



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:08 PM UTC

PDB ID : 9QCR / pdb_00009qcr
EMDB ID : EMD-53025
Title : DNA-PK bound to 153 bp H2AX nucleosome model 2
Authors : Hall, C.; Chaplin, A.
Deposited on : 2025-03-05
Resolution : 4.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

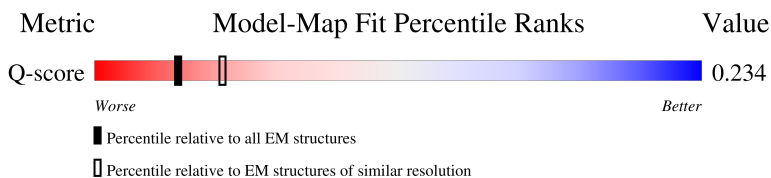
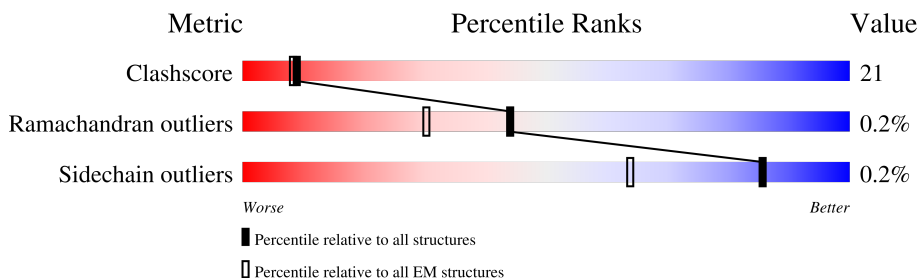
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.37 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.



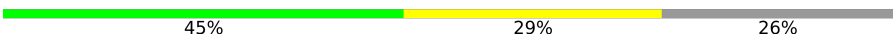
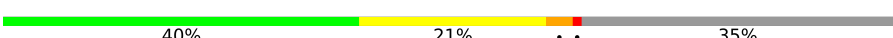
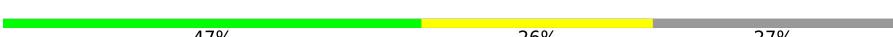
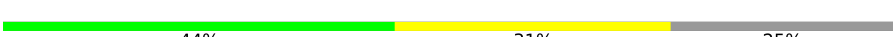
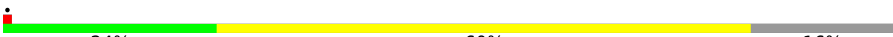
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3738 (3.87 - 4.87)

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	K	609	 50% 31% 19%
2	L	732	 39% 31% 29%
3	O	4128	 49% 36% 15%
4	C	143	 34% 30% 36%

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Mol	Chain	Length	Quality of chain
4	G	143	
5	D	126	
5	H	126	
6	A	136	
6	E	136	
7	B	103	
7	F	103	
8	I	153	
9	J	153	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 46641 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	493	Total	C	N	O	S	0	0
			3886	2489	647	732	18		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	517	Total	C	N	O	S	0	0
			4051	2599	678	751	23		

- Molecule 3 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	3527	Total	C	N	O	S	0	0
			27819	17843	4673	5117	186		

- Molecule 4 is a protein called Histone H2AX.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	92	Total	C	N	O	0	0
			707	445	139	123		
4	G	97	Total	C	N	O	0	0
			738	463	145	130		

- Molecule 5 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	93	Total	C	N	O	S	0	0
			705	443	126	135	1		
5	H	92	Total	C	N	O	S	0	0
			718	453	127	136	2		

- Molecule 6 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	96	Total	C	N	O	S	0	0
			794	500	154	136	4		
6	E	88	Total	C	N	O	S	0	0
			705	447	130	124	4		

- Molecule 7 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	75	Total	C	N	O	S	0	0
			595	377	116	101	1		
7	F	77	Total	C	N	O	S	0	0
			608	382	118	107	1		

- Molecule 8 is a DNA chain called 153 bp DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	129	Total	C	N	O	P	0	0
			2624	1247	481	769	127		

- Molecule 9 is a DNA chain called 153 bp DNA.

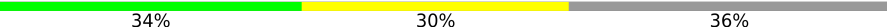
Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	131	Total	C	N	O	P	0	0
			2691	1275	504	783	129		

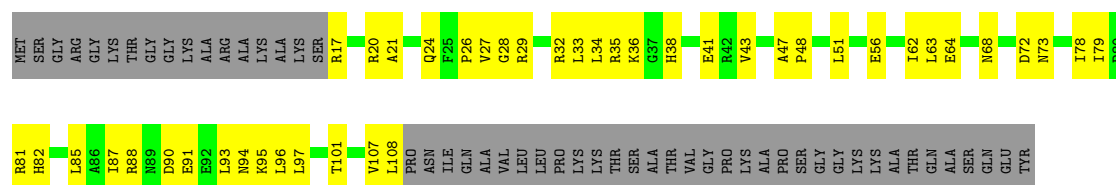
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W1632	L1633	A1644	V1645	L1646	I1652	L1653	Q1654	I1655	D1656	F1661	H1665	Y1675	L1678	L1684	D1685	L1686	H1687	L1688	K1689	G1690	V1691	M1692	V1693	F1699	THR	SER	LEU	THR	GLY	GLY	F1605	R1606	E1607	L1710	L1711	F1805	D1808	ASP	PRO	ARG	LEU	SER	PHE	T1815	R1816	Q1817	F1819	V1820								
L1358	L1359	K1360	K1361	D1362	L1363	C1364	N1365	L1366	H1367	L1368	M1369	R1370	V1371	L1372	V1373	Q1374	E1378	P1379	A1380	S1381	I1382	G1383	F1384	V1389	Q1390	L1402	M1403	K1404	A1405	L1406	Y1411	K1412	D1413	I1414	L1415	E1416	T1417	H1418	L1419	R1420	I1423	A1518	F1519	A1520	F1521	G1522	C1523	L1524	C1525	E1526	L1533	C1629				
R1445	V1452	L1458	L1463	L1464	H1465	H1466	I1467	L1468	Q1471	L1475	H1476	L1483	L1486	V1487	A1492	PRO	GLY	ASP	GLU	ARG	L1402	M1403	K1404	A1405	L1406	Y1411	K1412	D1413	I1414	L1415	E1416	T1417	H1418	L1419	R1420	I1423	A1518	F1519	A1520	F1521	G1522	C1523	L1524	C1525	E1526	L1533	C1629									
L1286	Q1287	S1288	S1289	K1292	A1293	V1294	H1295	F1296	F1297	S1300	I1301	H1304	C1312	PHE	GLY	THR	GLY	THR	ALA	GLY	ASN	ARG	T1322	E1326	E1327	E1328	Y1329	Y1330	N1331	K1334	C1335	T1336	V1337	V1338	V1339	M1342	E1343	F1344	T1345	T1346	T1347	L1348	L1349	N1350	T1351	S1352	F1353	E1354	G1355	W1356	K1357					
Q1180	C1183	R1184	S1187	V1195	P1196	L1197	L1198	N1201	R1202	S1203	L1206	W1207	G1226	G1230	Q1231	Q1232	I1235	T1240	T1241	T1242	T1243	T1244	T1245	T1246	T1247	T1248	T1249	L1250	Q1251	A1252	T1253	W1256	L1257	L1260	L1261	A1262	E1265	C1266	Y1267	N1268	T1269	E1273	A1278	L1279	L1282											
V1096	E1097	Q1098	F1099	V1100	F1101	E1102	A1103	L1104	I1106	L1111	A1112	D1117	L1121	G1122	T1123	I1124	Q1125	G1127	C1128	D1129	A1130	I1131	H1133	L1134	I1137	K1141	H1142	N1146	K1147	A1148	K1149	K1150	R1151	R1155	S1162	L1163	C1164	L1165	L1166	D1167	L1168	V1169	K1170	L1172	R1178	P1179										
N997	N998	F1001	D1005	E1011	D1015	I1017	V1018	D1019	L1025	R1026	R1031	R1034	S1040	I1041	S1052	N1055	T1056	K1057	S1058	L1059	F1060	K1061	L1068	H1069	P1070	N1071	A1072	F1073	K1074	R1075	L1076	L1080	A1081	F1082	N1083	N1084	I1085	Y1086	N1087	E1088	R1089	I1090	E1091	E1092	L1095											
L911	P912	R913	V914	T915	E916	L917	A918	A921	R924	Q925	F926	K927	C931	E932	L933	N937	V938	N939	I1041	I1040	N941	S1052	K944	E950	G952	Q953	G954	A955	P956	P957	N958	Y959	G960	L961	N979	D886	D887	R888	E989	K890	R891	L892	S893	F894	F898	R899	E900	Y901	T902	Q903	L904	I905	D908	V909	F910	
SER	ASN	GLU	ALA	ILE	S847	L848	T851	R852	G853	R854	V855	V856	Q857	M858	L859	G860	S861	L862	G863	Q864	Q865	D867	L868	Y789	L800	S803	ALA	LEU	THR	ASP	ASP	GLU	THR	LYS	ASN	ASN	TRP	GLU	VAL	ALA	LEU	SER	ALA	LEU	SER	ARG	ALA	ALA	GLN	LYS	GLY	F826	L834	T837	L840	SER
G759	Y762	T763	P764	L765	A766	E767	V768	N771	E775	Y779	I780	M785	Y788	K789	L793	Y799	L800	S803	ALA	LEU	THR	ASP	ASP	GLU	THR	LYS	ASN	ASN	TRP	GLU	VAL	ALA	LEU	SER	ALA	LEU	SER	ARG	ALA	ALA	GLN	LYS	GLY	F826	L834	T837	L840	SER								
ALA	PRO	VAL	THR	TRP	MET	ILE	PRO	THR	ASP	PRO	ALA	A610	N611	L612	H613	K618	F623	I624	N625	L626	V627	C630	I633	E636	Q637	Q638	A639	E640	E643	P644	W645	Y647	S648	F649	S650	Y651	E652	L653	I654	I655	Q656	THR	VAL	GLY	GLN	ASN	GLY	ASP	S671							



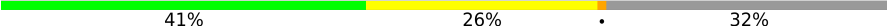
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K3257	L3258	L3259	L3262	R3269	W3272	R3281	R3282	L3283	S3284	H3285	C3286	R3287	S3288	R3289	S3290	Q3291	S3292	C3293	S3294	E3295	Q3296	V3297	L3298	T3299	V3300	L3301	V3304	N3311	S3314	K3318	N3319	I3320	L3321	A3322	F3323	R3324	I3328	T3332	T3333	Y3334	R3335	L3336	I3337	D3344	S3245	K3248	Q3249	N3250	L3132				
L3348	E3428	E3429	ASN	ALA	SER	VAL	ILE	ASP	SER	GLU	LEU	SER	SER	SER	E3371	K3372	V3373	I3374	L3377	A3381	F3382	L3385	Q3390	A3391	V3300	A3392	E3393	E3394	E3395	ALA	GLN	PRO	PRO	SER	TRP	CYS	GLY	PRO	ALA	Y3413	L3416	F3419	L3420	D3421	Q3422	Q3423	L3424	W3498	E3427				
K3502	V3503	A3504	L3505	L3506	D3507	K3508	A3513	Q3514	Q3515	V3518	E3519	T3522	D3523	T3529	V3530	V3531	P3532	F3533	I3534	I3535	S3536	S3537	E3538	S3539	T3545	S3546	T3547	Q3548	H3549	K3552	V3555	T3558	K3561	Q3577	L3578	W3588	V3592	R3593	L3594	E3595	LEU	ALA	LYS										
THR	PRO	VAL	ASN	LYS	K3604	N3605	L3606	E3607	K3608	M3609	Y3610	N3613	Y3614	L3617	G3618	L3625	R3629	P3632	I3633	F3636	G3637	F3640	D3641	K3642	G3645	LYS	GLY	GLY	SER	LYS	LEU	LEU	ARG	MET	LYS	LEU	ASP	PHE	N3660	D3661	L3662	M3665	L3666	K3669	D3675	P3676	V3764	V3770					
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M3771	N3772	Q3773	K3774	L3775	L3788	V3793	V3794	P3795	M3796	T3797	L3800	G3801	L3802	W3805	L3806	T3809	V3810	T3811	L3812	K3813	D3814	L3815	N3818	T3819	M3820	S3821	Q3822	E3823	E3824	K3825	R3833	A3834	P3835	P3836	C3837	E3838	I3839	K3840	D3842	L3843	THR	LYS	MET	SER	GLY	LYS	HIS	D3851	V3852	G3853			
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LYS	ASN	W4038	R4041	Q4042	K4043	I4044	C4045	Y4046	K4047	K4048	R4049	K4050	L4051	A4052	G4053	A4054	N4055	P4056	A4057	V4058	I4059	T4060	E4063	L4064	H4068	A4069	K4070	A4073	R4082	Y4077	V4080	A4081	G4083	D4086	H4087	N4088	A4091	G4097	E4100	D4109	Q4110	A4111	T4112	D4113	P4114	N4115	I4116	L4117					
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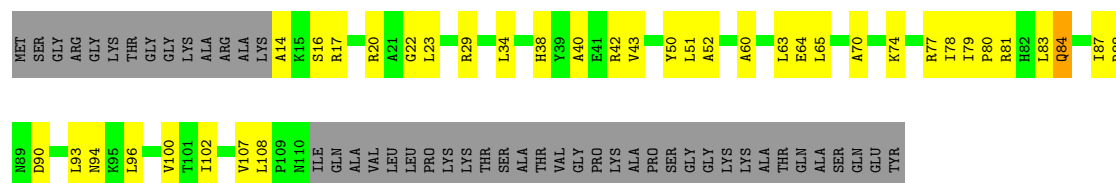
• Molecule 4: Histone H2AX

Chain C:  34% 30% 36%

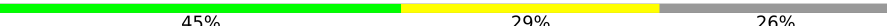


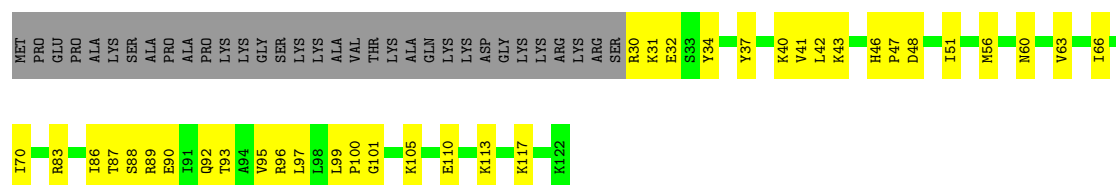
• Molecule 4: Histone H2AX

Chain G:  41% 26% 32%



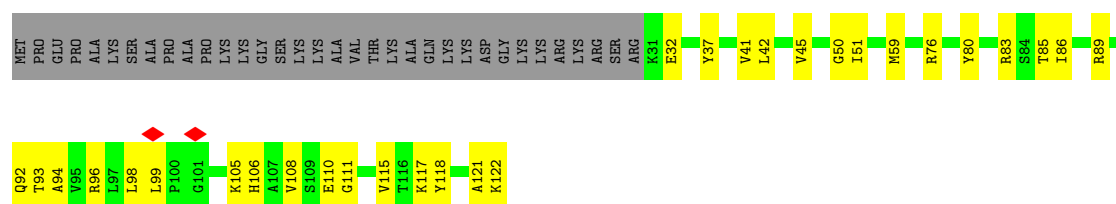
• Molecule 5: Histone H2B type 1-J

Chain D:  45% 29% 26%



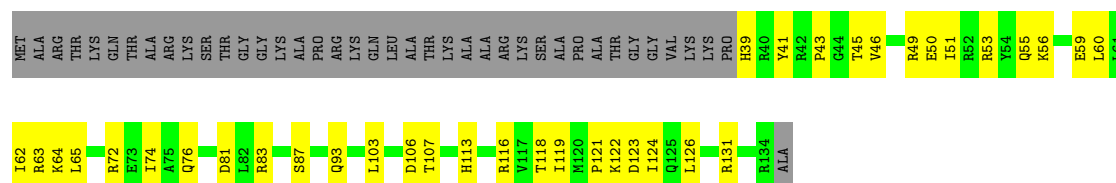
• Molecule 5: Histone H2B type 1-J

Chain H:  49% 24% 27%

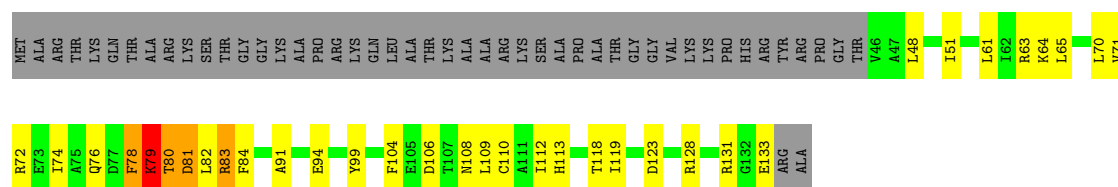


• Molecule 6: Histone H3.1

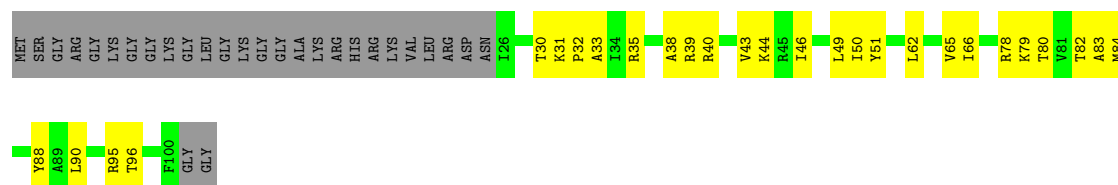
Chain A:  43% 27% 29%



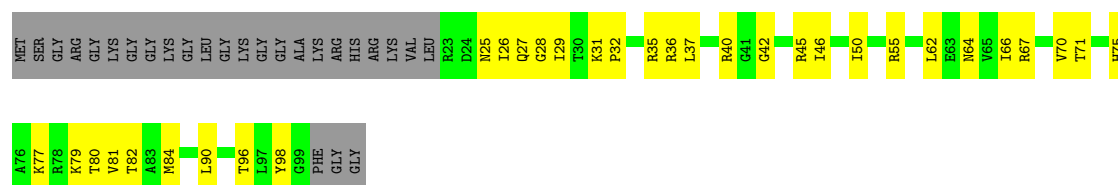
• Molecule 6: Histone H3.1



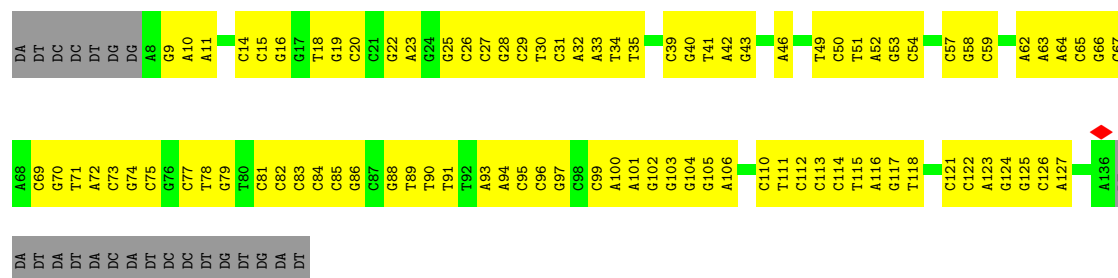
Chain B: 47% 26% 27%



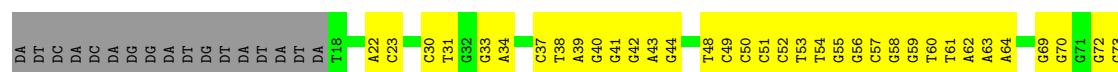
Chain F: 44% 31% 25%



Chain I: 24% 60% 16%



Chain J: 39% 47% 14%



A74	C75	A76	G79	C80	G81	T82	A83	G89	T90	T91	T92	A93	A94	G97	C101	T102	A103	G104	A105	G106	C107	T108	A113	T122	G125	C126	G127	G128	C129	C130	T131	C132	G133	G134	C135	A136	C137	C138	G139	G140	G141	C147	C148	DA	DG	DG	DG	DA	DT
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15518	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 ($e^-/\text{\AA}^2$)	48.59	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.875	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	692.16, 692.16, 692.16	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6479999, 1.6479999, 1.6479999	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	K	0.11	0/3962	0.27	0/5354
2	L	0.13	0/4131	0.35	0/5585
3	O	0.12	0/28365	0.36	0/38383
4	C	0.10	0/716	0.26	0/965
4	G	0.10	0/748	0.29	0/1010
5	D	0.12	0/714	0.32	0/961
5	H	0.10	0/729	0.28	0/979
6	A	0.11	0/805	0.30	0/1079
6	E	0.26	0/713	0.52	0/958
7	B	0.11	0/601	0.26	0/805
7	F	0.11	0/614	0.30	0/825
8	I	0.19	0/2940	0.36	0/4530
9	J	0.18	0/3020	0.36	0/4661
All	All	0.13	0/48058	0.35	0/66095

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	K	3886	0	3875	166	0
2	L	4051	0	4049	186	0
3	O	27819	0	27772	1141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	707	0	744	38	0
4	G	738	0	769	40	0
5	D	705	0	719	33	0
5	H	718	0	740	26	0
6	A	794	0	831	43	0
6	E	705	0	726	44	0
7	B	595	0	640	29	0
7	F	608	0	639	45	0
8	I	2624	0	1449	118	0
9	J	2691	0	1472	92	0
All	All	46641	0	44425	1799	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 21.

All (1799) 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)
3:O:3868:VAL:HG12	3:O:4117:LEU:HB2	1.57	0.86
7:F:90:LEU:HB3	7:F:96:THR:HA	1.60	0.84
3:O:1172:LEU:HD11	3:O:1187:SER:HB2	1.62	0.82
6:E:128:ARG:HG3	6:E:133:GLU:HG3	1.62	0.82
3:O:196:LEU:HD13	3:O:227:LEU:HD11	1.61	0.81
6:E:83:ARG:HB2	7:F:80:THR:HG22	1.62	0.80
3:O:4116:ILE:HA	3:O:4124:TRP:HH2	1.47	0.80
3:O:364:ARG:HH12	3:O:415:GLN:HB2	1.47	0.79
3:O:2187:VAL:HB	3:O:2728:LEU:HD21	1.64	0.79
3:O:3163:THR:HB	3:O:3167:ARG:HH22	1.46	0.79
8:I:111:DT:H1'	9:J:44:DG:H22	1.48	0.79
1:K:507:THR:HB	2:L:394:ARG:HD3	1.63	0.78
3:O:3717:VAL:HG23	3:O:3743:HIS:H	1.49	0.78
2:L:251:LEU:HB2	2:L:261:ILE:HG12	1.66	0.78
3:O:393:LYS:HA	3:O:397:LEU:HD23	1.64	0.78
1:K:39:ILE:HG22	1:K:84:ALA:HB3	1.67	0.76
3:O:1169:VAL:HG21	3:O:1198:LEU:HD11	1.66	0.76
2:L:253:ILE:HD11	2:L:342:VAL:HG23	1.67	0.76
4:C:28:GLY:HA3	8:I:33:DA:H3'	1.67	0.75
9:J:41:DG:H2''	9:J:42:DG:N7	2.01	0.75
3:O:925:GLN:HG3	3:O:2800:ARG:HH12	1.52	0.75
3:O:1380:ALA:HA	3:O:1384:PHE:HA	1.69	0.75
3:O:2415:LEU:HB3	3:O:2420:PHE:HB2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:4125:GLU:HB2	3:O:4128:MET:HE1	1.67	0.74
6:E:72:ARG:NH2	8:I:54:DC:OP1	2.20	0.74
1:K:95:ASN:HD22	1:K:95:ASN:N	1.82	0.74
3:O:893:SER:O	3:O:944:LYS:NZ	2.20	0.74
3:O:663:ILE:HG22	3:O:665:GLY:H	1.53	0.74
7:B:82:THR:HG22	7:B:84:MET:H	1.52	0.74
3:O:124:LYS:HZ2	8:I:11:DA:H3'	1.52	0.73
3:O:3535:ILE:HG23	3:O:3797:THR:HA	1.70	0.73
2:L:44:ARG:NH2	2:L:240:ILE:O	2.21	0.73
2:L:337:GLY:HA2	2:L:399:LYS:HA	1.69	0.73
3:O:1932:GLN:HB2	3:O:1937:ARG:HE	1.53	0.73
1:K:400:TYR:O	1:K:408:PRO:HA	1.90	0.72
3:O:1068:LEU:HD21	3:O:1106:ILE:HD12	1.71	0.72
3:O:1686:LEU:HD11	3:O:1738:ASN:HB3	1.71	0.72
3:O:901:MET:HG2	3:O:903:PRO:HD3	1.71	0.72
6:A:39:HIS:HB2	8:I:86:DG:H21	1.54	0.72
3:O:914:VAL:HG11	3:O:937:MET:HE1	1.72	0.71
1:K:299:LYS:NZ	2:L:296:CYS:O	2.22	0.71
6:A:113:HIS:NE2	6:E:123:ASP:OD1	2.23	0.71
7:F:31:LYS:HG3	7:F:32:PRO:HD3	1.72	0.71
6:E:82:LEU:O	6:E:83:ARG:C	2.33	0.71
3:O:1589:ASN:HD21	3:O:1592:MET:HB2	1.55	0.71
3:O:3681:LYS:NZ	3:O:3683:CYS:SG	2.63	0.71
3:O:271:GLY:O	3:O:274:LEU:HB2	1.91	0.71
7:F:25:ASN:HB3	7:F:29:ILE:HG12	1.71	0.71
2:L:362:LEU:HB2	2:L:421:TYR:HB3	1.73	0.71
3:O:867:ASN:HB3	3:O:3129:LEU:HD11	1.73	0.71
2:L:391:ALA:HB3	2:L:408:ALA:HB3	1.73	0.70
3:O:3069:MET:HA	3:O:3075:LYS:HB2	1.71	0.70
3:O:730:LEU:HD11	3:O:765:LEU:HD22	1.72	0.70
3:O:3156:PRO:O	3:O:3159:ARG:NH1	2.24	0.70
6:E:108:ASN:ND2	7:F:42:GLY:O	2.24	0.70
4:C:43:VAL:HG23	5:D:86:ILE:HB	1.72	0.69
3:O:771:ASN:OD1	3:O:854:ARG:NH2	2.26	0.69
3:O:2327:LEU:O	3:O:2333:ARG:NH1	2.26	0.69
9:J:69:DG:H2''	9:J:70:DG:C8	2.27	0.69
3:O:1034:ARG:HD2	3:O:1084:ASN:HB2	1.74	0.69
3:O:2357:GLU:HA	3:O:2360:PHE:HB3	1.75	0.69
1:K:172:GLU:HA	1:K:207:LYS:HE3	1.75	0.69
3:O:3969:ASN:HA	3:O:3972:LEU:HG	1.75	0.69
1:K:420:LEU:HG	1:K:426:GLN:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:500:PRO:O	1:K:502:GLN:NE2	2.26	0.68
3:O:3130:GLN:NE2	3:O:3174:ASP:OD1	2.26	0.68
3:O:172:GLU:HB2	3:O:219:VAL:HG12	1.75	0.68
4:G:40:ALA:HB3	5:H:86:ILE:HD11	1.75	0.68
1:K:358:LYS:HA	2:L:353:ARG:HH12	1.58	0.68
1:K:264:ASN:HB2	2:L:530:LEU:HD22	1.75	0.67
6:E:74:ILE:HG23	7:F:66:ILE:HD13	1.76	0.67
3:O:1817:GLN:OE1	3:O:1936:ARG:NH2	2.27	0.67
1:K:300:THR:H	3:O:164:LYS:HZ2	1.43	0.67
2:L:248:PRO:HB2	2:L:262:ALA:HB1	1.75	0.67
3:O:1011:GLU:O	3:O:1015:ASP:N	2.27	0.67
3:O:2507:ILE:HD11	3:O:2545:LEU:HD12	1.77	0.67
3:O:2365:ASN:ND2	3:O:2399:GLU:OE1	2.27	0.67
4:G:84:GLN:HB3	4:G:102:ILE:HD11	1.75	0.67
3:O:275:PHE:HA	3:O:282:PHE:HE2	1.60	0.67
3:O:2461:PHE:HB2	3:O:2473:MET:HE3	1.77	0.67
6:A:116:ARG:NH1	6:A:118:THR:O	2.28	0.67
3:O:1568:ASN:HA	3:O:1600:MET:HE1	1.75	0.67
1:K:430:PRO:HG2	2:L:438:LEU:HD12	1.78	0.66
3:O:532:ARG:NH1	3:O:636:GLU:OE2	2.27	0.66
3:O:2361:ILE:HD11	3:O:2393:LEU:HD23	1.77	0.66
3:O:3531:TYR:OH	3:O:3796:MET:SD	2.51	0.66
4:G:23:LEU:HD21	4:G:52:ALA:HB3	1.76	0.66
3:O:1359:LEU:O	3:O:1362:ASP:HB2	1.94	0.66
7:B:78:ARG:NH2	7:B:80:THR:OG1	2.29	0.66
3:O:165:LYS:NZ	9:J:139:DG:N7	2.41	0.66
3:O:3314:SER:HB2	3:O:3318:LYS:HB3	1.78	0.66
2:L:111:LEU:HD22	2:L:150:ILE:HG12	1.78	0.66
3:O:297:LEU:HD13	3:O:316:LEU:HA	1.77	0.66
3:O:2407:GLY:HA3	3:O:2411:LEU:HD11	1.76	0.66
3:O:3291:GLN:HG2	3:O:3293:CYS:H	1.59	0.66
3:O:862:LEU:HB3	3:O:866:ILE:HD11	1.77	0.66
3:O:3693:GLU:HG3	3:O:3696:ARG:HH21	1.61	0.66
2:L:489:ARG:NH2	2:L:506:PRO:O	2.29	0.66
3:O:1475:LEU:HD22	3:O:1523:GLY:HA2	1.78	0.66
3:O:653:LEU:HD23	3:O:670:LEU:HD22	1.78	0.65
1:K:254:ARG:NH1	8:I:14:DC:OP1	2.29	0.65
3:O:2225:HIS:H	3:O:2231:PHE:HB2	1.61	0.65
3:O:4004:VAL:HG22	3:O:4005:PHE:H	1.62	0.65
4:C:85:LEU:HD23	4:C:108:LEU:HD21	1.79	0.65
3:O:1417:THR:O	3:O:1420:ARG:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:56:MET:O	5:D:60:ASN:ND2	2.29	0.65
3:O:2195:SER:O	3:O:2722:ARG:NH1	2.30	0.65
3:O:3739:ILE:HG23	3:O:3749:PRO:HB3	1.78	0.65
1:K:444:ARG:NH2	2:L:244:SER:OG	2.30	0.65
3:O:200:PHE:HE2	3:O:227:LEU:HD22	1.62	0.65
3:O:2446:LEU:HG	3:O:2450:GLU:HG3	1.78	0.65
3:O:3015:SER:HA	3:O:3044:MET:HE1	1.79	0.65
3:O:418:ALA:HB2	3:O:464:VAL:HG12	1.77	0.65
1:K:76:ILE:HG21	1:K:248:ALA:HA	1.77	0.65
3:O:469:ALA:HA	3:O:475:LEU:HD12	1.79	0.65
3:O:2165:LEU:HD11	3:O:2200:ALA:HB1	1.78	0.65
3:O:2287:PRO:HB3	3:O:2326:ILE:HD12	1.77	0.65
3:O:2531:LEU:HG	3:O:2538:ARG:HG3	1.79	0.65
3:O:4114:PRO:HA	3:O:4117:LEU:HG	1.78	0.65
3:O:1155:ARG:NH2	3:O:3689:ASP:OD1	2.30	0.64
3:O:1389:VAL:HG22	3:O:1390:GLN:H	1.61	0.64
4:C:20:ARG:NH1	8:I:35:DT:OP1	2.30	0.64
4:G:77:ARG:NH2	5:H:51:ILE:O	2.30	0.64
1:K:376:ILE:HB	2:L:540:ILE:HG13	1.77	0.64
3:O:1331:ASN:HA	3:O:1334:LYS:HE2	1.80	0.64
3:O:3870:SER:HB2	3:O:3874:ARG:HH21	1.61	0.64
1:K:94:LYS:H	1:K:103:TYR:HA	1.62	0.64
2:L:11:VAL:HB	2:L:132:ILE:HG12	1.79	0.64
3:O:3172:LYS:HG3	3:O:3173:MET:HG3	1.80	0.64
3:O:3838:GLU:OE2	3:O:3874:ARG:NH1	2.30	0.64
3:O:1445:ARG:NH2	3:O:1507:CYS:SG	2.70	0.64
3:O:1607:GLU:OE2	3:O:1614:GLN:NE2	2.31	0.64
9:J:104:DG:H2"	9:J:105:DA:C8	2.33	0.64
3:O:415:GLN:HA	3:O:463:LYS:HD2	1.79	0.64
3:O:2216:LEU:HD13	3:O:2241:LEU:HD23	1.80	0.64
4:G:81:ARG:NH1	4:G:107:VAL:O	2.24	0.64
2:L:250:ARG:NH1	2:L:252:THR:OG1	2.31	0.64
2:L:493:CYS:HB2	2:L:505:LEU:HD13	1.80	0.64
2:L:64:THR:HG22	2:L:69:SER:HB2	1.79	0.64
3:O:3311:ASN:HB3	3:O:3314:SER:HA	1.79	0.63
7:F:26:ILE:HG13	7:F:27:GLN:H	1.63	0.63
3:O:2367:VAL:O	3:O:2371:PHE:N	2.30	0.63
2:L:250:ARG:NH2	2:L:338:LYS:O	2.31	0.63
3:O:670:LEU:HB3	3:O:732:PHE:CE1	2.34	0.63
3:O:1445:ARG:NH2	3:O:1506:SER:OG	2.32	0.63
4:G:77:ARG:HA	5:H:50:GLY:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:289:TYR:HD2	1:K:292:THR:H	1.47	0.63
3:O:1458:LEU:HD22	3:O:1463:LEU:HD12	1.78	0.63
8:I:88:DG:H2''	8:I:89:DT:H5''	1.79	0.63
3:O:1851:LEU:HD13	3:O:1870:LYS:HD3	1.81	0.63
3:O:197:PHE:O	3:O:201:LEU:HG	1.98	0.63
3:O:3681:LYS:HG2	3:O:3724:GLU:HG2	1.79	0.63
6:E:82:LEU:C	7:F:80:THR:HA	2.24	0.63
3:O:2391:GLY:O	3:O:2431:ARG:NH2	2.32	0.63
8:I:9:DG:N2	9:J:147:DC:O2	2.32	0.63
1:K:275:ASN:ND2	1:K:278:GLN:OE1	2.32	0.62
3:O:174:VAL:O	3:O:177:LEU:HB2	1.99	0.62
3:O:1073:PHE:HE1	3:O:1121:LEU:HD22	1.64	0.62
5:D:101:GLY:O	5:D:105:LYS:NZ	2.32	0.62
1:K:48:MET:HA	1:K:59:PRO:HG2	1.79	0.62
3:O:956:PRO:HA	3:O:959:TYR:HB2	1.81	0.62
3:O:1071:ASN:ND2	3:O:1073:PHE:H	1.96	0.62
3:O:2353:GLN:HB3	3:O:2360:PHE:HB2	1.80	0.62
1:K:338:LYS:NZ	8:I:18:DT:OP1	2.31	0.62
2:L:316:TYR:HB3	2:L:319:ASP:HB2	1.81	0.62
2:L:347:LYS:HG3	2:L:349:SER:H	1.64	0.62
3:O:2356:MET:SD	3:O:2359:LYS:NZ	2.66	0.62
2:L:10:VAL:HB	2:L:54:ILE:HG13	1.81	0.62
3:O:1833:LEU:HD23	3:O:1835:ALA:H	1.65	0.62
1:K:95:ASN:N	1:K:95:ASN:ND2	2.47	0.62
3:O:2310:VAL:HG11	3:O:2359:LYS:HD2	1.81	0.62
4:C:87:ILE:HA	4:C:93:LEU:HD12	1.82	0.62
6:A:59:GLU:O	7:B:40:ARG:NH1	2.33	0.62
2:L:65:ASP:HB3	2:L:78:THR:HG23	1.82	0.62
3:O:3066:ASP:HA	3:O:3069:MET:SD	2.40	0.62
8:I:25:DG:H4'	8:I:26:DC:H5'	1.81	0.62
1:K:203:MET:HE1	1:K:241:ASP:HB2	1.81	0.62
3:O:396:PHE:HE2	3:O:441:MET:HG2	1.65	0.62
3:O:3759:ARG:HA	3:O:3762:GLN:HG2	1.81	0.62
1:K:484:GLN:O	1:K:488:ARG:HG2	1.99	0.61
3:O:2122:LEU:O	3:O:2127:LYS:NZ	2.32	0.61
3:O:1766:LEU:HD23	3:O:1775:GLU:HG3	1.82	0.61
3:O:2587:GLN:O	3:O:2777:HIS:N	2.33	0.61
6:A:106:ASP:OD2	6:A:131:ARG:NH2	2.32	0.61
2:L:465:LYS:O	2:L:474:GLU:N	2.33	0.61
3:O:914:VAL:O	3:O:918:ALA:N	2.30	0.61
3:O:1632:TRP:CD1	3:O:1645:VAL:HG21	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2386:LEU:HD12	3:O:2418:LYS:HG3	1.82	0.61
1:K:407:PRO:HG2	2:L:486:ARG:HD2	1.82	0.61
3:O:655:LEU:HB3	3:O:659:ARG:HH12	1.65	0.61
3:O:1301:ILE:H	3:O:1301:ILE:HD12	1.66	0.61
2:L:461:MET:HB3	2:L:526:SER:HB3	1.82	0.61
3:O:23:ASP:OD2	3:O:70:ARG:NH1	2.34	0.61
3:O:2524:PHE:O	3:O:2530:ARG:NH1	2.27	0.61
2:L:7:LYS:HB2	2:L:51:LYS:HB3	1.83	0.61
2:L:264:TYR:HB2	2:L:363:LYS:HB3	1.83	0.61
3:O:990:GLN:NE2	3:O:2778:GLY:O	2.33	0.61
3:O:1820:VAL:HG23	3:O:1824:LEU:HB2	1.83	0.61
3:O:2808:LEU:HD23	3:O:2812:LEU:HD23	1.81	0.61
3:O:305:ASN:O	3:O:308:LEU:N	2.34	0.61
3:O:1452:VAL:HA	3:O:1517:LEU:HD11	1.83	0.61
5:D:83:ARG:NH1	8:I:43:DG:OP2	2.34	0.61
3:O:1725:GLN:O	3:O:1768:ARG:NH2	2.34	0.60
3:O:2125:TRP:O	3:O:2129:LEU:N	2.29	0.60
3:O:2404:ARG:O	3:O:2441:LYS:NZ	2.34	0.60
3:O:767:GLU:O	3:O:771:ASN:ND2	2.35	0.60
3:O:3720:ALA:HB3	3:O:3743:HIS:HA	1.82	0.60
4:G:100:VAL:HG12	7:F:96:THR:HG22	1.83	0.60
2:L:93:ASP:O	2:L:97:LYS:HB2	2.01	0.60
3:O:971:ARG:HG3	3:O:1025:LEU:HD11	1.83	0.60
3:O:1831:CYS:SG	3:O:1883:ARG:NH1	2.74	0.60
3:O:2136:PRO:O	3:O:2143:ARG:NH2	2.33	0.60
3:O:2538:ARG:NH2	3:O:2565:MET:HE3	2.16	0.60
3:O:164:LYS:HB2	3:O:166:ILE:HG12	1.83	0.60
8:I:57:DC:H1'	9:J:97:DG:H22	1.65	0.60
1:K:173:ASP:OD1	1:K:207:LYS:NZ	2.30	0.60
1:K:325:ARG:NH2	2:L:498:ALA:O	2.35	0.60
3:O:1367:HIS:HA	3:O:1370:ARG:HH11	1.67	0.60
4:C:101:THR:OG1	7:B:96:THR:O	2.20	0.60
8:I:20:DC:N4	9:J:134:DG:O6	2.35	0.60
3:O:1072:ALA:HB1	3:O:1123:THR:HG21	1.84	0.60
3:O:2097:LEU:HD11	3:O:2149:LEU:HD22	1.83	0.60
3:O:1602:ASP:O	3:O:1606:ARG:N	2.35	0.60
3:O:3960:PRO:HD3	3:O:4111:ALA:HB1	1.84	0.60
8:I:104:DG:N2	9:J:51:DC:O2	2.35	0.60
1:K:469:LEU:HD11	1:K:518:LEU:HD11	1.84	0.60
3:O:848:LEU:HB3	3:O:852:ARG:HH22	1.67	0.60
5:D:92:GLN:OE1	5:D:96:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:GLY:O	2:L:21:SER:N	2.32	0.60
3:O:207:GLN:HG3	3:O:217:LEU:HD13	1.84	0.60
3:O:2278:GLY:O	3:O:2282:ALA:N	2.35	0.60
1:K:52:GLN:NE2	1:K:206:LYS:O	2.34	0.59
8:I:62:DA:H1'	8:I:63:DA:H5'	1.84	0.59
3:O:225:LYS:HE3	3:O:270:ALA:HB3	1.83	0.59
3:O:2544:SER:HA	3:O:2842:ARG:HH22	1.68	0.59
3:O:2843:PHE:O	3:O:2847:THR:OG1	2.20	0.59
1:K:413:LEU:HD12	1:K:432:PHE:HB3	1.85	0.59
3:O:908:ASP:HA	3:O:911:LEU:HD23	1.84	0.59
3:O:1727:ARG:NH2	3:O:1771:GLN:O	2.36	0.59
4:G:90:ASP:HB2	4:G:93:LEU:HB2	1.85	0.59
3:O:393:LYS:NZ	3:O:1685:ASP:OD2	2.35	0.59
3:O:2988:GLU:HA	3:O:2991:LYS:HE2	1.84	0.59
3:O:3190:LEU:HB3	3:O:3231:ILE:HG23	1.84	0.59
2:L:448:GLU:HA	2:L:451:LEU:HD12	1.84	0.59
3:O:415:GLN:NE2	3:O:460:ALA:HB2	2.17	0.59
3:O:950:GLU:OE1	3:O:950:GLU:N	2.33	0.59
8:I:117:DG:N2	9:J:38:DT:O2	2.35	0.59
3:O:3011:LEU:HB3	3:O:3047:SER:HB3	1.83	0.59
7:B:39:ARG:NH1	7:B:44:LYS:O	2.36	0.59
3:O:953:GLN:OE1	3:O:953:GLN:N	2.36	0.59
3:O:1083:ASN:ND2	3:O:1126:GLN:OE1	2.34	0.59
3:O:1583:MET:HG3	3:O:1625:HIS:HB3	1.85	0.59
3:O:3593:ARG:HH21	3:O:3660:ASN:HD22	1.51	0.59
7:F:35:ARG:HG3	7:F:46:ILE:HD11	1.83	0.59
8:I:97:DG:N1	9:J:57:DC:N3	2.50	0.59
2:L:315:ARG:HA	2:L:320:ILE:HA	1.85	0.59
3:O:3666:LEU:HA	3:O:3669:LYS:HD2	1.83	0.59
1:K:492:ALA:HA	1:K:497:LEU:HD13	1.83	0.58
2:L:54:ILE:HD13	2:L:86:PRO:HG3	1.84	0.58
3:O:584:GLU:O	3:O:613:HIS:N	2.34	0.58
3:O:4004:VAL:H	3:O:4007:LYS:HZ1	1.51	0.58
1:K:488:ARG:NH2	1:K:491:GLU:OE2	2.36	0.58
2:L:352:GLN:HB3	2:L:354:ARG:HG2	1.84	0.58
3:O:793:LEU:HB3	3:O:870:LEU:HA	1.84	0.58
3:O:3319:ASN:O	3:O:3322:ALA:N	2.32	0.58
3:O:3606:ILE:HA	3:O:3609:MET:HE2	1.84	0.58
3:O:1096:VAL:O	3:O:1100:VAL:HG13	2.03	0.58
3:O:2452:ARG:HB2	3:O:2498:ILE:HD11	1.85	0.58
9:J:73:DG:H2''	9:J:74:DA:N7	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:288:LEU:N	2:L:311:ILE:O	2.36	0.58
3:O:3416:LEU:HD22	3:O:3449:LYS:HE3	1.86	0.58
3:O:3880:ALA:O	3:O:3885:ARG:NH2	2.34	0.58
3:O:243:GLN:NE2	3:O:281:GLN:O	2.36	0.58
3:O:3909:ALA:HB1	3:O:3984:MET:HE3	1.86	0.58
4:C:17:ARG:HH21	4:C:27:VAL:HG12	1.67	0.58
3:O:958:MET:HB2	3:O:961:LEU:HB2	1.85	0.58
6:A:59:GLU:H	7:B:40:ARG:HH12	1.52	0.58
2:L:21:SER:HB2	2:L:100:PRO:HB2	1.86	0.58
3:O:1365:ASN:OD1	3:O:1370:ARG:NH1	2.37	0.58
3:O:2266:ASN:O	3:O:2311:ARG:NH1	2.36	0.58
8:I:124:DG:N2	9:J:31:DT:O2	2.37	0.58
9:J:133:DG:H2'	9:J:134:DG:C8	2.39	0.58
2:L:153:SER:HA	2:L:156:LYS:HG2	1.85	0.58
3:O:734:LEU:HD11	3:O:768:VAL:HB	1.85	0.58
3:O:1112:ALA:HB1	3:O:1180:GLN:HE21	1.69	0.58
3:O:3135:LEU:O	3:O:3138:ILE:HG22	2.04	0.58
3:O:3301:LEU:HD12	3:O:3304:VAL:HG23	1.86	0.58
4:C:79:ILE:HG22	4:C:81:ARG:H	1.67	0.58
2:L:165:LEU:O	2:L:227:PHE:N	2.35	0.58
3:O:1069:HIS:HB3	3:O:1074:LYS:HD2	1.85	0.58
3:O:1464:LEU:HD11	3:O:1521:PHE:HA	1.85	0.58
3:O:3471:ILE:HA	3:O:3474:ARG:HB2	1.85	0.58
4:G:16:SER:HA	9:J:34:DA:H4'	1.85	0.58
3:O:1230:GLY:O	3:O:1292:LYS:NZ	2.33	0.58
3:O:3993:SER:OG	3:O:3994:ASP:N	2.33	0.58
1:K:388:LYS:HE3	2:L:451:LEU:HB3	1.85	0.57
3:O:201:LEU:HD22	3:O:249:PHE:HD2	1.69	0.57
3:O:1304:HIS:O	3:O:1334:LYS:NZ	2.31	0.57
3:O:1841:SER:HA	3:O:1844:VAL:HG23	1.84	0.57
3:O:3974:MET:N	3:O:3974:MET:SD	2.77	0.57
3:O:4055:ASN:HD21	3:O:4057:ALA:HB3	1.69	0.57
4:G:84:GLN:HA	4:G:87:ILE:HG12	1.86	0.57
8:I:41:DT:H2''	8:I:42:DA:C8	2.40	0.57
8:I:94:DA:H2''	8:I:95:DC:H5''	1.85	0.57
1:K:416:GLN:NE2	1:K:417:GLU:O	2.37	0.57
3:O:860:GLY:HA3	3:O:3136:THR:HG21	1.86	0.57
3:O:2594:ASP:HB3	3:O:2596:ARG:HD3	1.86	0.57
8:I:102:DG:H2''	8:I:103:DG:C8	2.40	0.57
2:L:496:HIS:CG	2:L:506:PRO:HD3	2.39	0.57
2:L:193:PRO:HD2	2:L:195:LYS:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:225:LYS:HB3	3:O:274:LEU:HD21	1.86	0.57
3:O:1961:PHE:CE1	3:O:2100:LEU:HD21	2.40	0.57
3:O:3875:GLU:HG3	3:O:3965:ARG:HE	1.70	0.57
6:E:70:LEU:HD22	7:F:25:ASN:HB2	1.87	0.57
1:K:192:ASP:OD1	3:O:2380:ASN:ND2	2.37	0.57
3:O:93:LEU:HD23	3:O:136:GLN:HG3	1.85	0.57
3:O:2322:VAL:HA	3:O:2325:LEU:HD12	1.85	0.57
3:O:2773:ARG:HG2	3:O:2789:SER:HB2	1.85	0.57
3:O:3321:LEU:HG	3:O:3324:ARG:HH21	1.70	0.57
3:O:3750:PHE:HB3	3:O:3802:LEU:HD11	1.86	0.57
8:I:103:DG:N2	9:J:52:DC:O2	2.38	0.57
1:K:299:LYS:HG3	2:L:294:VAL:HG23	1.86	0.57
2:L:130:ARG:NH2	2:L:157:CYS:O	2.38	0.57
3:O:2196:TRP:HB2	3:O:2199:LEU:HB2	1.87	0.57
3:O:3636:PHE:O	3:O:3640:PHE:N	2.32	0.57
4:G:43:VAL:HA	5:H:86:ILE:HB	1.86	0.57
8:I:53:DG:O6	9:J:101:DC:N4	2.38	0.57
1:K:194:ARG:NH1	1:K:219:ASP:O	2.37	0.57
3:O:1201:ASN:OD1	3:O:1207:TRP:N	2.34	0.57
3:O:2543:ASN:OD1	3:O:2544:SER:N	2.38	0.57
3:O:3281:CYS:O	3:O:3285:HIS:ND1	2.37	0.57
3:O:3662:ILE:HA	3:O:3665:MET:HE2	1.87	0.57
3:O:1075:ARG:NH2	3:O:1117:ASP:OD2	2.38	0.57
4:C:41:GLU:OE1	4:G:38:HIS:NE2	2.37	0.57
8:I:96:DC:H42	9:J:57:DC:H41	1.53	0.57
9:J:43:DA:H2''	9:J:44:DG:C8	2.40	0.57
1:K:369:TYR:OH	2:L:436:SER:O	2.21	0.57
2:L:316:TYR:N	2:L:319:ASP:O	2.38	0.57
3:O:724:GLU:HB3	3:O:2600:THR:HA	1.85	0.57
1:K:157:VAL:O	3:O:2388:LYS:NZ	2.37	0.56
3:O:3360:LEU:HB2	3:O:3373:VAL:HG21	1.86	0.56
4:C:17:ARG:NH1	8:I:34:DT:OP2	2.37	0.56
5:H:83:ARG:NH2	9:J:44:DG:OP2	2.38	0.56
1:K:147:LEU:HD12	1:K:189:LYS:HB3	1.86	0.56
1:K:403:ARG:HD2	9:J:140:DG:H4'	1.87	0.56
1:K:459:VAL:HG12	1:K:463:LYS:HE3	1.87	0.56
2:L:245:ILE:N	9:J:131:DT:OP1	2.37	0.56
3:O:1420:ARG:NH2	3:O:1466:ASN:O	2.38	0.56
3:O:2161:ALA:HA	3:O:2164:TRP:HB2	1.86	0.56
4:C:29:ARG:NH1	5:D:32:GLU:O	2.38	0.56
1:K:40:PHE:HB3	1:K:169:PHE:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:300:THR:HA	2:L:293:THR:HA	1.87	0.56
1:K:349:GLY:HA3	2:L:463:LEU:HG	1.85	0.56
2:L:51:LYS:NZ	8:I:27:DC:O2	2.33	0.56
3:O:220:LEU:HD23	3:O:224:LEU:HD23	1.87	0.56
3:O:331:ALA:O	3:O:334:HIS:ND1	2.38	0.56
3:O:1428:ILE:HA	3:O:1431:LEU:HB2	1.87	0.56
3:O:1711:ARG:NH1	3:O:1760:GLU:OE2	2.38	0.56
3:O:1805:PHE:HD1	3:O:1819:PHE:HB2	1.70	0.56
3:O:2168:LEU:O	3:O:2172:ALA:N	2.37	0.56
3:O:4055:ASN:HD22	3:O:4058:VAL:HG23	1.70	0.56
4:C:96:LEU:HD13	5:D:100:PRO:HD3	1.87	0.56
2:L:139:SER:HA	2:L:201:GLN:HG2	1.88	0.56
2:L:194:LEU:HD22	2:L:202:LYS:HE2	1.88	0.56
3:O:1369:MET:SD	3:O:1370:ARG:NH1	2.79	0.56
3:O:2938:VAL:HG22	3:O:3979:LEU:HD21	1.87	0.56
3:O:3578:LEU:HD13	3:O:3676:PRO:HA	1.87	0.56
3:O:527:TYR:O	3:O:530:LEU:HB3	2.06	0.56
3:O:1261:LEU:HD11	3:O:1336:THR:HG22	1.87	0.56
3:O:2167:PRO:O	3:O:2171:LEU:N	2.34	0.56
3:O:3737:ARG:HA	3:O:3751:LEU:HB2	1.88	0.56
3:O:346:TYR:HB3	3:O:349:ILE:HD11	1.87	0.56
3:O:971:ARG:HA	3:O:1025:LEU:HD21	1.88	0.56
3:O:3239:LYS:HG3	3:O:3262:LEU:HD21	1.88	0.56
2:L:47:PHE:HE2	2:L:495:LEU:HG	1.70	0.56
3:O:361:ILE:O	3:O:364:ARG:HB3	2.06	0.56
3:O:958:MET:N	3:O:958:MET:SD	2.79	0.56
3:O:1614:GLN:HA	3:O:1617:LYS:HE2	1.88	0.56
3:O:1825:LEU:HD21	3:O:1875:LYS:HD3	1.88	0.56
3:O:3838:GLU:O	3:O:3842:TRP:NE1	2.39	0.56
9:J:58:DG:C8	9:J:58:DG:H5'	2.41	0.56
1:K:469:LEU:HD21	1:K:518:LEU:HG	1.87	0.56
1:K:469:LEU:HD22	1:K:514:MET:HG3	1.86	0.56
2:L:326:VAL:O	2:L:329:GLU:HG3	2.06	0.56
8:I:114:DC:O2	9:J:41:DG:N2	2.38	0.56
2:L:253:ILE:HD13	2:L:340:PHE:CD2	2.41	0.56
3:O:367:GLY:HA3	3:O:416:SER:HA	1.88	0.56
3:O:998:ASN:HA	3:O:1001:PHE:HB2	1.88	0.56
3:O:1594:SER:O	3:O:1598:ASN:ND2	2.38	0.56
4:G:107:VAL:H	7:F:40:ARG:HH21	1.52	0.56
9:J:102:DT:H1'	9:J:103:DA:C5	2.41	0.56
3:O:360:SER:O	3:O:363:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1583:MET:HA	3:O:1586:SER:HB3	1.88	0.56
3:O:3988:LEU:HD23	3:O:4100:GLU:HA	1.87	0.56
1:K:264:ASN:HB3	1:K:267:ILE:H	1.71	0.55
3:O:91:ILE:HG21	3:O:834:LEU:HD23	1.89	0.55
3:O:612:LEU:HD11	3:O:2602:LEU:HD11	1.88	0.55
3:O:3794:VAL:HG11	3:O:3802:LEU:HD23	1.88	0.55
3:O:108:LYS:HE3	3:O:148:LYS:HE3	1.87	0.55
3:O:1413:ASP:OD1	3:O:1414:ILE:N	2.39	0.55
3:O:1771:GLN:OE1	3:O:1775:GLU:N	2.39	0.55
3:O:3048:LYS:HB3	3:O:3061:LEU:HD13	1.89	0.55
3:O:3588:TRP:HE1	3:O:3609:MET:HG3	1.71	0.55
5:D:37:TYR:HA	5:D:40:LYS:HE3	1.88	0.55
3:O:715:ALA:HA	3:O:718:MET:HE2	1.86	0.55
3:O:2410:GLU:HG3	3:O:2413:PHE:HB3	1.87	0.55
3:O:2890:ILE:HD13	3:O:2893:LEU:HD21	1.88	0.55
4:C:26:PRO:HG2	4:C:29:ARG:HB3	1.88	0.55
6:A:72:ARG:NH2	9:J:54:DT:OP2	2.39	0.55
2:L:41:PHE:HA	2:L:238:LYS:HZ3	1.72	0.55
3:O:415:GLN:HE21	3:O:460:ALA:HB2	1.71	0.55
3:O:1476:HIS:ND1	3:O:1476:HIS:O	2.38	0.55
3:O:1793:THR:O	3:O:1797:LEU:HG	2.06	0.55
3:O:3176:MET:HE1	3:O:3249:GLN:NE2	2.21	0.55
5:D:89:ARG:O	5:D:92:GLN:NE2	2.30	0.55
3:O:864:GLY:HA2	3:O:867:ASN:HB2	1.87	0.55
3:O:1436:LEU:HD22	3:O:1445:ARG:HG2	1.89	0.55
3:O:2327:LEU:HD11	3:O:2342:CYS:SG	2.47	0.55
6:E:83:ARG:HB3	8:I:53:DG:H4'	1.87	0.55
1:K:74:LYS:HG3	1:K:83:LEU:HD11	1.89	0.55
1:K:418:GLU:HG3	1:K:430:PRO:HD3	1.89	0.55
2:L:405:VAL:O	2:L:423:GLN:NE2	2.40	0.55
3:O:3236:PHE:HB3	3:O:3272:TRP:CH2	2.42	0.55
3:O:3446:VAL:HG23	3:O:3468:LEU:HD11	1.89	0.55
6:A:53:ARG:HA	6:A:56:LYS:HE2	1.88	0.55
3:O:334:HIS:O	3:O:337:LYS:HB3	2.06	0.55
3:O:892:LEU:HA	3:O:944:LYS:HE3	1.89	0.55
3:O:2824:LYS:O	3:O:2829:LYS:NZ	2.39	0.55
3:O:414:LEU:HD12	3:O:464:VAL:HG11	1.87	0.55
3:O:2093:CYS:O	3:O:2094:MET:HE2	2.07	0.55
3:O:3814:ASP:O	3:O:3818:ASN:ND2	2.39	0.55
2:L:108:LEU:O	2:L:112:ILE:HD12	2.06	0.55
3:O:894:PHE:HB2	3:O:940:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:103:DG:H2''	8:I:104:DG:O5'	2.06	0.55
1:K:327:ILE:HG23	2:L:497:ARG:HG2	1.89	0.55
2:L:266:SER:HB2	2:L:361:VAL:HG12	1.89	0.55
3:O:639:ALA:H	3:O:679:LYS:HZ3	1.55	0.55
3:O:2260:PHE:HA	3:O:2270:ASN:HB2	1.88	0.55
3:O:2295:GLN:HG2	3:O:2297:SER:H	1.70	0.55
3:O:3533:PHE:O	3:O:3537:SER:OG	2.23	0.55
3:O:3864:ARG:O	3:O:3868:VAL:HG13	2.07	0.55
3:O:3882:LEU:H	3:O:3966:GLN:HE22	1.53	0.55
3:O:4041:ARG:HE	3:O:4044:ILE:HD11	1.72	0.55
6:E:81:ASP:O	6:E:82:LEU:C	2.51	0.54
1:K:416:GLN:O	1:K:430:PRO:HA	2.07	0.54
3:O:2105:HIS:NE2	3:O:2156:VAL:O	2.39	0.54
1:K:404:ARG:HD2	3:O:213:ARG:HG3	1.89	0.54
3:O:1226:GLY:O	3:O:1230:GLY:N	2.35	0.54
3:O:1610:ASN:OD1	3:O:1611:GLN:N	2.41	0.54
3:O:2425:ARG:NH1	3:O:2460:GLU:OE2	2.39	0.54
3:O:3288:SER:HB2	3:O:3296:GLN:HG2	1.89	0.54
6:E:61:LEU:HD23	7:F:36:ARG:HB3	1.90	0.54
8:I:14:DC:H42	9:J:140:DG:H1	1.54	0.54
4:C:96:LEU:HD13	5:D:99:LEU:HA	1.90	0.54
6:A:83:ARG:HB3	9:J:53:DT:H4'	1.88	0.54
6:A:83:ARG:HB2	7:B:80:THR:HA	1.89	0.54
8:I:40:DG:O6	9:J:113:DA:N6	2.40	0.54
3:O:2561:PHE:O	3:O:2565:MET:HG3	2.08	0.54
6:E:82:LEU:HA	7:F:80:THR:HA	1.90	0.54
1:K:241:ASP:O	1:K:244:ARG:NH1	2.33	0.54
2:L:119:GLN:HA	2:L:122:THR:HB	1.89	0.54
3:O:240:GLU:HG2	3:O:243:GLN:HG2	1.90	0.54
3:O:2225:HIS:CD2	3:O:2226:PRO:HD2	2.43	0.54
3:O:3382:PHE:HD2	3:O:3419:PHE:HE2	1.55	0.54
3:O:3879:PRO:HB2	3:O:3882:LEU:HD21	1.90	0.54
8:I:101:DA:H2''	8:I:102:DG:C8	2.42	0.54
3:O:234:PHE:HD1	3:O:235:THR:HG23	1.73	0.54
3:O:332:GLU:O	3:O:335:LYS:NZ	2.40	0.54
3:O:1722:PHE:HZ	3:O:1742:CYS:HB2	1.73	0.54
3:O:3588:TRP:NE1	3:O:3609:MET:HG3	2.23	0.54
3:O:3980:MET:N	3:O:3980:MET:SD	2.81	0.54
8:I:69:DC:H2''	8:I:70:DG:C5	2.43	0.54
3:O:79:ARG:HA	3:O:119:ARG:HH21	1.73	0.54
3:O:1606:ARG:HH11	3:O:2042:GLN:HG2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1632:TRP:HD1	3:O:1633:TRP:HB3	1.72	0.54
8:I:65:DC:H2"	8:I:66:DG:H8	1.73	0.54
3:O:639:ALA:H	3:O:679:LYS:NZ	2.06	0.54
3:O:2298:GLU:HA	3:O:2301:GLN:HG2	1.89	0.54
3:O:2568:MET:SD	3:O:2568:MET:N	2.80	0.54
3:O:3292:GLY:HA2	3:O:3297:VAL:HG11	1.89	0.54
4:G:17:ARG:HG2	4:G:20:ARG:HH21	1.73	0.54
1:K:299:LYS:HA	3:O:164:LYS:NZ	2.23	0.54
1:K:522:VAL:HG11	2:L:256:ASN:HB2	1.89	0.54
3:O:12:LEU:HD21	3:O:44:LEU:HD22	1.88	0.54
3:O:4005:PHE:O	3:O:4007:LYS:N	2.41	0.54
4:G:83:LEU:HD13	5:H:59:MET:HE3	1.90	0.54
3:O:2891:ARG:NH2	3:O:2895:GLU:OE2	2.41	0.53
3:O:3796:MET:HB3	3:O:3801:GLY:HA2	1.89	0.53
4:C:90:ASP:O	4:C:94:ASN:ND2	2.41	0.53
2:L:44:ARG:HD3	2:L:239:LYS:HD3	1.89	0.53
2:L:460:SER:HB2	2:L:525:LYS:HB3	1.90	0.53
3:O:1747:LEU:HD21	3:O:1781:SER:OG	2.08	0.53
3:O:2575:PRO:HA	3:O:2786:LYS:HA	1.90	0.53
3:O:3333:THR:O	3:O:3337:ILE:HG12	2.08	0.53
3:O:3679:ASN:N	3:O:3724:GLU:O	2.41	0.53
6:A:107:THR:HG22	6:A:124:ILE:HA	1.88	0.53
2:L:464:ALA:HB1	2:L:473:LEU:HB3	1.91	0.53
3:O:71:LYS:HG3	3:O:73:LEU:H	1.74	0.53
3:O:726:LEU:HG	3:O:730:LEU:HD23	1.90	0.53
4:C:72:ASP:OD1	4:C:73:ASN:N	2.41	0.53
4:G:88:ARG:HH21	4:G:94:ASN:HA	1.73	0.53
3:O:3259:LEU:HD11	3:O:3283:LEU:HD13	1.89	0.53
6:E:82:LEU:O	7:F:81:VAL:HG12	2.08	0.53
3:O:664:SER:HB3	3:O:725:LEU:HD12	1.89	0.53
3:O:790:LYS:HA	3:O:869:ASN:HB3	1.89	0.53
3:O:2263:LYS:HA	3:O:2309:PHE:HZ	1.74	0.53
3:O:4014:LYS:HG2	3:O:4015:ASN:H	1.74	0.53
4:C:107:VAL:O	6:A:55:GLN:NE2	2.42	0.53
3:O:710:PHE:O	3:O:714:VAL:HG12	2.08	0.53
3:O:865:GLN:HE22	3:O:3172:LYS:HB3	1.74	0.53
3:O:1423:ILE:HD11	3:O:1427:SER:HB3	1.91	0.53
3:O:3588:TRP:HZ2	3:O:3610:TYR:HB2	1.74	0.53
3:O:3637:GLY:O	3:O:3641:ASP:N	2.41	0.53
5:H:105:LYS:HA	5:H:108:VAL:HG12	1.90	0.53
8:I:57:DC:H2"	8:I:58:DG:C5	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:111:DT:H71	8:I:112:DC:H42	1.74	0.53
2:L:64:THR:HG23	2:L:76:ASN:H	1.74	0.53
3:O:1837:ARG:O	3:O:1840:PHE:HB3	2.08	0.53
3:O:3610:TYR:O	3:O:3614:TYR:HB3	2.08	0.53
4:G:42:ARG:NH2	8:I:114:DC:O2	2.42	0.53
3:O:746:ARG:HE	3:O:788:TYR:HE1	1.56	0.53
3:O:1354:GLU:HA	3:O:1357:LYS:HB3	1.90	0.53
3:O:1836:LEU:O	3:O:1840:PHE:N	2.34	0.53
3:O:2251:ILE:HD12	3:O:2252:PRO:HD2	1.91	0.53
3:O:4064:LEU:O	3:O:4068:HIS:N	2.38	0.53
3:O:169:THR:HG23	3:O:170:VAL:HG23	1.90	0.53
3:O:1288:SER:O	3:O:1292:LYS:N	2.32	0.53
3:O:3030:ILE:HG13	3:O:3067:LYS:HD2	1.91	0.53
3:O:4053:GLY:O	3:O:4097:GLY:N	2.42	0.53
4:C:62:ILE:HG13	4:C:63:LEU:HD12	1.91	0.53
4:C:88:ARG:NH2	4:C:94:ASN:OD1	2.41	0.53
5:D:92:GLN:HB2	5:D:96:ARG:HH21	1.74	0.53
2:L:40:MET:SD	2:L:238:LYS:NZ	2.73	0.53
3:O:528:VAL:HG23	3:O:633:ILE:HD13	1.91	0.53
4:G:79:ILE:HG13	4:G:80:PRO:HD2	1.89	0.53
6:E:71:VAL:HA	6:E:74:ILE:HG22	1.90	0.53
8:I:116:DA:H61	9:J:38:DT:H3	1.57	0.53
3:O:449:TYR:CD2	3:O:453:MET:HE1	2.43	0.52
3:O:643:GLU:HA	3:O:646:VAL:HG23	1.91	0.52
6:A:50:GLU:HG3	6:A:53:ARG:HH21	1.73	0.52
1:K:362:LEU:HD11	2:L:269:GLN:HB2	1.92	0.52
3:O:31:GLY:O	3:O:35:ILE:HG12	2.10	0.52
3:O:477:ASN:OD1	3:O:478:CYS:N	2.42	0.52
3:O:1374:GLN:O	3:O:1378:GLU:N	2.36	0.52
3:O:3975:LYS:HG3	3:O:3977:THR:H	1.74	0.52
8:I:51:DT:H2"	8:I:52:DA:N7	2.24	0.52
2:L:20:MET:HE1	2:L:30:PRO:HB2	1.92	0.52
2:L:235:CYS:O	2:L:237:PHE:N	2.41	0.52
2:L:431:ARG:NH1	8:I:15:DC:OP1	2.36	0.52
3:O:648:SER:O	3:O:651:TYR:N	2.43	0.52
3:O:1751:GLU:HA	3:O:1785:ILE:HD12	1.92	0.52
3:O:2332:GLU:O	3:O:2334:LYS:NZ	2.41	0.52
3:O:3139:GLN:HA	3:O:3142:ILE:HG12	1.91	0.52
1:K:403:ARG:HB3	3:O:213:ARG:HH12	1.72	0.52
3:O:714:VAL:HG11	3:O:733:LEU:HD21	1.92	0.52
3:O:1080:LEU:O	3:O:1084:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2151:ILE:HD11	3:O:2189:ILE:HG22	1.92	0.52
3:O:2254:ARG:NH1	3:O:2292:CYS:SG	2.82	0.52
3:O:2322:VAL:O	3:O:2326:ILE:HG12	2.08	0.52
3:O:2589:TYR:HB2	3:O:2777:HIS:HB2	1.91	0.52
3:O:3535:ILE:HD12	3:O:3797:THR:N	2.25	0.52
3:O:3701:ILE:HG12	3:O:3717:VAL:HG13	1.91	0.52
6:E:83:ARG:CB	7:F:80:THR:HG22	2.37	0.52
8:I:118:DT:N3	9:J:37:DC:O2	2.43	0.52
3:O:486:GLY:O	3:O:490:ILE:HG12	2.09	0.52
3:O:1057:LYS:O	3:O:1061:LYS:HG2	2.10	0.52
3:O:1743:MET:HG3	3:O:1773:VAL:HG11	1.91	0.52
3:O:2169:LEU:HB3	3:O:2211:LEU:HD11	1.91	0.52
3:O:3453:ALA:O	3:O:3458:SER:OG	2.28	0.52
3:O:3460:GLU:O	3:O:3464:LYS:HG2	2.10	0.52
8:I:116:DA:H2"	8:I:117:DG:C8	2.45	0.52
2:L:361:VAL:HG13	2:L:420:VAL:HG13	1.90	0.52
3:O:899:ARG:HD2	3:O:2569:SER:N	2.25	0.52
3:O:1104:LEU:HD22	3:O:1134:LEU:HD21	1.92	0.52
3:O:1775:GLU:N	3:O:1775:GLU:OE1	2.42	0.52
3:O:3002:TYR:HD2	3:O:3014:CYS:HB3	1.73	0.52
1:K:213:ILE:O	1:K:218:ARG:N	2.43	0.52
3:O:225:LYS:O	3:O:274:LEU:HD11	2.10	0.52
3:O:3546:SER:O	3:O:3549:HIS:NE2	2.43	0.52
1:K:90:THR:O	1:K:101:ASN:ND2	2.39	0.52
3:O:176:GLU:HG3	3:O:223:CYS:HA	1.92	0.52
3:O:222:GLY:HA2	3:O:225:LYS:HE2	1.90	0.52
3:O:941:MET:HG2	3:O:958:MET:HE2	1.91	0.52
3:O:2129:LEU:HA	3:O:2132:LYS:HE3	1.91	0.52
3:O:3450:MET:O	3:O:3454:LEU:N	2.41	0.52
3:O:3605:ASN:HA	3:O:3608:LYS:HG2	1.91	0.52
3:O:3922:ASP:OD2	3:O:3927:ASN:ND2	2.43	0.52
5:D:93:THR:O	5:D:96:ARG:HG2	2.09	0.52
1:K:38:LEU:O	1:K:83:LEU:HA	2.09	0.52
2:L:246:HIS:CD2	2:L:264:TYR:HD1	2.28	0.52
3:O:1327:GLY:O	3:O:1331:ASN:ND2	2.43	0.52
3:O:1406:LEU:HD13	3:O:1415:LEU:HG	1.91	0.52
3:O:1815:THR:O	3:O:1818:SER:OG	2.26	0.52
6:A:45:THR:HG22	6:A:49:ARG:HH12	1.75	0.52
1:K:297:LYS:HG2	2:L:297:LEU:HD12	1.92	0.52
2:L:85:LEU:HD12	2:L:86:PRO:HD2	1.92	0.52
3:O:85:ILE:O	3:O:89:LEU:N	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:473:PRO:O	3:O:477:ASN:ND2	2.43	0.52
3:O:931:CYS:O	3:O:984:TYR:OH	2.23	0.52
3:O:1711:ARG:HG3	3:O:1761:LEU:HD11	1.93	0.52
3:O:2349:LEU:HB3	3:O:2360:PHE:HE1	1.75	0.52
4:C:21:ALA:O	5:D:117:LYS:NZ	2.42	0.52
4:G:14:ALA:HB3	8:I:122:DC:H4'	1.91	0.52
4:G:17:ARG:HG3	9:J:34:DA:H3'	1.92	0.52
1:K:147:LEU:HA	1:K:150:CYS:SG	2.49	0.51
2:L:295:TYR:HB2	2:L:304:GLU:HB2	1.92	0.51
3:O:307:GLU:HA	3:O:310:LYS:HE3	1.92	0.51
3:O:1605:PHE:HE2	3:O:2042:GLN:HA	1.75	0.51
4:C:64:GLU:O	4:C:68:ASN:ND2	2.43	0.51
3:O:638:GLN:HG3	3:O:640:GLU:HG3	1.92	0.51
3:O:1835:ALA:O	3:O:1838:GLU:HG2	2.11	0.51
3:O:4124:TRP:CZ3	3:O:4126:PRO:HG3	2.45	0.51
8:I:49:DT:H4'	8:I:50:DC:H5'	1.93	0.51
8:I:110:DC:H2''	8:I:111:DT:O4'	2.10	0.51
1:K:252:ARG:NE	8:I:14:DC:OP2	2.44	0.51
3:O:217:LEU:HG	3:O:221:ALA:HB2	1.93	0.51
3:O:397:LEU:HD21	3:O:438:LEU:HD21	1.91	0.51
3:O:2186:VAL:HA	3:O:2189:ILE:HG12	1.91	0.51
3:O:2473:MET:O	3:O:2477:LEU:HG	2.10	0.51
9:J:125:DG:H1'	9:J:126:DC:H5'	1.91	0.51
9:J:136:DA:H2'	9:J:137:DC:C6	2.45	0.51
1:K:95:ASN:HD22	1:K:95:ASN:H	1.55	0.51
3:O:341:PHE:O	3:O:342:MET:HE2	2.10	0.51
3:O:1588:ASP:OD1	3:O:1589:ASN:N	2.43	0.51
3:O:1727:ARG:NH1	3:O:1772:HIS:O	2.44	0.51
3:O:3269:ARG:O	3:O:3272:TRP:N	2.42	0.51
1:K:287:LYS:HA	2:L:312:GLN:HA	1.91	0.51
2:L:496:HIS:NE2	2:L:504:PRO:O	2.43	0.51
3:O:1052:SER:O	3:O:1055:ASN:ND2	2.38	0.51
6:E:48:LEU:HD13	6:E:51:ILE:HD12	1.91	0.51
1:K:319:SER:N	2:L:277:THR:O	2.37	0.51
1:K:189:LYS:O	1:K:193:LEU:HG	2.10	0.51
3:O:643:GLU:HG3	3:O:644:PRO:HD3	1.91	0.51
3:O:899:ARG:HH12	3:O:2566:THR:HG23	1.76	0.51
3:O:1282:LEU:HA	3:O:1286:ALA:HB2	1.92	0.51
3:O:2287:PRO:HG3	3:O:2326:ILE:HG23	1.93	0.51
3:O:2571:ASP:O	3:O:2787:HIS:ND1	2.43	0.51
3:O:3158:LYS:HB2	3:O:3162:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:27:DC:H3'	8:I:28:DG:C8	2.46	0.51
8:I:71:DT:H72	8:I:72:DA:H61	1.76	0.51
1:K:262:LYS:HE2	1:K:346:MET:HB3	1.92	0.51
3:O:251:PHE:O	3:O:255:ALA:N	2.44	0.51
3:O:955:ALA:N	3:O:956:PRO:HD3	2.26	0.51
3:O:3390:GLN:HA	3:O:3393:GLU:HG2	1.91	0.51
7:B:32:PRO:HG2	9:J:64:DA:H2'	1.91	0.51
9:J:138:DC:H2''	9:J:139:DG:C8	2.45	0.51
3:O:762:TYR:HD2	3:O:765:LEU:HG	1.75	0.51
3:O:1414:ILE:HD12	3:O:1417:THR:HB	1.92	0.51
3:O:2886:GLN:H	3:O:2886:GLN:CD	2.19	0.51
3:O:3479:THR:HA	3:O:3482:LEU:HD12	1.93	0.51
6:A:126:LEU:HD22	6:E:113:HIS:CG	2.45	0.51
2:L:364:VAL:HB	2:L:419:LEU:HB2	1.92	0.51
2:L:457:LEU:HD13	2:L:529:PRO:HB2	1.93	0.51
3:O:1414:ILE:O	3:O:1418:HIS:N	2.34	0.51
3:O:1963:GLN:HA	3:O:2125:TRP:CE2	2.46	0.51
3:O:2098:THR:O	3:O:2102:LYS:HD3	2.11	0.51
6:A:116:ARG:HH21	6:A:122:LYS:HE3	1.75	0.51
1:K:142:SER:HB3	1:K:182:LYS:HE2	1.93	0.50
2:L:206:GLU:HA	2:L:209:LYS:HD2	1.92	0.50
2:L:306:LEU:HG	2:L:308:GLU:H	1.75	0.50
3:O:859:LEU:O	3:O:867:ASN:ND2	2.41	0.50
3:O:3103:ILE:HG23	3:O:3135:LEU:HD11	1.93	0.50
4:C:63:LEU:HD22	5:D:41:VAL:HG23	1.92	0.50
4:C:88:ARG:HB2	4:C:108:LEU:HD23	1.92	0.50
6:E:63:ARG:NH2	8:I:63:DA:O4'	2.43	0.50
3:O:43:VAL:O	3:O:46:SER:OG	2.27	0.50
3:O:526:ASP:OD1	3:O:526:ASP:N	2.44	0.50
3:O:1104:LEU:HG	3:O:1168:LEU:HD11	1.93	0.50
3:O:2040:MET:HA	3:O:2040:MET:HE3	1.91	0.50
3:O:3295:GLU:O	3:O:3299:THR:N	2.43	0.50
3:O:3420:CYS:O	3:O:3424:LEU:HG	2.10	0.50
3:O:3592:VAL:HG12	3:O:3606:ILE:HD12	1.94	0.50
3:O:966:PHE:CD2	3:O:1011:GLU:HG2	2.47	0.50
3:O:1921:ASP:OD1	3:O:1922:ALA:N	2.44	0.50
3:O:3029:LYS:HB2	3:O:3033:GLU:HA	1.92	0.50
2:L:154:LEU:HD13	2:L:215:LEU:HD11	1.93	0.50
3:O:1073:PHE:O	3:O:1076:LEU:HG	2.12	0.50
3:O:2602:LEU:HG	3:O:2603:THR:HG23	1.93	0.50
3:O:3085:GLU:OE1	3:O:3085:GLU:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3339:ASN:O	3:O:3343:SER:OG	2.27	0.50
3:O:3577:GLN:HA	3:O:3617:LEU:HD11	1.93	0.50
8:I:26:DC:O2	9:J:128:DG:N2	2.44	0.50
1:K:74:LYS:O	1:K:78:SER:N	2.44	0.50
3:O:1090:ARG:HA	3:O:1137:ILE:HD11	1.94	0.50
3:O:1372:LEU:HD21	3:O:1415:LEU:HD11	1.94	0.50
3:O:2538:ARG:HH21	3:O:2565:MET:HE3	1.75	0.50
3:O:2576:MET:N	3:O:2576:MET:SD	2.85	0.50
4:G:34:LEU:HD11	4:G:51:LEU:HD12	1.94	0.50
2:L:251:LEU:HD11	2:L:340:PHE:CE2	2.47	0.50
3:O:1142:HIS:CG	3:O:1197:LEU:HD12	2.47	0.50
3:O:1411:TYR:O	3:O:1414:ILE:HG22	2.10	0.50
3:O:2555:LEU:HD11	3:O:2854:PHE:HA	1.93	0.50
6:E:82:LEU:HA	7:F:79:LYS:O	2.12	0.50
3:O:1016:GLY:O	3:O:1026:ARG:HG2	2.12	0.50
3:O:1198:LEU:O	3:O:1202:ARG:NH2	2.34	0.50
3:O:1445:ARG:HE	3:O:1510:LEU:HD11	1.77	0.50
3:O:3506:LEU:HD11	3:O:3518:VAL:HG11	1.94	0.50
3:O:4088:ASN:ND2	3:O:4109:ASP:O	2.44	0.50
4:C:17:ARG:N	8:I:34:DT:H5'	2.26	0.50
4:G:96:LEU:HD13	5:H:99:LEU:HD12	1.94	0.50
8:I:14:DC:N3	9:J:141:DG:N2	2.60	0.50
9:J:33:DG:C2	9:J:34:DA:C6	3.00	0.50
3:O:394:GLN:HE21	3:O:1738:ASN:CG	2.19	0.50
3:O:847:SER:OG	3:O:848:LEU:N	2.45	0.50
3:O:848:LEU:HD13	3:O:851:ILE:HD11	1.94	0.50
3:O:898:PHE:HB3	3:O:2535:THR:HG21	1.93	0.50
3:O:2949:THR:N	3:O:2990:GLU:OE2	2.36	0.50
3:O:3728:VAL:HG23	3:O:3734:ARG:HD2	1.94	0.50
1:K:329:LEU:HD23	1:K:334:THR:HG22	1.94	0.50
2:L:329:GLU:OE2	2:L:330:GLN:NE2	2.45	0.50
3:O:180:LEU:HD23	3:O:189:MET:HE3	1.92	0.50
3:O:3451:LEU:O	3:O:3454:LEU:HB2	2.12	0.50
4:C:78:ILE:HB	5:D:51:ILE:HA	1.94	0.50
6:A:41:TYR:HB2	8:I:86:DG:H4'	1.93	0.50
8:I:121:DC:H1'	9:J:33:DG:H22	1.76	0.50
1:K:36:ASP:O	1:K:81:ASP:HA	2.12	0.49
3:O:672:ILE:HG22	3:O:676:ASN:HD21	1.78	0.49
3:O:1081:ALA:HA	3:O:1084:ASN:HD21	1.76	0.49
3:O:1330:TYR:CZ	3:O:1334:LYS:HD3	2.46	0.49
3:O:3618:GLY:H	3:O:3629:ARG:HG3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:59:GLU:H	7:B:40:ARG:HH22	1.60	0.49
8:I:62:DA:H2''	8:I:63:DA:N7	2.27	0.49
9:J:30:DC:H2''	9:J:31:DT:C5	2.47	0.49
1:K:466:VAL:O	1:K:470:ARG:N	2.45	0.49
3:O:1267:TYR:HB3	3:O:1344:PHE:CE1	2.47	0.49
3:O:1684:LEU:O	3:O:1689:LYS:NZ	2.35	0.49
3:O:1779:GLN:O	3:O:1783:ARG:HG2	2.12	0.49
3:O:3007:GLU:HA	3:O:3257:LYS:HE3	1.94	0.49
3:O:3545:THR:HB	3:O:3548:GLY:HA3	1.93	0.49
6:A:107:THR:HG21	6:A:124:ILE:HG12	1.94	0.49
2:L:110:ALA:HA	2:L:113:VAL:HG12	1.94	0.49
2:L:168:SER:HB3	2:L:226:SER:HB2	1.93	0.49
2:L:529:PRO:HA	2:L:532:LYS:HG2	1.94	0.49
3:O:742:GLU:HB3	3:O:780:ILE:HD12	1.93	0.49
3:O:1180:GLN:OE1	3:O:1180:GLN:N	2.45	0.49
3:O:1251:GLN:OE1	3:O:1251:GLN:N	2.34	0.49
3:O:2476:ILE:O	3:O:2480:ILE:HG12	2.12	0.49
3:O:2980:ASP:N	3:O:2980:ASP:OD1	2.42	0.49
3:O:3192:LYS:O	3:O:3195:GLU:HG3	2.12	0.49
3:O:3916:TRP:HZ2	3:O:4056:PRO:HB3	1.77	0.49
3:O:3965:ARG:HA	3:O:3968:ILE:HD12	1.94	0.49
7:F:80:THR:N	9:J:105:DA:OP1	2.45	0.49
3:O:1722:PHE:CE2	3:O:1743:MET:HE3	2.47	0.49
3:O:1949:ILE:HG12	3:O:2100:LEU:HD13	1.94	0.49
3:O:2592:ASP:OD1	3:O:2593:SER:N	2.45	0.49
5:D:30:ARG:HA	9:J:125:DG:H4'	1.95	0.49
6:A:62:ILE:HA	7:B:33:ALA:HB1	1.94	0.49
6:E:82:LEU:CA	7:F:80:THR:HA	2.41	0.49
2:L:18:PHE:N	2:L:104:GLN:OE1	2.46	0.49
3:O:651:TYR:CZ	3:O:655:LEU:HD11	2.47	0.49
3:O:1301:ILE:HD11	3:O:1334:LYS:HB3	1.93	0.49
3:O:2510:LEU:HD21	3:O:2525:TRP:CD1	2.47	0.49
3:O:3337:ILE:HB	3:O:3377:LEU:HD21	1.95	0.49
1:K:91:GLU:OE1	1:K:137:HIS:N	2.45	0.49
3:O:785:MET:N	3:O:785:MET:SD	2.85	0.49
3:O:1261:LEU:HD12	3:O:1337:VAL:HA	1.95	0.49
3:O:1370:ARG:O	3:O:1374:GLN:NE2	2.46	0.49
3:O:2548:PRO:HB2	3:O:2848:PHE:CD1	2.47	0.49
3:O:2817:LEU:HA	3:O:2820:MET:HG3	1.95	0.49
3:O:3448:GLU:O	3:O:3451:LEU:HG	2.12	0.49
5:D:43:LYS:HD3	5:D:47:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:19:DG:N2	9:J:136:DA:H2	2.11	0.49
8:I:104:DG:H2''	8:I:105:DG:H8	1.77	0.49
3:O:535:LEU:HD12	3:O:637:LYS:HE3	1.95	0.49
3:O:1515:LEU:HD12	3:O:1519:PHE:CZ	2.48	0.49
3:O:3046:ARG:NH2	3:O:3181:ASP:OD2	2.45	0.49
3:O:3320:ILE:O	3:O:3324:ARG:HG3	2.12	0.49
7:F:79:LYS:HB2	9:J:104:DG:H3'	1.95	0.49
8:I:66:DG:H1'	8:I:67:DC:H5'	1.94	0.49
9:J:22:DA:H2''	9:J:23:DC:C6	2.47	0.49
1:K:263:LEU:HD23	1:K:347:LEU:HD22	1.94	0.49
2:L:246:HIS:CD2	2:L:248:PRO:HD3	2.47	0.49
3:O:52:ALA:O	3:O:56:SER:OG	2.28	0.49
3:O:1361:LYS:NZ	3:O:1366:THR:OG1	2.45	0.49
3:O:3123:GLN:OE1	3:O:3123:GLN:N	2.36	0.49
3:O:3469:LEU:HA	3:O:3472:ILE:HD12	1.95	0.49
3:O:3505:LEU:HD13	3:O:3514:VAL:HG21	1.94	0.49
6:E:80:THR:O	6:E:81:ASP:C	2.56	0.49
1:K:65:GLN:HG2	1:K:123:LYS:HE3	1.95	0.49
1:K:147:LEU:HB3	1:K:193:LEU:HD11	1.95	0.49
2:L:404:GLN:HB3	2:L:423:GLN:HE22	1.77	0.49
3:O:759:GLY:O	3:O:799:TYR:OH	2.31	0.49
3:O:1471:GLN:HB2	3:O:1476:HIS:HA	1.95	0.49
3:O:1685:ASP:HB3	3:O:1688:LEU:HG	1.95	0.49
3:O:2373:PRO:HA	3:O:2404:ARG:HH22	1.77	0.49
3:O:3916:TRP:O	3:O:4050:LYS:NZ	2.46	0.49
4:C:34:LEU:HD12	4:C:48:PRO:HG3	1.95	0.49
6:E:106:ASP:OD2	6:E:131:ARG:NH2	2.44	0.49
9:J:73:DG:H2''	9:J:74:DA:C5	2.48	0.49
1:K:263:LEU:HA	1:K:347:LEU:HB3	1.95	0.49
2:L:11:VAL:HG22	2:L:55:ALA:HB3	1.94	0.49
2:L:163:PHE:O	2:L:225:TYR:N	2.45	0.49
3:O:304:THR:OG1	3:O:305:ASN:N	2.46	0.49
3:O:2351:GLN:O	3:O:2352:HIS:ND1	2.46	0.49
3:O:3235:LYS:HA	3:O:3238:MET:SD	2.53	0.49
3:O:3842:TRP:CD1	3:O:3858:MET:HE3	2.47	0.49
3:O:585:ILE:HA	3:O:612:LEU:HA	1.95	0.48
3:O:2303:LEU:HD13	3:O:2323:LEU:HD21	1.94	0.48
3:O:3090:TYR:HB3	3:O:3095:ASP:HB2	1.95	0.48
3:O:3505:LEU:HA	3:O:3508:LYS:HG2	1.94	0.48
3:O:3870:SER:HB2	3:O:3874:ARG:NH2	2.28	0.48
2:L:261:ILE:HD11	2:L:263:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:404:GLN:NE2	2:L:423:GLN:OE1	2.45	0.48
3:O:583:LEU:HD13	3:O:612:LEU:HB2	1.95	0.48
3:O:1348:LEU:O	3:O:1352:SER:OG	2.31	0.48
3:O:4042:GLN:OE1	3:O:4042:GLN:N	2.41	0.48
4:G:102:ILE:HA	7:F:98:TYR:HB2	1.95	0.48
2:L:106:ASP:HB3	2:L:109:ASP:HB2	1.95	0.48
3:O:78:PHE:O	3:O:82:ARG:HG2	2.13	0.48
3:O:1178:ARG:HH22	3:O:1187:SER:HB3	1.77	0.48
3:O:1412:LYS:O	3:O:1415:LEU:HB2	2.14	0.48
3:O:1961:PHE:CD2	3:O:2124:SER:HA	2.47	0.48
6:A:119:ILE:HG13	7:B:43:VAL:HG13	1.95	0.48
4:G:29:ARG:HG3	9:J:33:DG:OP1	2.13	0.48
1:K:462:MET:HA	1:K:465:ILE:HD12	1.96	0.48
3:O:82:ARG:HH21	3:O:85:ILE:HD12	1.78	0.48
3:O:463:LYS:HA	3:O:466:LEU:HD12	1.95	0.48
3:O:1178:ARG:NH2	3:O:1183:CYS:SG	2.66	0.48
3:O:2175:GLU:N	3:O:2175:GLU:OE1	2.47	0.48
3:O:3090:TYR:HA	3:O:3093:GLN:HG2	1.94	0.48
3:O:3588:TRP:CZ2	3:O:3610:TYR:HB2	2.47	0.48
8:I:91:DT:O4	9:J:62:DA:N6	2.46	0.48
9:J:93:DA:H1'	9:J:94:DA:C8	2.49	0.48
2:L:107:PHE:HZ	2:L:140:SER:H	1.61	0.48
2:L:261:ILE:HA	2:L:367:ALA:H	1.78	0.48
2:L:394:ARG:NH1	2:L:404:GLN:H	2.12	0.48
3:O:1278:ALA:HB1	3:O:1282:LEU:HD12	1.95	0.48
3:O:2382:VAL:O	3:O:2386:LEU:HG	2.14	0.48
3:O:3089:LEU:HA	3:O:3092:LEU:HD12	1.95	0.48
3:O:3123:GLN:H	3:O:3123:GLN:CD	2.18	0.48
3:O:3413:TYR:CD1	3:O:3449:LYS:HG3	2.47	0.48
3:O:4113:ASP:N	3:O:4114:PRO:HD2	2.29	0.48
3:O:175:TYR:HA	3:O:178:LEU:HD12	1.96	0.48
3:O:430:VAL:HG11	3:O:1644:ALA:HB2	1.96	0.48
3:O:921:ALA:HB3	3:O:927:LYS:HB2	1.94	0.48
3:O:1358:LEU:O	3:O:1362:ASP:N	2.47	0.48
3:O:1725:GLN:HB2	3:O:1728:GLU:HB3	1.95	0.48
3:O:3171:ALA:HB1	3:O:3245:SER:HB2	1.94	0.48
3:O:3837:CYS:O	3:O:3840:LYS:HG3	2.14	0.48
3:O:3908:HIS:HA	3:O:3937:VAL:HG21	1.96	0.48
6:A:63:ARG:NH1	9:J:63:DA:H5''	2.29	0.48
9:J:140:DG:H2''	9:J:141:DG:C8	2.48	0.48
2:L:6:ASN:ND2	8:I:27:DC:OP1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:467:ASP:N	2:L:467:ASP:OD1	2.45	0.48
3:O:180:LEU:H	3:O:231:LEU:HD21	1.79	0.48
3:O:1082:PHE:HD2	3:O:1130:ALA:HB1	1.77	0.48
3:O:1092:GLU:O	3:O:1096:VAL:HG12	2.14	0.48
3:O:1142:HIS:O	3:O:1146:ASN:N	2.43	0.48
3:O:2962:ARG:HA	3:O:3989:ARG:NH1	2.29	0.48
3:O:3820:MET:SD	3:O:3824:GLU:HG3	2.53	0.48
1:K:254:ARG:NH1	8:I:14:DC:O4'	2.47	0.48
2:L:43:GLN:HB2	2:L:495:LEU:HD21	1.96	0.48
2:L:204:GLY:O	2:L:207:ILE:HG22	2.14	0.48
2:L:359:ASN:CG	2:L:360:GLN:HG3	2.39	0.48
2:L:457:LEU:O	2:L:461:MET:HG3	2.13	0.48
3:O:1257:LEU:HA	3:O:1260:LEU:HD12	1.95	0.48
3:O:2295:GLN:HG3	3:O:2298:GLU:H	1.79	0.48
3:O:2311:ARG:H	3:O:2315:VAL:HG21	1.78	0.48
3:O:2826:LEU:HA	3:O:2829:LYS:HE2	1.96	0.48
3:O:3467:ARG:O	3:O:3471:ILE:HG12	2.14	0.48
1:K:41:LEU:HD13	1:K:86:VAL:HB	1.96	0.48
1:K:57:LEU:HB2	1:K:62:MET:HE3	1.94	0.48
1:K:403:ARG:HG2	3:O:213:ARG:HH22	1.78	0.48
1:K:471:PHE:CE2	2:L:344:GLY:HA3	2.48	0.48
3:O:1605:PHE:HB2	3:O:1655:ILE:HD11	1.96	0.48
3:O:1629:CYS:HB2	3:O:1632:TRP:CH2	2.49	0.48
3:O:2225:HIS:CG	3:O:2226:PRO:HD2	2.49	0.48
3:O:3805:TRP:CG	3:O:3806:LEU:H	2.32	0.48
3:O:3930:VAL:HG12	3:O:3937:VAL:HG12	1.95	0.48
1:K:438:PRO:HB2	1:K:442:ASP:HB2	1.96	0.48
2:L:11:VAL:HG11	2:L:114:SER:HB2	1.95	0.48
2:L:512:ILE:HA	2:L:515:MET:HG2	1.94	0.48
3:O:1653:LEU:HA	3:O:1656:ASP:HB3	1.96	0.48
3:O:4083:GLY:HA2	3:O:4088:ASN:HB3	1.96	0.48
6:A:46:VAL:N	8:I:86:DG:OP1	2.41	0.48
7:F:25:ASN:O	7:F:55:ARG:NH2	2.38	0.48
1:K:286:ILE:O	2:L:313:GLY:N	2.47	0.47
2:L:341:SER:H	2:L:394:ARG:HB2	1.78	0.47
3:O:1041:ILE:HD11	3:O:1056:THR:HG21	1.96	0.47
3:O:1082:PHE:HA	3:O:1085:ILE:HG12	1.95	0.47
3:O:2957:LEU:HD21	3:O:2993:PHE:HZ	1.78	0.47
3:O:3029:LYS:HZ2	3:O:3074:GLN:HB2	1.79	0.47
8:I:25:DG:N1	9:J:129:DC:N3	2.62	0.47
8:I:28:DG:H2'	8:I:28:DG:OP2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:479:GLU:HG2	2:L:427:MET:HG3	1.96	0.47
3:O:213:ARG:NH2	9:J:141:DG:OP1	2.47	0.47
3:O:1005:ASP:OD1	3:O:1005:ASP:N	2.47	0.47
3:O:1147:LYS:HZ2	3:O:1149:LYS:HB3	1.78	0.47
3:O:1595:ALA:HA	3:O:1598:ASN:HD21	1.79	0.47
3:O:2931:ARG:HB2	3:O:2939:LEU:HD11	1.95	0.47
3:O:3729:MET:O	3:O:3734:ARG:HG3	2.13	0.47
3:O:2958:LEU:O	3:O:2962:ARG:NH1	2.48	0.47
5:D:34:TYR:HB3	5:D:37:TYR:HD2	1.79	0.47
8:I:99:DC:N3	8:I:100:DA:N6	2.63	0.47
3:O:399:GLN:H	3:O:1744:LYS:NZ	2.13	0.47
3:O:1300:SER:HB3	3:O:1301:ILE:HD12	1.95	0.47
3:O:1415:LEU:O	3:O:1419:LEU:HG	2.14	0.47
3:O:2274:ILE:HD13	3:O:2319:ALA:HB2	1.96	0.47
3:O:2574:ASN:O	3:O:2787:HIS:ND1	2.47	0.47
3:O:3811:THR:HG22	3:O:3813:LYS:H	1.78	0.47
4:C:24:GLN:N	4:C:56:GLU:OE2	2.47	0.47
6:E:82:LEU:HA	7:F:79:LYS:C	2.39	0.47
7:F:32:PRO:HB2	8:I:64:DA:P	2.54	0.47
8:I:34:DT:H2'	8:I:35:DT:C6	2.49	0.47
9:J:136:DA:H2'	9:J:137:DC:H6	1.78	0.47
3:O:67:VAL:HG21	3:O:82:ARG:NH1	2.29	0.47
3:O:586:GLN:OE1	3:O:586:GLN:N	2.47	0.47
3:O:1772:HIS:ND1	3:O:1773:VAL:HG23	2.29	0.47
3:O:3058:ASP:OD2	3:O:3060:SER:OG	2.28	0.47
3:O:3150:ASN:HD21	3:O:3157:LEU:HD21	1.79	0.47
3:O:3515:GLN:O	3:O:3519:GLU:N	2.36	0.47
3:O:3822:GLN:HA	3:O:3825:LYS:HE3	1.97	0.47
3:O:3860:LYS:HG3	3:O:4073:ALA:HB2	1.97	0.47
3:O:250:ASN:O	3:O:254:LYS:N	2.39	0.47
3:O:1782:PHE:HA	3:O:1785:ILE:HG22	1.96	0.47
3:O:2385:LEU:HD13	3:O:2388:LYS:HG3	1.96	0.47
3:O:2725:LEU:HA	3:O:2728:LEU:HB3	1.95	0.47
3:O:3039:THR:O	3:O:3042:PRO:HD2	2.14	0.47
3:O:3244:ASP:OD1	3:O:3245:SER:N	2.47	0.47
3:O:3357:ARG:HD2	3:O:3360:LEU:HD21	1.96	0.47
3:O:3724:GLU:OE1	3:O:3724:GLU:N	2.47	0.47
6:A:119:ILE:HB	7:B:46:ILE:HG22	1.95	0.47
9:J:135:DC:H2''	9:J:136:DA:O5'	2.14	0.47
1:K:481:PRO:HB2	2:L:333:TYR:CE2	2.50	0.47
3:O:170:VAL:HA	3:O:219:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:746:ARG:NH2	3:O:788:TYR:OH	2.48	0.47
3:O:914:VAL:HA	3:O:917:LEU:HD12	1.96	0.47
3:O:1085:ILE:O	3:O:1089:PHE:HB2	2.14	0.47
3:O:1269:THR:O	3:O:1273:GLU:HB2	2.14	0.47
3:O:1585:SER:OG	3:O:1588:ASP:OD1	2.29	0.47
3:O:1868:THR:HG22	3:O:1936:ARG:NH1	2.30	0.47
3:O:1927:MET:SD	3:O:1927:MET:N	2.86	0.47
3:O:2122:LEU:HB2	3:O:2126:MET:HG2	1.96	0.47
3:O:2147:ALA:O	3:O:2151:ILE:HG12	2.15	0.47
3:O:2255:LEU:O	3:O:2259:LYS:HB2	2.15	0.47
3:O:2349:LEU:HB3	3:O:2360:PHE:CE1	2.50	0.47
3:O:3103:ILE:HD12	3:O:3142:ILE:HD13	1.97	0.47
3:O:3995:PRO:O	3:O:3999:THR:N	2.48	0.47
9:J:79:DG:H2''	9:J:80:DC:H5'	1.97	0.47
3:O:129:ASP:HA	3:O:132:ILE:HG12	1.96	0.47
3:O:1015:ASP:N	3:O:1015:ASP:OD1	2.46	0.47
3:O:2965:TYR:O	3:O:2969:ALA:N	2.39	0.47
3:O:3000:ASP:O	3:O:3004:HIS:ND1	2.48	0.47
3:O:3321:LEU:HA	3:O:3324:ARG:HE	1.79	0.47
7:F:26:ILE:O	7:F:55:ARG:HG3	2.15	0.47
8:I:29:DC:N4	9:J:125:DG:O6	2.47	0.47
9:J:54:DT:N3	9:J:55:DG:O6	2.48	0.47
1:K:330:GLU:N	1:K:333:GLU:OE1	2.40	0.47
2:L:59:PHE:HB2	2:L:105:ALA:HB3	1.97	0.47
2:L:296:CYS:HB3	2:L:300:ASP:HA	1.96	0.47
3:O:738:HIS:HA	3:O:741:ILE:HB	1.97	0.47
3:O:738:HIS:CE1	3:O:779:TYR:HB3	2.49	0.47
3:O:2133:LEU:HD22	3:O:2171:LEU:HD11	1.96	0.47
3:O:3236:PHE:HB3	3:O:3272:TRP:CZ2	2.50	0.47
3:O:3300:VAL:HG11	3:O:3359:ILE:HD11	1.96	0.47
5:D:90:GLU:HG3	7:F:75:HIS:CE1	2.50	0.47
6:E:83:ARG:HD3	9:J:104:DG:H4'	1.96	0.47
9:J:61:DT:H2''	9:J:62:DA:N7	2.30	0.47
3:O:650:SER:O	3:O:654:ILE:HG12	2.15	0.47
3:O:1350:ASN:OD1	3:O:1351:THR:N	2.48	0.47
3:O:2455:LEU:HD21	3:O:2498:ILE:HG12	1.96	0.47
3:O:2792:THR:OG1	3:O:2793:PRO:HD3	2.15	0.47
3:O:3478:GLU:OE1	3:O:3478:GLU:N	2.48	0.47
3:O:3490:VAL:HG23	3:O:3494:GLN:HB2	1.96	0.47
4:C:33:LEU:HA	4:C:36:LYS:HG2	1.96	0.47
8:I:82:DC:H1'	8:I:83:DC:C2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:529:PRO:HA	2:L:532:LYS:HE3	1.95	0.46
3:O:128:LEU:HD22	3:O:170:VAL:HG12	1.97	0.46
3:O:2155:GLU:HA	3:O:2158:ARG:HG3	1.96	0.46
3:O:2196:TRP:CD1	3:O:2200:ALA:HB3	2.50	0.46
3:O:2328:ARG:NH2	3:O:2370:SER:O	2.48	0.46
3:O:2356:MET:HG2	3:O:2358:ASP:H	1.80	0.46
3:O:3065:ILE:HG22	3:O:3069:MET:HE1	1.96	0.46
3:O:3625:LEU:N	3:O:3683:CYS:O	2.48	0.46
4:G:87:ILE:HA	4:G:93:LEU:HB3	1.96	0.46
1:K:472:THR:HG23	2:L:350:GLN:NE2	2.30	0.46
2:L:251:LEU:CB	2:L:261:ILE:HG12	2.43	0.46
3:O:206:THR:HG22	3:O:212:VAL:HG21	1.98	0.46
3:O:2253:TYR:HA	3:O:2256:ILE:HD12	1.97	0.46
3:O:2443:MET:HE1	3:O:2479:TRP:CE3	2.50	0.46
3:O:3192:LYS:C	3:O:3196:LYS:HZ2	2.23	0.46
4:G:108:LEU:HD23	4:G:108:LEU:H	1.79	0.46
5:H:89:ARG:O	5:H:92:GLN:NE2	2.48	0.46
3:O:30:ALA:HA	3:O:33:GLN:HG2	1.97	0.46
3:O:887:ASP:OD2	3:O:890:LYS:N	2.48	0.46
3:O:1016:GLY:HA2	3:O:1019:ASP:HB3	1.98	0.46
3:O:1164:CYS:SG	3:O:1165:LEU:N	2.89	0.46
3:O:1354:GLU:HB3	3:O:1357:LYS:HD3	1.97	0.46
3:O:2225:HIS:CD2	3:O:2230:VAL:HB	2.50	0.46
3:O:3296:GLN:HB2	3:O:3301:LEU:HD23	1.97	0.46
3:O:3614:TYR:HB2	3:O:3640:PHE:HE2	1.80	0.46
3:O:3833:ARG:NH2	3:O:3835:PRO:HD3	2.29	0.46
8:I:122:DC:H2''	8:I:123:DA:N7	2.30	0.46
2:L:13:CYS:HB3	2:L:134:ILE:HA	1.98	0.46
2:L:57:VAL:HG22	2:L:79:VAL:HG13	1.97	0.46
2:L:531:SER:HA	2:L:534:LYS:HE2	1.97	0.46
3:O:31:GLY:HA2	3:O:77:GLU:OE1	2.16	0.46
3:O:332:GLU:OE1	3:O:332:GLU:N	2.44	0.46
3:O:953:GLN:HG2	3:O:954:GLY:H	1.79	0.46
3:O:1149:LYS:HE2	3:O:1151:ARG:HD2	1.96	0.46
3:O:1287:GLN:HG3	3:O:1289:SER:H	1.81	0.46
3:O:2531:LEU:HD23	3:O:2538:ARG:HH11	1.81	0.46
7:B:30:THR:HG21	9:J:64:DA:H5''	1.98	0.46
7:B:84:MET:HG3	7:B:88:TYR:CZ	2.50	0.46
8:I:82:DC:O2	9:J:72:DG:N1	2.31	0.46
1:K:252:ARG:CZ	8:I:14:DC:H4'	2.45	0.46
2:L:7:LYS:HE3	2:L:127:PHE:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:865:GLN:HG2	3:O:3170:ASP:HA	1.96	0.46
3:O:1201:ASN:CG	3:O:1206:LEU:HB2	2.41	0.46
3:O:1440:ASP:OD1	3:O:1440:ASP:N	2.47	0.46
6:A:65:LEU:HD12	8:I:94:DA:H2'	1.96	0.46
6:E:80:THR:O	6:E:82:LEU:N	2.49	0.46
8:I:121:DC:H2''	8:I:122:DC:C2	2.51	0.46
1:K:71:TYR:CE2	1:K:115:ARG:HD3	2.50	0.46
2:L:386:ASP:OD1	2:L:387:LEU:N	2.49	0.46
2:L:479:THR:O	2:L:482:ILE:HG22	2.16	0.46
3:O:71:LYS:HD2	3:O:75:SER:HB2	1.98	0.46
3:O:1442:GLN:HA	3:O:1445:ARG:HD3	1.96	0.46
3:O:2433:LYS:NZ	3:O:2437:ASP:OD1	2.49	0.46
3:O:3250:ASN:HA	3:O:3286:CYS:SG	2.55	0.46
3:O:3810:VAL:N	3:O:3930:VAL:O	2.43	0.46
7:F:82:THR:HB	7:F:84:MET:HG3	1.98	0.46
2:L:197:ILE:HG23	2:L:202:LYS:HE3	1.96	0.46
3:O:88:PHE:O	3:O:92:PHE:N	2.33	0.46
3:O:573:LEU:HA	3:O:576:VAL:HG22	1.97	0.46
3:O:3796:MET:HG3	3:O:3800:LEU:HB3	1.98	0.46
3:O:3985:VAL:HG12	3:O:3989:ARG:NE	2.30	0.46
4:C:91:GLU:HA	4:C:94:ASN:HD22	1.80	0.46
1:K:297:LYS:HZ2	2:L:297:LEU:HA	1.81	0.46
1:K:320:GLN:HB3	1:K:322:TYR:CE1	2.51	0.46
1:K:372:GLU:CD	1:K:377:GLY:H	2.22	0.46
2:L:324:SER:O	2:L:328:GLU:N	2.45	0.46
3:O:114:VAL:O	3:O:119:ARG:HB2	2.16	0.46
3:O:180:LEU:HG	3:O:185:HIS:CE1	2.50	0.46
3:O:736:LEU:HD21	3:O:740:ILE:HB	1.97	0.46
3:O:1417:THR:HA	3:O:1420:ARG:HG2	1.98	0.46
3:O:2724:ASP:N	3:O:2724:ASP:OD1	2.46	0.46
3:O:3770:VAL:O	3:O:3774:ILE:HG23	2.15	0.46
3:O:4060:THR:O	3:O:4064:LEU:HD23	2.16	0.46
6:E:64:LYS:HG3	6:E:65:LEU:HD12	1.98	0.46
8:I:57:DC:H1'	9:J:97:DG:H1	1.81	0.46
1:K:130:ARG:HB3	1:K:134:MET:HE1	1.98	0.46
1:K:399:ARG:HH12	2:L:517:ASN:HA	1.80	0.46
3:O:148:LYS:HG2	3:O:151:GLU:OE2	2.16	0.46
3:O:414:LEU:HB3	3:O:460:ALA:HB1	1.98	0.46
3:O:441:MET:O	3:O:445:SER:N	2.49	0.46
3:O:933:LEU:HG	3:O:937:MET:HE2	1.98	0.46
3:O:996:THR:HG23	3:O:1040:SER:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3529:ILE:O	3:O:3532:PRO:HD2	2.15	0.46
7:F:66:ILE:HG13	7:F:67:ARG:N	2.31	0.46
2:L:212:MET:HE2	2:L:220:GLY:HA2	1.97	0.46
2:L:357:MET:N	2:L:357:MET:SD	2.87	0.46
3:O:86:LEU:HA	3:O:89:LEU:HD12	1.98	0.46
3:O:374:LYS:HD3	3:O:423:TYR:HB3	1.98	0.46
3:O:2773:ARG:NH2	3:O:2785:ILE:HG21	2.31	0.46
3:O:3450:MET:HG2	3:O:3468:LEU:HD12	1.97	0.46
6:E:104:PHE:HE2	7:F:37:LEU:HB3	1.80	0.46
9:J:48:DT:H2''	9:J:49:DC:H5'	1.98	0.46
1:K:91:GLU:OE1	1:K:91:GLU:N	2.49	0.45
3:O:1235:ILE:HG23	3:O:1296:PHE:HZ	1.81	0.45
3:O:2330:VAL:HG12	3:O:2335:ASN:HB3	1.98	0.45
3:O:3700:GLU:HA	3:O:3718:ARG:HA	1.97	0.45
5:D:56:MET:HE3	5:D:60:ASN:HD21	1.80	0.45
6:A:43:PRO:HA	8:I:86:DG:H5''	1.98	0.45
6:E:83:ARG:HH21	8:I:53:DG:H5'	1.81	0.45
8:I:114:DC:H2''	8:I:115:DT:C6	2.51	0.45
1:K:478:PHE:O	2:L:427:MET:HG2	2.17	0.45
2:L:261:ILE:HA	2:L:367:ALA:N	2.31	0.45
3:O:248:ILE:HA	3:O:251:PHE:CD2	2.52	0.45
3:O:288:ASP:OD1	3:O:288:ASP:N	2.47	0.45
3:O:1330:TYR:O	3:O:1334:LYS:HG3	2.16	0.45
3:O:1412:LYS:HA	3:O:1415:LEU:HB2	1.98	0.45
3:O:2120:ARG:HA	3:O:2159:PRO:HB2	1.98	0.45
3:O:2166:SER:OG	3:O:2167:PRO:HD3	2.16	0.45
3:O:2819:GLU:O	3:O:2822:LYS:HG2	2.16	0.45
3:O:2837:LEU:HD11	3:O:2870:SER:HB2	1.97	0.45
3:O:2940:ARG:NH1	3:O:2961:ALA:HA	2.32	0.45
3:O:2999:LEU:HD23	3:O:3014:CYS:HB2	1.97	0.45
3:O:3151:LEU:HD11	3:O:3196:LYS:HD3	1.97	0.45
3:O:3152:SER:O	3:O:3154:GLN:NE2	2.49	0.45
3:O:3760:GLN:O	3:O:3764:VAL:HG23	2.16	0.45
3:O:4055:ASN:ND2	3:O:4058:VAL:HG23	2.31	0.45
7:B:46:ILE:HB	7:B:50:ILE:HG13	1.97	0.45
7:F:26:ILE:HG13	7:F:27:GLN:N	2.30	0.45
9:J:50:DC:H4'	9:J:51:DC:H5'	1.97	0.45
1:K:300:THR:H	3:O:164:LYS:NZ	2.11	0.45
3:O:1031:ARG:O	3:O:1034:ARG:HG2	2.16	0.45
3:O:1231:GLN:HA	3:O:1292:LYS:HD3	1.97	0.45
3:O:1508:LYS:NZ	3:O:1562:LEU:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2518:GLN:HA	3:O:2521:ILE:HG22	1.99	0.45
3:O:2551:GLU:OE2	3:O:2851:PHE:N	2.47	0.45
3:O:3446:VAL:HA	3:O:3449:LYS:HE2	1.99	0.45
4:C:38:HIS:O	4:G:38:HIS:HB3	2.16	0.45
6:A:123:ASP:OD1	6:A:124:ILE:N	2.49	0.45
8:I:22:DG:H1'	8:I:23:DA:C8	2.52	0.45
1:K:382:PHE:HE1	1:K:431:GLY:HA2	1.82	0.45
1:K:412:ALA:HB2	1:K:437:LEU:HD11	1.98	0.45
1:K:509:PRO:HG2	2:L:341:SER:HB3	1.98	0.45
2:L:359:ASN:OD1	2:L:360:GLN:HG3	2.16	0.45
3:O:490:ILE:HD12	3:O:527:TYR:CE2	2.52	0.45
3:O:886:TRP:NE1	3:O:912:PRO:HB3	2.31	0.45
3:O:1661:PHE:HA	3:O:1665:HIS:HD2	1.81	0.45
3:O:1747:LEU:O	3:O:1750:LEU:HG	2.17	0.45
3:O:2206:PRO:O	3:O:2210:VAL:HG12	2.16	0.45
3:O:2806:LYS:HG3	3:O:2857:CYS:HB2	1.98	0.45
5:D:83:ARG:HH11	8:I:43:DG:H2'	1.81	0.45
8:I:73:DC:H2''	8:I:74:DG:C8	2.51	0.45
1:K:463:LYS:O	1:K:466:VAL:N	2.49	0.45
2:L:251:LEU:HD21	2:L:253:ILE:HB	1.98	0.45
3:O:363:ILE:O	3:O:366:TYR:HB2	2.17	0.45
3:O:768:VAL:HA	3:O:771:ASN:HD22	1.80	0.45
3:O:1723:PRO:HB2	3:O:1725:GLN:OE1	2.16	0.45
3:O:2869:LEU:HB3	3:O:2896:ALA:HA	1.99	0.45
3:O:3183:ILE:HG13	3:O:3242:MET:SD	2.56	0.45
3:O:3381:ALA:O	3:O:3385:LEU:HG	2.17	0.45
3:O:3898:LEU:C	3:O:3900:LEU:H	2.24	0.45
6:A:83:ARG:HG3	7:B:79:LYS:HG3	1.98	0.45
1:K:304:ASN:OD1	1:K:305:THR:N	2.49	0.45
1:K:371:GLU:OE2	1:K:373:SER:OG	2.29	0.45
3:O:450:SER:HG	3:O:453:MET:HG3	1.81	0.45
3:O:475:LEU:O	3:O:479:ILE:HG12	2.17	0.45
3:O:853:ILE:HA	3:O:856:VAL:HG12	1.97	0.45
3:O:2245:TRP:HD1	3:O:2249:LEU:HD11	1.82	0.45
3:O:2424:MET:HE1	3:O:2457:PRO:HB2	1.98	0.45
3:O:3421:ASP:OD1	3:O:3467:ARG:NE	2.49	0.45
4:G:63:LEU:HD22	5:H:42:LEU:HD13	1.97	0.45
4:G:64:GLU:HB2	5:H:45:VAL:HB	1.99	0.45
6:E:91:ALA:HA	6:E:94:GLU:CD	2.41	0.45
1:K:256:LEU:HB2	1:K:273:ILE:O	2.17	0.45
3:O:712:LYS:NZ	3:O:748:TYR:OH	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1675:TYR:OH	3:O:1693:VAL:HA	2.16	0.45
8:I:32:DA:H2	9:J:122:DT:H3	1.65	0.45
1:K:329:LEU:HG	1:K:333:GLU:HB2	1.99	0.45
1:K:422:ASP:OD2	1:K:423:GLN:NE2	2.50	0.45
3:O:257:ARG:HD2	3:O:260:ILE:HD11	1.99	0.45
3:O:488:ILE:HA	3:O:491:CYS:SG	2.57	0.45
3:O:682:TYR:CZ	3:O:700:LYS:HD3	2.52	0.45
3:O:771:ASN:O	3:O:775:GLU:HG2	2.16	0.45
3:O:1766:LEU:HA	3:O:1772:HIS:CE1	2.52	0.45
3:O:3128:LYS:O	3:O:3132:VAL:HG13	2.17	0.45
3:O:3533:PHE:O	3:O:3537:SER:N	2.49	0.45
3:O:4091:ALA:HB3	3:O:4110:GLN:OE1	2.16	0.45
5:D:42:LEU:O	5:D:46:HIS:N	2.38	0.45
5:D:48:ASP:N	5:D:48:ASP:OD1	2.49	0.45
8:I:104:DG:H2''	8:I:105:DG:C8	2.52	0.45
3:O:58:VAL:HG23	3:O:61:ARG:HE	1.82	0.45
3:O:493:LYS:HD3	3:O:524:TYR:HD1	1.82	0.45
3:O:888:ARG:HB3	3:O:3889:ARG:NE	2.31	0.45
3:O:1934:LEU:HD22	3:O:1937:ARG:HD2	1.99	0.45
3:O:2421:VAL:O	3:O:2425:ARG:N	2.49	0.45
3:O:2429:ASP:HA	3:O:2432:GLN:NE2	2.32	0.45
3:O:2964:ASP:OD2	3:O:2967:GLU:HB3	2.17	0.45
3:O:3681:LYS:H	3:O:3724:GLU:HB2	1.82	0.45
3:O:3693:GLU:HG3	3:O:3696:ARG:NH2	2.28	0.45
5:H:115:VAL:HA	5:H:118:TYR:CE2	2.52	0.45
1:K:299:LYS:HA	3:O:164:LYS:HZ1	1.82	0.45
2:L:285:LYS:HB3	2:L:287:GLU:HG2	1.99	0.45
3:O:483:VAL:HG21	3:O:567:GLU:HG3	1.99	0.45
3:O:905:ILE:HG23	3:O:2811:SER:HB2	1.98	0.45
3:O:1249:SER:O	3:O:1253:THR:N	2.40	0.45
3:O:1560:TYR:CZ	3:O:1596:VAL:HA	2.51	0.45
3:O:1709:GLU:CD	3:O:1709:GLU:H	2.25	0.45
3:O:1757:MET:SD	3:O:1758:LEU:N	2.90	0.45
3:O:1818:SER:HA	3:O:1821:ASP:HB2	1.98	0.45
3:O:2392:VAL:O	3:O:2396:LEU:HG	2.15	0.45
3:O:2409:THR:C	3:O:2411:LEU:H	2.24	0.45
3:O:2987:THR:HG23	3:O:2990:GLU:H	1.81	0.45
3:O:3049:LEU:HD21	3:O:3088:LEU:HD12	1.99	0.45
3:O:3498:TRP:O	3:O:3502:MET:HG2	2.17	0.45
3:O:3718:ARG:H	3:O:3743:HIS:CG	2.35	0.45
8:I:58:DG:H1'	8:I:59:DC:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:97:DG:O6	9:J:57:DC:N4	2.50	0.45
1:K:476:ASP:OD1	1:K:476:ASP:N	2.47	0.44
3:O:20:SER:HA	3:O:70:ARG:HH12	1.81	0.44
3:O:80:GLU:O	3:O:83:GLU:HB2	2.17	0.44
3:O:485:GLN:HA	3:O:488:ILE:HG22	1.99	0.44
3:O:653:LEU:HB3	3:O:670:LEU:HD21	1.99	0.44
3:O:800:LEU:HB3	3:O:3114:TYR:CD1	2.52	0.44
3:O:891:ARG:NE	3:O:957:PRO:O	2.32	0.44
3:O:1349:LEU:HB3	3:O:1405:ALA:HB1	2.00	0.44
3:O:3226:ASP:O	3:O:3229:SER:OG	2.24	0.44
3:O:3283:LEU:O	3:O:3287:ARG:HG2	2.17	0.44
3:O:3493:TRP:HB2	3:O:3708:ARG:O	2.16	0.44
7:B:49:LEU:HD23	7:B:49:LEU:H	1.82	0.44
9:J:39:DA:H2''	9:J:40:DG:C8	2.51	0.44
9:J:105:DA:H2''	9:J:106:DG:C8	2.52	0.44
1:K:352:PRO:HG3	2:L:473:LEU:HD22	1.98	0.44
3:O:149:ILE:HD13	3:O:180:LEU:HD11	1.99	0.44
3:O:1279:LEU:HD13	3:O:1356:TRP:HE1	1.82	0.44
3:O:2396:LEU:O	3:O:2400:VAL:HG23	2.17	0.44
3:O:2429:ASP:OD1	3:O:2430:GLU:N	2.51	0.44
3:O:2866:ALA:HA	3:O:2869:LEU:HG	1.99	0.44
3:O:2897:LEU:HD11	3:O:2923:TRP:CE2	2.53	0.44
3:O:3771:MET:O	3:O:3775:LEU:HG	2.17	0.44
3:O:3839:TYR:HA	3:O:3842:TRP:CD1	2.52	0.44
3:O:3858:MET:HB3	3:O:3862:ALA:HB2	1.99	0.44
6:A:60:LEU:HD13	6:A:93:GLN:HG2	1.98	0.44
6:A:113:HIS:HE1	6:E:110:CYS:HB3	1.81	0.44
8:I:14:DC:N3	9:J:140:DG:N2	2.55	0.44
8:I:112:DC:H4'	8:I:113:DC:C2	2.52	0.44
2:L:245:ILE:HG22	2:L:246:HIS:H	1.81	0.44
2:L:450:GLN:HG2	2:L:536:LEU:HB3	1.99	0.44
3:O:391:ARG:HD3	3:O:391:ARG:HA	1.81	0.44
3:O:425:ASP:N	3:O:425:ASP:OD1	2.49	0.44
3:O:489:ARG:O	3:O:492:SER:OG	2.24	0.44
3:O:931:CYS:HB3	3:O:984:TYR:HE2	1.82	0.44
3:O:3424:LEU:HD21	3:O:3443:PRO:HB3	1.98	0.44
3:O:1335:CYS:O	3:O:1339:VAL:HG13	2.16	0.44
3:O:2430:GLU:N	3:O:2430:GLU:OE1	2.46	0.44
3:O:2773:ARG:NH1	3:O:2775:TYR:HA	2.32	0.44
3:O:2865:HIS:HB2	3:O:2868:LEU:HD12	1.99	0.44
3:O:3002:TYR:CD2	3:O:3014:CYS:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3762:GLN:HB2	3:O:3793:VAL:HG11	1.99	0.44
4:G:77:ARG:HE	5:H:50:GLY:HA3	1.82	0.44
1:K:111:PRO:HA	1:K:115:ARG:HD2	1.99	0.44
1:K:446:MET:HE3	1:K:447:PRO:HG2	1.98	0.44
2:L:151:ILE:HG12	2:L:211:VAL:HG13	1.98	0.44
3:O:358:GLU:O	3:O:361:ILE:HG12	2.17	0.44
3:O:618:LYS:HE2	3:O:618:LYS:HB2	1.87	0.44
3:O:640:GLU:O	3:O:643:GLU:HG3	2.18	0.44
3:O:727:ALA:HB1	3:O:765:LEU:HD21	1.98	0.44
3:O:1151:ARG:HB2	3:O:1163:LEU:HD12	2.00	0.44
3:O:1487:VAL:HG12	3:O:1559:PHE:CE1	2.53	0.44
3:O:1820:VAL:O	3:O:1825:LEU:HG	2.16	0.44
3:O:2197:THR:HG23	3:O:2722:ARG:HH12	1.83	0.44
3:O:2855:VAL:O	3:O:2859:GLN:HG2	2.16	0.44
3:O:3239:LYS:HB3	3:O:3262:LEU:HD11	1.98	0.44
9:J:56:DG:H2''	9:J:57:DC:C5	2.52	0.44
1:K:122:PHE:HB3	1:K:131:PHE:HB2	2.00	0.44
1:K:248:ALA:C	1:K:249:LYS:HD3	2.43	0.44
1:K:254:ARG:N	2:L:433:TYR:OH	2.50	0.44
2:L:539:LEU:HD23	2:L:539:LEU:HA	1.79	0.44
3:O:175:TYR:O	3:O:227:LEU:HD12	2.16	0.44
3:O:442:GLN:NE2	3:O:442:GLN:O	2.50	0.44
3:O:524:TYR:HD2	3:O:525:LYS:HD3	1.83	0.44
3:O:1288:SER:O	3:O:1288:SER:OG	2.36	0.44
3:O:1363:LEU:C	3:O:1365:ASN:H	2.25	0.44
3:O:1590:THR:OG1	3:O:1591:LYS:NZ	2.35	0.44
3:O:2364:LEU:HA	3:O:2367:VAL:HG12	2.00	0.44
3:O:2382:VAL:HG23	3:O:2397:CYS:HB2	1.99	0.44
3:O:2405:VAL:HG23	3:O:2441:LYS:HD3	2.00	0.44
3:O:2965:TYR:HB3	3:O:3001:CYS:HB2	2.00	0.44
3:O:3183:ILE:HG13	3:O:3242:MET:CE	2.48	0.44
3:O:3424:LEU:O	3:O:3427:GLU:HG2	2.16	0.44
8:I:65:DC:H2''	8:I:66:DG:C8	2.51	0.44
8:I:81:DC:H1'	9:J:73:DG:H22	1.82	0.44
9:J:90:DT:H2''	9:J:91:DT:H5'	1.99	0.44
1:K:36:ASP:HB2	1:K:81:ASP:CG	2.42	0.44
2:L:74:TYR:CD1	2:L:113:VAL:HB	2.53	0.44
2:L:167:PHE:HB3	2:L:192:PHE:HD2	1.81	0.44
3:O:290:TYR:HE2	3:O:340:TYR:HB3	1.83	0.44
3:O:561:ASN:HA	3:O:564:LEU:HG	1.98	0.44
3:O:1017:ILE:HG13	3:O:1080:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1102:GLU:H	3:O:1102:GLU:CD	2.25	0.44
3:O:2304:VAL:O	3:O:2307:MET:HB2	2.18	0.44
3:O:3332:THR:HG23	3:O:3335:ARG:NH1	2.33	0.44
3:O:3360:LEU:O	3:O:3364:GLY:N	2.43	0.44
3:O:3460:GLU:H	3:O:3460:GLU:CD	2.24	0.44
3:O:3464:LYS:HE2	3:O:3998:LEU:HD21	1.98	0.44
3:O:3613:MET:SD	3:O:3614:TYR:N	2.90	0.44
6:A:74:ILE:HG22	7:B:66:ILE:HG21	2.00	0.44
9:J:89:DG:H21	9:J:91:DT:H5''	1.83	0.44
3:O:19:LEU:HD13	3:O:34:LEU:HG	2.00	0.44
3:O:200:PHE:HB3	3:O:224:LEU:HD22	2.00	0.44
3:O:1710:LEU:HD23	3:O:1710:LEU:H	1.83	0.44
3:O:3772:ASN:HD21	3:O:3788:LEU:HB3	1.83	0.44
6:E:61:LEU:HB2	7:F:37:LEU:HD23	1.99	0.44
6:E:76:GLN:C	6:E:78:PHE:N	2.76	0.44
3:O:468:LEU:HD13	3:O:478:CYS:SG	2.58	0.44
3:O:682:TYR:O	3:O:700:LYS:NZ	2.37	0.44
3:O:1017:ILE:HD11	3:O:1081:ALA:HB2	2.00	0.44
3:O:1034:ARG:HA	3:O:1085:ILE:HG22	2.00	0.44
3:O:1034:ARG:HH21	3:O:1087:ARG:HB2	1.82	0.44
3:O:1092:GLU:OE1	3:O:1095:LEU:HB2	2.18	0.44
3:O:2402:LEU:HA	3:O:2438:ILE:HG12	1.99	0.44
3:O:3519:GLU:O	3:O:3523:ASP:N	2.46	0.44
3:O:3851:ASP:OD1	3:O:3852:VAL:N	2.51	0.44
3:O:3865:THR:O	3:O:3868:VAL:HG22	2.18	0.44
6:E:118:THR:HA	7:F:45:ARG:O	2.18	0.44
8:I:126:DC:H2'	8:I:127:DA:C8	2.53	0.44
9:J:92:DT:H2''	9:J:93:DA:H5'	1.99	0.44
1:K:76:ILE:HG12	1:K:248:ALA:HB1	2.00	0.43
1:K:523:ASP:O	1:K:527:GLU:HG2	2.17	0.43
2:L:261:ILE:HG13	2:L:262:ALA:N	2.33	0.43
2:L:261:ILE:HD13	2:L:364:VAL:HG13	1.99	0.43
2:L:312:GLN:NE2	2:L:313:GLY:N	2.66	0.43
3:O:676:ASN:O	3:O:680:ILE:HG13	2.19	0.43
3:O:1184:ARG:NH2	3:O:1262:ALA:HA	2.33	0.43
3:O:1750:LEU:HD13	3:O:1759:LEU:HD23	1.99	0.43
3:O:1773:VAL:O	3:O:1773:VAL:HG12	2.18	0.43
3:O:2928:LYS:HA	3:O:2931:ARG:NH1	2.33	0.43
3:O:3552:LYS:HA	3:O:3555:VAL:HG12	1.99	0.43
3:O:3970:LEU:O	3:O:3971:MET:HE2	2.18	0.43
3:O:174:VAL:HA	3:O:177:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:291:VAL:HG12	3:O:340:TYR:CG	2.52	0.43
3:O:385:TYR:O	3:O:389:ILE:HG12	2.18	0.43
3:O:966:PHE:HD2	3:O:1011:GLU:HG2	1.83	0.43
3:O:995:PHE:HB3	3:O:1005:ASP:HB3	1.99	0.43
3:O:2234:ASN:HA	3:O:2237:ILE:HD12	2.00	0.43
3:O:3132:VAL:O	3:O:3136:THR:HG23	2.18	0.43
3:O:3530:VAL:O	3:O:3534:ILE:HG13	2.19	0.43
6:A:121:PRO:HG2	7:B:49:LEU:HG	2.00	0.43
7:B:62:LEU:HA	7:B:65:VAL:HG22	1.99	0.43
5:H:99:LEU:HD12	5:H:99:LEU:HA	1.89	0.43
8:I:90:DT:H2"	8:I:91:DT:H5"	1.99	0.43
1:K:143:LEU:O	1:K:147:LEU:HG	2.17	0.43
1:K:468:LYS:O	1:K:517:ARG:NH2	2.50	0.43
2:L:14:MET:SD	2:L:38:ILE:HG13	2.58	0.43
2:L:14:MET:HB2	2:L:58:LEU:HB3	2.00	0.43
2:L:37:VAL:HG22	2:L:231:LEU:HB2	1.98	0.43
2:L:107:PHE:CZ	2:L:138:LEU:HA	2.52	0.43
3:O:181:LEU:HD23	3:O:234:PHE:HD2	1.82	0.43
3:O:270:ALA:O	3:O:273:ARG:HG2	2.18	0.43
3:O:395:MET:HE1	3:O:410:MET:HE1	2.00	0.43
3:O:789:TYR:O	3:O:793:LEU:HB2	2.18	0.43
3:O:1876:ILE:O	3:O:1880:MET:HG3	2.18	0.43
3:O:2139:PRO:O	3:O:2143:ARG:HG3	2.17	0.43
3:O:2415:LEU:O	3:O:2419:ASP:N	2.52	0.43
3:O:2532:PRO:HD2	3:O:2538:ARG:HA	2.00	0.43
3:O:3588:TRP:O	3:O:3592:VAL:HG13	2.18	0.43
3:O:3822:GLN:NE2	3:O:3822:GLN:O	2.51	0.43
3:O:3946:PHE:HZ	3:O:4047:ALA:HB2	1.83	0.43
3:O:3958:LEU:HD11	3:O:4081:ALA:HB2	1.99	0.43
3:O:4010:SER:O	3:O:4014:LYS:HB3	2.19	0.43
6:A:103:LEU:O	6:A:107:THR:HG23	2.18	0.43
4:G:60:ALA:HB1	5:H:45:VAL:HG11	2.00	0.43
4:G:77:ARG:HH12	9:J:23:DC:H5"	1.83	0.43
5:H:94:ALA:O	5:H:98:LEU:HB2	2.18	0.43
8:I:10:DA:H2"	8:I:11:DA:C8	2.53	0.43
1:K:44:ALA:HB3	1:K:89:GLY:C	2.44	0.43
1:K:278:GLN:O	2:L:429:ASP:HA	2.18	0.43
3:O:714:VAL:CG1	3:O:733:LEU:HD21	2.48	0.43
3:O:912:PRO:O	3:O:915:THR:HB	2.18	0.43
3:O:1056:THR:HA	3:O:1059:LEU:HG	1.99	0.43
3:O:1458:LEU:HB3	3:O:1463:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2572:TYR:HA	3:O:2787:HIS:HB2	2.00	0.43
3:O:2918:PRO:HB2	3:O:2919:ASP:H	1.62	0.43
3:O:3192:LYS:HG3	3:O:3196:LYS:NZ	2.34	0.43
3:O:3894:PRO:HA	3:O:3897:PHE:HB3	1.99	0.43
5:D:63:VAL:HA	5:D:66:ILE:HG12	1.99	0.43
5:D:92:GLN:HA	5:D:95:VAL:HG22	2.01	0.43
6:A:64:LYS:H	8:I:95:DC:P	2.41	0.43
4:G:17:ARG:HA	4:G:20:ARG:HE	1.84	0.43
7:F:46:ILE:HB	7:F:50:ILE:HD11	2.00	0.43
7:F:66:ILE:O	7:F:70:VAL:HG23	2.17	0.43
1:K:350:PHE:CE2	2:L:458:ILE:HG12	2.52	0.43
3:O:357:LYS:NZ	3:O:1732:GLY:HA3	2.33	0.43
3:O:1195:VAL:HG12	3:O:1203:SER:HA	1.99	0.43
3:O:1428:ILE:HG12	3:O:1432:CYS:HB3	2.01	0.43
3:O:1646:LEU:HD11	3:O:1692:ALA:HB2	2.00	0.43
3:O:2185:MET:N	3:O:2185:MET:SD	2.91	0.43
3:O:2562:LEU:O	3:O:2566:THR:OG1	2.34	0.43
3:O:3139:GLN:NE2	3:O:3139:GLN:O	2.52	0.43
3:O:3371:GLU:HA	3:O:3374:ILE:HG12	1.99	0.43
3:O:3522:THR:HB	3:O:3561:LYS:HD2	2.01	0.43
3:O:4009:PRO:HA	3:O:4012:ASP:HB2	2.00	0.43
5:D:110:GLU:HA	5:D:113:LYS:HE3	1.99	0.43
8:I:105:DG:H2"	8:I:106:DA:C8	2.53	0.43
1:K:157:VAL:HG22	1:K:159:PHE:H	1.84	0.43
2:L:7:LYS:NZ	2:L:125:LYS:O	2.35	0.43
2:L:148:ASP:OD1	2:L:148:ASP:N	2.51	0.43
3:O:319:PHE:O	3:O:323:VAL:HG13	2.18	0.43
3:O:1423:ILE:O	3:O:1467:ILE:HD11	2.19	0.43
3:O:1611:GLN:HB2	3:O:1613:HIS:ND1	2.33	0.43
3:O:3235:LYS:O	3:O:3238:MET:HG2	2.18	0.43
3:O:3324:ARG:HG2	3:O:3391:ALA:HB3	2.00	0.43
1:K:270:SER:H	1:K:375:VAL:HB	1.82	0.43
2:L:347:LYS:HB2	2:L:347:LYS:HE2	1.76	0.43
3:O:136:GLN:NE2	3:O:140:SER:OG	2.52	0.43
3:O:925:GLN:O	3:O:925:GLN:NE2	2.51	0.43
3:O:1125:GLN:HA	3:O:1128:CYS:SG	2.59	0.43
3:O:3467:ARG:HB2	3:O:3997:LEU:CD1	2.48	0.43
3:O:3993:SER:C	3:O:3995:PRO:HD3	2.44	0.43
3:O:4121:TRP:HB3	3:O:4124:TRP:HB2	2.01	0.43
4:G:29:ARG:NH2	5:H:32:GLU:OE1	2.52	0.43
4:G:77:ARG:HA	5:H:50:GLY:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:654:ILE:HD12	3:O:710:PHE:CG	2.54	0.43
3:O:672:ILE:O	3:O:676:ASN:ND2	2.51	0.43
3:O:1128:CYS:HA	3:O:1131:ILE:HG12	2.01	0.43
3:O:1518:ALA:HB1	3:O:1524:LEU:HD21	2.00	0.43
3:O:1576:ASP:OD1	3:O:1576:ASP:N	2.52	0.43
3:O:2269:ASP:OD1	3:O:2269:ASP:N	2.52	0.43
3:O:3447:VAL:HA	3:O:3450:MET:HG3	2.01	0.43
3:O:3796:MET:HE3	3:O:3797:THR:HG22	2.00	0.43
5:D:87:THR:HG22	5:D:88:SER:H	1.84	0.43
6:A:62:ILE:HD11	6:A:93:GLN:HE22	1.84	0.43
4:G:50:TYR:CZ	5:H:111:GLY:HA3	2.54	0.43
7:F:67:ARG:O	7:F:71:THR:HG22	2.18	0.43
8:I:125:DG:H1'	8:I:126:DC:C2	2.53	0.43
9:J:59:DG:H2''	9:J:60:DT:C6	2.54	0.43
1:K:332:GLU:OE1	3:O:205:LYS:NZ	2.47	0.43
3:O:359:LEU:O	3:O:362:ALA:HB3	2.19	0.43
3:O:460:ALA:O	3:O:464:VAL:HG13	2.18	0.43
3:O:1432:CYS:HB2	3:O:1486:LEU:HD11	2.01	0.43
3:O:2245:TRP:CD1	3:O:2249:LEU:HD11	2.54	0.43
3:O:2325:LEU:N	3:O:2370:SER:OG	2.52	0.43
3:O:2544:SER:HA	3:O:2842:ARG:NH2	2.33	0.43
3:O:3239:LYS:O	3:O:3243:ILE:HG12	2.19	0.43
8:I:22:DG:N1	9:J:133:DG:C2	2.86	0.43
1:K:35:ARG:O	1:K:164:LYS:NZ	2.50	0.43
1:K:166:ILE:HG23	1:K:200:LEU:HA	2.00	0.43
1:K:349:GLY:HA2	2:L:461:MET:HE1	2.00	0.43
2:L:306:LEU:HD23	2:L:309:ASP:HB2	2.00	0.43
3:O:217:LEU:HB2	3:O:220:LEU:HB3	2.00	0.43
3:O:886:TRP:HE1	3:O:912:PRO:HB3	1.84	0.43
3:O:888:ARG:HD2	3:O:3889:ARG:HG2	2.00	0.43
3:O:913:ARG:NH1	3:O:916:GLU:OE1	2.51	0.43
3:O:1102:GLU:O	3:O:1106:ILE:HG12	2.18	0.43
3:O:1437:TYR:HA	3:O:1507:CYS:SG	2.59	0.43
3:O:1632:TRP:CG	3:O:1645:VAL:HG11	2.54	0.43
3:O:2257:PHE:CE1	3:O:2299:TYR:HA	2.53	0.43
3:O:3172:LYS:HA	3:O:3172:LYS:HD2	1.87	0.43
3:O:3810:VAL:O	3:O:3930:VAL:N	2.50	0.43
3:O:3882:LEU:H	3:O:3966:GLN:NE2	2.14	0.43
3:O:3995:PRO:HD2	3:O:4051:LEU:HD21	2.00	0.43
7:B:31:LYS:HG2	7:B:51:TYR:CE1	2.54	0.43
1:K:376:ILE:N	2:L:540:ILE:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:261:ILE:HB	2:L:365:PHE:O	2.18	0.42
3:O:540:MET:HE2	3:O:540:MET:HA	2.01	0.42
3:O:764:PRO:O	3:O:768:VAL:HG22	2.18	0.42
3:O:975:ASP:O	3:O:981:ARG:HD2	2.19	0.42
3:O:1111:LEU:HD11	3:O:1131:ILE:HD13	2.01	0.42
3:O:2301:GLN:HA	3:O:2304:VAL:HG22	2.00	0.42
3:O:2310:VAL:HG13	3:O:2316:TYR:CE2	2.54	0.42
3:O:2405:VAL:HA	3:O:2441:LYS:HD3	2.00	0.42
3:O:3052:LEU:HD11	3:O:3061:LEU:HD21	2.01	0.42
3:O:3504:ALA:O	3:O:3508:LYS:NZ	2.47	0.42
5:D:31:LYS:O	9:J:125:DG:H5''	2.18	0.42
5:D:110:GLU:HA	5:D:113:LYS:HG2	2.00	0.42
7:F:77:LYS:HE3	7:F:77:LYS:HB2	1.77	0.42
8:I:102:DG:N2	9:J:52:DC:O2	2.52	0.42
3:O:143:LEU:HG	3:O:182:GLY:HA2	2.00	0.42
3:O:478:CYS:SG	3:O:479:ILE:N	2.91	0.42
3:O:665:GLY:HA2	3:O:668:LYS:HD2	2.02	0.42
3:O:1069:HIS:CD2	3:O:1070:PRO:HD2	2.54	0.42
3:O:1069:HIS:CG	3:O:1070:PRO:HD2	2.55	0.42
3:O:1776:GLU:O	3:O:1779:GLN:HG3	2.19	0.42
3:O:2295:GLN:HE21	3:O:2295:GLN:HB3	1.70	0.42
3:O:3451:LEU:HD22	3:O:3486:GLU:HB3	2.00	0.42
3:O:3462:ARG:O	3:O:3465:PHE:HB3	2.19	0.42
3:O:3515:GLN:O	3:O:3519:GLU:HG2	2.19	0.42
7:B:90:LEU:HB3	7:B:95:ARG:O	2.18	0.42
6:E:51:ILE:HD13	7:F:42:GLY:HA2	2.00	0.42
3:O:382:ASP:OD1	3:O:424:LEU:HD11	2.18	0.42
3:O:1100:VAL:HG23	3:O:1101:PHE:N	2.34	0.42
3:O:1366:THR:O	3:O:1368:LEU:N	2.52	0.42
3:O:1755:SER:HB3	3:O:1758:LEU:HB2	2.01	0.42
3:O:3815:LEU:HA	3:O:3818:ASN:HD21	1.85	0.42
3:O:3822:GLN:HA	3:O:3825:LYS:HG2	2.00	0.42
4:C:91:GLU:HG2	4:C:95:LYS:HE2	2.02	0.42
6:A:76:GLN:OE1	6:A:81:ASP:N	2.49	0.42
8:I:74:DG:H1'	8:I:75:DC:C2	2.54	0.42
8:I:77:DC:H1'	8:I:78:DT:H5'	2.01	0.42
3:O:924:ARG:NH2	3:O:977:ASP:OD1	2.43	0.42
3:O:1560:TYR:OH	3:O:1599:GLY:HA3	2.19	0.42
3:O:1632:TRP:CD1	3:O:1633:TRP:HB3	2.52	0.42
3:O:3172:LYS:HA	3:O:3248:LYS:HZ1	1.84	0.42
3:O:4086:ASP:OD1	3:O:4086:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:4120:THR:HA	3:O:4124:TRP:CZ3	2.53	0.42
5:H:85:THR:OG1	9:J:43:DA:OP1	2.27	0.42
5:H:93:THR:HA	5:H:96:ARG:HE	1.85	0.42
6:E:78:PHE:O	6:E:80:THR:N	2.52	0.42
3:O:86:LEU:HD13	3:O:129:ASP:HB3	2.01	0.42
3:O:108:LYS:O	3:O:112:THR:HG22	2.19	0.42
3:O:371:GLY:O	3:O:374:LYS:N	2.52	0.42
3:O:1150:LYS:HD3	3:O:1162:SER:HA	2.01	0.42
3:O:2164:TRP:O	3:O:2167:PRO:HD2	2.19	0.42
3:O:2398:LEU:HD23	3:O:2434:VAL:HG13	2.00	0.42
3:O:3123:GLN:O	3:O:3126:LEU:HG	2.19	0.42
3:O:3161:LEU:HG	3:O:3166:ASN:ND2	2.34	0.42
3:O:3552:LYS:HA	3:O:3552:LYS:HD3	1.92	0.42
6:E:99:TYR:OH	6:E:133:GLU:OE1	2.28	0.42
2:L:342:VAL:HG22	2:L:393:VAL:HG12	2.02	0.42
3:O:131:LEU:HB3	3:O:177:LEU:HD21	2.01	0.42
3:O:643:GLU:HB3	3:O:680:ILE:HD13	2.02	0.42
3:O:1122:GLY:C	3:O:1124:ILE:H	2.27	0.42
3:O:1942:CYS:HB2	3:O:2094:MET:SD	2.60	0.42
3:O:2120:ARG:O	3:O:2160:TYR:HB2	2.19	0.42
3:O:2280:VAL:HG11	3:O:2287:PRO:HA	2.01	0.42
3:O:2773:ARG:HD2	3:O:2775:TYR:CE1	2.55	0.42
3:O:3161:LEU:HD11	3:O:3186:ARG:HH12	1.84	0.42
3:O:3291:GLN:HG2	3:O:3293:CYS:N	2.30	0.42
3:O:3522:THR:HG21	3:O:3558:ILE:HD12	2.01	0.42
3:O:3833:ARG:HG2	3:O:3834:ALA:H	1.83	0.42
1:K:333:GLU:HA	1:K:336:GLU:HG3	2.01	0.42
1:K:465:ILE:HG12	1:K:521:LEU:HB3	2.02	0.42
2:L:147:LEU:O	2:L:151:ILE:HG13	2.19	0.42
3:O:294:PHE:O	3:O:298:LEU:HG	2.20	0.42
3:O:364:ARG:NH1	3:O:415:GLN:HB2	2.25	0.42
3:O:442:GLN:HG2	3:O:461:ILE:HD11	2.02	0.42
3:O:468:LEU:HD22	3:O:478:CYS:SG	2.59	0.42
3:O:472:GLY:O	3:O:475:LEU:HB3	2.20	0.42
3:O:979:VAL:HA	3:O:982:GLN:HG2	2.00	0.42
3:O:1379:PRO:O	3:O:1382:ILE:HG12	2.19	0.42
3:O:1483:LEU:HD11	3:O:1515:LEU:HD22	2.00	0.42
3:O:2153:THR:HG21	3:O:2157:PHE:HE2	1.85	0.42
3:O:2268:LYS:HB3	3:O:2311:ARG:HD3	2.01	0.42
3:O:3034:PRO:HB2	3:O:3037:GLN:HG3	2.02	0.42
5:H:106:HIS:O	5:H:110:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:119:ILE:HD11	7:F:46:ILE:HG22	2.01	0.42
8:I:31:DC:H2''	8:I:32:DA:C5	2.55	0.42
1:K:109:ASP:HB3	1:K:115:ARG:HH12	1.84	0.42
1:K:332:GLU:O	1:K:335:GLU:HG3	2.20	0.42
2:L:17:GLY:HA2	2:L:103:GLN:O	2.19	0.42
2:L:326:VAL:HG12	2:L:330:GLN:HE22	1.84	0.42
3:O:68:PHE:CE1	3:O:117:LYS:HG3	2.55	0.42
3:O:416:SER:O	3:O:420:VAL:HG23	2.20	0.42
3:O:1711:ARG:HD2	3:O:1757:MET:HB2	2.00	0.42
3:O:1839:PHE:O	3:O:1842:THR:HB	2.20	0.42
3:O:2153:THR:HG22	3:O:2154:GLU:H	1.84	0.42
3:O:2279:ILE:O	3:O:2282:ALA:HB3	2.19	0.42
3:O:2385:LEU:HD12	3:O:2389:PHE:CZ	2.55	0.42
3:O:2503:LYS:O	3:O:2507:ILE:HG12	2.19	0.42
3:O:3419:PHE:O	3:O:3422:GLN:HG2	2.20	0.42
3:O:3737:ARG:HA	3:O:3751:LEU:CB	2.49	0.42
4:C:95:LYS:HB2	4:C:95:LYS:HE3	1.79	0.42
6:E:82:LEU:O	6:E:84:PHE:N	2.53	0.42
8:I:46:DA:H61	9:J:108:DT:H3	1.67	0.42
8:I:78:DT:H2''	8:I:79:DG:C8	2.54	0.42
9:J:102:DT:H4'	9:J:103:DA:O4'	2.20	0.42
2:L:7:LYS:HE2	2:L:7:LYS:HB3	1.54	0.42
2:L:528:ILE:HB	2:L:529:PRO:HD3	2.02	0.42
3:O:95:LYS:HD2	3:O:837:THR:HG22	2.00	0.42
3:O:164:LYS:HD3	3:O:164:LYS:N	2.34	0.42
3:O:888:ARG:HB3	3:O:3889:ARG:HE	1.84	0.42
3:O:1346:THR:HG22	3:O:1402:LEU:HA	2.00	0.42
3:O:1360:LYS:O	3:O:1363:LEU:HB2	2.20	0.42
3:O:1601:LEU:HD11	3:O:1652:ILE:HG13	2.01	0.42
3:O:2959:ALA:HA	3:O:2962:ARG:HH22	1.85	0.42
3:O:3447:VAL:O	3:O:3450:MET:HG3	2.19	0.42
3:O:3508:LYS:HE3	3:O:3508:LYS:HB3	1.80	0.42
3:O:3712:LEU:HB3	3:O:3716:HIS:CD2	2.54	0.42
8:I:111:DT:H5''	8:I:112:DC:C5	2.54	0.42
1:K:189:LYS:HD2	1:K:189:LYS:HA	1.80	0.42
2:L:213:ILE:HA	2:L:217:GLY:HA2	2.01	0.42
3:O:33:GLN:HG3	3:O:34:LEU:HD12	2.01	0.42
3:O:465:PHE:HD1	3:O:468:LEU:HD21	1.84	0.42
3:O:891:ARG:HH21	3:O:958:MET:HA	1.85	0.42
3:O:1071:ASN:ND2	3:O:1072:ALA:N	2.68	0.42
3:O:1071:ASN:HD21	3:O:1073:PHE:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1445:ARG:HB3	3:O:1510:LEU:HD11	2.02	0.42
3:O:1596:VAL:O	3:O:1600:MET:HG2	2.19	0.42
3:O:3289:ARG:H	3:O:3289:ARG:HD3	1.85	0.42
3:O:4070:LYS:HE2	3:O:4070:LYS:HB2	1.92	0.42
8:I:39:DC:H2''	8:I:40:DG:C4	2.55	0.42
1:K:144:SER:HB2	1:K:185:ARG:HG3	2.02	0.41
2:L:165:LEU:HB2	2:L:167:PHE:O	2.20	0.41
3:O:183:GLU:O	3:O:185:HIS:ND1	2.53	0.41
3:O:584:GLU:N	3:O:613:HIS:O	2.38	0.41
3:O:789:TYR:HA	3:O:792:ILE:HG12	2.02	0.41
3:O:910:PHE:O	3:O:914:VAL:HG12	2.19	0.41
3:O:938:VAL:O	3:O:941:MET:HB3	2.20	0.41
3:O:2145:PHE:O	3:O:2149:LEU:HG	2.19	0.41
3:O:2426:HIS:O	3:O:2432:GLN:OE1	2.38	0.41
3:O:2549:LYS:HB2	3:O:2549:LYS:HE3	1.79	0.41
3:O:3061:LEU:O	3:O:3065:ILE:HG12	2.20	0.41
3:O:3704:GLN:N	3:O:3704:GLN:HE21	2.18	0.41
3:O:3927:ASN:OD1	3:O:3940:ILE:N	2.50	0.41
7:B:35:ARG:HH22	8:I:85:DC:H2'	1.84	0.41
8:I:15:DC:H2''	8:I:16:DG:C8	2.55	0.41
1:K:115:ARG:O	1:K:119:LEU:HG	2.20	0.41
1:K:153:LEU:HD23	1:K:153:LEU:HA	1.88	0.41
1:K:259:LEU:HD23	1:K:259:LEU:HA	1.89	0.41
2:L:14:MET:HE1	2:L:135:PHE:CD1	2.55	0.41
3:O:191:ASN:O	3:O:195:ASN:OD1	2.38	0.41
3:O:623:PHE:HE2	3:O:665:GLY:HA3	1.85	0.41
3:O:932:GLU:HG3	3:O:2793:PRO:HB3	2.01	0.41
3:O:1483:LEU:HD22	3:O:1518:ALA:CB	2.50	0.41
3:O:1729:PHE:CZ	3:O:1735:ARG:HD2	2.54	0.41
3:O:2153:THR:HG22	3:O:2154:GLU:N	2.35	0.41
3:O:2186:VAL:O	3:O:2189:ILE:HG12	2.20	0.41
3:O:2193:ILE:HD13	3:O:2196:TRP:HZ2	1.85	0.41
3:O:2514:ASN:HB3	3:O:2517:LEU:HG	2.02	0.41
3:O:2776:ARG:HG3	3:O:2782:ASP:OD2	2.21	0.41
3:O:2825:THR:N	3:O:2828:GLU:OE1	2.48	0.41
3:O:3238:MET:O	3:O:3242:MET:HG2	2.19	0.41
3:O:3772:ASN:OD1	3:O:3788:LEU:N	2.53	0.41
3:O:3946:PHE:CZ	3:O:4047:ALA:HB2	2.55	0.41
7:F:62:LEU:O	7:F:66:ILE:HG12	2.20	0.41
2:L:543:LYS:HA	2:L:543:LYS:HD3	1.85	0.41
3:O:229:SER:HB3	3:O:274:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1294:VAL:HG21	3:O:1363:LEU:HG	2.03	0.41
3:O:1464:LEU:O	3:O:1468:LEU:N	2.50	0.41
3:O:2438:ILE:O	3:O:2442:MET:HG3	2.19	0.41
3:O:2470:ARG:NH1	3:O:2513:GLU:OE2	2.53	0.41
3:O:3069:MET:HB2	3:O:3075:LYS:HD3	2.02	0.41
3:O:3348:LEU:O	3:O:3352:GLU:N	2.46	0.41
3:O:3719:ILE:C	3:O:3743:HIS:HB2	2.45	0.41
3:O:3840:LYS:NZ	3:O:3874:ARG:HH22	2.18	0.41
3:O:4077:TYR:HA	3:O:4080:VAL:HG22	2.03	0.41
4:C:51:LEU:HD11	5:D:70:ILE:HG21	2.02	0.41
5:D:92:GLN:NE2	5:D:93:THR:OG1	2.54	0.41
1:K:49:PHE:CE2	1:K:137:HIS:HB2	2.55	0.41
1:K:330:GLU:O	1:K:334:THR:HG23	2.21	0.41
1:K:413:LEU:HB3	1:K:432:PHE:CD1	2.55	0.41
2:L:7:LYS:HG3	2:L:52:ASP:HA	2.02	0.41
2:L:237:PHE:CE2	2:L:511:HIS:HB3	2.55	0.41
3:O:717:LYS:HD2	3:O:717:LYS:HA	1.75	0.41
3:O:1322:THR:O	3:O:1327:GLY:N	2.41	0.41
3:O:1633:TRP:HB2	3:O:1678:LEU:HD21	2.02	0.41
3:O:1808:ASP:O	3:O:1816:ARG:NE	2.50	0.41
3:O:2965:TYR:HB2	3:O:3005:LEU:HD21	2.01	0.41
3:O:3725:ARG:O	3:O:3738:ILE:HA	2.21	0.41
3:O:3740:ILE:H	3:O:3749:PRO:HA	1.84	0.41
5:D:93:THR:HG21	7:F:75:HIS:HB2	2.01	0.41
6:A:103:LEU:HA	6:A:131:ARG:HH22	1.85	0.41
6:E:51:ILE:HG21	7:F:42:GLY:HA2	2.01	0.41
9:J:50:DC:H1'	9:J:51:DC:C2	2.55	0.41
1:K:248:ALA:O	1:K:249:LYS:HD3	2.20	0.41
1:K:252:ARG:HH22	1:K:254:ARG:HB2	1.85	0.41
1:K:350:PHE:HB3	1:K:394:VAL:HG21	2.03	0.41
3:O:349:ILE:H	3:O:391:ARG:NH2	2.18	0.41
3:O:2459:VAL:HA	3:O:2473:MET:HE2	2.01	0.41
3:O:2794:LEU:HG	3:O:2808:LEU:HD11	2.03	0.41
3:O:2806:LYS:HG3	3:O:2857:CYS:CB	2.50	0.41
3:O:3173:MET:HE2	3:O:3173:MET:O	2.21	0.41
3:O:3467:ARG:NH2	3:O:3471:ILE:HD11	2.35	0.41
3:O:3577:GLN:NE2	3:O:3629:ARG:HD2	2.36	0.41
8:I:126:DC:H2'	8:I:127:DA:H8	1.84	0.41
1:K:440:ALA:HB2	2:L:481:LYS:C	2.45	0.41
1:K:478:PHE:N	2:L:427:MET:HE2	2.34	0.41
3:O:238:MET:HE3	3:O:283:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:320:LEU:HB3	3:O:368:LEU:HD23	2.02	0.41
3:O:327:VAL:HG12	3:O:333:MET:HB3	2.02	0.41
3:O:359:LEU:O	3:O:363:ILE:HG23	2.21	0.41
3:O:488:ILE:HD11	3:O:2036:LEU:HA	2.02	0.41
3:O:1086:TYR:CD1	3:O:1133:HIS:HB3	2.56	0.41
3:O:1196:PRO:HB3	3:O:1203:SER:HB3	2.02	0.41
3:O:1504:ASP:OD1	3:O:1505:LEU:N	2.52	0.41
3:O:2571:ASP:HA	3:O:2574:ASN:HB2	2.02	0.41
3:O:3719:ILE:HD11	3:O:3722:PHE:CZ	2.56	0.41
3:O:3950:THR:OG1	3:O:4063:GLU:OE2	2.32	0.41
5:H:37:TYR:O	5:H:41:VAL:HG23	2.21	0.41
7:F:64:ASN:HA	7:F:67:ARG:NH1	2.35	0.41
1:K:418:GLU:HB2	1:K:430:PRO:HB3	2.03	0.41
3:O:73:LEU:N	3:O:118:ASP:OD2	2.54	0.41
3:O:1533:LEU:HD13	3:O:1585:SER:HB3	2.02	0.41
3:O:3193:ILE:HA	3:O:3196:LYS:HG2	2.02	0.41
3:O:3677:PRO:O	3:O:3681:LYS:HD3	2.20	0.41
3:O:3717:VAL:HG23	3:O:3743:HIS:HB3	2.03	0.41
7:B:38:ALA:HB1	7:B:43:VAL:HB	2.01	0.41
4:G:65:LEU:HD13	4:G:93:LEU:HD11	2.02	0.41
1:K:351:LYS:HE3	1:K:351:LYS:HB2	1.67	0.41
3:O:173:LYS:HA	3:O:223:CYS:HB3	2.02	0.41
3:O:381:VAL:HG12	3:O:424:LEU:HD13	2.03	0.41
3:O:1141:LYS:HG3	3:O:1141:LYS:O	2.20	0.41
3:O:1184:ARG:HH22	3:O:1265:GLU:HB2	1.86	0.41
3:O:1256:TRP:CE2	3:O:1260:LEU:HD11	2.56	0.41
3:O:1300:SER:HB3	3:O:1301:ILE:H	1.61	0.41
3:O:1504:ASP:HB3	3:O:1507:CYS:SG	2.60	0.41
3:O:1619:ALA:HA	3:O:1622:ILE:HG22	2.03	0.41
3:O:2126:MET:HA	3:O:2129:LEU:HD12	2.02	0.41
3:O:2344:LEU:O	3:O:2347:LYS:HG2	2.21	0.41
3:O:2418:LYS:HD3	3:O:2418:LYS:HA	1.83	0.41
3:O:3368:GLU:HA	3:O:3372:LYS:HD2	2.02	0.41
3:O:3642:LYS:HA	3:O:3642:LYS:HD3	1.93	0.41
3:O:3809:THR:HG1	3:O:3930:VAL:C	2.27	0.41
4:C:32:ARG:N	4:C:35:ARG:HH21	2.19	0.41
6:A:83:ARG:HB2	7:B:80:THR:HG22	2.03	0.41
7:F:25:ASN:HD22	7:F:28:GLY:HA3	1.85	0.41
8:I:79:DG:N2	9:J:76:DA:N1	2.69	0.41
1:K:71:TYR:HE2	1:K:115:ARG:HD3	1.86	0.41
1:K:264:ASN:OD1	1:K:265:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:421:ASP:HB3	1:K:425:ILE:HB	2.03	0.41
1:K:459:VAL:O	1:K:463:LYS:HG3	2.20	0.41
2:L:155:LYS:HE3	2:L:215:LEU:HD23	2.02	0.41
2:L:523:THR:O	2:L:527:GLN:HG3	2.20	0.41
3:O:55:THR:HA	3:O:58:VAL:HG12	2.02	0.41
3:O:82:ARG:HG2	3:O:82:ARG:HH11	1.85	0.41
3:O:142:ARG:H	3:O:144:MET:HE1	1.86	0.41
3:O:320:LEU:HA	3:O:323:VAL:HG22	2.02	0.41
3:O:410:MET:N	3:O:411:PRO:HD2	2.36	0.41
3:O:446:PHE:CZ	3:O:530:LEU:HB2	2.56	0.41
3:O:671:SER:HA	3:O:674:VAL:HG12	2.03	0.41
3:O:714:VAL:O	3:O:718:MET:N	2.53	0.41
3:O:854:ARG:O	3:O:857:GLN:HG3	2.20	0.41
3:O:910:PHE:HB3	3:O:2804:ILE:HD11	2.03	0.41
3:O:1112:ALA:HA	3:O:1180:GLN:HG2	2.03	0.41
3:O:1342:MET:O	3:O:1346:THR:HG23	2.20	0.41
3:O:1526:GLU:OE1	3:O:1526:GLU:N	2.54	0.41
3:O:1754:GLN:HA	3:O:1785:ILE:HD11	2.02	0.41
3:O:1919:CYS:SG	3:O:1948:ALA:HB2	2.61	0.41
3:O:1935:GLU:O	3:O:1939:LEU:HG	2.20	0.41
3:O:2160:TYR:HD2	3:O:2164:TRP:NE1	2.18	0.41
3:O:2227:LYS:HG3	3:O:2228:ARG:H	1.86	0.41
3:O:2398:LEU:HA	3:O:2401:VAL:HG22	2.03	0.41
3:O:2404:ARG:C	3:O:2441:LYS:HZ3	2.27	0.41
3:O:2938:VAL:O	3:O:2942:ILE:HG12	2.21	0.41
3:O:3353:GLU:HA	3:O:3357:ARG:HG3	2.03	0.41
3:O:3447:VAL:HG12	3:O:3468:LEU:HD13	2.03	0.41
3:O:3483:MET:HE1	3:O:3513:ALA:HB3	2.02	0.41
3:O:3813:LYS:HD3	3:O:3925:LEU:HD12	2.01	0.41
3:O:3814:ASP:OD1	3:O:3815:LEU:N	2.54	0.41
3:O:3843:LEU:H	3:O:3843:LEU:HD23	1.85	0.41
5:D:93:THR:O	5:D:97:LEU:HD23	2.21	0.41
6:A:87:SER:C	7:B:83:ALA:HB2	2.45	0.41
6:E:109:LEU:HD23	6:E:112:ILE:HD11	2.03	0.41
8:I:41:DT:H6	8:I:41:DT:H2'	1.62	0.41
8:I:93:DA:H2''	8:I:94:DA:C8	2.56	0.41
8:I:113:DC:O2	9:J:42:DG:N2	2.54	0.41
9:J:51:DC:H2''	9:J:52:DC:C6	2.55	0.41
9:J:80:DC:H1'	9:J:81:DG:C4	2.56	0.41
1:K:64:ILE:O	1:K:67:ILE:HG22	2.21	0.41
1:K:484:GLN:O	1:K:488:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:712:LYS:HA	3:O:712:LYS:HD3	1.96	0.41
3:O:1057:LYS:HE2	3:O:1057:LYS:HB2	1.85	0.41
3:O:1756:PRO:HA	3:O:1759:LEU:HD12	2.02	0.41
3:O:1835:ALA:HA	3:O:1838:GLU:CD	2.46	0.41
3:O:2599:SER:OG	3:O:2600:THR:N	2.53	0.41
3:O:2817:LEU:HD12	3:O:2865:HIS:CE1	2.56	0.41
3:O:3531:TYR:O	3:O:3535:ILE:HG12	2.20	0.41
3:O:3558:ILE:HD13	3:O:3558:ILE:HA	1.90	0.41
6:A:113:HIS:CE1	6:E:110:CYS:HB3	2.55	0.41
4:G:22:GLY:HA3	5:H:117:LYS:HZ2	1.87	0.41
8:I:84:DC:H2''	8:I:85:DC:C5	2.56	0.41
1:K:46:LYS:HA	1:K:49:PHE:HD2	1.86	0.40
2:L:64:THR:HG23	2:L:76:ASN:N	2.36	0.40
3:O:1098:GLN:HA	3:O:1151:ARG:HE	1.85	0.40
3:O:1403:MET:HB3	3:O:1463:LEU:HD11	2.03	0.40
3:O:1736:PHE:O	3:O:1740:VAL:HG13	2.21	0.40
3:O:3614:TYR:HB2	3:O:3640:PHE:CE2	2.56	0.40
6:A:51:ILE:HG13	7:B:39:ARG:HD2	2.02	0.40
5:H:121:ALA:HB3	5:H:122:LYS:HE2	2.03	0.40
8:I:49:DT:H2''	8:I:50:DC:C5	2.56	0.40
1:K:420:LEU:HA	1:K:427:VAL:H	1.85	0.40
2:L:395:TYR:O	2:L:404:GLN:HB2	2.22	0.40
3:O:78:PHE:O	3:O:82:ARG:NH1	2.55	0.40
3:O:186:PRO:O	3:O:190:ILE:HG12	2.21	0.40
3:O:385:TYR:CZ	3:O:421:LEU:HD13	2.56	0.40
3:O:627:VAL:HA	3:O:630:CYS:SG	2.61	0.40
3:O:1297:PHE:HA	3:O:1300:SER:OG	2.21	0.40
3:O:1366:THR:C	3:O:1368:LEU:H	2.29	0.40
3:O:2350:LYS:HD2	3:O:2350:LYS:HA	1.86	0.40
3:O:2957:LEU:HD23	3:O:2957:LEU:HA	1.84	0.40
4:C:29:ARG:HG3	4:C:32:ARG:HH21	1.86	0.40
4:C:93:LEU:O	4:C:97:LEU:HG	2.21	0.40
5:H:76:ARG:NE	5:H:80:TYR:OH	2.54	0.40
6:E:82:LEU:HB3	7:F:81:VAL:HG12	2.03	0.40
8:I:30:DT:H1'	8:I:31:DC:C4	2.56	0.40
9:J:30:DC:H1'	9:J:31:DT:C2	2.56	0.40
1:K:206:LYS:HB2	1:K:237:SER:HA	2.04	0.40
2:L:226:SER:HB3	2:L:229:GLU:HG2	2.03	0.40
3:O:13:LEU:HB2	3:O:59:PHE:CE2	2.57	0.40
3:O:363:ILE:HA	3:O:366:TYR:CD2	2.56	0.40
3:O:559:SER:OG	3:O:560:LEU:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:886:TRP:HE3	3:O:961:LEU:HD13	1.86	0.40
3:O:1442:GLN:HG2	3:O:1445:ARG:HD3	2.02	0.40
3:O:1849:ASP:OD1	3:O:1850:VAL:N	2.54	0.40
3:O:1963:GLN:HA	3:O:2125:TRP:NE1	2.36	0.40
3:O:2312:TYR:O	3:O:2315:VAL:HG22	2.20	0.40
3:O:2335:ASN:HD21	3:O:2337:LEU:HG	1.85	0.40
3:O:2339:GLU:OE1	3:O:2339:GLU:N	2.53	0.40
3:O:3048:LYS:HA	3:O:3048:LYS:HD3	1.83	0.40
3:O:3609:MET:O	3:O:3613:MET:HG3	2.22	0.40
3:O:3681:LYS:O	3:O:3688:SER:OG	2.37	0.40
3:O:3738:ILE:H	3:O:3751:LEU:HA	1.87	0.40
1:K:90:THR:OG1	1:K:135:MET:O	2.38	0.40
2:L:291:LYS:HB2	2:L:291:LYS:HE2	1.83	0.40
2:L:406:GLY:HA2	2:L:424:LEU:HG	2.04	0.40
3:O:201:LEU:HB3	3:O:249:PHE:CE2	2.56	0.40
3:O:225:LYS:HE2	3:O:225:LYS:HB2	1.87	0.40
3:O:275:PHE:CE1	3:O:319:PHE:HB2	2.57	0.40
3:O:392:CYS:SG	3:O:413:PHE:HD2	2.45	0.40
3:O:990:GLN:HB3	3:O:2781:PRO:HD3	2.02	0.40
3:O:1098:GLN:HE22	3:O:1151:ARG:HG2	1.86	0.40
3:O:1326:GLU:OE2	3:O:1329:ARG:HG3	2.21	0.40
3:O:2104:MET:HE1	3:O:2122:LEU:HD22	2.02	0.40
3:O:2873:PRO:C	3:O:2925:GLU:HG3	2.46	0.40
3:O:2945:SER:OG	3:O:3975:LYS:HE2	2.21	0.40
3:O:3029:LYS:NZ	3:O:3074:GLN:HB2	2.36	0.40
3:O:3675:LYS:O	3:O:3677:PRO:HD3	2.20	0.40
4:C:47:ALA:HB3	4:C:48:PRO:HD3	2.04	0.40
6:A:59:GLU:N	7:B:40:ARG:HH12	2.17	0.40
6:A:62:ILE:HG22	7:B:33:ALA:HB1	2.03	0.40
4:G:78:ILE:HD13	4:G:78:ILE:HA	1.93	0.40
6:E:79:LYS:HD2	6:E:79:LYS:HA	1.62	0.40
7:F:45:ARG:HE	9:J:83:DA:H5'	1.86	0.40
8:I:103:DG:H4'	8:I:104:DG:OP1	2.22	0.40
9:J:137:DC:H2'	9:J:138:DC:C6	2.57	0.40
1:K:38:LEU:HD12	1:K:39:ILE:H	1.87	0.40
1:K:42:VAL:HB	1:K:87:PHE:CD2	2.57	0.40
1:K:67:ILE:HD11	1:K:85:VAL:HG22	2.04	0.40
2:L:35:LYS:HE2	2:L:98:ILE:HG22	2.03	0.40
2:L:108:LEU:HD12	2:L:143:SER:O	2.21	0.40
2:L:408:ALA:HA	2:L:420:VAL:O	2.20	0.40
3:O:169:THR:HG21	8:I:10:DA:H5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:524:TYR:OH	3:O:625:ASN:O	2.27	0.40
3:O:653:LEU:HD21	3:O:669:LEU:HB3	2.03	0.40
3:O:714:VAL:O	3:O:718:MET:HG3	2.22	0.40
3:O:1166:LEU:C	3:O:1170:LYS:HZ3	2.29	0.40
3:O:2260:PHE:HE1	3:O:2302:ALA:HB3	1.86	0.40
3:O:3328:ILE:HD13	3:O:3328:ILE:HA	1.94	0.40
3:O:3356:ALA:HA	3:O:3359:ILE:HG12	2.02	0.40
3:O:3853:GLY:HA2	3:O:4121:TRP:CZ2	2.56	0.40
3:O:4045:CYS:HA	3:O:4048:LYS:HE2	2.03	0.40
3:O:4116:ILE:HA	3:O:4124:TRP:CH2	2.39	0.40
4:C:82:HIS:HA	4:C:85:LEU:HD12	2.04	0.40
4:G:70:ALA:O	4:G:74:LYS:N	2.54	0.40
8:I:18:DT:H2''	8:I:19:DG:OP1	2.19	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	K	489/609 (80%)	466 (95%)	23 (5%)	0	100	100
2	L	513/732 (70%)	451 (88%)	62 (12%)	0	100	100
3	O	3455/4128 (84%)	3118 (90%)	331 (10%)	6 (0%)	43	77
4	C	90/143 (63%)	87 (97%)	3 (3%)	0	100	100
4	G	95/143 (66%)	89 (94%)	6 (6%)	0	100	100
5	D	91/126 (72%)	88 (97%)	3 (3%)	0	100	100
5	H	90/126 (71%)	88 (98%)	2 (2%)	0	100	100
6	A	94/136 (69%)	87 (93%)	7 (7%)	0	100	100
6	E	86/136 (63%)	76 (88%)	6 (7%)	4 (5%)	2	16
7	B	73/103 (71%)	72 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F	75/103 (73%)	73 (97%)	2 (3%)	0	100	100
All	All	5151/6485 (79%)	4695 (91%)	446 (9%)	10 (0%)	44	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	O	76	ILE
6	E	79	LYS
6	E	81	ASP
6	E	83	ARG
3	O	1956	PHE
3	O	3250	ASN
3	O	3633	ILE
6	E	80	THR
3	O	1925	GLU
3	O	956	PRO

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	K	427/548 (78%)	426 (100%)	1 (0%)	87	85
2	L	445/649 (69%)	443 (100%)	2 (0%)	84	82
3	O	3045/3671 (83%)	3041 (100%)	4 (0%)	88	88
4	C	70/106 (66%)	70 (100%)	0	100	100
4	G	73/106 (69%)	72 (99%)	1 (1%)	59	71
5	D	74/105 (70%)	74 (100%)	0	100	100
5	H	78/105 (74%)	78 (100%)	0	100	100
6	A	84/111 (76%)	84 (100%)	0	100	100
6	E	73/111 (66%)	71 (97%)	2 (3%)	39	59
7	B	61/79 (77%)	61 (100%)	0	100	100
7	F	62/79 (78%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4492/5670 (79%)	4482 (100%)	10 (0%)	85	85

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

Mol	Chain	Res	Type
1	K	95	ASN
2	L	312	GLN
2	L	360	GLN
3	O	1691	GLN
3	O	2295	GLN
3	O	2432	GLN
3	O	3704	GLN
4	G	84	GLN
6	E	78	PHE
6	E	79	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	95	ASN
2	L	312	GLN
2	L	360	GLN
2	L	500	HIS
3	O	136	GLN
3	O	1568	ASN
3	O	2295	GLN
3	O	3166	ASN
3	O	3278	GLN
7	B	64	ASN
4	G	110	ASN
7	F	25	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

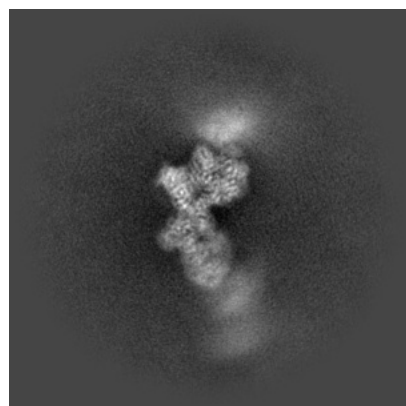
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53025. These allow visual inspection of the internal detail of the map and identification of artifacts.

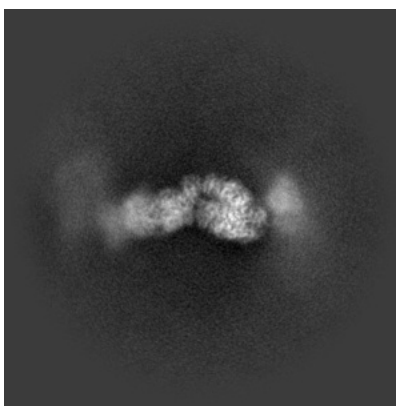
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

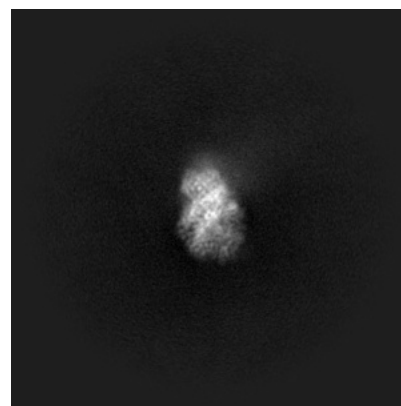
6.1.1 Primary map



X

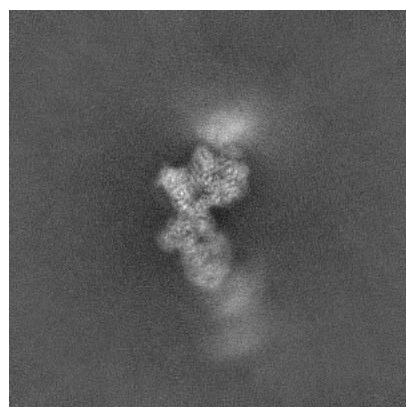


Y

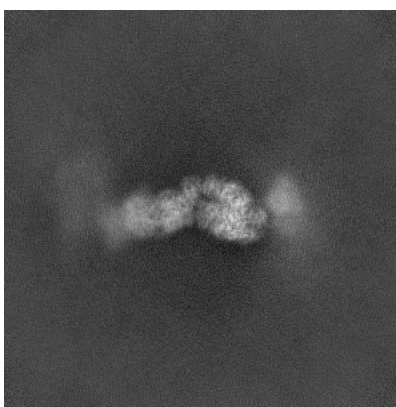


Z

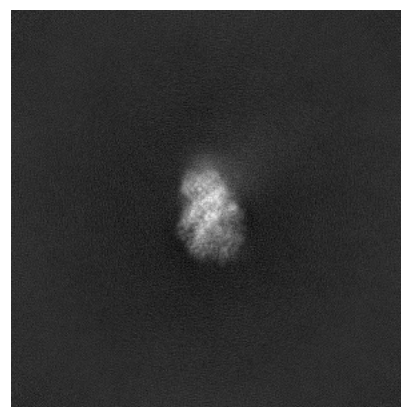
6.1.2 Raw map



X



Y

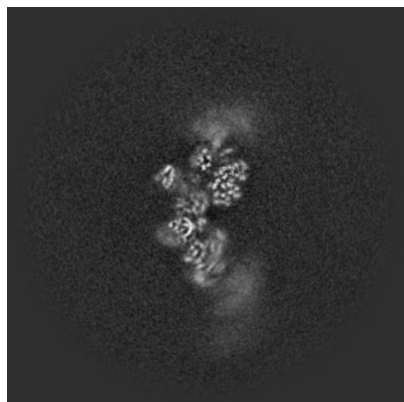


Z

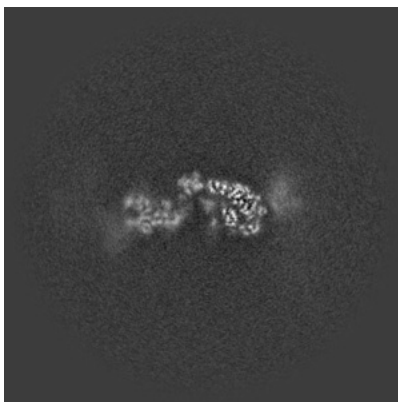
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

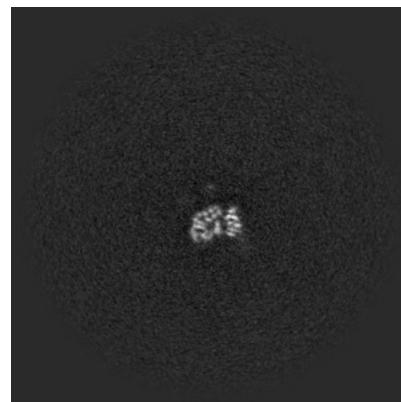
6.2.1 Primary map



X Index: 210

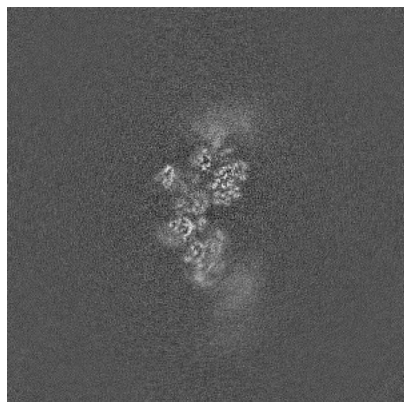


Y Index: 210

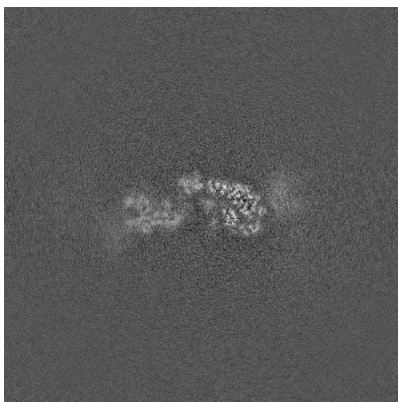


Z Index: 210

6.2.2 Raw map



X Index: 210



Y Index: 210

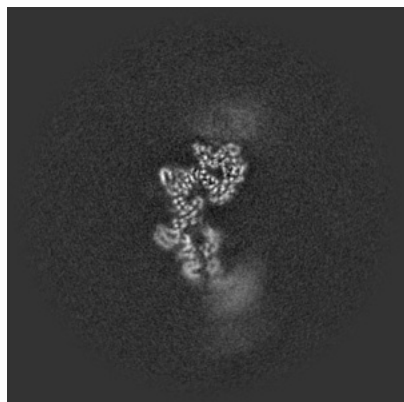


Z Index: 210

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

6.3 Largest variance slices [i](#)

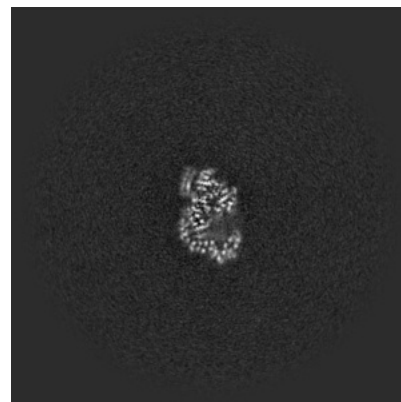
6.3.1 Primary map



X Index: 201

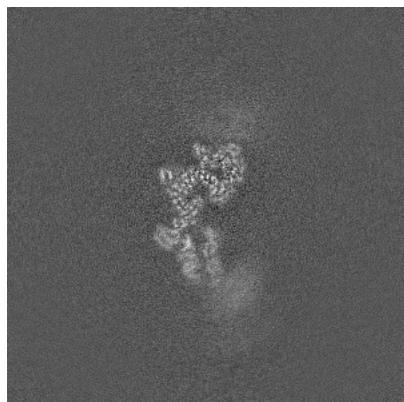


Y Index: 206



Z Index: 238

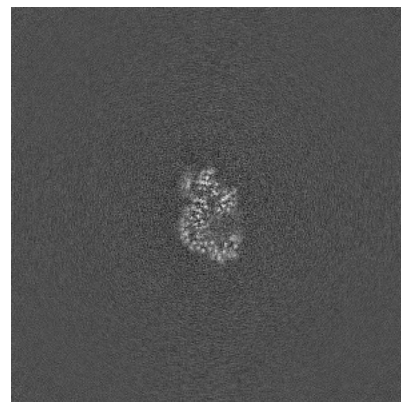
6.3.2 Raw map



X Index: 200



Y Index: 206

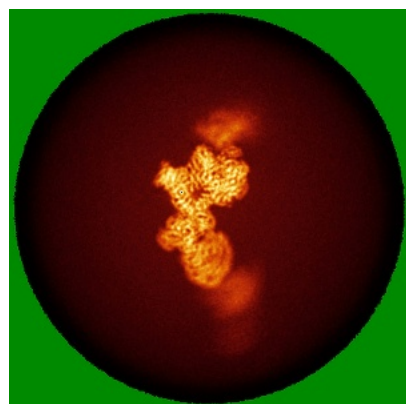


Z Index: 239

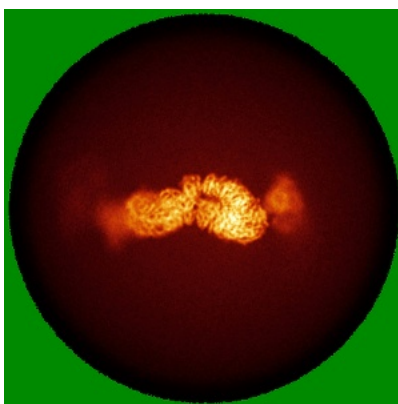
The images above show the largest variance slices of the map in three orthogonal directions.

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

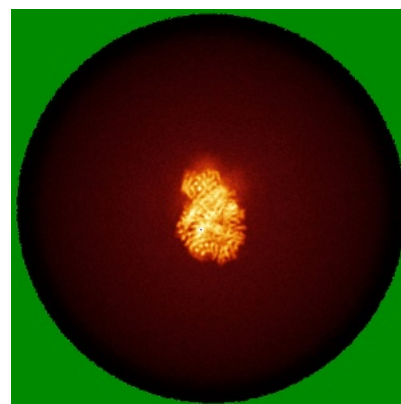
6.4.1 Primary map



X

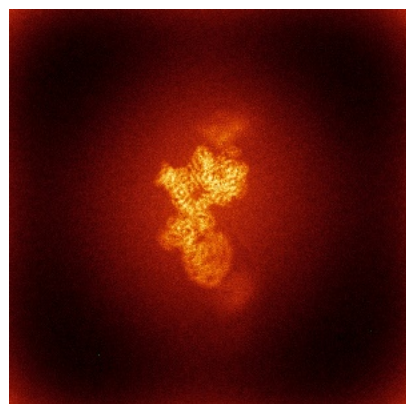


Y

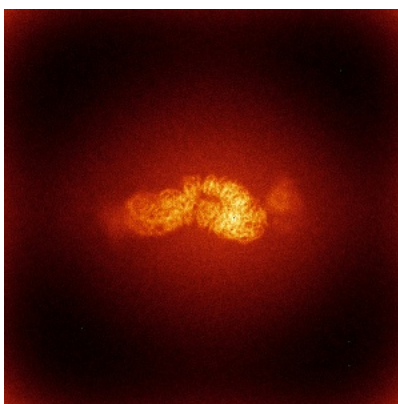


Z

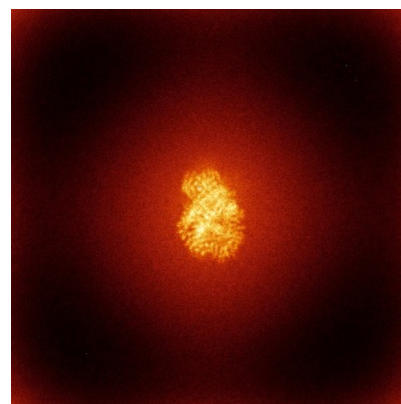
6.4.2 Raw map



X



Y

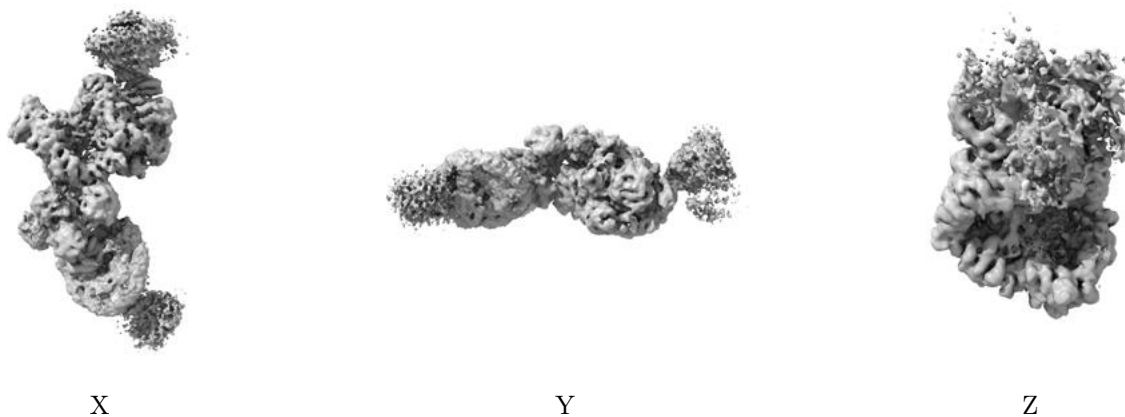


Z

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.

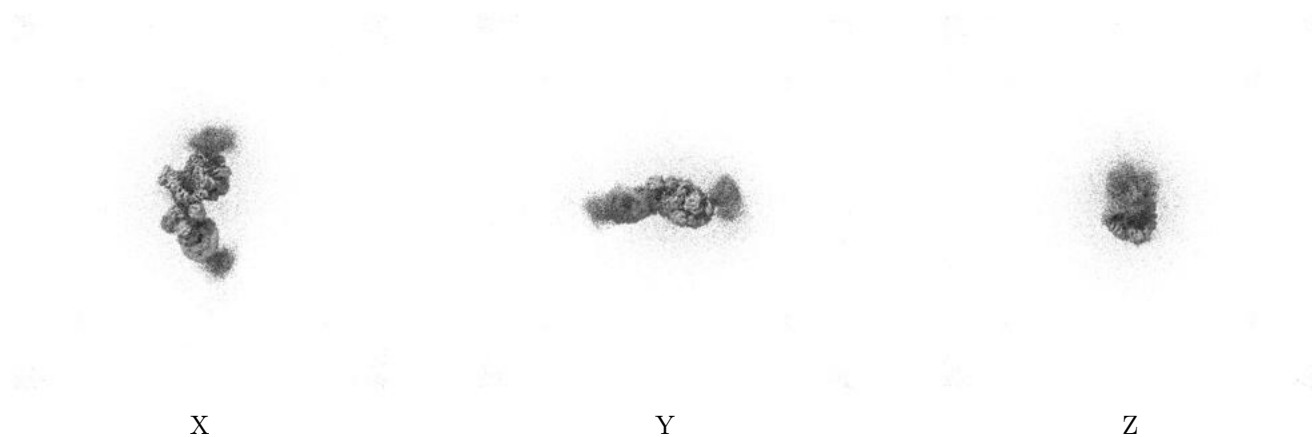
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

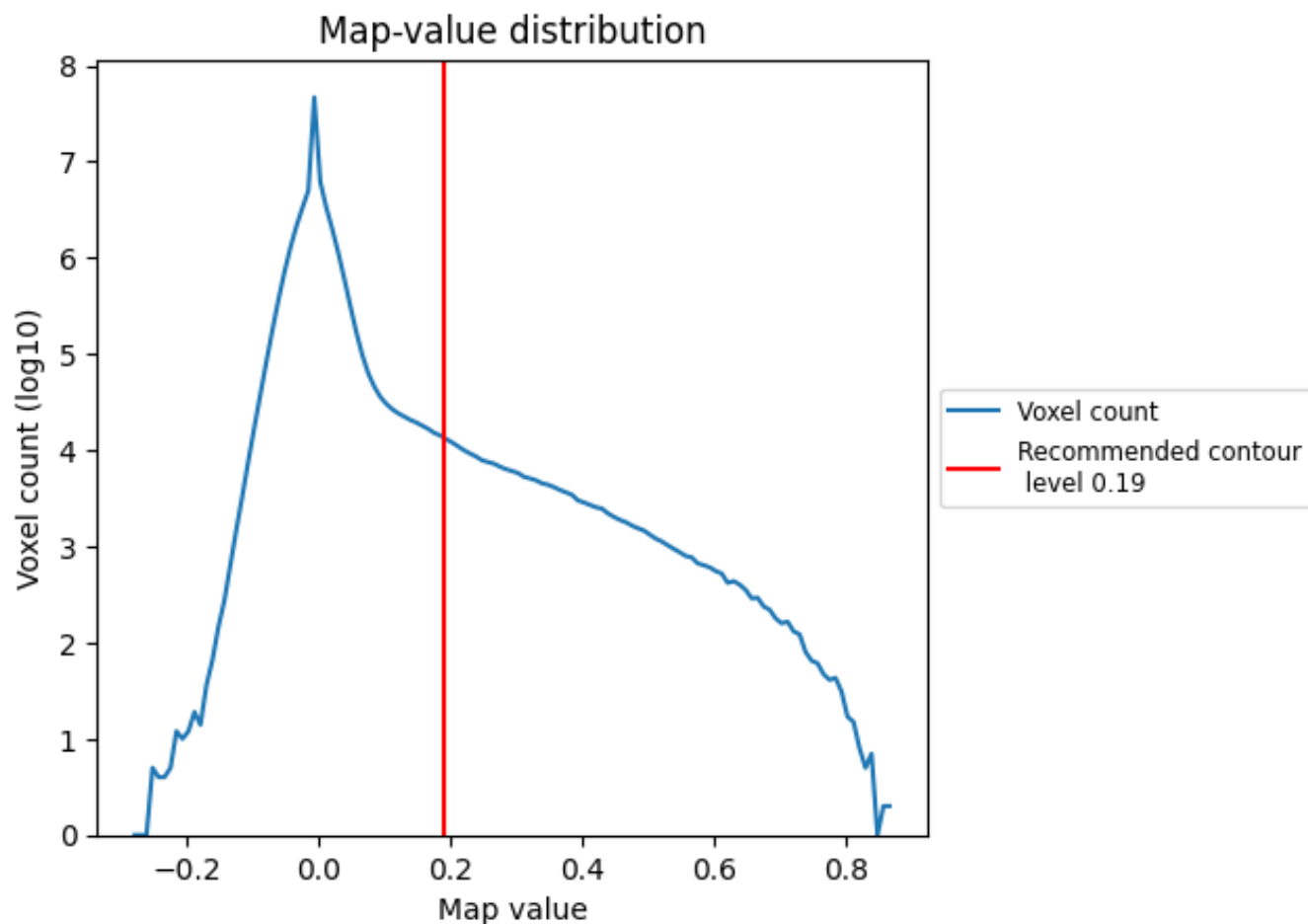
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

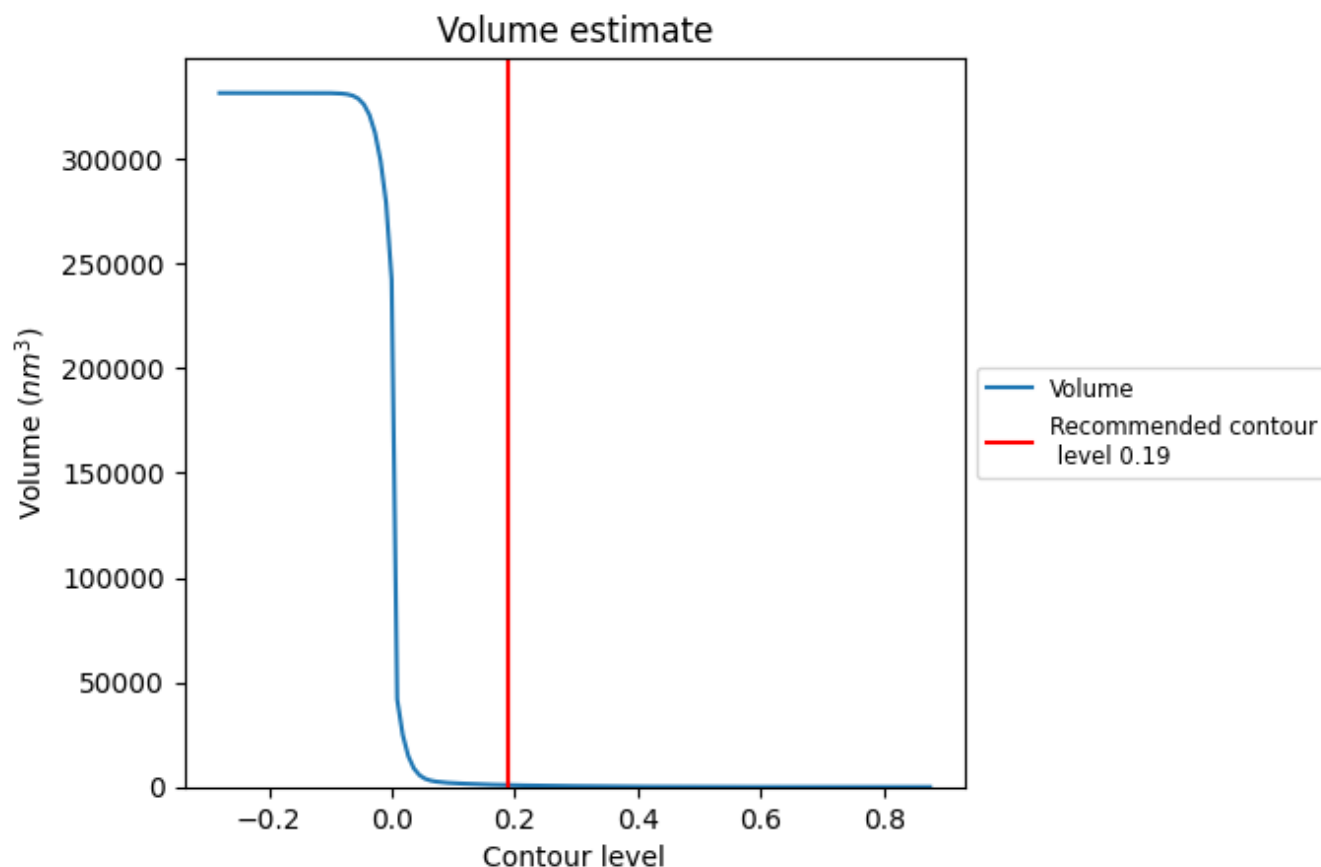
This section contains the results of statistical analysis of the map.

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.

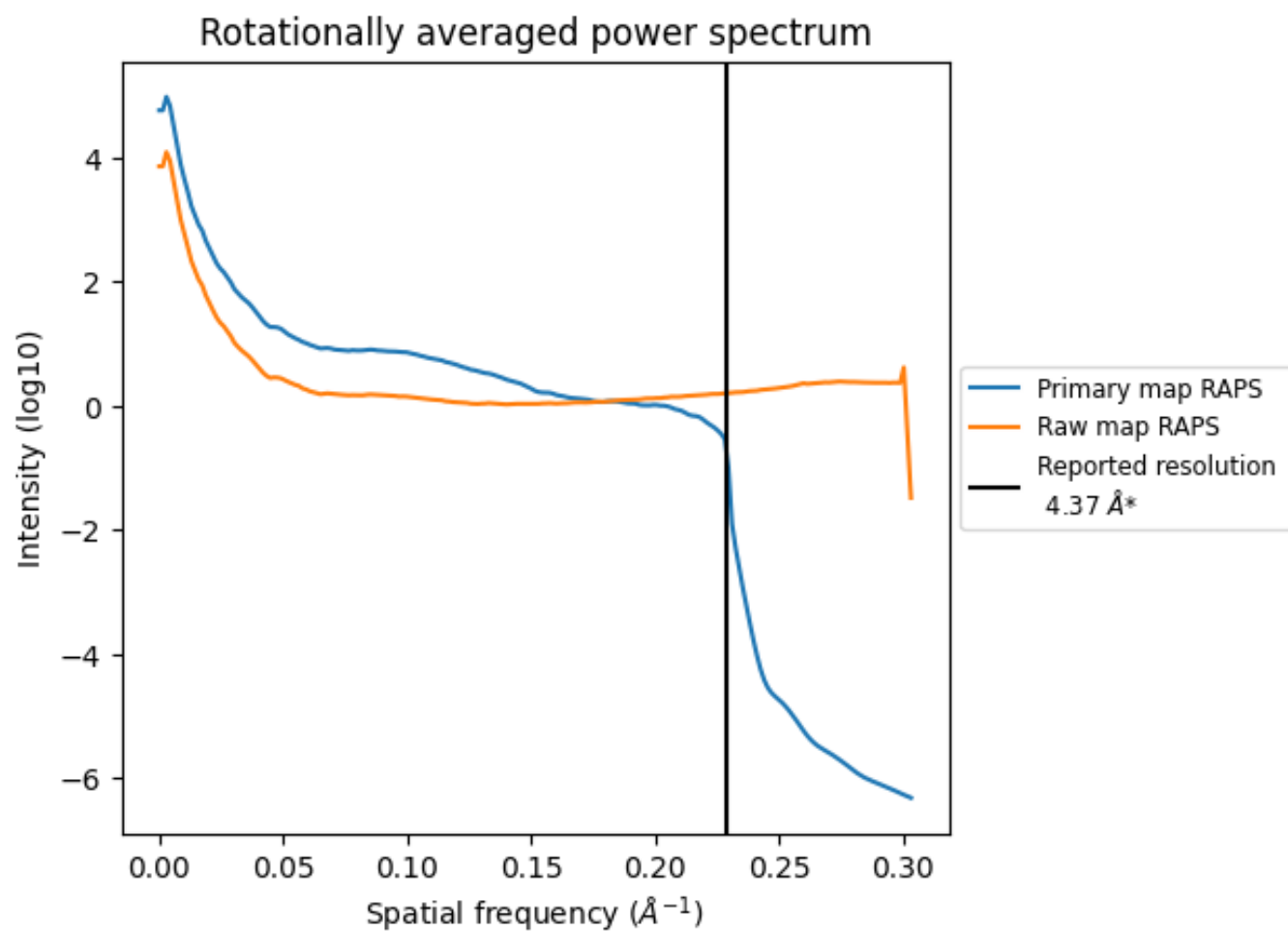
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 880 nm^3 ; this corresponds to an approximate mass of 795 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 ⓘ

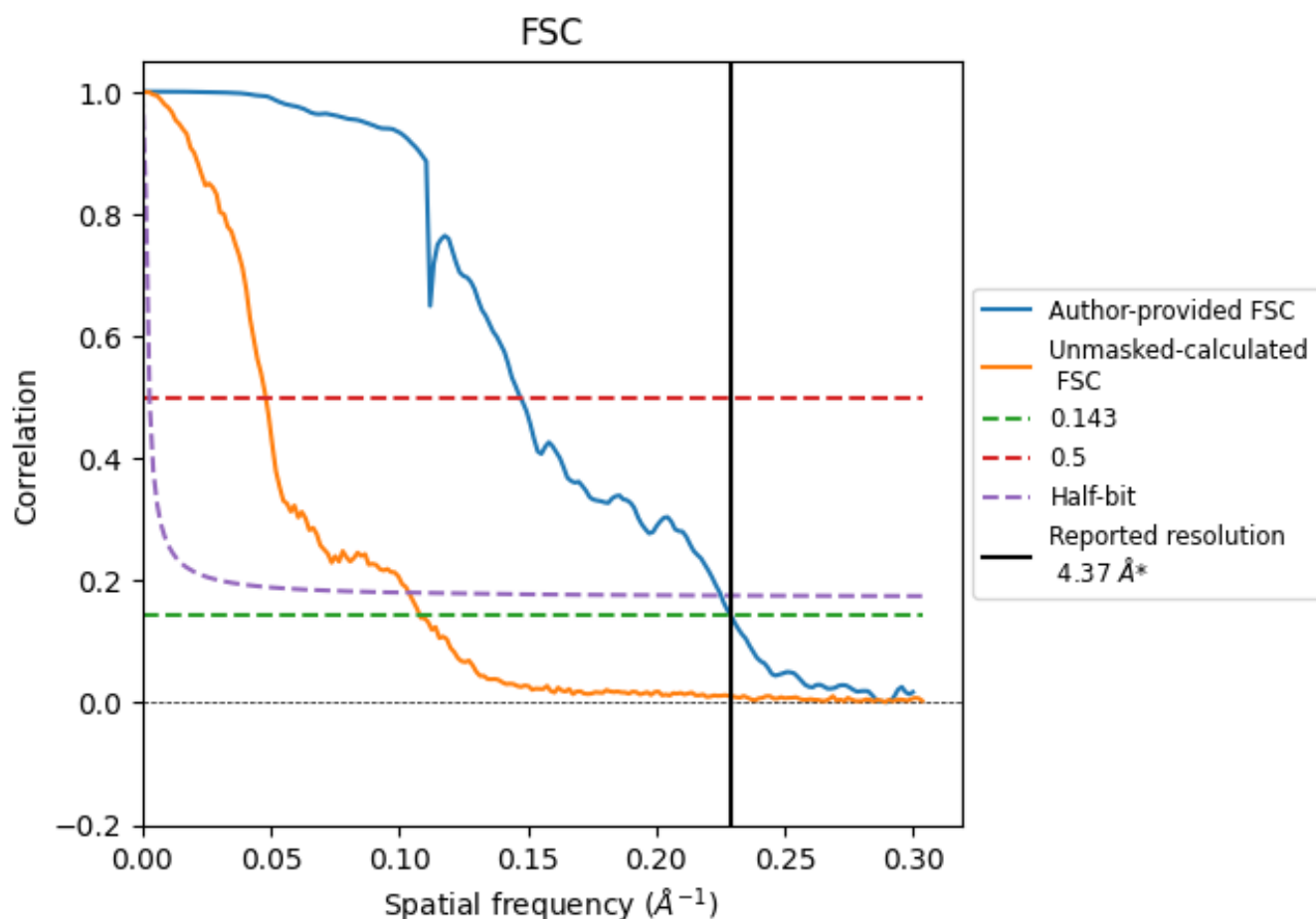


*Reported resolution corresponds to spatial frequency of 0.229 Å⁻¹

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 0.229 Å⁻¹

8.2 Resolution estimates [i](#)

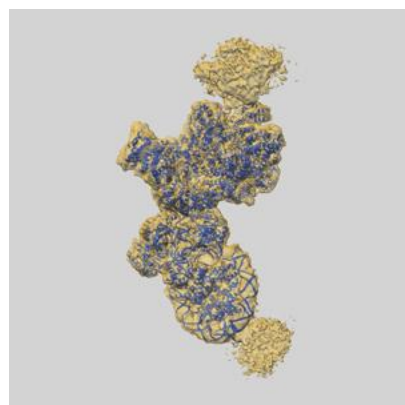
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.37	-	-
Author-provided FSC curve	4.37	6.80	4.44
Unmasked-calculated*	9.27	20.83	9.63

*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 9.27 differs from the reported value 4.37 by more than 10 %

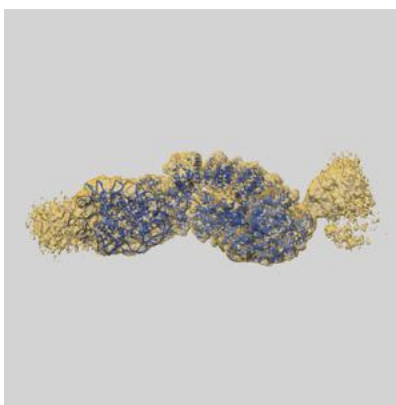
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53025 and PDB model 9QCR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

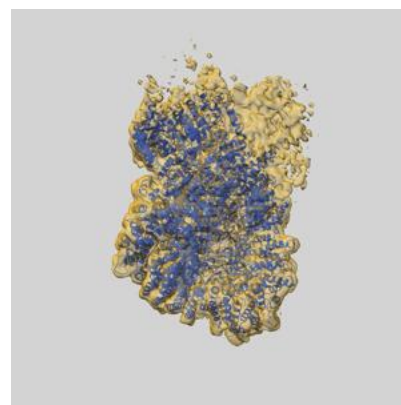
9.1 Map-model overlay [i](#)



X



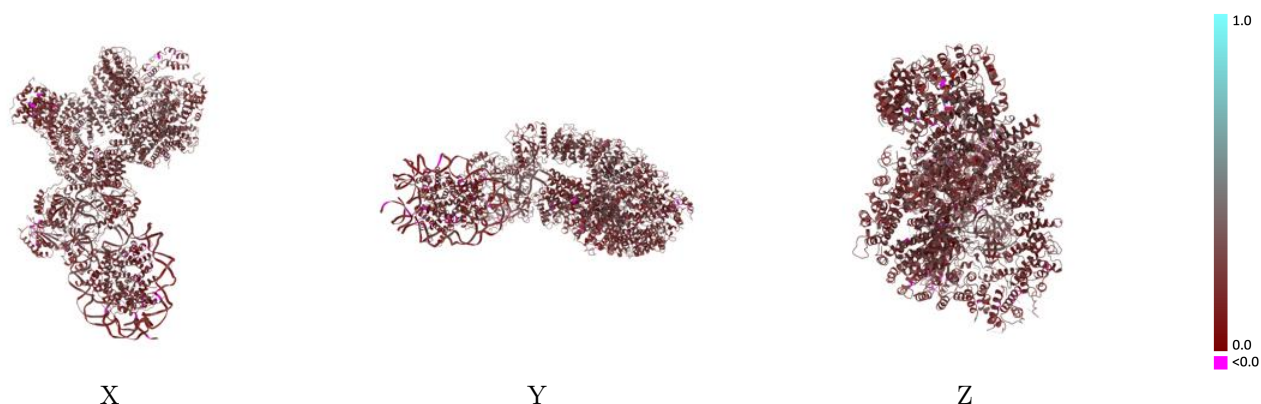
Y



Z

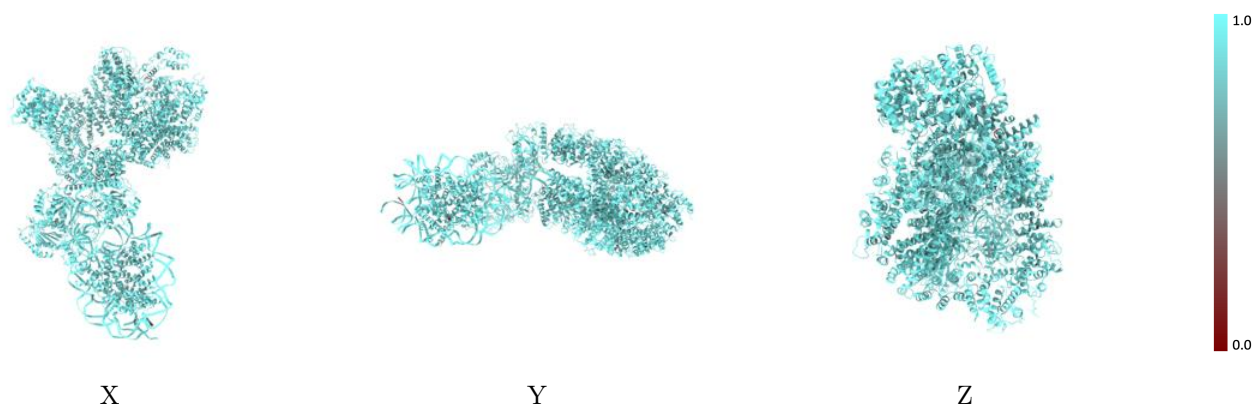
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



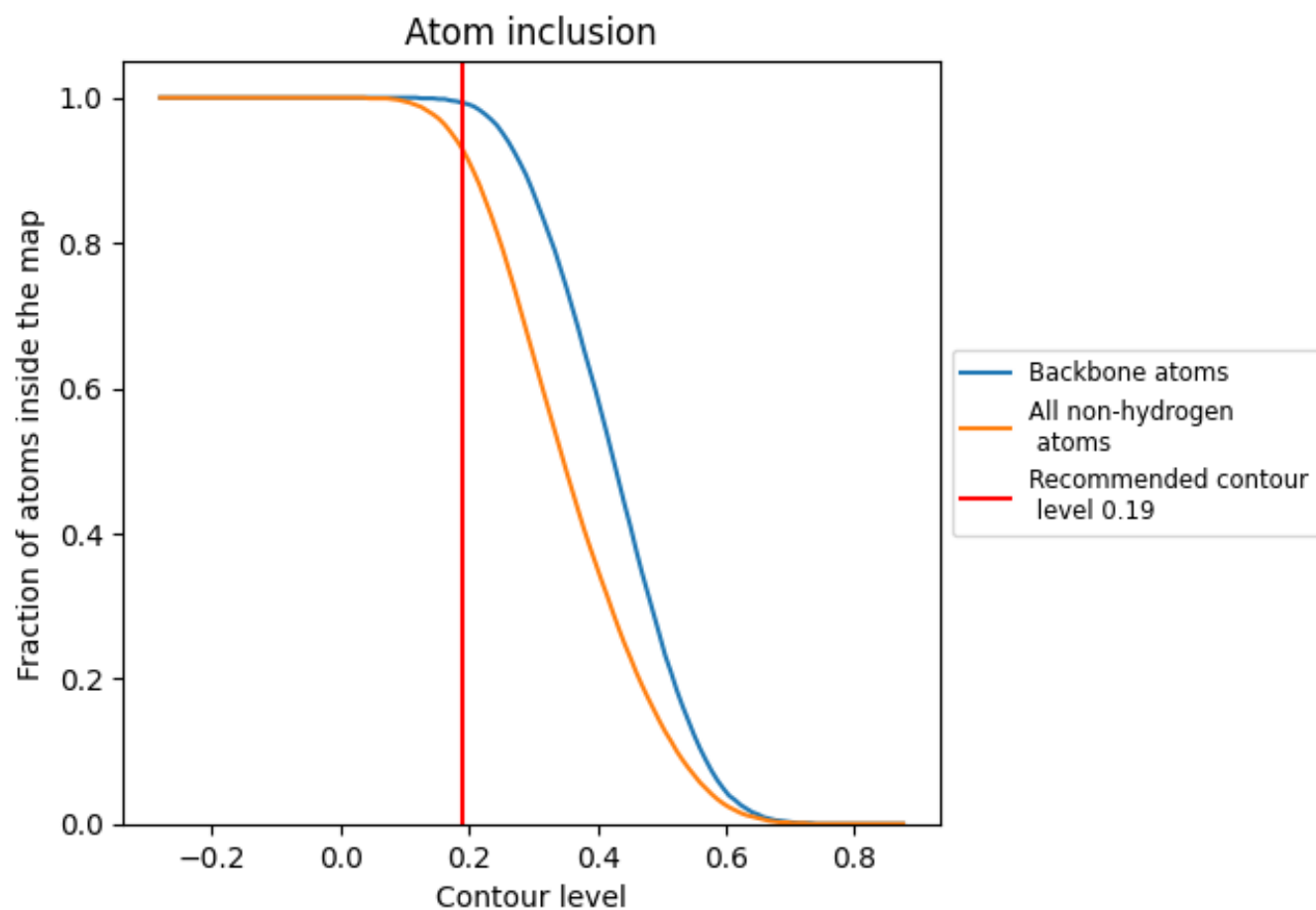
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.2340
A	 0.9520	 0.1650
B	 0.9440	 0.1770
C	 0.9430	 0.2150
D	 0.9520	 0.2240
E	 0.9650	 0.1840
F	 0.9620	 0.1930
G	 0.9440	 0.1620
H	 0.9090	 0.1850
I	 0.9730	 0.2120
J	 0.9620	 0.2030
K	 0.9360	 0.2470
L	 0.9460	 0.2260
O	 0.9140	 0.2470

