:1601:LEU:HD12	2:Y:1601:LEU:HA	1.83	0.44
2:Y:1783:SER:O	2:Y:1817:ARG:NH1	2.50	0.44
2:Y:1829:MET:HE3	2:Y:1830:GLN:N	2.32	0.44
2:y:348:LEU:HD21	2:y:363:TYR:HE2	1.83	0.44
2:y:764:TRP:CH2	2:y:803:LEU:HB3	2.52	0.44
2:y:1487:VAL:HB	2:y:1589:MET:SD	2.58	0.44
2:Y:27:LEU:O	2:Y:478:ARG:NE	2.49	0.44
2:Y:699:PHE:CE2	2:Y:736:VAL:HG22	2.52	0.44
2:Y:945:MET:O	2:Y:948:VAL:HG22	2.17	0.44
2:Y:1016:MET:SD	2:Y:1017:PRO:HD2	2.58	0.44
2:y:152:LEU:HD23	2:y:152:LEU:HA	1.79	0.44
2:y:203:GLN:HG2	2:y:205:LEU:HG	2.00	0.44
2:y:1381:TYR:HB3	2:y:1460:PHE:HD1	1.82	0.44
2:Y:1085:GLN:O	2:Y:1088:GLU:HG3	2.17	0.44
2:y:723:PRO:HA	2:y:726:ILE:HG12	2.00	0.44
2:y:839:ASP:O	2:y:842:THR:OG1	2.25	0.44
2:y:1813:MET:SD	2:y:1813:MET:N	2.90	0.44
2:y:1930:TRP:CD1	2:y:2103:ALA:HB1	2.53	0.44
2:Y:784:SER:O	2:Y:787:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:71:MET:SD	2:y:93:PRO:HD3	2.57	0.44
2:y:181:LEU:HD23	2:y:181:LEU:HA	1.85	0.44
2:y:615:ILE:HD12	2:y:615:ILE:HA	1.86	0.44
2:Y:89:LYS:HE2	2:Y:89:LYS:HB2	1.87	0.44
2:Y:1718:GLN:HA	2:Y:1721:ASN:HB2	2.00	0.44
2:y:126:MET:HE3	2:y:169:TRP:CE3	2.53	0.44
2:Y:830:ILE:HD13	2:Y:859:LYS:HB2	1.99	0.44
2:Y:1245:THR:HG23	2:Y:1247:LEU:HB2	1.98	0.44
2:y:620:GLU:HA	2:y:635:PHE:HE2	1.83	0.43
2:y:667:ARG:HB3	2:y:1063:LEU:HD11	1.98	0.43
2:y:1261:ALA:HA	2:y:1264:GLN:HG3	2.00	0.43
2:y:1526:CYS:SG	2:y:1554:HIS:CE1	3.11	0.43
2:y:1911:PRO:HA	2:y:2087:ARG:HH22	1.82	0.43
2:Y:337:ILE:HD11	2:Y:367:GLN:HG3	2.00	0.43
2:y:386:LEU:HD12	2:y:387:LEU:N	2.33	0.43
2:y:735:MET:H	2:y:735:MET:CE	2.31	0.43
2:y:746:ALA:O	2:y:749:ILE:HG12	2.19	0.43
2:y:902:GLN:N	2:y:905:ASP:OD2	2.49	0.43
2:y:994:LEU:O	2:y:1010:LYS:NZ	2.37	0.43
2:y:1047:ILE:HG23	2:y:1056:TRP:CD1	2.52	0.43
2:y:1953:PRO:HD2	2:y:1996:ASN:O	2.18	0.43
2:Y:98:LEU:HA	2:Y:101:TRP:NE1	2.32	0.43
2:Y:580:ARG:HH11	1:G:20:DA:H5'	1.82	0.43
2:Y:1245:THR:OG1	2:Y:1246:VAL:N	2.51	0.43
2:y:27:LEU:HB3	2:y:29:LEU:HD23	2.00	0.43
2:Y:729:LEU:HD22	2:Y:750:LEU:HD21	2.00	0.43
2:Y:854:TRP:CH2	2:Y:948:VAL:HG12	2.52	0.43
2:y:1203:ASP:OD1	2:y:1203:ASP:N	2.51	0.43
2:y:1453:ARG:O	2:y:1580:TRP:HD1	2.02	0.43
2:y:1910:GLY:O	2:y:2087:ARG:NH1	2.51	0.43
2:y:1953:PRO:HG2	2:y:1994:LEU:HD12	2.00	0.43
2:Y:794:THR:OG1	2:Y:797:GLN:OE1	2.24	0.43
2:Y:1609:ARG:NE	2:Y:1634:THR:OG1	2.52	0.43
2:y:96:HIS:CE1	2:y:97:GLN:HG3	2.53	0.43
2:y:582:ASN:OD1	2:y:582:ASN:N	2.44	0.43
2:y:672:GLN:HG3	2:y:1066:LYS:HZ3	1.82	0.43
2:y:863:ASP:O	2:y:867:ARG:HB2	2.18	0.43
2:y:1679:LEU:HD21	2:y:1708:ALA:HB3	2.01	0.43
2:Y:423:ARG:HH21	2:Y:1137:GLY:HA3	1.84	0.43
2:Y:492:GLU:O	2:Y:493:MET:HE2	2.19	0.43
2:Y:809:ARG:HH11	2:Y:811:PRO:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:170:THR:HG23	2:Y:202:GLU:HG3	1.99	0.43
2:Y:193:ILE:O	2:Y:197:GLN:N	2.51	0.43
2:Y:1219:GLN:HA	2:Y:1222:ARG:HG2	2.01	0.43
2:y:667:ARG:NH2	2:y:816:THR:HA	2.33	0.43
2:y:734:PRO:HG2	2:Y:731:ILE:HG23	1.99	0.43
2:y:1935:THR:O	2:y:1937:HIS:ND1	2.51	0.43
2:y:390:ALA:O	2:y:394:TRP:N	2.41	0.43
2:Y:143:SER:OG	2:Y:178:ARG:NH2	2.46	0.43
2:Y:654:SER:HB3	2:Y:1100:ASN:HD22	1.84	0.43
2:Y:762:MET:HE2	2:Y:762:MET:HB3	1.78	0.43
2:Y:843:LEU:HD21	2:Y:930:ILE:HD11	2.00	0.43
2:Y:1086:PHE:HD1	2:Y:1089:LYS:HE3	1.84	0.43
2:Y:1274:LEU:HD12	2:Y:1274:LEU:O	2.18	0.43
1:i:1:DT:H1'	1:i:2:DA:C4	2.54	0.43
2:y:1092:LYS:HE2	2:y:1111:ILE:HG12	2.01	0.43
2:Y:265:ALA:O	2:Y:268:LEU:HG	2.19	0.43
2:Y:1107:MET:SD	2:Y:1107:MET:N	2.91	0.43
2:y:721:LEU:HD22	2:y:725:ASP:HB3	2.01	0.43
2:y:873:PHE:HB2	2:y:964:GLN:HB3	2.01	0.43
2:Y:493:MET:HE1	2:Y:499:ASN:OD1	2.18	0.43
2:y:793:LEU:HD12	2:y:797:GLN:HB3	2.01	0.42
2:y:1057:SER:N	2:y:1060:SER:OG	2.52	0.42
2:y:1263:MET:HE2	2:y:1263:MET:HA	2.00	0.42
2:y:1270:TRP:HZ3	2:y:1274:LEU:HD22	1.84	0.42
2:y:1302:TYR:OH	2:y:1350:ALA:HB3	2.19	0.42
2:Y:575:SER:HB2	2:Y:582:ASN:HB3	2.00	0.42
2:Y:729:LEU:O	2:Y:733:GLU:HG3	2.19	0.42
2:Y:1525:ILE:O	2:Y:1576:HIS:N	2.48	0.42
1:i:3:DA:N3	1:i:3:DA:H2'	2.34	0.42
2:y:305:LEU:O	2:y:309:VAL:HG12	2.19	0.42
2:y:547:ILE:HD13	2:y:567:GLU:HA	2.01	0.42
2:y:1233:GLN:HG2	2:y:1234:LEU:N	2.34	0.42
2:Y:405:LEU:HA	2:Y:408:LEU:HD23	2.00	0.42
2:Y:1256:LEU:HA	2:Y:1256:LEU:HD23	1.84	0.42
2:y:668:ALA:HA	2:y:1063:LEU:HD13	2.00	0.42
2:y:700:SER:HA	2:y:708:ILE:HG12	2.01	0.42
2:Y:339:HIS:HB2	2:Y:363:TYR:CE1	2.54	0.42
2:Y:865:PHE:CZ	2:Y:909:PRO:HD3	2.53	0.42
1:i:3:DA:H2''	1:i:4:DA:C8	2.54	0.42
2:y:347:SER:O	2:y:351:LEU:HG	2.20	0.42
2:y:783:GLY:O	2:y:787:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:2043:VAL:O	2:y:2051:HIS:HB2	2.20	0.42
2:Y:155:LEU:HD22	2:Y:1107:MET:HE2	2.02	0.42
2:Y:827:TYR:HB2	2:Y:830:ILE:HG13	2.01	0.42
2:y:615:ILE:HG22	2:y:616:PRO:HD3	2.02	0.42
2:y:1618:GLY:HA2	2:y:1674:TYR:CD2	2.54	0.42
2:y:1902:ILE:HG23	2:y:2101:ILE:HG13	2.01	0.42
2:y:1903:ASN:HB3	2:y:2098:ARG:HH21	1.84	0.42
2:y:1950:LEU:HD12	2:y:1950:LEU:HA	1.90	0.42
2:Y:570:LEU:HD23	2:Y:570:LEU:HA	1.87	0.42
2:y:254:HIS:HB3	2:y:294:ILE:HG22	2.00	0.42
2:y:534:GLN:O	2:y:537:ARG:NH1	2.37	0.42
2:y:891:MET:HG3	2:y:893:GLN:OE1	2.20	0.42
2:Y:1044:ASN:OD1	2:Y:1047:ILE:N	2.41	0.42
2:Y:1462:THR:OG1	2:Y:1463:ASP:N	2.52	0.42
2:y:183:ASN:OD1	2:y:185:GLU:HG2	2.19	0.42
2:y:248:ILE:CG2	2:y:287:ILE:HD12	2.50	0.42
2:y:1123:PRO:HD2	2:y:1129:TYR:HB2	2.01	0.42
2:y:1910:GLY:HA2	2:y:2089:ARG:HG3	2.02	0.42
2:y:2078:GLN:OE1	2:y:2078:GLN:N	2.51	0.42
2:Y:766:THR:O	2:Y:770:GLN:HG2	2.20	0.42
2:y:58:PHE:CE2	2:y:424:MET:HB2	2.55	0.42
2:y:89:LYS:HE2	2:y:89:LYS:HB2	1.82	0.42
2:y:984:TYR:CZ	2:y:1000:LEU:HD13	2.55	0.42
2:y:1066:LYS:HZ3	2:y:1066:LYS:HB2	1.84	0.42
2:y:1095:LYS:HA	2:y:1095:LYS:HD3	1.89	0.42
2:y:1104:THR:O	2:y:1107:MET:HG2	2.20	0.42
2:y:2075:ARG:H	2:y:2078:GLN:HE22	1.64	0.42
2:Y:111:LEU:HD11	2:Y:323:VAL:CG2	2.47	0.42
2:Y:1157:MET:SD	2:Y:1157:MET:N	2.93	0.42
2:Y:1180:SER:HB3	2:Y:1658:ALA:HA	2.02	0.42
2:Y:1839:VAL:HG12	2:Y:1848:TRP:HZ3	1.83	0.42
2:y:699:PHE:CE1	2:Y:703:PRO:HD2	2.55	0.42
2:y:704:LEU:CD1	2:Y:739:LEU:HA	2.50	0.42
2:y:945:MET:HA	2:y:948:VAL:HG12	2.01	0.42
2:y:1189:ASN:HB3	2:y:1321:PHE:CZ	2.54	0.42
2:y:1594:LEU:HD23	2:y:1594:LEU:HA	1.86	0.42
2:y:1609:ARG:HD2	2:y:1699:TYR:CE2	2.55	0.42
2:Y:5:GLN:OE1	2:Y:1142:SER:OG	2.29	0.42
2:Y:130:LEU:HD23	2:Y:130:LEU:HA	1.74	0.42
2:Y:966:ASP:OD1	2:Y:966:ASP:N	2.44	0.42
2:Y:1787:ASN:HA	2:Y:1817:ARG:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1874:LYS:HE2	2:Y:1874:LYS:HB3	1.93	0.42
2:y:101:TRP:HA	2:y:104:ILE:CG2	2.49	0.42
2:y:348:LEU:HA	2:y:351:LEU:HD12	2.02	0.42
2:y:349:LYS:HA	2:y:411:ARG:NH2	2.32	0.42
2:y:786:LYS:HA	2:y:786:LYS:HD3	1.76	0.42
2:y:837:PRO:O	2:y:841:LYS:HG3	2.20	0.42
2:y:909:PRO:HD2	2:y:945:MET:HE1	2.00	0.42
2:y:1613:VAL:HG13	2:y:1691:LEU:HD22	2.01	0.42
2:Y:72:GLU:OE2	2:Y:75:ARG:NH2	2.53	0.42
2:Y:1207:LEU:HD13	2:Y:1211:TRP:CZ3	2.55	0.42
2:Y:1729:PHE:CE2	2:Y:1849:ALA:HB3	2.55	0.42
2:y:860:ILE:HD13	2:y:860:ILE:HA	1.90	0.41
2:y:942:ASN:O	2:y:946:ILE:HG12	2.20	0.41
2:y:1071:ARG:HG3	2:y:1096:VAL:HG23	2.02	0.41
2:Y:71:MET:HE1	2:Y:72:GLU:HG2	2.02	0.41
2:Y:246:LYS:HA	2:Y:285:VAL:HG23	2.01	0.41
2:Y:864:PHE:O	2:Y:868:GLU:HG2	2.20	0.41
2:Y:1753:TYR:CD2	2:Y:1841:ARG:HB2	2.55	0.41
2:Y:1772:TRP:HD1	2:Y:1773:PRO:HD2	1.85	0.41
2:y:338:ARG:HG3	2:y:339:HIS:ND1	2.35	0.41
2:y:988:ALA:HB2	2:y:1055:LEU:HD22	2.03	0.41
2:y:1771:GLN:OE1	2:y:1860:GLU:N	2.52	0.41
2:y:1912:LEU:HA	2:y:1915:PHE:CE2	2.55	0.41
2:Y:182:TYR:HD2	2:Y:224:MET:HB3	1.85	0.41
2:Y:1119:MET:HE1	2:Y:1129:TYR:CD1	2.55	0.41
2:Y:1170:THR:OG1	2:Y:1171:ALA:N	2.53	0.41
2:Y:1376:THR:O	2:Y:1380:GLU:HG3	2.20	0.41
2:Y:1519:PHE:HB3	2:Y:1521:HIS:CE1	2.55	0.41
2:y:109:LYS:HA	2:y:319:ASP:OD1	2.20	0.41
2:y:539:ILE:HB	2:y:568:ILE:HD11	2.03	0.41
2:y:677:ILE:HG12	2:y:1022:ARG:HH21	1.85	0.41
2:y:1248:MET:HE2	2:y:1248:MET:N	2.35	0.41
2:y:1547:ASN:HB3	2:y:1550:ARG:HB2	2.03	0.41
2:y:2075:ARG:NE	2:y:2077:PRO:HD2	2.33	0.41
2:Y:64:TRP:HB2	2:Y:94:PHE:CZ	2.55	0.41
2:Y:165:ARG:HB3	2:Y:169:TRP:CZ3	2.55	0.41
2:Y:1224:LEU:HD22	2:Y:1260:GLN:HG2	2.02	0.41
2:Y:1315:LYS:O	2:Y:1318:SER:OG	2.34	0.41
2:y:493:MET:HE1	2:y:499:ASN:HB3	2.02	0.41
2:y:733:GLU:HA	2:y:747:MET:SD	2.60	0.41
2:y:870:SER:O	2:y:870:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:893:GLN:HG3	2:y:907:LEU:HD23	2.03	0.41
2:y:1654:ASN:OD1	2:y:1654:ASN:O	2.37	0.41
2:y:2000:ASN:HB3	2:y:2003:ASP:HB3	2.02	0.41
2:Y:153:TYR:CD2	2:Y:159:ILE:HG23	2.55	0.41
2:Y:683:LYS:NZ	2:Y:684:LEU:HD12	2.35	0.41
2:y:235:ALA:HB2	2:y:1198:ARG:HD3	2.02	0.41
2:y:500:TRP:CE2	2:y:557:LYS:HB2	2.55	0.41
2:Y:423:ARG:HB2	2:Y:1144:SER:HB3	2.02	0.41
2:y:228:MET:HA	2:y:234:ASP:OD2	2.20	0.41
2:y:646:SER:OG	2:y:647:ARG:N	2.54	0.41
2:y:1801:ASP:OD1	2:y:1801:ASP:N	2.53	0.41
2:y:1832:LYS:HE2	2:y:1832:LYS:HB2	1.81	0.41
2:Y:100:ALA:HB1	2:Y:111:LEU:HD21	2.03	0.41
2:Y:253:ALA:HB3	2:Y:291:SER:HB2	2.01	0.41
2:Y:831:ASP:OD1	2:Y:831:ASP:N	2.52	0.41
2:Y:1108:GLY:HA2	2:Y:1135:ARG:NH1	2.35	0.41
2:y:1603:ARG:HH21	2:y:1644:THR:C	2.28	0.41
2:y:1967:VAL:HG11	2:y:2021:TRP:CD1	2.55	0.41
2:y:2011:LEU:HD12	2:y:2080:VAL:HG13	2.03	0.41
2:y:1277:LEU:HA	2:y:1280:ASN:ND2	2.36	0.41
2:Y:250:LEU:HD21	2:Y:256:TYR:CE2	2.48	0.41
2:Y:1452:LYS:HG3	2:Y:1580:TRP:HZ2	1.85	0.41
2:y:62:PHE:CZ	2:y:420:THR:HA	2.56	0.41
2:y:270:ARG:HG2	2:y:1241:LEU:HD11	2.02	0.41
2:y:622:SER:HB3	2:y:638:ARG:HB3	2.01	0.41
2:y:762:MET:SD	2:y:766:THR:HG23	2.60	0.41
2:y:1508:SER:O	2:y:1508:SER:OG	2.29	0.41
2:y:1696:SER:HA	2:y:1699:TYR:HB2	2.03	0.41
2:y:1940:ILE:HA	2:y:2045:PHE:HA	2.02	0.41
2:Y:235:ALA:N	2:Y:236:PRO:HD2	2.36	0.41
2:Y:291:SER:OG	2:Y:292:ALA:N	2.54	0.41
2:Y:647:ARG:CZ	2:Y:1372:ARG:HH11	2.34	0.41
2:Y:732:ILE:HA	2:Y:735:MET:HE3	2.02	0.41
2:Y:1154:ALA:HA	2:Y:1157:MET:HG2	2.03	0.41
2:Y:1205:THR:OG1	2:Y:1206:LYS:N	2.54	0.41
2:Y:1207:LEU:HB2	2:Y:1312:LEU:HD12	2.02	0.41
2:y:278:GLY:O	2:y:281:THR:HG22	2.21	0.41
2:y:634:PRO:HG3	2:y:780:ARG:HE	1.85	0.41
2:y:1389:LEU:HD12	2:y:1389:LEU:O	2.20	0.41
2:y:1545:LEU:HA	2:y:1545:LEU:HD23	1.87	0.41
2:Y:270:ARG:HH22	2:Y:1190:ALA:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:712:LYS:HA	2:Y:715:MET:HG2	2.02	0.41
2:Y:810:ARG:NE	2:Y:818:GLU:OE1	2.53	0.41
2:y:779:ASP:OD1	2:y:780:ARG:HG3	2.21	0.40
2:y:1196:PHE:CE2	2:y:1223:PHE:HB2	2.55	0.40
2:y:1607:ALA:HB2	2:y:1707:HIS:HB3	2.02	0.40
2:y:1627:ASN:OD1	2:y:1627:ASN:N	2.51	0.40
2:Y:806:GLU:HB3	2:Y:807:PHE:CD2	2.56	0.40
2:y:573:PRO:HG3	2:y:584:PHE:CZ	2.56	0.40
2:y:595:LYS:H	2:y:595:LYS:HG2	1.69	0.40
2:y:855:ARG:O	2:y:858:LEU:HG	2.21	0.40
2:y:1038:LEU:O	2:y:1042:GLU:HG2	2.21	0.40
2:y:1401:LEU:HD21	2:y:1405:LEU:N	2.36	0.40
2:Y:218:MET:HE2	2:Y:220:THR:OG1	2.20	0.40
2:Y:551:GLU:C	2:Y:553:THR:H	2.29	0.40
2:Y:1628:THR:HA	2:Y:1694:TYR:CZ	2.56	0.40
2:Y:1848:TRP:NE1	2:Y:1872:THR:HB	2.36	0.40
2:y:98:LEU:HD12	2:y:101:TRP:HE1	1.85	0.40
2:y:735:MET:H	2:y:735:MET:HE3	1.86	0.40
2:y:1589:MET:HE2	2:y:1589:MET:HB2	1.94	0.40
2:y:1769:PHE:HB3	2:y:1775:PHE:CD1	2.56	0.40
2:Y:746:ALA:C	2:Y:747:MET:HE2	2.46	0.40
2:Y:933:GLU:N	2:Y:933:GLU:OE1	2.55	0.40
2:Y:944:LEU:O	2:Y:948:VAL:HG13	2.21	0.40
2:y:121:LYS:HA	2:y:124:CYS:HB3	2.04	0.40
2:y:1215:GLY:O	2:y:1218:SER:OG	2.26	0.40
2:Y:167:ARG:O	2:Y:171:ARG:HG2	2.21	0.40
2:Y:387:LEU:HD13	2:Y:391:ARG:HH21	1.85	0.40
2:Y:904:ARG:O	2:Y:904:ARG:HG2	2.22	0.40
2:Y:1195:LEU:HD23	2:Y:1195:LEU:HA	1.90	0.40
2:y:903:LYS:HD3	2:y:904:ARG:HB3	2.03	0.40
2:y:945:MET:O	2:y:948:VAL:HG12	2.21	0.40
2:y:1300:ILE:HD12	2:y:1300:ILE:HA	1.88	0.40
2:y:1392:LYS:HG2	2:y:1468:ALA:HB1	2.03	0.40
2:y:1754:ASP:OD1	2:y:1754:ASP:N	2.52	0.40
2:Y:642:THR:HA	2:Y:1118:ALA:O	2.21	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	
2	Y	1835/2108 (87%)	1755 (96%)	80 (4%)	0	100	100
2	y	2038/2108 (97%)	1946 (96%)	92 (4%)	0	100	100
All	All	3873/4216 (92%)	3701 (96%)	172 (4%)	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	
2	Y	1572/1795 (88%)	1556 (99%)	16 (1%)	68	74
2	y	1745/1795 (97%)	1715 (98%)	30 (2%)	53	67
All	All	3317/3590 (92%)	3271 (99%)	46 (1%)	57	70

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	y	27	LEU
2	y	61	THR
2	y	73	ASP
2	y	106	GLU
2	y	124	CYS
2	y	150	ILE
2	y	248	ILE
2	y	469	CYS

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Mol	Chain	Res	Type
2	y	554	THR
2	y	612	ASN
2	y	650	THR
2	y	756	ASN
2	y	763	SER
2	y	766	THR
2	y	774	SER
2	y	775	VAL
2	y	803	LEU
2	y	872	VAL
2	y	922	LEU
2	y	1072	LEU
2	y	1096	VAL
2	y	1122	VAL
2	y	1213	PHE
2	y	1251	THR
2	y	1331	VAL
2	y	1332	VAL
2	y	1416	HIS
2	y	1590	VAL
2	y	1828	LEU
2	y	2016	TYR
2	Y	102	ARG
2	Y	159	ILE
2	Y	619	LEU
2	Y	705	LYS
2	Y	732	ILE
2	Y	736	VAL
2	Y	781	MET
2	Y	794	THR
2	Y	908	TRP
2	Y	1111	ILE
2	Y	1148	THR
2	Y	1264	GLN
2	Y	1332	VAL
2	Y	1420	PHE
2	Y	1433	THR
2	Y	1451	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	y	14	GLN
2	y	41	GLN
2	y	44	GLN
2	y	136	GLN
2	y	203	GLN
2	y	286	GLN
2	y	379	GLN
2	y	569	ASN
2	y	597	ASN
2	y	676	ASN
2	y	753	ASN
2	y	876	ASN
2	y	893	GLN
2	y	906	GLN
2	y	1090	GLN
2	y	1185	GLN
2	y	1422	HIS
2	y	1435	HIS
2	y	1535	GLN
2	y	1667	HIS
2	y	1721	ASN
2	y	1827	GLN
2	y	1903	ASN
2	y	2085	ASN
2	Y	156	ASN
2	Y	339	HIS
2	Y	838	GLN
2	Y	1049	HIS
2	Y	1078	GLN
2	Y	1087	ASN
2	Y	1120	ASN
2	Y	1467	GLN
2	Y	1513	HIS
2	Y	1521	HIS
2	Y	1697	GLN

5.3.3 RNA ⓘ

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](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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$
4	AGS	Y	2206	-	29,33,33	0.47	1 (3%)	39,52,52	0.65	1 (2%)
4	AGS	y	2201	-	29,33,33	0.47	1 (3%)	39,52,52	0.67	1 (2%)

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
4	AGS	Y	2206	-	-	2/21/38/38	0/3/3/3
4	AGS	y	2201	-	-	9/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	2206	AGS	PG-S1G	2.16	1.95	1.90
4	y	2201	AGS	PG-S1G	2.14	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	y	2201	AGS	PA-O3A-PB	-3.40	121.17	132.83
4	Y	2206	AGS	PA-O3A-PB	-3.23	121.75	132.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

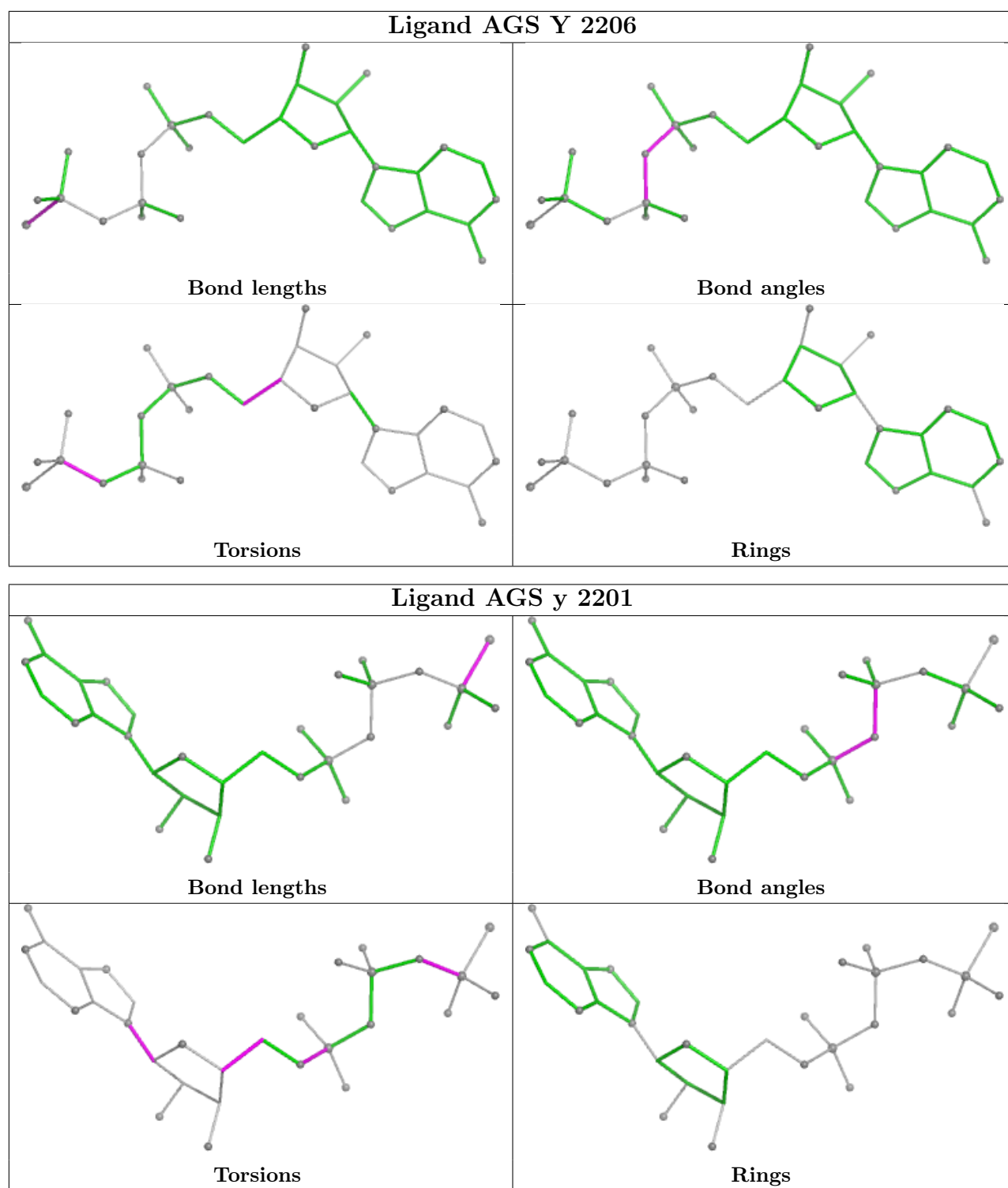
Mol	Chain	Res	Type	Atoms
4	y	2201	AGS	PB-O3B-PG-O2G
4	y	2201	AGS	PB-O3B-PG-O3G
4	y	2201	AGS	C5'-O5'-PA-O1A
4	y	2201	AGS	O4'-C4'-C5'-O5'
4	y	2201	AGS	C2'-C1'-N9-C8
4	y	2201	AGS	C5'-O5'-PA-O3A
4	y	2201	AGS	C5'-O5'-PA-O2A
4	y	2201	AGS	C2'-C1'-N9-C4
4	Y	2206	AGS	PB-O3B-PG-O3G
4	y	2201	AGS	O4'-C1'-N9-C8
4	Y	2206	AGS	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	2206	AGS	3	0
4	y	2201	AGS	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

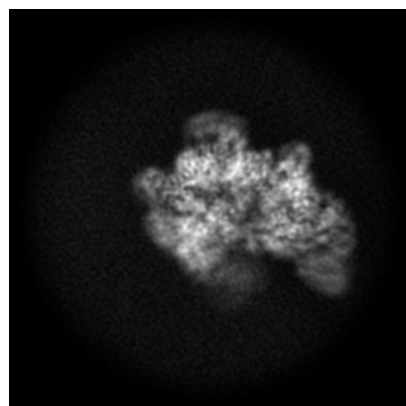
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56255. These allow visual inspection of the internal detail of the map and identification of artifacts.

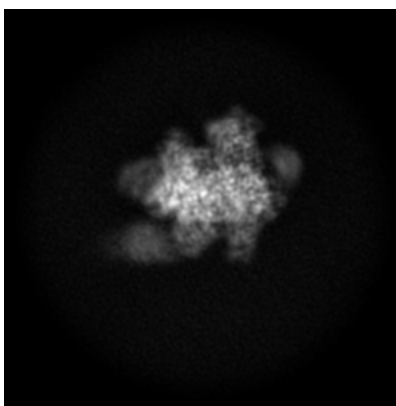
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

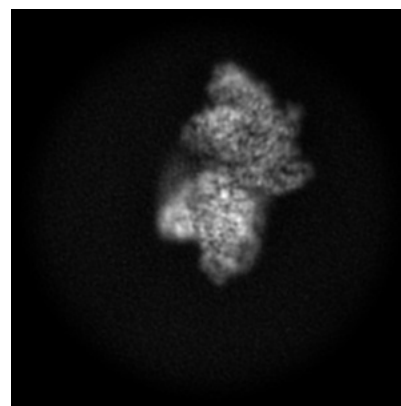
6.1.1 Primary map



X

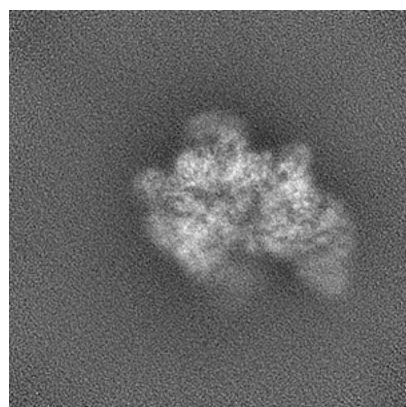


Y

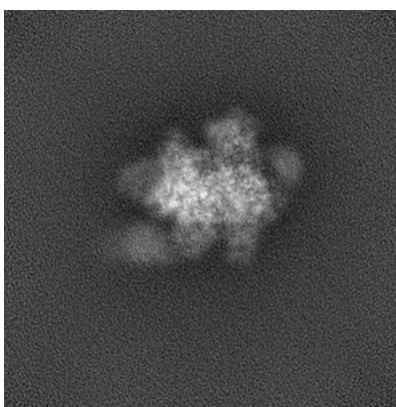


Z

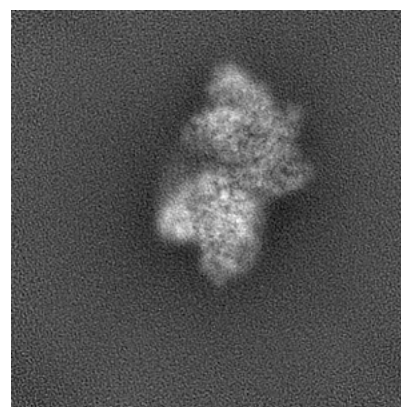
6.1.2 Raw map



X



Y

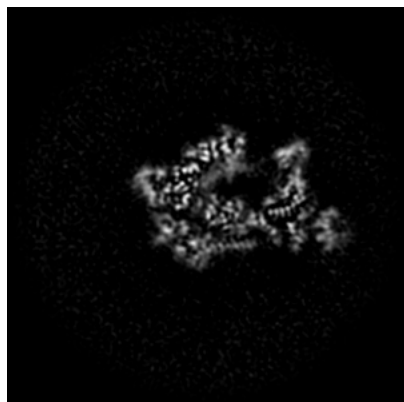


Z

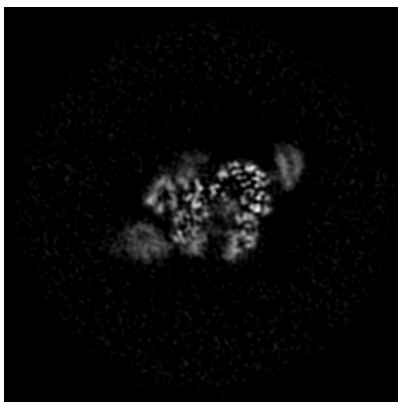
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

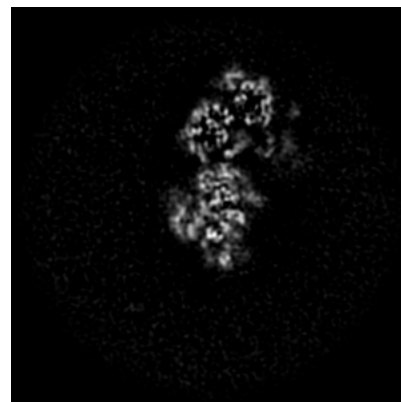
6.2.1 Primary map



X Index: 144

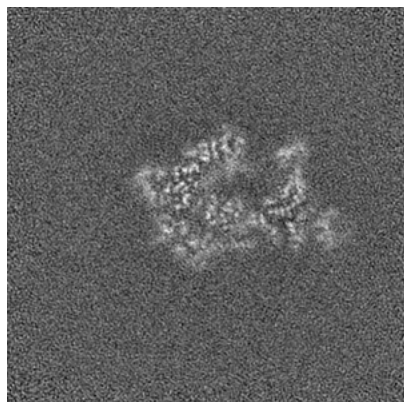


Y Index: 144

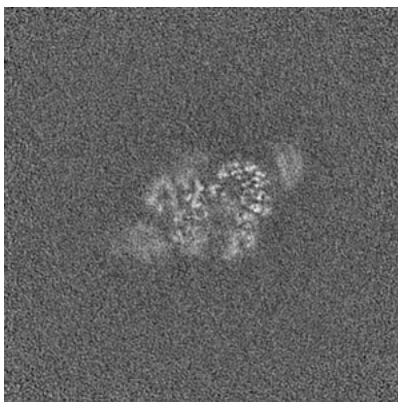


Z Index: 144

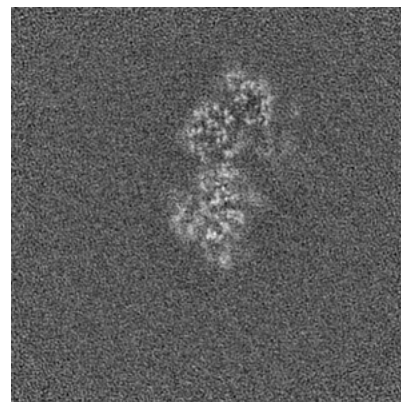
6.2.2 Raw map



X Index: 144



Y Index: 144

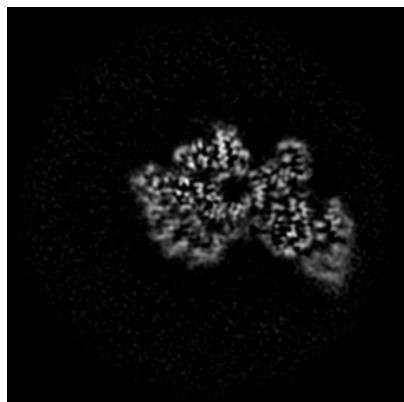


Z Index: 144

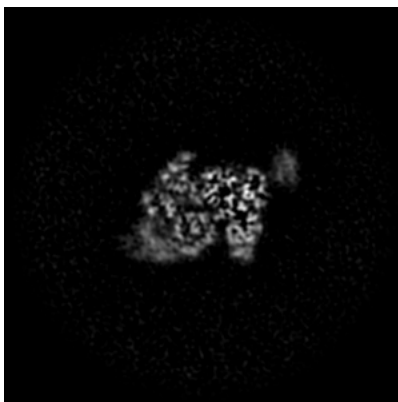
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

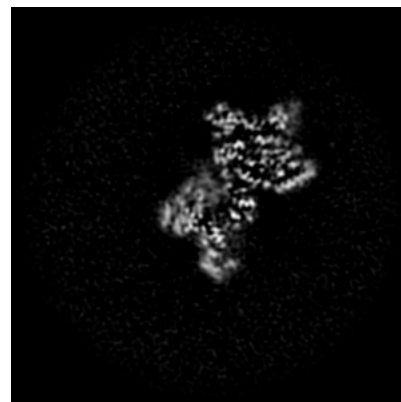
6.3.1 Primary map



X Index: 154

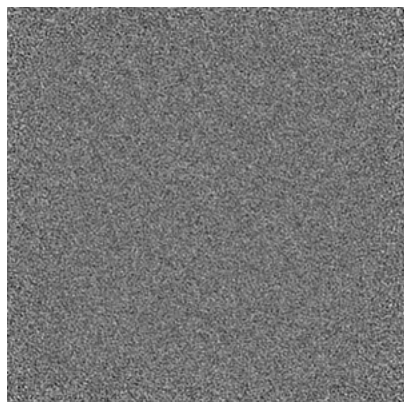


Y Index: 132

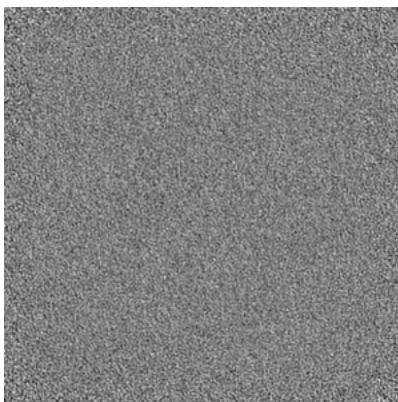


Z Index: 168

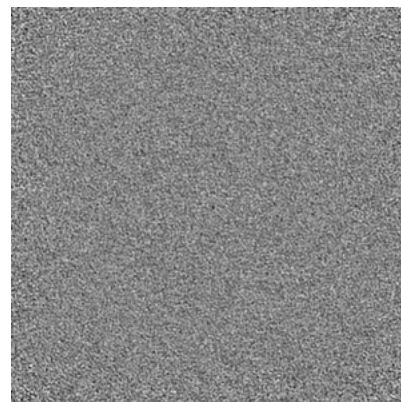
6.3.2 Raw map



X Index: 0



Y Index: 0

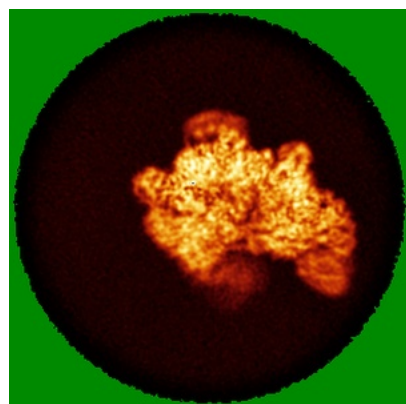


Z Index: 0

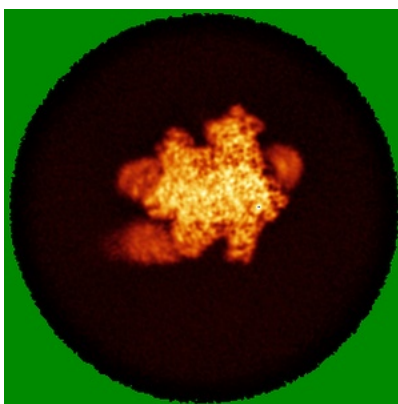
The images above show the largest variance slices of the map in three orthogonal directions.

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

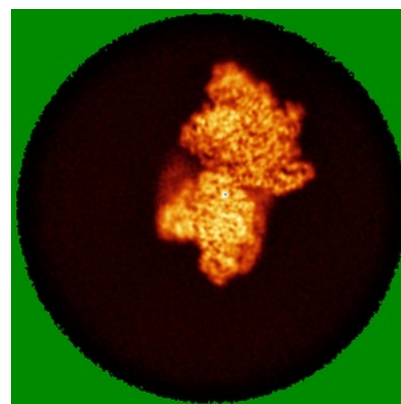
6.4.1 Primary map



X

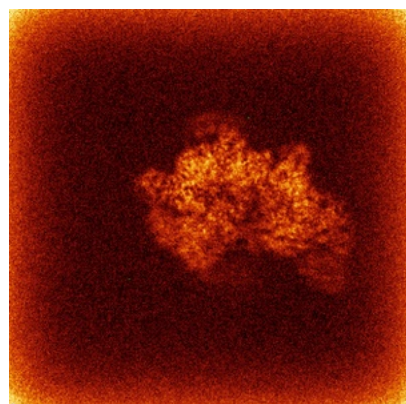


Y

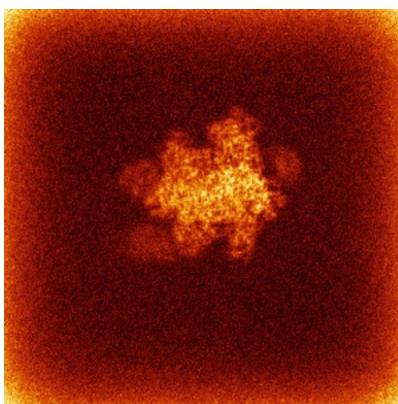


Z

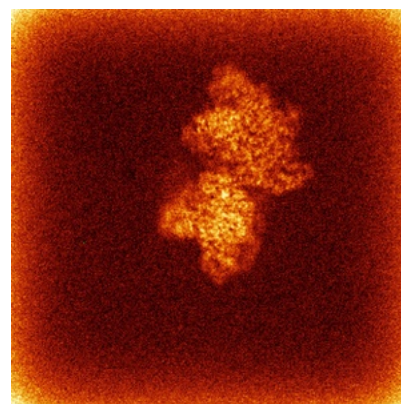
6.4.2 Raw map



X



Y



Z

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

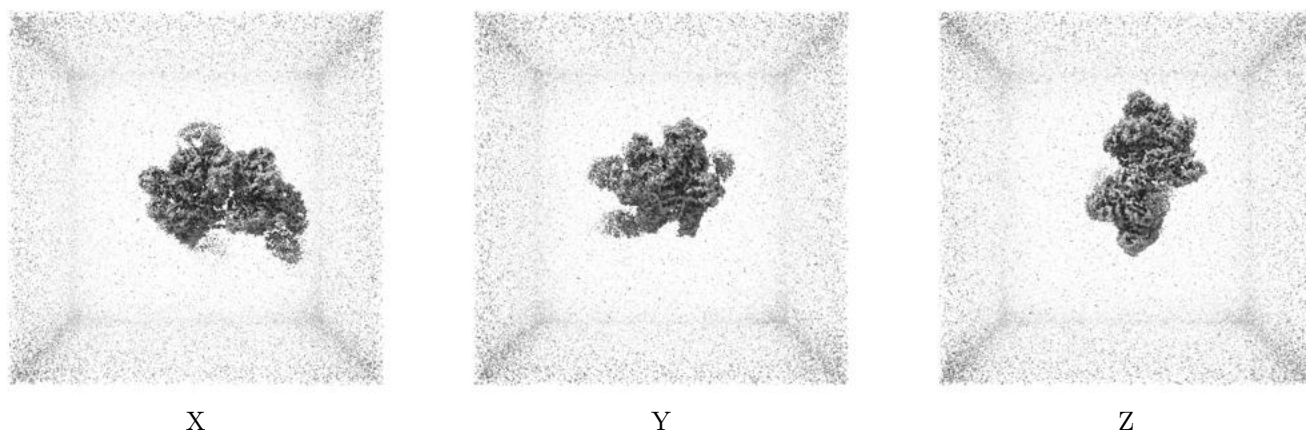
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

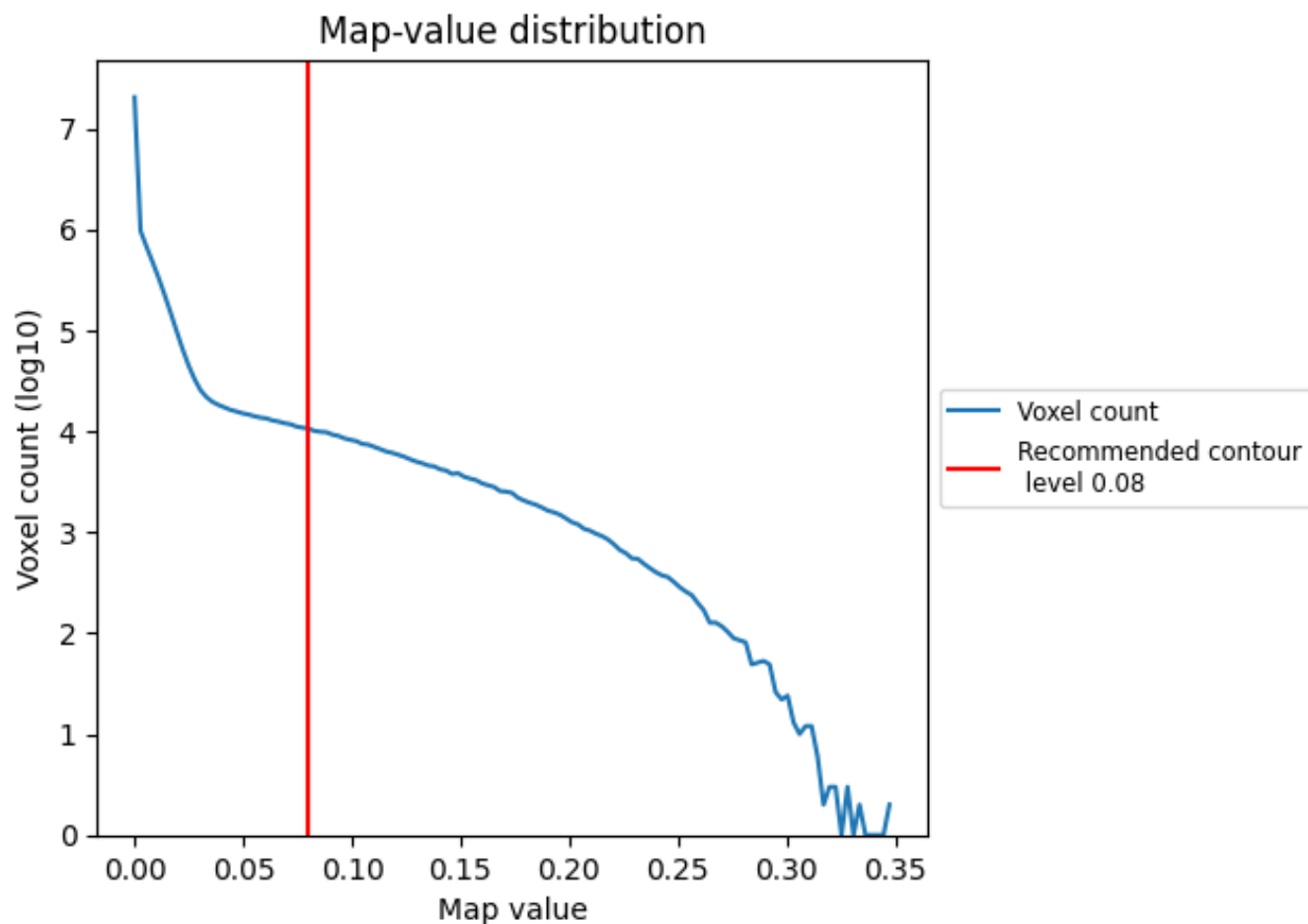
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

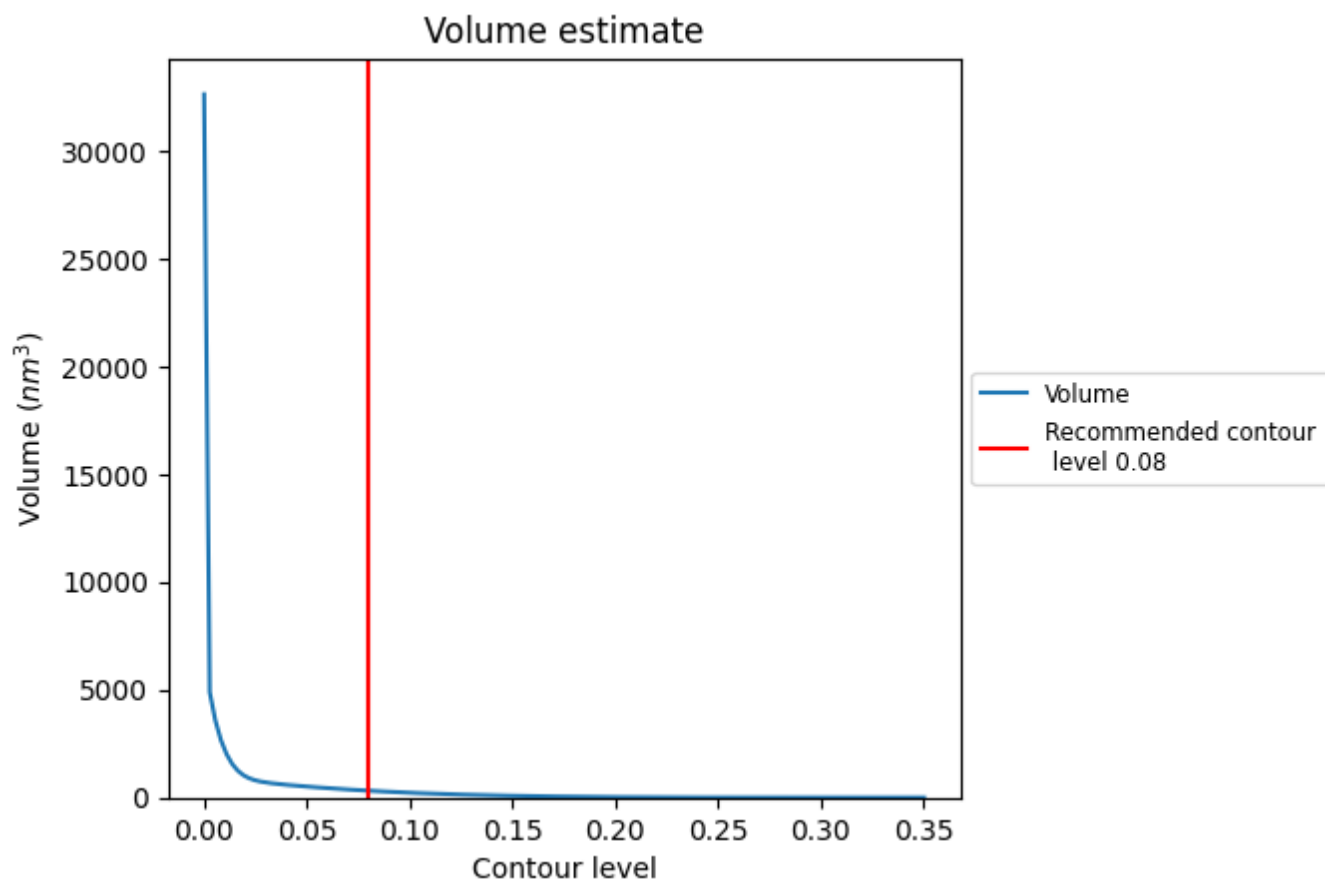
This section contains the results of statistical analysis of the map.

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.

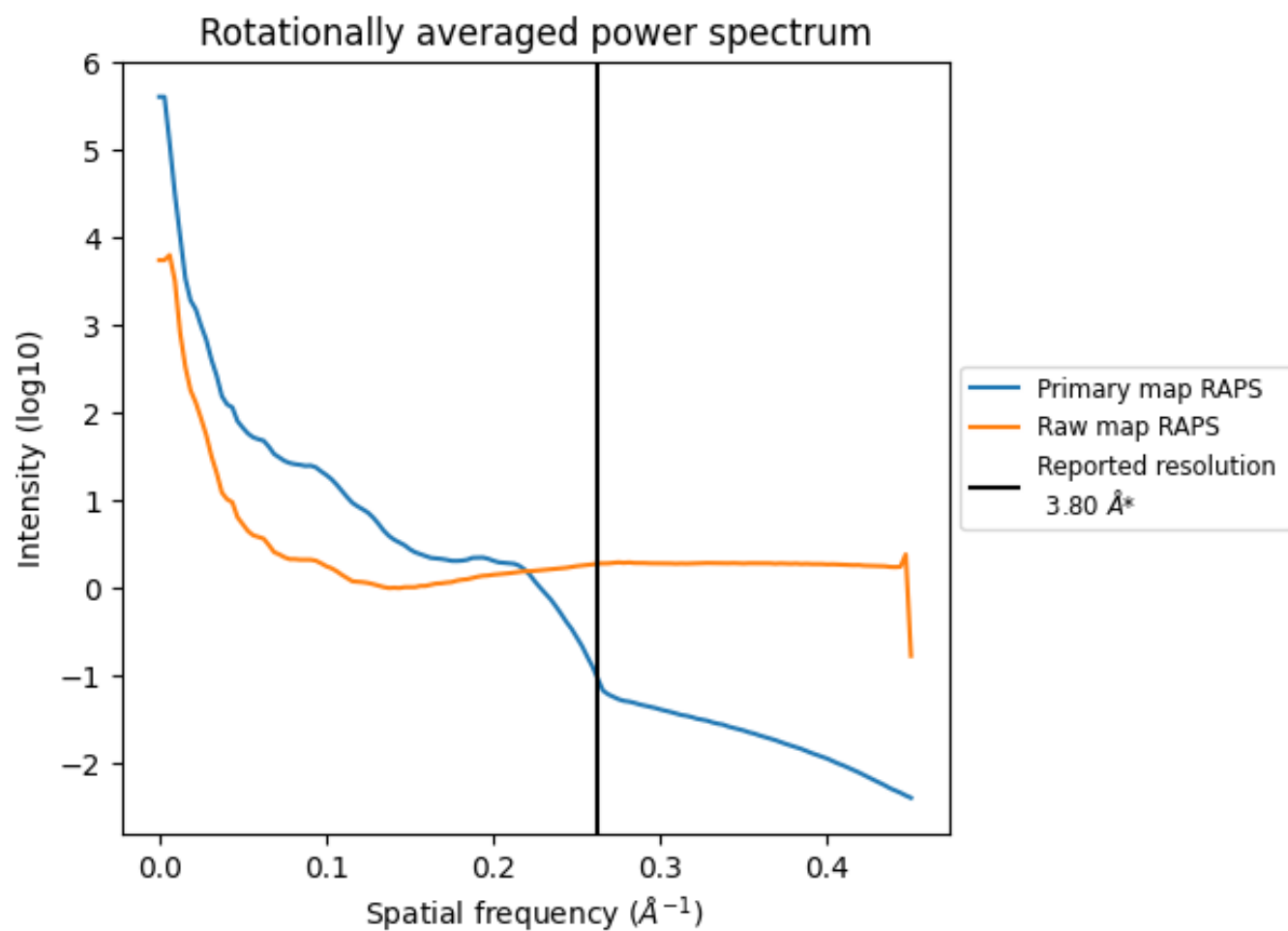
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 318 nm^3 ; this corresponds to an approximate mass of 287 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 ⓘ

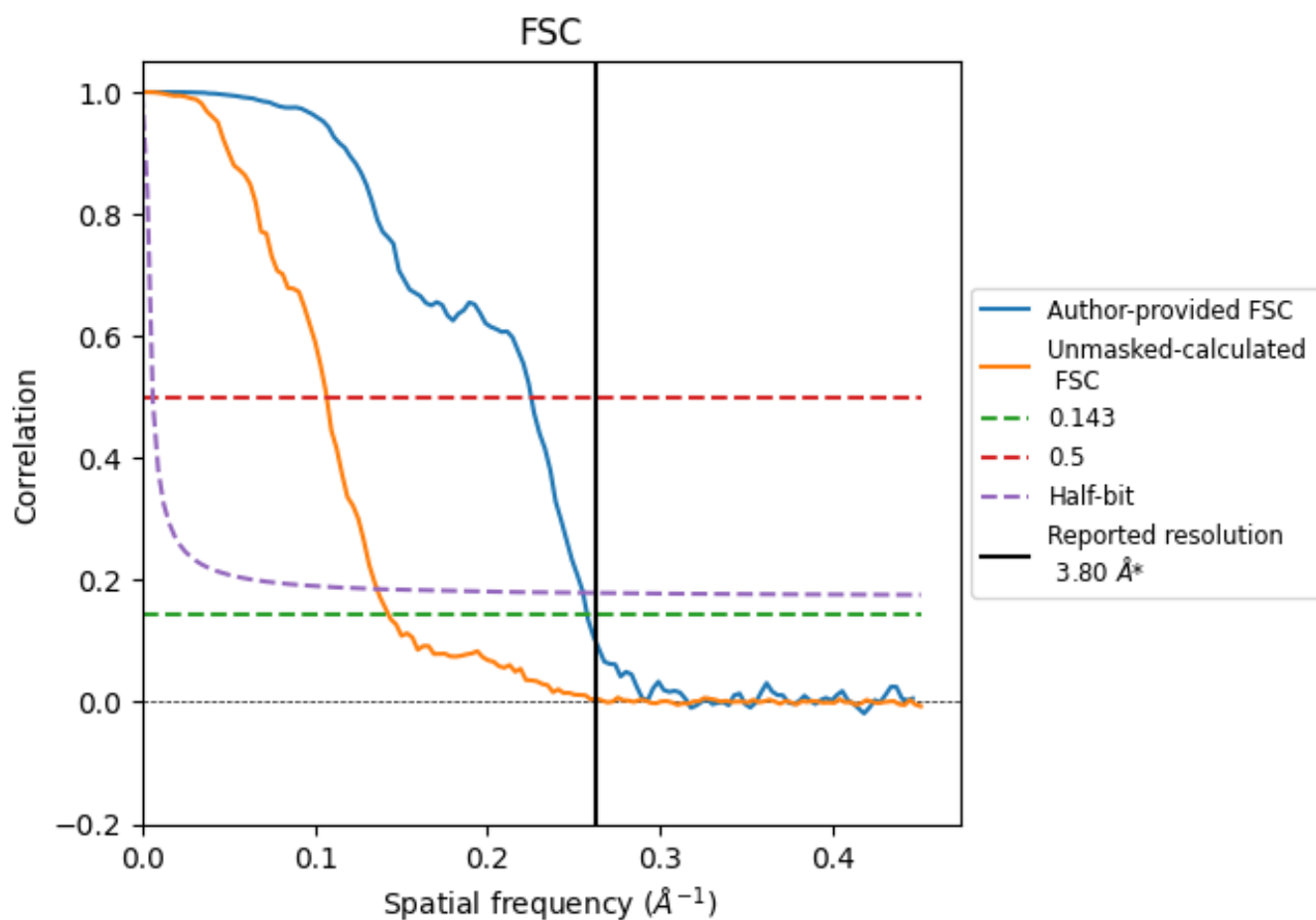


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

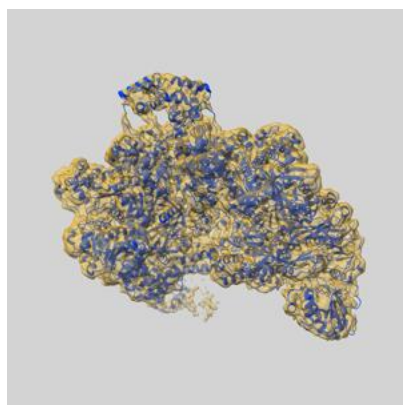
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.88	4.44	3.92
Unmasked-calculated*	7.01	9.35	7.35

*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 7.01 differs from the reported value 3.8 by more than 10 %

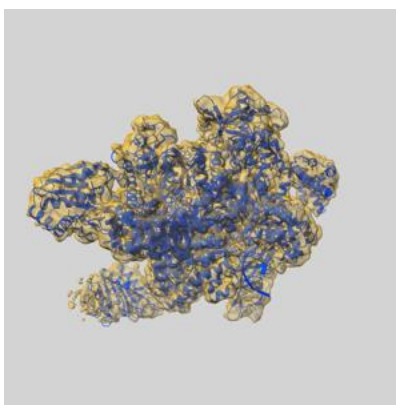
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56255 and PDB model 9TUB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

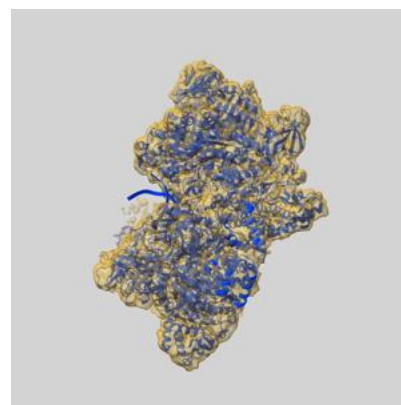
9.1 Map-model overlay [i](#)



X



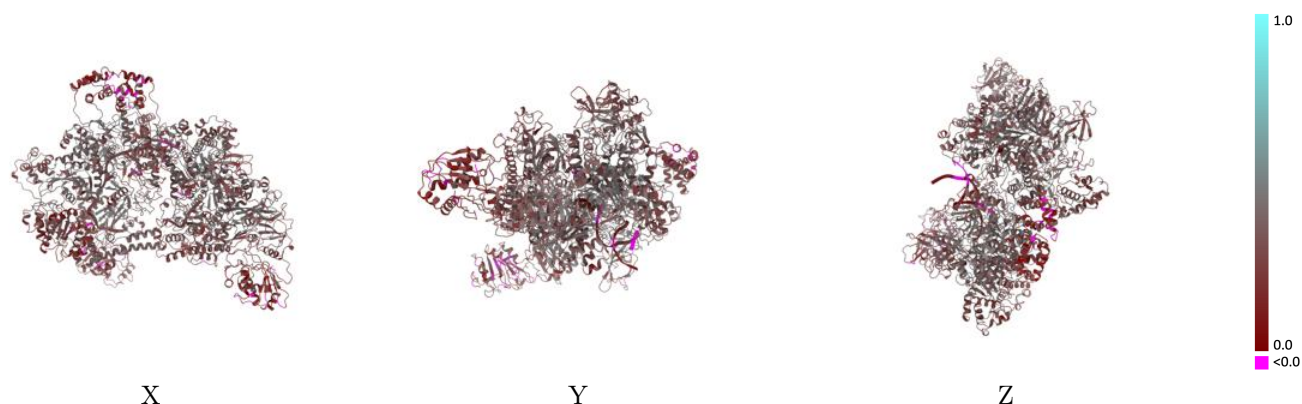
Y



Z

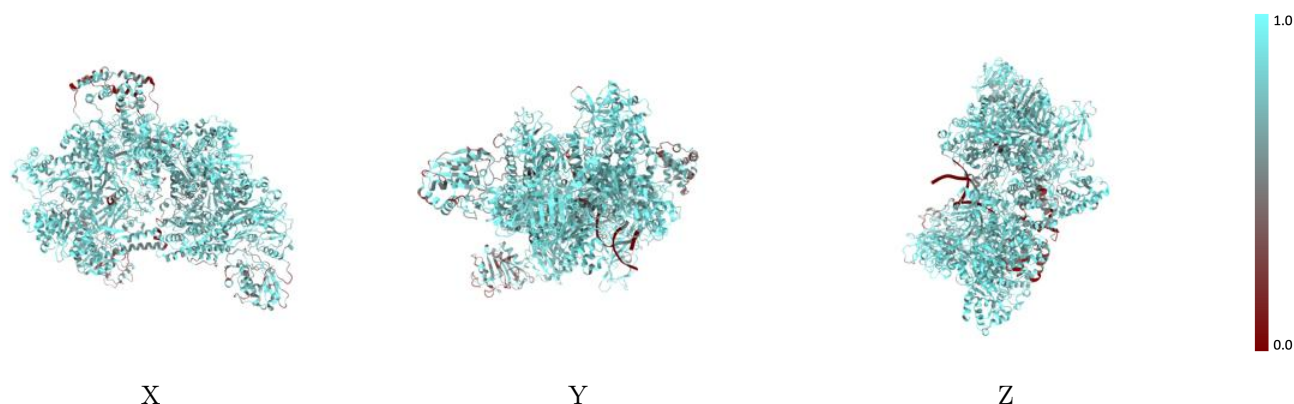
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



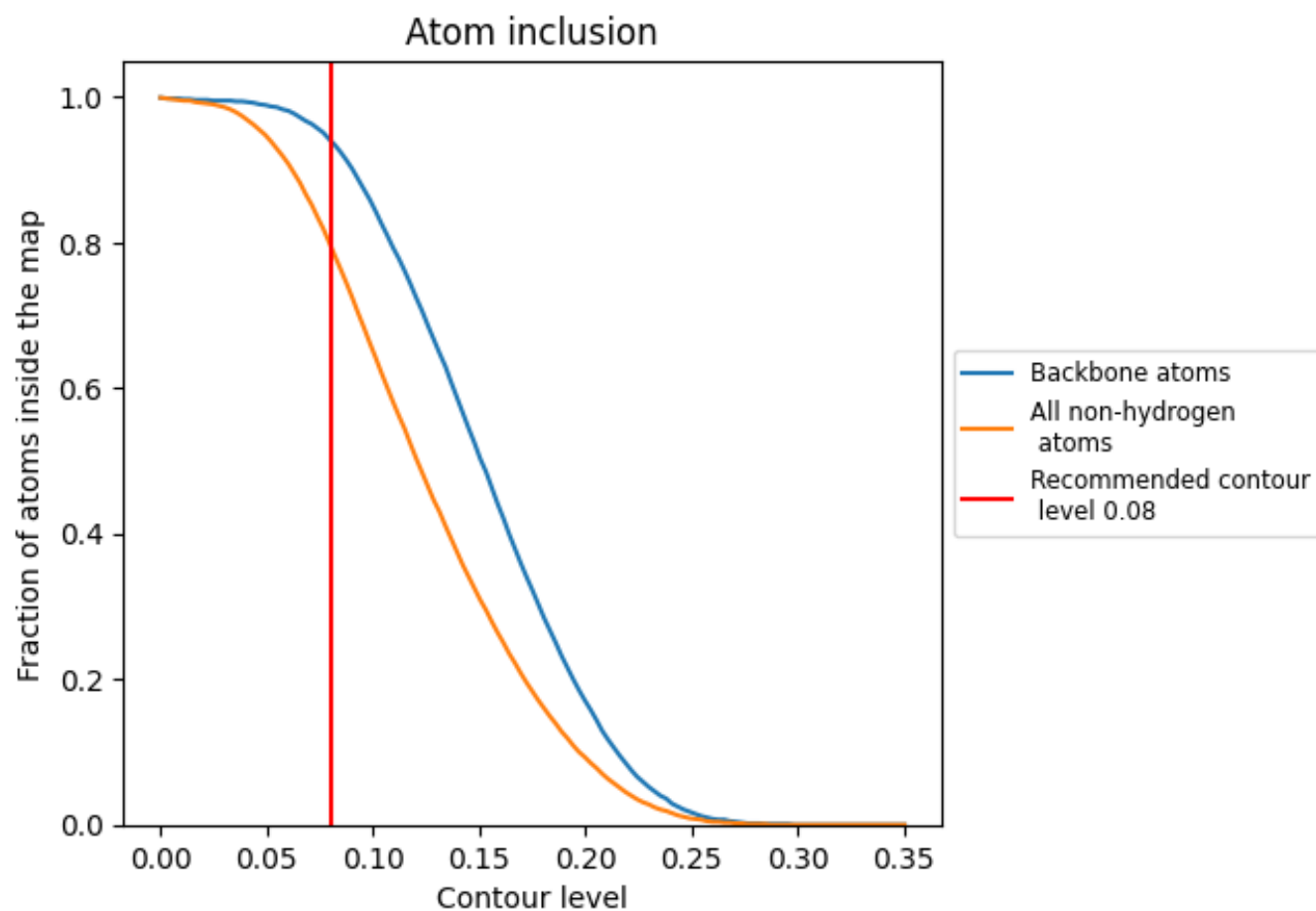
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.3290
G	0.1570	0.0490
I	0.6170	0.2430
Y	0.8230	0.3280
i	0.8330	0.3070
y	0.7860	0.3360

