



Full wwPDB EM Validation Report ⓘ

Jul 28, 2025 – 01:29 pm BST

PDB ID : 9G9L / pdb_00009g9l
EMDB ID : EMD-51156
Title : DNA-PK + Polymerase lambda
Authors : Chaplin, A.K.; Amin, H.; Zahid, S.; Hardwick, S.W.
Deposited on : 2024-07-25
Resolution : 4.63 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

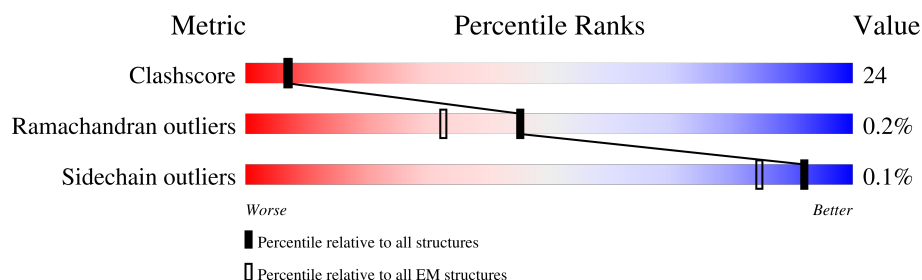
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4128	
2	B	609	
3	C	732	
4	F	575	
5	M	204	
6	D	24	
7	E	23	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 39800 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3688	Total	C	N	O	S	0	0
			29010	18609	4895	5318	188		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	488	Total	C	N	O	S	0	0
			3825	2453	645	709	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	647	Total	C	N	O	S	0	0
			5093	3248	849	970	26		

- Molecule 4 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	98	Total	C	N	O	S	0	0
			755	482	141	129	3		

- Molecule 5 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	23	Total	C	N	O	S	0	0
			155	99	25	30	1		

- Molecule 6 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	24	Total	C	N	O	P	0	0
			488	238	89	138	23		

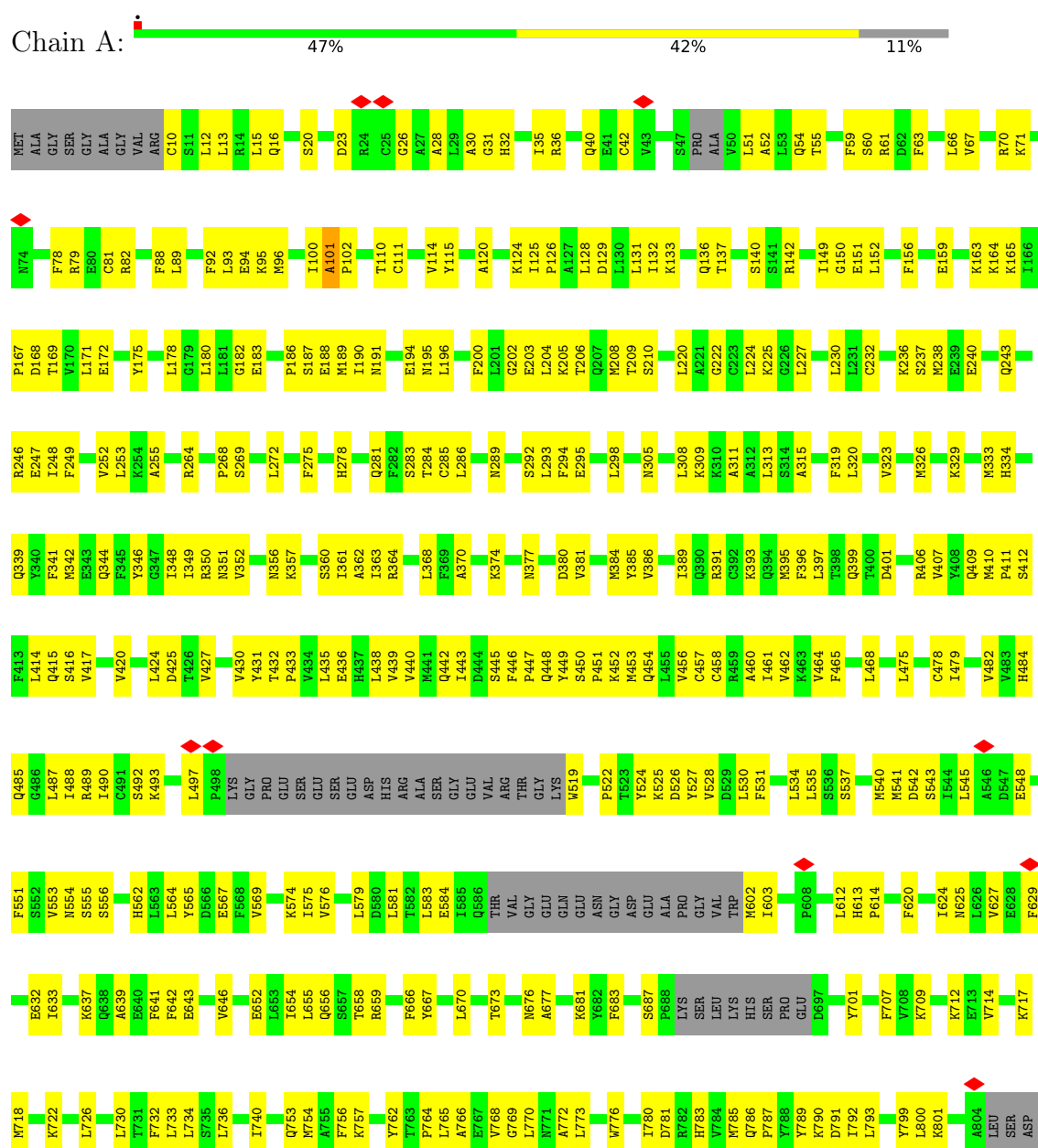
- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	23	Total	C	N	O	P	0	0
			474	230	79	142	23		

3 Residue-property plots

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

- Molecule 1: DNA-dependent protein kinase catalytic subunit

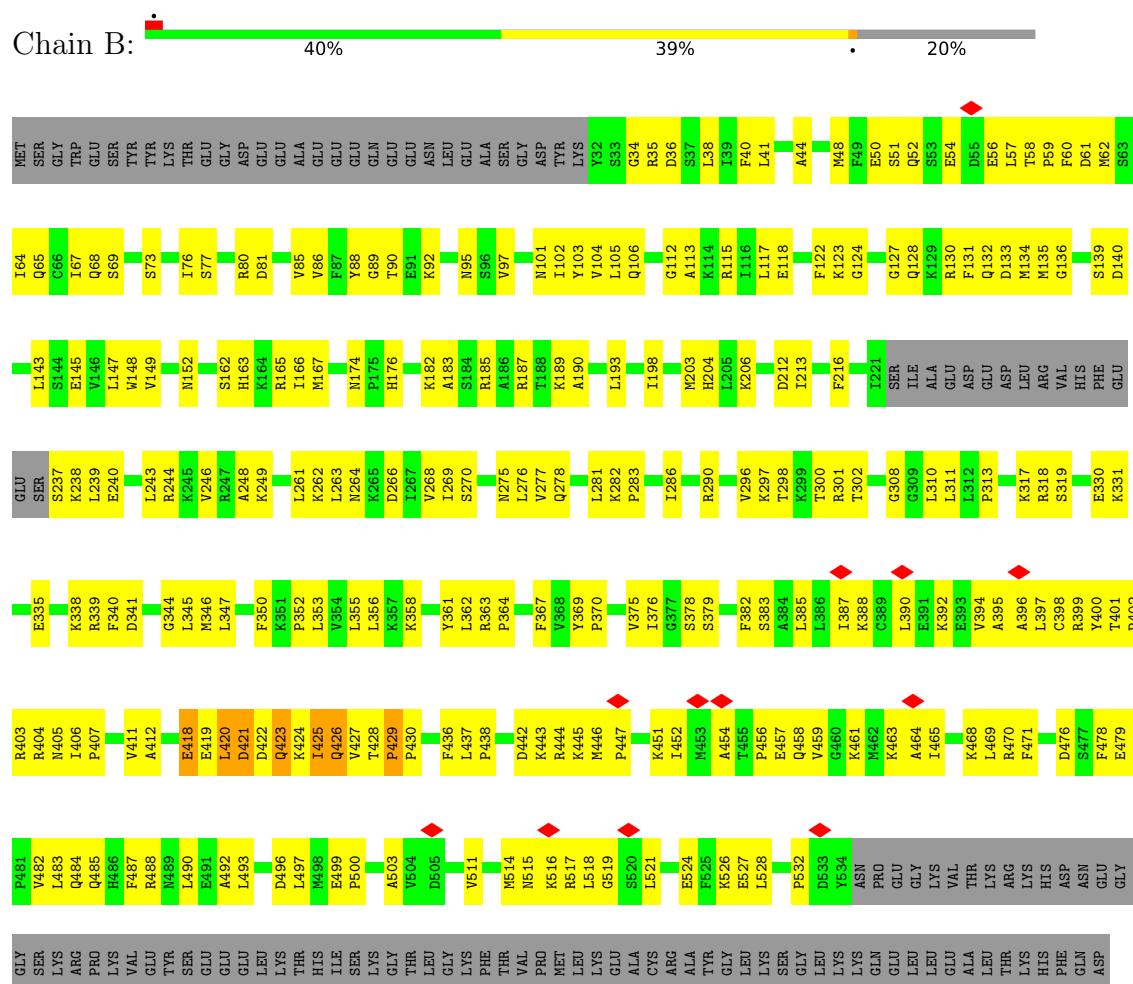


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E1860	F1778	H1687	M1593	G1514	E1421	T1345	F1271	H1185	F1106	P1020	M940	L871	LYS
L1861	Q1779	L1688	V1593	E1516	K1422	L1346	R1270	H1186	M1108	V1021	F940	ASN	ASN
F1862	S1780	K1689	V1596	L1517	T1423	L1347	R1271	S1187	E1109	D1022	M941	TRP	TRP
D1863	S1781	K1690	V1597	L1518	T1424	L1348	R1272	I1188	E1110	L1025	D877	GLU	GLU
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K1869	R1787	F1698	S1603	R1527	V1434	D1362	S1289	F1194	S1120	R1031	S882	ARG	ARG
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G1872	V1792	V1713	Q1614	V1537	Y1437	M1365	K1293	R1202	Q1126	F1036	V885	GLN	GLN
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P1810	R1811	R1811	V1645	H1555	Q1471	V1389	ALA	G1229	R1151	R1062	F906	LEU	LEU
L1812	S1812	S1812	L1648	Y1558	H1476	Q1390	ALA	G1230	R1152	L1066	C974	SER	SER
S1813	M1740	V1740	L1649	F1559	H1477	V1391	ALA	Q1231	P1154	P1070	F910	ASN	ASN
R1816	M1743	M1743	A1650	L1562	S1478	M1392	G1319	T1235	F1157	F1073	L911	A845	GLU
Q1817	D1748	D1748	K1651	L1563	V1479	A1393	R1320	T1236	L1163	K1074	P912	I846	THR
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D1821	P1756	P1756	Q1654	T1567	E1482	P1396	P1324	L1242	L1166	T915	T915	E849	ASN
R1822	L1757	L1757	I1655	L1567	L1483	P1397	Q1324	L1243	D1167	E916	E916	E850	ASN
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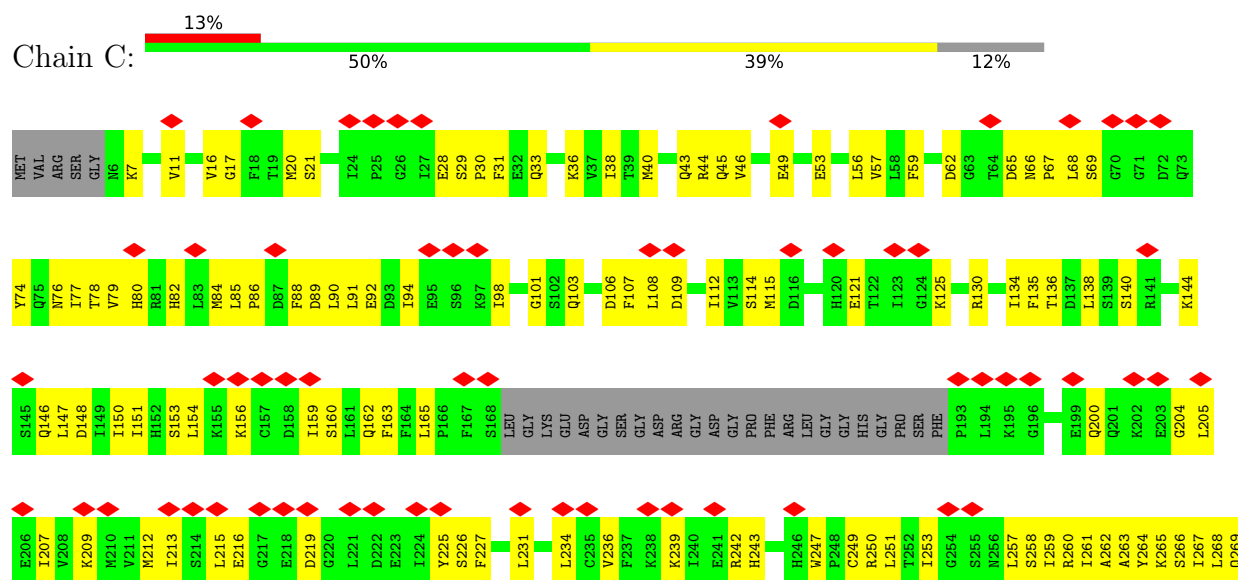
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		ALA	K2835	LYS	PRO	THR	M2565	R2485	E2321	T2153		ALA	
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		ARG	Q2838	GLU	PHE	GLN	D2570	R2404	Y2252	R2158		GLU	
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		LYS	D2919	LYS	ARG	PHE	N2574	S2495	E2410	F2257		GLY	
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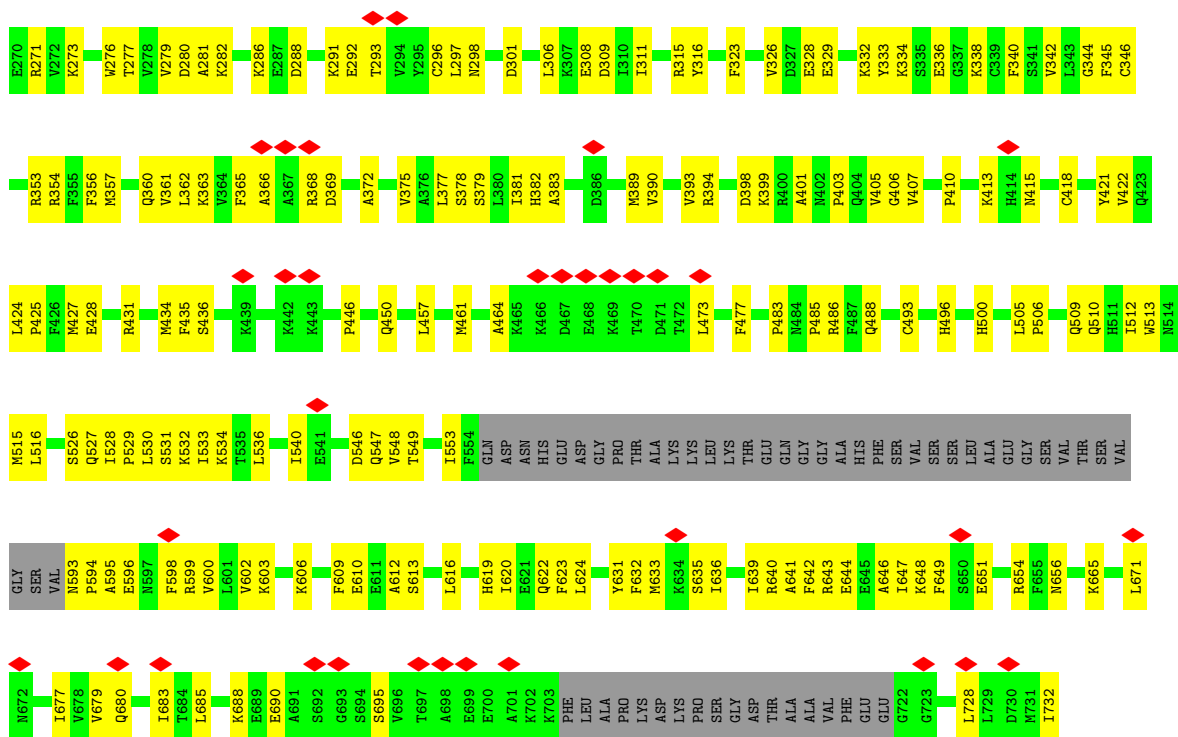
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	L4066	L3998	R3923	L3843	K3766	R3696	M3609	N3524		V3276	GLU	
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	H4068	N4000	L3925	K3845	K3769	E3698	R3612	P3526		Y3280	ASP	
	A4069	N3926	N3926	N3846	V3770	L3699	M3613	A3528			ASN	
	N4070	N3927	N3927	K3847	N3771	E3700		K3449		R3287	SER	
	K4071	F3928	F3928	G3848	N3772	T3701	K3621	V3530		Q3291	MET	
	A4072	V4004	V3929			P3702	A3622	P3532		K3380	ASN	
	P4073	V4005	V3930		L3775	G3703	P3623	F3533		S3294	VAL	
	F4074	A4006	A3931	K3856	L3786	Q3704	G3624			K3384	GLN	
		K4075	M3932	L3857	Q3787	Y3705	L3625			L3385	ASP	
	D4076	E4008	E3853	K3858	K3788	D3706	G3626			E3295	ASP	
	Y4077	P4009	T3934	K3859	K3789	G3707				Q3296	GLY	
		F4011	G3935	K3860	T3790	R3708				V3297	ASP	
	V4080	D4012	G3936	G3861	Y3791					L3298	PRO	
	A4081	K4013	V3937	K3862	Y3792	E3714	R3630			T3299	SER	
	R4082	K4014	I3938	N3863	V3793	Y3715	K3631			V3300	ARG	
		N4015	D3941	R3864	V3794	H3716	T3635			L3301	GLU	
		M4020	T3950	V3868	P3795	Y3717				V3304	MET	
		L4021	Q3951	R3872	N3796	R3718	K3638			Q3139	GLU	
		K4022	F3952			I3719	K3642			F3144		
		G4025	L3953	E3875	L3800	D3723	K3646			L3307	GLN	
		S4026	P3954	K3876	G3801	E3724	G3647			D3308	GLN	
		W4027	V3955	K3877	L3802	R3725				E3309	GLU	
		L4028	P3956	V3878	I3803	V3726	L3651			R3310	GLU	
			E3957	P3879	W3804	T3727	L3652			Y3315	D3226	
			L3958	A3880	W3805	V3728	R3653			S3229	S3229	
			P3959	D3881	E3807	M3729				L3290	L3290	
			M3960	L3882	N3808	A3730	Q3564			I3231	I3231	
			F3961	L3883	T3809					R3232	R3232	
			R3962	K3884	V3810		F3659			S3233	S3233	
			L3963	R3885			N3660			C3234	C3234	
			T3964	A3886	K3813		D3661			K3235	K3235	
			R3965	F3887	D3814		I3662			F3236	F3236	
			Q3966	V3888	L3815		T3663			S3237	S3237	
			F3967	R3889	L3816		N3664			M3238	M3238	
			I3968	N3890	L3817		M3665			R3335	R3335	
			N3969	S3891	N3818		L3666			A3171	A3171	
			L3870		T3819		L3667			M3240	M3240	
			M3971		K3820		L3668			K3241	K3241	
			R3972		S3821		K3669			I3337	I3337	
			P3973		E3742		M3670			A3340	A3340	
			K3974		H3743		N3671			Q3249	Q3249	
			S3975		E3744		K3672			F3252	F3252	
			K3975		E3745					S3343	S3343	
					R3746							

• Molecule 2: X-ray repair cross-complementing protein 6

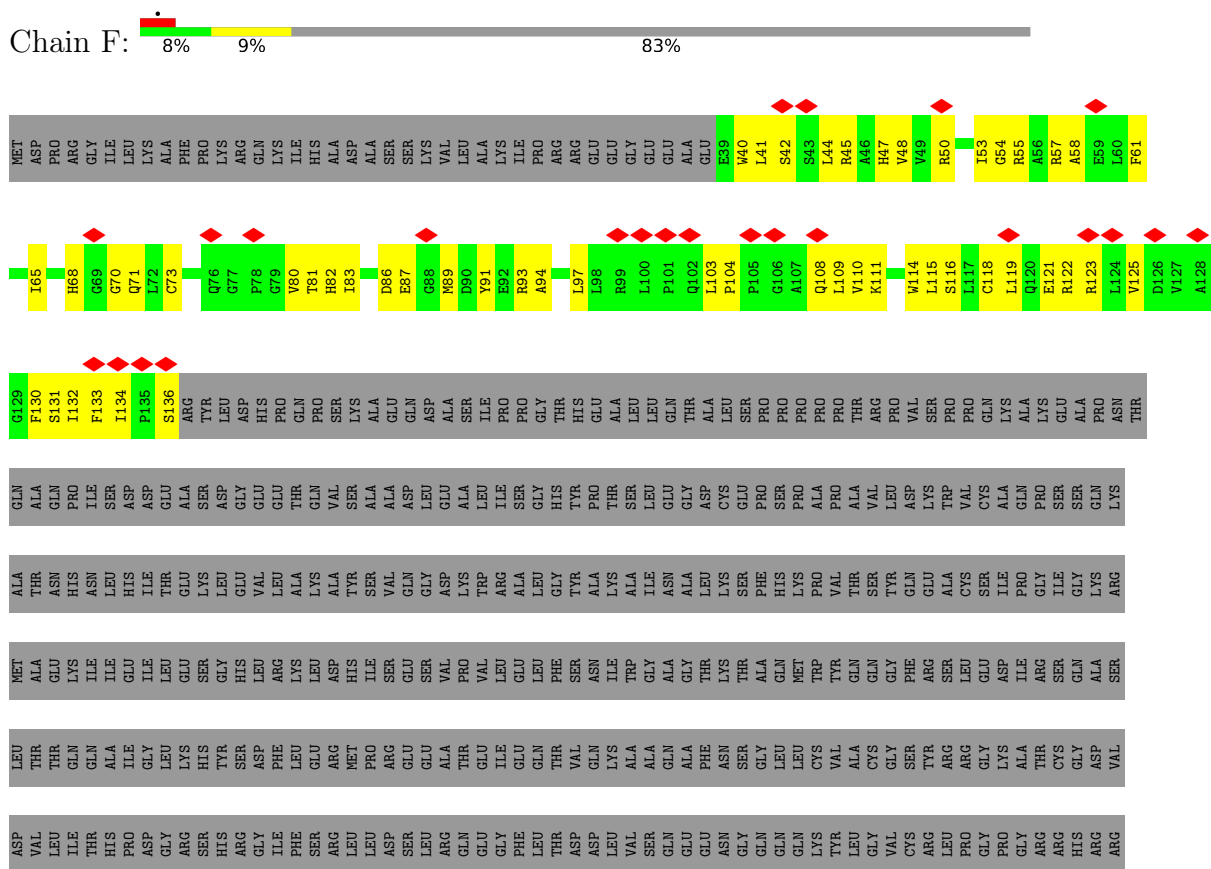


• Molecule 3: X-ray repair cross-complementing protein 5





- Molecule 4: DNA polymerase lambda

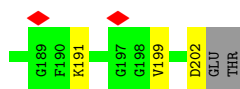


ARG	VAL	LEU	PRO	THR	THR	GLU	LYS	ASP	VAL	PHE	ARG	LEU	LEU	GLY	LEU	PRO	TYR	ARG	GLU	PRO	ALA	GLU	ARG	ASP	TRP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain M: 10% 89%

LYS ALA ARG ARG PHE GLY LEU SER SER ALA ALA ALA ALA ASP ASP THR THR PRO PRO ARG ARG PHE ARG ARG ARG ALA ALA ALA CYS GLU GLU GLN GLN VAL VAL ALA ALA LEU LEU THR THR LEU LEU GLN GLU GLU ASP ASP ARG ARG ALA ALA SER SER LEU LEU THR THR LEU LEU SER SER SER SER GLY GLY GLY PRO PRO SER SER ALA ALA LEU LEU ALA ALA PHE PHE ASP ASP LEU LEU SER SER LYS LYS VAL VAL PRO PRO GLY GLY PRO PRO GLU GLU ALA ALA ALA ALA PRO PRO

LEU	ARG	ALA	ALA	LEU	THR	LEU	GLY	LEU	ALA	ALA	LYS	ARG	VAL	TRP	SER	LEU	GLY	ARG	ARG	LEU	ALA	VAL	SER	PRO	ARG	LYS	SER	PRO	ARG	ARG	PRO	ALA	ALA	PRO	GLY	GLN	LEU	PHE	LEU	LEU	ASP	PRO	ASP	PRO	GLN	ARG	GLY	GLY	PRO	GLY	PRO	GLY	VAL	ARG	ARG	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



Chain D: 17% 83%

T20	A21		A24	A25	A26	C27	T28	A29	A30	A31	A32	A33	C34	T35	A36	T37	T38	A39	T40	T41	A42	T43
-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain E: 17% 83%

A15	A16	T17	A18	A19	T20	A21	G22	T23	T24	T25	T26	T27	A28	G29	T30	T31	T32	A33	T34	T35	A36	G37
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.96	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.640	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	417.28, 417.28, 417.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.18	0/29602	0.46	2/40074 (0.0%)
2	B	0.24	0/3900	0.49	2/5268 (0.0%)
3	C	0.15	0/5185	0.39	0/6998
4	F	0.27	0/771	0.50	0/1046
5	M	0.09	0/159	0.34	0/216
6	D	0.23	0/548	0.49	0/843
7	E	0.24	0/530	0.49	0/817
All	All	0.19	0/40695	0.46	4/55262 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	PRO	N-CA-CB	6.58	110.57	103.33
1	A	2297	SER	N-CA-C	-5.35	107.77	114.56
2	B	281	LEU	CA-C-N	5.24	130.90	120.94
2	B	281	LEU	C-N-CA	5.24	130.90	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29010	0	28916	1364	0
2	B	3825	0	3813	248	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5093	0	5039	247	0
4	F	755	0	767	54	0
5	M	155	0	135	3	0
6	D	488	0	275	39	0
7	E	474	0	266	29	0
All	All	39800	0	39211	1882	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1882) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LEU:HA	2:B:426:GLN:CA	1.78	1.12
2:B:420:LEU:CA	2:B:426:GLN:HA	1.79	1.11
1:A:3226:ASP:N	1:A:3229:SER:HG	1.69	0.89
1:A:3868:VAL:HG12	1:A:3872:ARG:HE	1.38	0.88
2:B:407:PRO:HG2	3:C:486:ARG:HD2	1.54	0.88
1:A:2806:LYS:HG2	1:A:2857:CYS:HB3	1.54	0.87
3:C:362:LEU:H	3:C:421:TYR:HB3	1.39	0.87
1:A:924:ARG:HH12	1:A:2769:VAL:HG12	1.40	0.87
1:A:865:GLN:HB3	1:A:3170:ASP:HB2	1.56	0.87
1:A:252:VAL:HA	3:C:553:ILE:HD11	1.54	0.86
2:B:35:ARG:H	2:B:162:SER:H	1.23	0.84
2:B:457:GLU:HG3	2:B:458:GLN:HE21	1.44	0.83
1:A:1766:LEU:HD13	1:A:1778:PHE:HD2	1.43	0.82
3:C:690:GLU:H	3:C:695:SER:HB3	1.43	0.82
6:D:42:DA:H2'	7:E:16:DA:N3	1.95	0.82
1:A:1359:LEU:H	1:A:1361:LYS:HZ3	1.23	0.81
1:A:3999:THR:HA	1:A:4002:MET:HE2	1.62	0.81
1:A:3503:VAL:O	1:A:3506:LEU:HB2	1.81	0.80
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	1.64	0.80
1:A:3729:MET:HE1	1:A:3737:ARG:HG2	1.65	0.79
2:B:379:SER:HA	2:B:382:PHE:HB2	1.65	0.79
1:A:1179:PRO:HA	1:A:1262:ALA:HB2	1.65	0.79
1:A:60:SER:HA	1:A:63:PHE:HB3	1.66	0.78
1:A:2873:PRO:HB2	1:A:2925:GLU:HG3	1.66	0.78
1:A:3593:ARG:HD2	1:A:3660:ASN:HB2	1.66	0.78
2:B:345:LEU:HB3	2:B:400:TYR:HD1	1.50	0.77
3:C:361:VAL:HG13	3:C:421:TYR:H	1.49	0.77
2:B:261:LEU:HB3	2:B:269:ILE:HG22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:406:GLY:HA2	3:C:424:LEU:HD23	1.67	0.77
1:A:447:PRO:HG3	1:A:522:PRO:HB3	1.67	0.77
1:A:2455:LEU:HD21	1:A:2501:LEU:HD23	1.67	0.77
1:A:1328:GLU:HG2	1:A:1329:ARG:HE	1.50	0.76
2:B:318:ARG:HD2	3:C:276:TRP:HB3	1.68	0.76
1:A:3503:VAL:HA	1:A:3506:LEU:HD23	1.66	0.76
4:F:45:ARG:HB2	4:F:81:THR:H	1.49	0.76
4:F:110:VAL:HA	4:F:131:SER:HA	1.69	0.75
2:B:51:SER:HA	2:B:58:THR:HG22	1.65	0.75
2:B:261:LEU:O	2:B:268:VAL:HA	1.86	0.75
1:A:1452:VAL:HA	1:A:1517:LEU:HD11	1.67	0.74
1:A:3235:LYS:HA	1:A:3238:MET:HE2	1.68	0.74
1:A:255:ALA:HB3	3:C:553:ILE:HD12	1.67	0.74
1:A:3130:GLN:HB3	1:A:3178:ILE:HG12	1.70	0.74
1:A:2405:VAL:HG21	1:A:2441:LYS:HG3	1.70	0.74
1:A:2538:ARG:NH1	1:A:2565:MET:SD	2.61	0.74
1:A:264:ARG:HB3	1:A:305:ASN:HB2	1.70	0.74
1:A:1976:LEU:HD13	1:A:2145:PHE:HD2	1.52	0.74
1:A:2891:ARG:HH22	1:A:3898:LEU:HB3	1.50	0.74
1:A:3240:MET:HE3	1:A:3262:LEU:HD22	1.69	0.74
1:A:1890:HIS:H	1:A:1894:SER:HB2	1.52	0.73
3:C:59:PHE:HB3	3:C:77:ILE:HD13	1.70	0.73
1:A:93:LEU:O	1:A:136:GLN:NE2	2.20	0.73
1:A:1070:PRO:HD3	1:A:3741:ARG:HH11	1.52	0.73
1:A:1384:PHE:HB2	1:A:1386:ILE:HG23	1.68	0.73
1:A:2411:LEU:HD21	1:A:2442:MET:HB2	1.70	0.73
1:A:551:PHE:HA	1:A:554:ASN:HB3	1.71	0.73
1:A:4082:ARG:HH12	1:A:4091:ALA:HA	1.54	0.73
3:C:493:CYS:HA	3:C:506:PRO:HD2	1.71	0.73
6:D:28:DT:O2	7:E:29:DG:N2	2.20	0.73
1:A:3104:GLN:O	1:A:3108:GLN:NE2	2.21	0.73
2:B:64:ILE:HG22	2:B:68:GLN:HE22	1.53	0.73
2:B:521:LEU:HA	2:B:524:GLU:HG2	1.70	0.73
1:A:714:VAL:HG13	1:A:733:LEU:HD11	1.69	0.73
1:A:3518:VAL:HA	1:A:3521:ILE:HG22	1.69	0.73
1:A:734:LEU:HD21	1:A:769:GLY:HA2	1.71	0.73
2:B:296:VAL:HA	3:C:298:ASN:H	1.54	0.73
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.70	0.72
1:A:1872:GLY:HA2	1:A:1875:LYS:HE2	1.70	0.72
1:A:881:LYS:HG2	1:A:883:TYR:H	1.55	0.72
1:A:1222:ASN:O	1:A:1231:GLN:NE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:ARG:H	5:M:202:ASP:H	1.36	0.72
2:B:61:ASP:O	2:B:65:GLN:NE2	2.22	0.72
1:A:222:GLY:HA2	1:A:225:LYS:HD2	1.71	0.72
1:A:2411:LEU:HA	1:A:2414:GLN:NE2	2.05	0.72
1:A:2589:TYR:HB2	1:A:2777:HIS:HB2	1.70	0.72
3:C:602:VAL:O	3:C:606:LYS:N	2.21	0.72
3:C:251:LEU:HA	3:C:340:PHE:HB2	1.72	0.71
1:A:1981:LEU:HB3	1:A:1984:LEU:HD21	1.71	0.71
1:A:3380:ARG:O	1:A:3384:HIS:ND1	2.21	0.71
1:A:2547:SER:HB3	1:A:2550:ILE:HG12	1.73	0.71
1:A:2504:ASP:O	1:A:2508:GLN:NE2	2.24	0.71
1:A:3707:GLY:O	1:A:3708:ARG:NH1	2.23	0.71
1:A:1436:LEU:O	1:A:1445:ARG:NH2	2.23	0.71
1:A:2271:SER:HB3	1:A:2315:VAL:HG12	1.72	0.71
3:C:640:ARG:HG3	3:C:685:LEU:HD12	1.71	0.71
1:A:2432:GLN:NE2	1:A:2469:CYS:SG	2.64	0.70
1:A:2219:LEU:O	1:A:2223:VAL:N	2.24	0.70
1:A:4006:VAL:HG22	1:A:4040:PRO:HB3	1.72	0.70
1:A:2330:VAL:C	1:A:2332:GLU:H	1.99	0.70
1:A:3183:ILE:HG13	1:A:3242:MET:HE3	1.73	0.70
2:B:528:LEU:HB3	3:C:372:ALA:HB1	1.72	0.70
1:A:3502:MET:O	1:A:3505:LEU:HB3	1.91	0.70
1:A:1927:MET:HE1	1:A:1974:ASN:HB2	1.73	0.70
1:A:2896:ALA:O	1:A:2900:LEU:HB2	1.92	0.70
1:A:3028:ASN:OD1	1:A:3029:LYS:N	2.22	0.70
1:A:2869:LEU:HD23	1:A:2892:LEU:HD12	1.74	0.70
1:A:2895:GLU:HA	1:A:2898:LEU:HG	1.74	0.70
1:A:1239:PRO:HB2	1:A:1292:LYS:HD2	1.73	0.69
2:B:73:SER:HB3	2:B:244:ARG:HH22	1.57	0.69
1:A:4035:GLU:OE1	1:A:4038:TRP:N	2.22	0.69
1:A:4113:ASP:HB3	1:A:4116:ILE:HD13	1.74	0.69
1:A:1982:ILE:HG23	1:A:2090:ARG:HD3	1.74	0.69
1:A:2254:ARG:HH21	1:A:2293:GLY:H	1.38	0.69
1:A:1764:GLU:HA	1:A:1819:PHE:HE1	1.57	0.69
1:A:3817:LEU:HD22	1:A:3825:LYS:HG3	1.74	0.69
1:A:433:PRO:O	1:A:436:GLU:HG3	1.93	0.69
1:A:895:ALA:HB1	1:A:902:LYS:HB3	1.73	0.69
1:A:1022:ASP:HB3	1:A:1025:LEU:HB3	1.74	0.69
1:A:1101:PHE:HB3	1:A:1154:PRO:HG3	1.75	0.69
1:A:1441:ALA:O	1:A:1445:ARG:NH1	2.25	0.69
3:C:407:VAL:HG12	3:C:424:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:PHE:HZ	1:A:707:PHE:HD2	1.37	0.68
1:A:1765:VAL:HA	1:A:1768:ARG:HH21	1.59	0.68
2:B:86:VAL:HG23	2:B:104:VAL:HG12	1.74	0.68
1:A:2893:LEU:HD21	1:A:2922:ARG:HB3	1.74	0.68
1:A:2840:PHE:HB2	1:A:2871:LEU:HD11	1.74	0.68
1:A:4090:ARG:N	1:A:4109:ASP:OD2	2.26	0.68
1:A:528:VAL:HA	1:A:633:ILE:HD11	1.75	0.68
1:A:1313:PHE:O	1:A:1319:GLY:N	2.26	0.68
2:B:383:SER:HB2	3:C:446:PRO:HD3	1.75	0.68
1:A:180:LEU:HA	1:A:230:LEU:HG	1.75	0.68
1:A:2820:MET:HE1	1:A:2829:LYS:HG2	1.76	0.68
3:C:20:MET:HE2	3:C:30:PRO:HG2	1.75	0.68
1:A:1178:ARG:HG2	1:A:1180:GLN:H	1.59	0.68
1:A:3716:HIS:O	1:A:3718:ARG:NH1	2.26	0.68
1:A:1102:GLU:HG3	1:A:1154:PRO:HA	1.76	0.67
1:A:3924:HIS:HE1	1:A:3926:ASN:HB2	1.59	0.67
1:A:913:ARG:HE	1:A:2803:ILE:HD11	1.59	0.67
1:A:3443:PRO:HA	1:A:3446:VAL:HG12	1.75	0.67
1:A:3183:ILE:HG23	1:A:3238:MET:HG3	1.77	0.67
1:A:4082:ARG:NH1	1:A:4091:ALA:HA	2.08	0.67
1:A:3751:LEU:HB3	1:A:3803:ILE:HG23	1.77	0.67
1:A:205:LYS:O	1:A:209:THR:N	2.26	0.67
1:A:1368:LEU:HG	1:A:1372:LEU:HD23	1.76	0.67
6:D:42:DA:N3	7:E:16:DA:H2'	2.10	0.67
1:A:3588:TRP:CD1	1:A:3613:MET:HE3	2.30	0.67
1:A:3680:LEU:HD12	1:A:3682:GLU:HG2	1.76	0.67
1:A:3796:MET:HE1	1:A:3802:LEU:HD23	1.75	0.67
1:A:1766:LEU:HD13	1:A:1778:PHE:CD2	2.29	0.67
6:D:35:DT:H2'	6:D:36:DA:C8	2.30	0.67
1:A:2803:ILE:HG22	1:A:2806:LYS:HD3	1.77	0.66
2:B:76:ILE:HD12	2:B:248:ALA:H	1.58	0.66
1:A:1772:HIS:HD2	1:A:1822:ARG:HH22	1.41	0.66
1:A:3924:HIS:HB3	1:A:4125:GLU:OE2	1.94	0.66
1:A:2216:LEU:HD22	1:A:2249:LEU:HD23	1.77	0.66
2:B:421:ASP:HB3	2:B:425:ILE:O	1.95	0.66
1:A:753:GLN:NE2	1:A:791:ASP:O	2.29	0.66
1:A:1572:LEU:HD11	1:A:1603:GLN:HG2	1.78	0.66
1:A:4054:ALA:HA	1:A:4096:SER:HA	1.78	0.66
1:A:16:GLN:O	1:A:20:SER:N	2.24	0.66
1:A:1775:GLU:OE2	1:A:1822:ARG:NH2	2.29	0.66
2:B:456:PRO:HA	2:B:459:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:ILE:HG23	1:A:1036:PHE:HD1	1.61	0.66
1:A:1784:ARG:HB3	1:A:1788:ARG:HH21	1.60	0.66
1:A:1985:LYS:HZ3	1:A:2180:GLU:HG2	1.61	0.66
2:B:490:LEU:HB3	3:C:316:TYR:HE2	1.61	0.66
3:C:66:ASN:ND2	3:C:68:LEU:O	2.29	0.66
3:C:483:PRO:HG2	3:C:488:GLN:HE22	1.62	0.65
1:A:1373:VAL:HG11	1:A:1422:LYS:HE2	1.78	0.65
1:A:3583:LEU:HD13	1:A:3733:ARG:HD3	1.78	0.65
2:B:290:ARG:NH1	3:C:308:GLU:O	2.27	0.65
2:B:427:VAL:O	2:B:428:THR:C	2.40	0.65
7:E:31:DT:C6	7:E:32:DT:H72	2.30	0.65
3:C:279:VAL:HG12	3:C:286:LYS:HD3	1.79	0.65
1:A:3168:TYR:CZ	1:A:3241:LYS:HE2	2.32	0.65
1:A:2252:PRO:O	1:A:2291:GLN:NE2	2.30	0.65
4:F:87:GLU:HA	4:F:132:ILE:HD12	1.78	0.65
1:A:2260:PHE:O	1:A:2306:ASN:ND2	2.30	0.65
1:A:2410:GLU:OE2	1:A:2413:PHE:N	2.28	0.65
3:C:728:LEU:HA	3:C:732:ILE:HA	1.79	0.65
1:A:1933:LEU:HG	1:A:1937:ARG:HB2	1.78	0.65
2:B:77:SER:HB3	2:B:249:LYS:HG3	1.79	0.65
4:F:48:VAL:HG21	4:F:61:PHE:HB3	1.78	0.65
7:E:30:DT:H2'	7:E:31:DT:C6	2.32	0.65
1:A:3518:VAL:HG22	1:A:3522:THR:HB	1.77	0.64
1:A:3624:GLY:HA2	1:A:3686:TRP:H	1.62	0.64
2:B:263:LEU:HA	2:B:347:LEU:HB3	1.78	0.64
1:A:1371:VAL:O	1:A:1374:GLN:HG3	1.97	0.64
1:A:2404:ARG:HH21	1:A:2406:GLU:HB2	1.63	0.64
2:B:458:GLN:HA	2:B:461:LYS:HE3	1.79	0.64
1:A:989:MET:HG3	1:A:993:HIS:CE1	2.31	0.64
2:B:278:GLN:HG2	3:C:431:ARG:HH12	1.63	0.64
1:A:3879:PRO:O	1:A:3966:GLN:NE2	2.29	0.64
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.30	0.64
2:B:445:LYS:N	3:C:242:ARG:O	2.30	0.64
1:A:3492:CYS:SG	1:A:3524:ASN:ND2	2.70	0.64
1:A:4037:ASN:HD22	1:A:4066:LEU:HD22	1.62	0.64
4:F:45:ARG:NE	4:F:81:THR:OG1	2.28	0.64
1:A:238:MET:SD	1:A:284:THR:OG1	2.56	0.64
1:A:722:LYS:O	1:A:726:LEU:N	2.26	0.64
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.78	0.64
1:A:92:PHE:HD1	1:A:96:MET:HE3	1.63	0.64
2:B:290:ARG:HH21	3:C:311:ILE:HD13	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3891:SER:HB2	1:A:3900:LEU:HD21	1.78	0.64
1:A:4014:LYS:HZ2	1:A:4033:VAL:HG12	1.63	0.64
3:C:378:SER:O	3:C:382:HIS:ND1	2.30	0.63
2:B:350:PHE:HB2	3:C:461:MET:HG3	1.81	0.63
2:B:468:LYS:HE3	2:B:521:LEU:HD21	1.80	0.63
1:A:1767:CYS:HA	1:A:1822:ARG:HH11	1.63	0.63
1:A:2205:VAL:HG12	1:A:2207:LYS:H	1.63	0.63
1:A:2365:ASN:OD1	1:A:2366:LYS:NZ	2.29	0.63
2:B:35:ARG:HG3	2:B:80:ARG:HE	1.63	0.63
1:A:2437:ASP:O	1:A:2441:LYS:HG2	1.99	0.63
4:F:40:TRP:HZ2	4:F:119:LEU:HA	1.63	0.63
1:A:2978:LYS:HE2	1:A:2981:TRP:HA	1.81	0.63
1:A:1115:HIS:CD2	1:A:1181:THR:H	2.17	0.63
1:A:2161:ALA:HA	1:A:2164:TRP:HB2	1.80	0.63
1:A:2543:ASN:ND2	1:A:2839:ASP:OD2	2.31	0.63
1:A:3183:ILE:HD12	1:A:3238:MET:HB2	1.81	0.63
1:A:1860:GLU:HG2	1:A:1862:THR:H	1.63	0.63
1:A:2357:GLU:O	1:A:2361:ILE:N	2.32	0.63
1:A:286:LEU:HD12	1:A:319:PHE:HD1	1.64	0.63
1:A:1147:LYS:HZ2	1:A:1149:LYS:HG2	1.64	0.63
4:F:54:GLY:H	4:F:57:ARG:HE	1.45	0.63
4:F:83:ILE:HD11	4:F:104:PRO:HG2	1.81	0.63
1:A:187:SER:O	1:A:191:ASN:ND2	2.33	0.62
1:A:1519:PHE:HE2	1:A:1566:THR:HB	1.65	0.62
2:B:444:ARG:N	3:C:266:SER:O	2.31	0.62
1:A:524:TYR:HB2	1:A:629:PHE:HD1	1.65	0.62
2:B:128:GLN:HG2	2:B:132:GLN:HE21	1.64	0.62
1:A:3924:HIS:CE1	1:A:3926:ASN:HB2	2.33	0.62
1:A:1027:ASP:O	1:A:1031:ARG:HG2	2.00	0.62
1:A:1300:SER:HA	1:A:1304:HIS:HB2	1.82	0.62
1:A:1583:MET:HE1	1:A:1628:LYS:HB2	1.81	0.62
1:A:2140:LEU:HA	1:A:2143:ARG:HD3	1.82	0.62
2:B:301:ARG:NH2	2:B:311:LEU:O	2.33	0.62
1:A:2474:TYR:O	1:A:2478:MET:HG2	2.00	0.62
1:A:2586:PHE:CZ	1:A:2782:ASP:HB3	2.35	0.62
2:B:454:ALA:HB3	3:C:379:SER:HB2	1.81	0.62
1:A:3568:ILE:HD11	1:A:3697:ASN:HD21	1.65	0.62
1:A:3769:GLN:HA	1:A:3772:ASN:HD22	1.64	0.62
2:B:346:MET:N	2:B:399:ARG:O	2.32	0.62
1:A:488:ILE:HD11	1:A:575:ILE:HG12	1.82	0.62
1:A:2902:PRO:HG2	1:A:2919:ASP:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3499:ILE:HG12	1:A:3529:ILE:HG22	1.82	0.62
2:B:419:GLU:O	2:B:420:LEU:C	2.43	0.62
2:B:526:LYS:HE2	2:B:528:LEU:HD12	1.80	0.62
1:A:658:THR:HG21	1:A:1388:ASP:HB2	1.82	0.61
3:C:381:ILE:HB	3:C:410:PRO:HG3	1.82	0.61
6:D:37:DT:H2'	6:D:38:DT:C2	2.35	0.61
1:A:2411:LEU:HA	1:A:2414:GLN:HE21	1.64	0.61
1:A:3834:ALA:O	1:A:3838:GLU:N	2.23	0.61
3:C:21:SER:HA	3:C:31:PHE:HB3	1.80	0.61
3:C:595:ALA:HA	3:C:598:PHE:CE2	2.35	0.61
1:A:2571:ASP:O	1:A:2787:HIS:ND1	2.30	0.61
1:A:3796:MET:N	1:A:3796:MET:SD	2.73	0.61
4:F:89:MET:HB2	4:F:93:ARG:HG2	1.82	0.61
1:A:1868:THR:HA	1:A:1871:MET:HG3	1.83	0.61
1:A:3037:GLN:HA	1:A:3040:TYR:CD2	2.36	0.61
3:C:160:SER:HB2	3:C:239:LYS:HG2	1.82	0.61
1:A:2580:PRO:HA	1:A:2783:ILE:HG12	1.83	0.61
2:B:286:ILE:HD12	3:C:315:ARG:HB2	1.81	0.61
1:A:111:CYS:HA	1:A:114:VAL:HG22	1.82	0.61
1:A:1356:TRP:NE1	1:A:1358:LEU:O	2.34	0.61
1:A:3679:ASN:OD1	1:A:3726:VAL:N	2.27	0.61
1:A:602:MET:SD	1:A:1087:ARG:NH1	2.74	0.61
1:A:3758:LEU:HD21	1:A:3793:VAL:HB	1.81	0.61
1:A:939:MET:HE3	1:A:2783:ILE:HA	1.82	0.61
1:A:1363:LEU:HB3	1:A:1367:HIS:HE1	1.65	0.61
1:A:2551:GLU:OE2	1:A:2850:PHE:N	2.34	0.61
2:B:352:PRO:HA	2:B:394:VAL:HG22	1.83	0.61
2:B:421:ASP:H	2:B:427:VAL:H	1.47	0.61
3:C:450:GLN:NE2	3:C:536:LEU:O	2.30	0.61
1:A:564:LEU:O	1:A:567:GLU:HG2	2.01	0.60
1:A:790:LYS:HA	1:A:869:ASN:HB3	1.82	0.60
1:A:1686:LEU:HD12	1:A:1721:HIS:HB3	1.83	0.60
1:A:2550:ILE:HB	1:A:2553:HIS:CE1	2.36	0.60
1:A:3030:ILE:O	1:A:3037:GLN:NE2	2.34	0.60
7:E:23:DT:H2'	7:E:24:DT:H71	1.83	0.60
1:A:717:LYS:NZ	1:A:1120:SER:OG	2.31	0.60
1:A:3592:VAL:HA	1:A:3595:GLU:HG2	1.83	0.60
2:B:425:ILE:HG23	5:M:191:LYS:HE3	1.83	0.60
3:C:656:ASN:HB3	3:C:688:LYS:HB2	1.82	0.60
1:A:1476:HIS:ND1	1:A:1522:GLY:O	2.25	0.60
1:A:2253:TYR:HB2	1:A:2291:GLN:HE22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:OD2	7:E:22:DG:H8	1.83	0.60
1:A:1101:PHE:HE2	1:A:1163:LEU:HB3	1.65	0.60
1:A:1108:MET:HE1	1:A:1178:ARG:HH22	1.67	0.60
3:C:108:LEU:HD13	3:C:150:ILE:HG21	1.81	0.60
1:A:2551:GLU:HA	1:A:2554:PHE:CD2	2.37	0.60
1:A:3500:SER:O	1:A:3504:ALA:N	2.30	0.60
3:C:280:ASP:OD1	3:C:281:ALA:N	2.34	0.60
1:A:79:ARG:O	1:A:82:ARG:HG2	2.02	0.60
1:A:399:GLN:HG3	1:A:401:ASP:H	1.66	0.60
1:A:439:VAL:HA	1:A:442:GLN:HG3	1.84	0.60
2:B:422:ASP:C	2:B:424:LYS:H	2.10	0.60
1:A:320:LEU:HG	1:A:368:LEU:HD22	1.81	0.60
1:A:1933:LEU:HB2	1:A:1936:ARG:HB2	1.83	0.60
1:A:2239:LYS:HZ3	1:A:2282:ALA:HB3	1.65	0.60
6:D:21:DA:H1'	7:E:36:DA:C2	2.35	0.60
1:A:542:ASP:OD1	1:A:543:SER:N	2.35	0.60
1:A:958:MET:HB3	1:A:961:LEU:HB3	1.84	0.60
1:A:1039:TRP:HA	1:A:1042:LYS:HG2	1.83	0.60
1:A:2820:MET:HE2	1:A:2824:LYS:HG3	1.82	0.60
1:A:3886:ALA:HA	1:A:3889:ARG:HD3	1.82	0.60
1:A:4062:ASP:HA	1:A:4065:LEU:HD12	1.84	0.60
1:A:718:MET:HE2	1:A:733:LEU:HD12	1.84	0.60
1:A:773:LEU:HA	1:A:776:TRP:NE1	2.17	0.60
1:A:3590:ASN:HB2	1:A:4022:LYS:HE3	1.84	0.60
2:B:458:GLN:NE2	2:B:527:GLU:OE1	2.34	0.60
3:C:328:GLU:O	3:C:332:LYS:N	2.34	0.60
1:A:3526:PRO:O	1:A:3527:GLN:HG3	2.01	0.59
2:B:485:GLN:HA	2:B:488:ARG:HE	1.65	0.59
2:B:353:LEU:HD13	2:B:395:ALA:HB2	1.83	0.59
1:A:584:GLU:N	1:A:613:HIS:O	2.32	0.59
1:A:1684:LEU:HA	1:A:1688:LEU:HD12	1.85	0.59
1:A:2529:THR:OG1	1:A:2530:ARG:NH1	2.35	0.59
1:A:3446:VAL:HA	1:A:3449:LYS:HG2	1.83	0.59
1:A:3883:LEU:HB2	1:A:3970:LEU:HD21	1.83	0.59
3:C:646:ALA:HA	3:C:651:GLU:HB3	1.85	0.59
1:A:3789:ARG:NH1	1:A:3790:THR:O	2.35	0.59
2:B:369:TYR:OH	3:C:436:SER:O	2.20	0.59
1:A:687:SER:HB3	1:A:701:TYR:HB2	1.83	0.59
1:A:3522:THR:HG23	1:A:3561:LYS:HE2	1.85	0.59
3:C:344:GLY:HA3	5:M:199:VAL:HG21	1.84	0.59
1:A:3642:LYS:O	1:A:3646:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3846:MET:HG2	1:A:3858:MET:SD	2.43	0.59
2:B:40:PHE:HD1	2:B:167:MET:HG2	1.67	0.59
2:B:73:SER:HB2	2:B:249:LYS:HD2	1.85	0.59
2:B:244:ARG:NH2	2:B:246:VAL:O	2.35	0.59
1:A:414:LEU:HB2	1:A:460:ALA:HB1	1.84	0.59
1:A:1359:LEU:H	1:A:1361:LYS:NZ	2.00	0.59
1:A:1651:LYS:O	1:A:1654:GLN:HG3	2.02	0.59
1:A:3496:ILE:HD12	1:A:3707:GLY:HA2	1.84	0.59
1:A:3856:MET:O	1:A:3860:LYS:NZ	2.36	0.59
3:C:66:ASN:HD21	3:C:69:SER:HA	1.67	0.59
1:A:28:ALA:O	1:A:32:HIS:ND1	2.36	0.59
1:A:531:PHE:O	1:A:535:LEU:N	2.31	0.59
1:A:652:GLU:O	1:A:655:LEU:HB2	2.02	0.59
1:A:2214:ARG:NH1	1:A:2214:ARG:O	2.36	0.59
1:A:2857:CYS:O	1:A:2861:ILE:HG12	2.03	0.59
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.85	0.58
1:A:1985:LYS:NZ	1:A:2180:GLU:O	2.36	0.58
1:A:3252:PHE:HB3	1:A:3256:MET:HE1	1.84	0.58
1:A:3509:ASP:CG	1:A:3548:GLY:H	2.11	0.58
1:A:204:LEU:O	1:A:208:MET:HB2	2.03	0.58
1:A:531:PHE:CD1	1:A:534:LEU:HD12	2.37	0.58
1:A:1793:THR:O	1:A:1797:LEU:HG	2.02	0.58
1:A:2813:PHE:HE2	1:A:2868:LEU:HD11	1.68	0.58
1:A:2815:GLY:O	1:A:2818:LYS:HG3	2.03	0.58
2:B:430:PRO:HD2	3:C:435:PHE:HB2	1.84	0.58
1:A:781:ASP:OD2	1:A:783:HIS:ND1	2.37	0.58
1:A:1876:ILE:HA	1:A:1879:VAL:HG12	1.84	0.58
1:A:2364:LEU:HA	1:A:2367:VAL:HG22	1.85	0.58
1:A:100:ILE:O	1:A:101:ALA:C	2.45	0.58
1:A:2181:GLY:HA3	1:A:2222:HIS:CD2	2.39	0.58
1:A:1505:LEU:HA	1:A:1508:LYS:HD2	1.86	0.58
1:A:3506:LEU:HD11	1:A:3554:PHE:HD2	1.69	0.58
1:A:323:VAL:HA	1:A:326:MET:HG2	1.86	0.58
1:A:2539:LEU:HA	1:A:2542:LEU:HD23	1.85	0.58
4:F:91:TYR:HE1	4:F:103:LEU:HD22	1.68	0.58
1:A:3468:LEU:HA	1:A:3471:ILE:HB	1.85	0.58
1:A:186:PRO:HG2	1:A:189:MET:HE1	1.85	0.58
1:A:934:LEU:HA	1:A:937:MET:HG3	1.85	0.58
1:A:998:ASN:OD1	1:A:999:LYS:N	2.37	0.58
1:A:3814:ASP:O	1:A:3818:ASN:ND2	2.36	0.58
1:A:449:TYR:HB3	1:A:453:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:LYS:HB3	1:A:1061:LYS:NZ	2.19	0.58
1:A:1274:ARG:NH2	1:A:1276:VAL:O	2.37	0.58
1:A:1409:SER:O	1:A:1412:LYS:NZ	2.33	0.58
1:A:3259:LEU:HG	1:A:3276:TRP:NE1	2.19	0.58
1:A:200:PHE:CE2	1:A:227:LEU:HD21	2.39	0.58
1:A:142:ARG:HE	1:A:182:GLY:HA3	1.69	0.57
1:A:4098:LEU:HB3	1:A:4102:THR:HG23	1.84	0.57
3:C:106:ASP:OD2	3:C:146:GLN:NE2	2.37	0.57
1:A:59:PHE:O	1:A:63:PHE:N	2.37	0.57
1:A:3029:LYS:O	1:A:3033:GLU:N	2.37	0.57
1:A:3008:TRP:O	1:A:3011:LEU:N	2.37	0.57
2:B:174:ASN:OD1	2:B:176:HIS:NE2	2.37	0.57
1:A:129:ASP:O	1:A:133:LYS:HG2	2.04	0.57
1:A:530:LEU:O	1:A:534:LEU:N	2.37	0.57
1:A:789:TYR:HA	1:A:792:ILE:HB	1.85	0.57
1:A:1727:ARG:HH22	1:A:1774:MET:H	1.53	0.57
2:B:471:PHE:HB3	3:C:346:CYS:HB3	1.86	0.57
1:A:395:MET:HG3	1:A:396:PHE:HD1	1.70	0.57
1:A:913:ARG:NE	1:A:2803:ILE:HD11	2.19	0.57
3:C:323:PHE:HE1	3:C:328:GLU:HG2	1.69	0.57
1:A:450:SER:O	1:A:454:GLN:N	2.36	0.57
1:A:1367:HIS:HA	1:A:1370:ARG:HG2	1.85	0.57
1:A:2157:PHE:O	1:A:2161:ALA:N	2.37	0.57
3:C:20:MET:O	3:C:29:SER:OG	2.20	0.57
1:A:3598:LYS:HG3	1:A:3599:THR:HG22	1.87	0.57
1:A:655:LEU:HD13	1:A:1388:ASP:HB3	1.86	0.57
1:A:2208:ASP:OD1	1:A:2209:GLU:N	2.37	0.57
1:A:2405:VAL:HG11	1:A:2441:LYS:HD3	1.86	0.57
1:A:3692:VAL:HG21	1:A:3720:ALA:HA	1.85	0.57
2:B:425:ILE:O	2:B:427:VAL:N	2.37	0.57
1:A:2866:ALA:HA	1:A:2869:LEU:HD12	1.87	0.57
1:A:3843:LEU:O	1:A:3847:SER:OG	2.22	0.57
2:B:362:LEU:HD21	2:B:438:PRO:HA	1.85	0.57
1:A:440:VAL:HG11	1:A:485:GLN:HB3	1.87	0.57
1:A:3450:MET:HE2	1:A:3468:LEU:HD21	1.86	0.57
1:A:3463:LEU:O	1:A:4000:ASN:ND2	2.38	0.57
2:B:296:VAL:HG12	3:C:297:LEU:HD12	1.87	0.57
1:A:754:MET:HA	1:A:757:LYS:HG2	1.87	0.56
1:A:801:LYS:NZ	1:A:3114:TYR:O	2.34	0.56
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.06	0.56
1:A:3483:MET:O	1:A:3487:ILE:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:28:DT:H2'	6:D:29:DA:C8	2.40	0.56
6:D:33:DA:H2''	6:D:34:DC:C4	2.40	0.56
1:A:435:LEU:O	1:A:438:LEU:HB2	2.05	0.56
1:A:865:GLN:OE1	1:A:865:GLN:N	2.37	0.56
1:A:2528:GLU:HA	1:A:2532:PRO:HA	1.87	0.56
1:A:462:VAL:HG11	1:A:540:MET:SD	2.45	0.56
1:A:677:ALA:O	1:A:681:LYS:N	2.37	0.56
1:A:870:LEU:HD23	1:A:870:LEU:H	1.70	0.56
1:A:2386:LEU:O	1:A:2394:LYS:NZ	2.34	0.56
1:A:3361:GLU:HG3	1:A:3373:VAL:HG21	1.87	0.56
3:C:65:ASP:H	3:C:78:THR:HG22	1.70	0.56
6:D:39:DA:C2	7:E:19:DA:C6	2.94	0.56
1:A:849:GLU:O	1:A:853:ILE:HG23	2.05	0.56
1:A:1070:PRO:HD3	1:A:3741:ARG:NH1	2.21	0.56
1:A:3897:PHE:CZ	1:A:3901:ARG:HD2	2.41	0.56
2:B:60:PHE:O	2:B:64:ILE:HG12	2.05	0.56
2:B:101:ASN:ND2	2:B:140:ASP:OD1	2.38	0.56
1:A:734:LEU:HD21	1:A:769:GLY:CA	2.35	0.56
3:C:253:ILE:HB	3:C:257:LEU:HD12	1.86	0.56
3:C:394:ARG:NE	3:C:403:PRO:HB3	2.20	0.56
6:D:20:DT:H1'	7:E:36:DA:C8	2.41	0.56
1:A:208:MET:HE3	1:A:208:MET:O	2.06	0.56
1:A:1364:CYS:SG	1:A:1365:ASN:N	2.79	0.56
1:A:2257:PHE:HA	1:A:2260:PHE:CE1	2.40	0.56
1:A:3572:ILE:HA	1:A:3575:LEU:HD12	1.86	0.56
1:A:3868:VAL:O	1:A:3872:ARG:HG3	2.05	0.56
1:A:397:LEU:HD21	1:A:438:LEU:HD23	1.87	0.56
1:A:892:LEU:HB2	1:A:907:LEU:H	1.71	0.56
2:B:64:ILE:O	2:B:68:GLN:NE2	2.39	0.56
1:A:89:LEU:O	1:A:133:LYS:NZ	2.27	0.56
1:A:1154:PRO:HD3	1:A:1163:LEU:HD11	1.88	0.56
1:A:1202:ARG:NH2	1:A:1210:ASP:OD1	2.39	0.56
3:C:271:ARG:O	3:C:273:LYS:NZ	2.38	0.56
6:D:27:DC:H2''	6:D:28:DT:C5	2.41	0.56
1:A:172:GLU:HG3	1:A:220:LEU:HA	1.87	0.56
1:A:3831:ASP:O	1:A:3833:ARG:N	2.39	0.56
2:B:145:GLU:O	2:B:148:TRP:HB3	2.06	0.56
2:B:147:LEU:HD13	2:B:189:LYS:HB3	1.88	0.56
2:B:344:GLY:N	2:B:401:THR:O	2.39	0.56
3:C:216:GLU:HB3	3:C:219:ASP:HB2	1.86	0.56
3:C:323:PHE:CE1	3:C:328:GLU:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:HG2	1:A:96:MET:HG3	1.88	0.55
1:A:1946:ASN:HA	1:A:1949:ILE:HD12	1.88	0.55
1:A:3170:ASP:HB3	1:A:3173:MET:HB3	1.87	0.55
1:A:3931:ALA:O	1:A:3935:GLY:N	2.38	0.55
1:A:583:LEU:HD13	1:A:612:LEU:HD13	1.87	0.55
1:A:639:ALA:HB2	1:A:676:ASN:HB3	1.87	0.55
1:A:2320:ALA:HB1	1:A:2366:LYS:HB2	1.88	0.55
1:A:2365:ASN:ND2	1:A:2399:GLU:OE2	2.36	0.55
2:B:403:ARG:HB3	2:B:406:ILE:HG13	1.86	0.55
3:C:33:GLN:HE22	3:C:231:LEU:HD22	1.70	0.55
1:A:1190:LEU:HA	1:A:1193:LYS:HD3	1.88	0.55
1:A:1758:LEU:HD23	1:A:1761:LEU:HD12	1.88	0.55
1:A:1870:LYS:HA	1:A:1873:TYR:HD2	1.71	0.55
1:A:2501:LEU:HD12	1:A:2504:ASP:HB2	1.88	0.55
4:F:109:LEU:HG	4:F:132:ILE:HB	1.87	0.55
1:A:1575:LEU:HD21	1:A:1617:LYS:HD2	1.89	0.55
1:A:2891:ARG:NH2	1:A:3894:PRO:O	2.40	0.55
1:A:309:LYS:O	1:A:313:LEU:HG	2.07	0.55
1:A:2319:ALA:HA	1:A:2322:VAL:HG22	1.89	0.55
1:A:2410:GLU:O	1:A:2414:GLN:NE2	2.33	0.55
1:A:3352:GLU:HG3	1:A:3356:ALA:H	1.72	0.55
1:A:3686:TRP:O	1:A:3690:PHE:N	2.40	0.55
2:B:308:GLY:O	4:F:57:ARG:HD3	2.07	0.55
2:B:363:ARG:HB2	2:B:436:PHE:HD2	1.70	0.55
2:B:80:ARG:NH2	2:B:81:ASP:OD1	2.40	0.55
3:C:378:SER:O	3:C:381:ILE:HG12	2.07	0.55
3:C:613:SER:OG	3:C:654:ARG:NH2	2.39	0.55
4:F:121:GLU:HG3	4:F:123:ARG:HB2	1.88	0.55
1:A:292:SER:HA	1:A:295:GLU:CD	2.32	0.55
1:A:3506:LEU:HD11	1:A:3554:PHE:CD2	2.41	0.55
1:A:855:VAL:HA	1:A:858:MET:HG3	1.88	0.55
1:A:862:LEU:HD12	1:A:866:ILE:HG21	1.87	0.55
1:A:1202:ARG:NE	1:A:1210:ASP:OD2	2.40	0.55
3:C:165:LEU:H	3:C:226:SER:HA	1.70	0.55
4:F:116:SER:HA	4:F:119:LEU:HD12	1.88	0.55
1:A:2373:PRO:O	1:A:2377:ARG:NH1	2.40	0.55
1:A:2944:THR:HG22	1:A:2957:LEU:HD13	1.89	0.55
1:A:3233:SER:HA	1:A:3272:TRP:HZ2	1.71	0.55
1:A:3739:ILE:HG22	1:A:3747:GLU:OE2	2.07	0.55
1:A:3748:HIS:HB2	1:A:3750:PHE:HE1	1.71	0.55
2:B:59:PRO:HA	2:B:62:MET:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HG2	3:C:431:ARG:NH1	2.22	0.55
2:B:492:ALA:HB2	2:B:500:PRO:HD3	1.88	0.55
1:A:2835:LYS:HD2	1:A:2838:GLN:HE21	1.72	0.55
1:A:3065:ILE:HA	1:A:3068:ALA:HB3	1.89	0.55
2:B:362:LEU:HD11	2:B:438:PRO:HB3	1.89	0.55
1:A:1537:VAL:HA	1:A:1554:SER:HA	1.89	0.54
2:B:41:LEU:HB3	2:B:88:TYR:HE1	1.72	0.54
4:F:111:LYS:HB2	4:F:130:PHE:HB3	1.89	0.54
1:A:489:ARG:O	1:A:492:SER:OG	2.23	0.54
1:A:1328:GLU:OE1	1:A:1328:GLU:N	2.41	0.54
1:A:3974:MET:HE2	1:A:3977:THR:C	2.33	0.54
2:B:446:MET:HG3	3:C:363:LYS:HG3	1.89	0.54
1:A:1760:GLU:HA	1:A:1763:THR:HG22	1.89	0.54
1:A:3123:GLN:O	1:A:3127:THR:HG23	2.06	0.54
1:A:3509:ASP:O	1:A:3551:ASN:ND2	2.41	0.54
1:A:2120:ARG:HD2	1:A:2163:HIS:NE2	2.22	0.54
1:A:2919:ASP:O	1:A:2923:TRP:N	2.39	0.54
1:A:3664:ASN:O	1:A:3667:LEU:HB3	2.07	0.54
3:C:144:LYS:HB3	3:C:207:ILE:HG21	1.89	0.54
3:C:363:LYS:HD2	3:C:418:CYS:HB2	1.88	0.54
1:A:1096:VAL:HA	1:A:1100:VAL:HG13	1.89	0.54
1:A:1400:VAL:HG23	1:A:1457:GLN:HE21	1.72	0.54
1:A:3274:VAL:HA	1:A:3277:VAL:HG22	1.90	0.54
3:C:112:ILE:HA	3:C:115:MET:HE2	1.90	0.54
1:A:272:LEU:HB2	1:A:311:ALA:HB1	1.89	0.54
1:A:1877:LEU:HA	1:A:1880:MET:SD	2.48	0.54
1:A:3041:LEU:HA	1:A:3044:MET:HE2	1.88	0.54
1:A:3122:HIS:HA	1:A:3125:ARG:HE	1.73	0.54
3:C:271:ARG:HH12	7:E:29:DG:H2'	1.72	0.54
1:A:1098:GLN:OE1	1:A:1152:ARG:N	2.40	0.54
1:A:1178:ARG:NH2	1:A:1229:CYS:SG	2.80	0.54
1:A:1391:VAL:HA	1:A:1394:HIS:CE1	2.43	0.54
1:A:3165:THR:HA	1:A:3168:TYR:CZ	2.42	0.54
1:A:3518:VAL:O	1:A:3522:THR:N	2.28	0.54
2:B:319:SER:N	3:C:277:THR:O	2.37	0.54
3:C:527:GLN:HA	3:C:530:LEU:HB2	1.89	0.54
1:A:381:VAL:HG23	1:A:424:LEU:HD13	1.89	0.54
1:A:396:PHE:CE1	1:A:406:ARG:HB2	2.43	0.54
1:A:2385:LEU:HD13	1:A:2388:LYS:HD2	1.90	0.54
1:A:3226:ASP:N	1:A:3229:SER:OG	2.38	0.54
2:B:89:GLY:O	2:B:139:SER:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4065:LEU:HD23	1:A:4074:PHE:CZ	2.42	0.54
2:B:296:VAL:HA	3:C:297:LEU:HA	1.89	0.54
1:A:417:VAL:HA	1:A:420:VAL:HG22	1.90	0.53
1:A:864:GLY:H	1:A:3169:PRO:HA	1.73	0.53
4:F:41:LEU:HD21	4:F:115:LEU:HD11	1.89	0.53
1:A:232:CYS:HB2	1:A:278:HIS:CE1	2.44	0.53
1:A:1019:ASP:O	1:A:1026:ARG:NH1	2.41	0.53
1:A:2254:ARG:HH12	1:A:2288:TYR:HE1	1.56	0.53
1:A:3724:GLU:HG3	1:A:3725:ARG:HH21	1.72	0.53
1:A:4002:MET:HE1	1:A:4048:LYS:HE3	1.88	0.53
2:B:276:LEU:HG	2:B:277:VAL:HG13	1.90	0.53
1:A:527:TYR:HB2	1:A:629:PHE:HE1	1.73	0.53
1:A:553:VAL:HB	1:A:1550:VAL:HG12	1.91	0.53
1:A:1184:ARG:HE	1:A:1265:GLU:HB2	1.73	0.53
1:A:2312:TYR:O	1:A:2315:VAL:HG22	2.09	0.53
1:A:2330:VAL:C	1:A:2332:GLU:N	2.66	0.53
1:A:3108:GLN:HA	1:A:3111:MET:HG2	1.89	0.53
1:A:4065:LEU:HD23	1:A:4074:PHE:HZ	1.74	0.53
3:C:162:GLN:NE2	3:C:163:PHE:O	2.41	0.53
3:C:215:LEU:HG	3:C:216:GLU:HG2	1.91	0.53
4:F:50:ARG:O	4:F:55:ARG:NH1	2.41	0.53
1:A:370:ALA:O	1:A:374:LYS:N	2.35	0.53
1:A:1149:LYS:H	1:A:1151:ARG:HH21	1.56	0.53
1:A:2519:LEU:O	1:A:2522:ARG:HG3	2.09	0.53
1:A:4065:LEU:O	1:A:4069:GLU:HG2	2.07	0.53
2:B:269:ILE:HA	2:B:375:VAL:HG11	1.90	0.53
1:A:465:PHE:HE2	1:A:564:LEU:HD21	1.74	0.53
1:A:1811:ARG:HD3	1:A:1819:PHE:CE2	2.44	0.53
1:A:2352:HIS:HB2	1:A:2356:MET:HG3	1.91	0.53
1:A:2429:ASP:OD1	1:A:2430:GLU:N	2.42	0.53
1:A:3580:ASN:HD21	1:A:3582:GLU:HB2	1.74	0.53
2:B:418:GLU:C	2:B:420:LEU:H	2.16	0.53
1:A:203:GLU:HG3	1:A:224:LEU:HD11	1.91	0.53
1:A:770:LEU:HD11	1:A:858:MET:HG2	1.91	0.53
1:A:776:TRP:CZ3	1:A:785:MET:HG2	2.44	0.53
1:A:1717:LEU:O	1:A:1721:HIS:ND1	2.40	0.53
1:A:3179:TRP:HB3	1:A:3242:MET:HE1	1.91	0.53
2:B:204:HIS:ND1	2:B:212:ASP:OD1	2.37	0.53
3:C:66:ASN:HB3	3:C:77:ILE:HG22	1.90	0.53
1:A:3864:ARG:HG3	1:A:4115:ASN:HB2	1.90	0.53
1:A:4009:PRO:O	1:A:4015:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:ILE:HD12	3:C:154:LEU:HD21	1.89	0.53
3:C:644:GLU:HA	3:C:647:ILE:HD12	1.91	0.53
1:A:389:ILE:HG22	1:A:393:LYS:NZ	2.24	0.53
1:A:962:TYR:HD2	1:A:1007:VAL:HG11	1.73	0.53
1:A:1291:LEU:HG	1:A:1363:LEU:HD11	1.90	0.53
1:A:1345:THR:HA	1:A:1348:LEU:HD12	1.90	0.53
1:A:2323:LEU:HA	1:A:2326:ILE:HG22	1.91	0.53
1:A:3744:ASP:O	1:A:3746:ARG:NH1	2.42	0.53
2:B:57:LEU:HD23	2:B:65:GLN:HE21	1.72	0.53
1:A:26:GLY:HA2	1:A:30:ALA:HB3	1.90	0.53
1:A:3154:GLN:HG2	1:A:3157:LEU:HD12	1.90	0.53
1:A:3443:PRO:O	1:A:3447:VAL:HG12	2.09	0.53
1:A:3595:GLU:HA	1:A:3598:LYS:HG2	1.91	0.53
1:A:3886:ALA:HA	1:A:3889:ARG:HH11	1.74	0.53
1:A:3966:GLN:O	1:A:3970:LEU:N	2.39	0.53
3:C:651:GLU:HG3	3:C:654:ARG:HD3	1.91	0.53
1:A:391:ARG:HH21	1:A:395:MET:HB3	1.73	0.53
1:A:667:TYR:HB3	1:A:732:PHE:HB2	1.90	0.53
1:A:855:VAL:HA	1:A:858:MET:CG	2.39	0.53
1:A:1115:HIS:HD2	1:A:1181:THR:HG22	1.74	0.53
1:A:1565:GLU:HA	1:A:1568:ASN:ND2	2.24	0.53
1:A:1760:GLU:OE1	1:A:1801:VAL:HA	2.09	0.53
1:A:3700:GLU:HG2	1:A:3718:ARG:HG3	1.89	0.53
1:A:3887:PHE:HA	1:A:3890:MET:SD	2.49	0.53
2:B:302:THR:HG23	2:B:311:LEU:HB2	1.91	0.53
2:B:341:ASP:OD2	2:B:346:MET:HE3	2.09	0.53
2:B:421:ASP:N	2:B:427:VAL:H	2.07	0.53
4:F:108:GLN:HE22	4:F:110:VAL:HB	1.74	0.53
1:A:391:ARG:HG3	1:A:395:MET:HE3	1.91	0.52
1:A:443:ILE:O	1:A:527:TYR:OH	2.20	0.52
1:A:959:TYR:CE1	1:A:1007:VAL:HB	2.44	0.52
1:A:1235:ILE:HG23	1:A:1259:LEU:HD11	1.91	0.52
1:A:4122:GLU:HG3	1:A:4127:TRP:HZ3	1.73	0.52
2:B:297:LYS:N	3:C:296:CYS:O	2.42	0.52
3:C:368:ARG:HE	3:C:369:ASP:H	1.56	0.52
1:A:128:LEU:O	1:A:132:ILE:HD12	2.09	0.52
1:A:407:VAL:HA	1:A:410:MET:HG2	1.91	0.52
1:A:938:VAL:HA	1:A:941:MET:HG3	1.91	0.52
1:A:4011:PHE:O	1:A:4038:TRP:NE1	2.32	0.52
2:B:122:PHE:HB3	2:B:131:PHE:HB2	1.92	0.52
3:C:624:LEU:HA	3:C:671:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:NH2	1:A:102:PRO:HB2	2.24	0.52
1:A:1298:LEU:HG	1:A:1367:HIS:HB3	1.91	0.52
1:A:1719:VAL:HB	3:C:631:TYR:HB2	1.92	0.52
1:A:2560:ASN:OD1	1:A:2561:PHE:N	2.43	0.52
1:A:3659:PHE:HA	1:A:3662:ILE:HD13	1.92	0.52
1:A:3934:THR:HG23	1:A:3936:GLY:H	1.73	0.52
1:A:4053:GLY:O	1:A:4098:LEU:N	2.38	0.52
2:B:443:LYS:HE3	2:B:445:LYS:HA	1.90	0.52
1:A:1976:LEU:HB3	1:A:2145:PHE:HE2	1.75	0.52
2:B:424:LYS:O	2:B:426:GLN:N	2.43	0.52
4:F:118:CYS:HB3	4:F:123:ARG:O	2.08	0.52
1:A:163:LYS:HD3	1:A:164:LYS:HB2	1.92	0.52
1:A:764:PRO:HG3	1:A:846:ILE:HG21	1.90	0.52
1:A:801:LYS:HA	1:A:3115:SER:HA	1.92	0.52
1:A:2866:ALA:O	1:A:2899:ARG:NH2	2.43	0.52
1:A:3332:THR:HA	1:A:3335:ARG:HG2	1.91	0.52
1:A:3588:TRP:CE2	1:A:3609:MET:HE3	2.45	0.52
1:A:3750:PHE:HA	1:A:3805:TRP:H	1.75	0.52
2:B:204:HIS:HA	2:B:213:ILE:HG13	1.91	0.52
4:F:41:LEU:HB2	4:F:68:HIS:HB2	1.92	0.52
1:A:1242:LEU:O	1:A:1311:LYS:NZ	2.42	0.52
6:D:30:DA:H2"	6:D:31:DA:N7	2.24	0.52
1:A:1576:ASP:OD1	1:A:1577:LEU:N	2.42	0.52
1:A:1871:MET:HE2	1:A:1940:TYR:HB2	1.92	0.52
1:A:2422:GLN:HA	1:A:2425:ARG:HE	1.75	0.52
2:B:166:ILE:HG12	2:B:198:ILE:HD11	1.92	0.52
2:B:298:THR:OG1	2:B:300:THR:OG1	2.20	0.52
2:B:300:THR:HA	3:C:293:THR:HB	1.92	0.52
2:B:463:LYS:HG3	3:C:383:ALA:HB1	1.91	0.52
1:A:475:LEU:O	1:A:479:ILE:HD12	2.10	0.52
1:A:2556:SER:HB2	1:A:2799:GLN:HA	1.92	0.52
1:A:2891:ARG:HH22	1:A:3898:LEU:HD23	1.74	0.52
1:A:4068:HIS:HB3	1:A:4071:ALA:HB3	1.92	0.52
2:B:511:VAL:HA	2:B:514:MET:HB3	1.92	0.52
1:A:63:PHE:HA	1:A:66:LEU:HD12	1.91	0.52
1:A:992:ILE:O	1:A:996:THR:HG22	2.10	0.52
1:A:1173:LEU:HA	1:A:1176:CYS:SG	2.50	0.52
1:A:1210:ASP:O	1:A:1213:LYS:NZ	2.37	0.52
1:A:1805:PHE:O	1:A:1816:ARG:NH1	2.43	0.52
1:A:2220:MET:HA	1:A:2223:VAL:HG12	1.91	0.52
1:A:3881:ASP:OD1	1:A:3884:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:493:CYS:O	3:C:505:LEU:HD22	2.10	0.52
3:C:602:VAL:HG21	3:C:642:PHE:HE1	1.75	0.52
4:F:42:SER:HA	4:F:70:GLY:HA2	1.91	0.52
1:A:412:SER:O	1:A:415:GLN:HG3	2.10	0.52
1:A:1863:PHE:HA	1:A:1866:GLN:HG2	1.91	0.52
1:A:2793:PRO:HA	1:A:2796:ALA:HB3	1.92	0.52
2:B:385:LEU:HA	2:B:392:LYS:HD3	1.92	0.52
1:A:16:GLN:HG2	1:A:59:PHE:HE1	1.75	0.51
1:A:1949:ILE:HG21	1:A:2096:PRO:HB3	1.92	0.51
1:A:2088:LEU:HA	1:A:2094:MET:HE2	1.93	0.51
1:A:2437:ASP:OD1	1:A:2472:GLN:HG2	2.09	0.51
1:A:2930:TYR:HB2	1:A:2939:LEU:HD22	1.91	0.51
1:A:2936:TYR:HA	1:A:2939:LEU:HB3	1.92	0.51
1:A:3000:ASP:O	1:A:3004:HIS:ND1	2.43	0.51
3:C:40:MET:O	3:C:43:GLN:HG3	2.09	0.51
3:C:262:ALA:N	3:C:365:PHE:O	2.38	0.51
3:C:596:GLU:HA	3:C:599:ARG:HE	1.75	0.51
1:A:1716:GLN:HA	1:A:1719:VAL:HG22	1.92	0.51
1:A:2143:ARG:NH2	1:A:2170:GLN:OE1	2.43	0.51
1:A:2991:LYS:HA	1:A:2994:TRP:CE3	2.44	0.51
1:A:3385:LEU:HB3	1:A:3416:LEU:HD21	1.92	0.51
1:A:3608:LYS:O	1:A:3612:ARG:HG2	2.11	0.51
4:F:50:ARG:NH2	4:F:55:ARG:O	2.43	0.51
1:A:167:PRO:HD2	1:A:171:LEU:HD13	1.92	0.51
1:A:1279:LEU:HD13	1:A:1282:LEU:HD11	1.93	0.51
1:A:1368:LEU:HA	1:A:1371:VAL:HG22	1.91	0.51
1:A:3061:LEU:O	1:A:3065:ILE:HG12	2.10	0.51
1:A:3259:LEU:HG	1:A:3276:TRP:CE2	2.45	0.51
2:B:92:LYS:NZ	2:B:133:ASP:O	2.40	0.51
3:C:140:SER:O	3:C:200:GLN:HG2	2.11	0.51
4:F:89:MET:HE1	4:F:94:ALA:HA	1.91	0.51
1:A:110:THR:O	1:A:114:VAL:HG13	2.10	0.51
1:A:446:PHE:HA	1:A:449:TYR:CD2	2.45	0.51
1:A:2413:PHE:HA	1:A:2416:LYS:HG2	1.92	0.51
1:A:3660:ASN:O	1:A:3663:THR:HB	2.10	0.51
1:A:3967:PHE:HA	1:A:3970:LEU:HG	1.92	0.51
2:B:469:LEU:HD22	3:C:345:PHE:H	1.75	0.51
1:A:537:SER:O	1:A:541:MET:HE3	2.11	0.51
1:A:1059:LEU:HD23	1:A:1062:ARG:HH21	1.74	0.51
1:A:2891:ARG:NH2	1:A:3898:LEU:HB3	2.22	0.51
1:A:2937:ASP:HB3	1:A:3979:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3986:HIS:O	1:A:3989:ARG:HD3	2.11	0.51
1:A:971:ARG:NH1	1:A:1022:ASP:OD2	2.44	0.51
1:A:1257:LEU:HD23	1:A:1260:LEU:HD12	1.92	0.51
1:A:2376:ASP:HB2	1:A:2377:ARG:HH11	1.75	0.51
1:A:3809:THR:HG22	1:A:3931:ALA:HA	1.93	0.51
1:A:3908:HIS:HA	1:A:3911:ILE:HG12	1.93	0.51
3:C:616:LEU:O	3:C:620:ILE:HG12	2.11	0.51
1:A:445:SER:OG	1:A:448:GLN:NE2	2.36	0.51
1:A:786:GLN:HA	1:A:789:TYR:CG	2.46	0.51
1:A:3955:VAL:HG21	1:A:4121:TRP:CD2	2.45	0.51
3:C:531:SER:HA	3:C:534:LYS:HG2	1.92	0.51
4:F:87:GLU:OE1	4:F:87:GLU:N	2.44	0.51
1:A:1807:LYS:NZ	1:A:1808:ASP:OD1	2.39	0.51
1:A:3064:PHE:O	1:A:3068:ALA:N	2.44	0.51
1:A:3659:PHE:O	1:A:3663:THR:N	2.36	0.51
3:C:74:TYR:HB3	3:C:77:ILE:HG13	1.92	0.51
1:A:448:GLN:HB3	1:A:519:TRP:CD1	2.46	0.51
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.11	0.51
1:A:2327:LEU:O	1:A:2328:ARG:C	2.54	0.51
1:A:3904:PHE:O	1:A:3908:HIS:HB2	2.10	0.51
1:A:850:GLU:O	1:A:853:ILE:HG12	2.11	0.51
1:A:1047:GLN:O	1:A:1051:LYS:HG2	2.11	0.51
1:A:1070:PRO:O	1:A:1075:ARG:NH1	2.44	0.51
1:A:1694:THR:HG23	1:A:1695:LEU:HD22	1.92	0.51
1:A:1764:GLU:O	1:A:1768:ARG:NH2	2.44	0.51
1:A:3626:GLY:O	1:A:3630:ARG:HG2	2.11	0.51
1:A:3978:GLY:N	1:A:3980:MET:SD	2.83	0.51
1:A:4089:ILE:N	1:A:4109:ASP:OD2	2.44	0.51
3:C:134:ILE:HB	3:C:163:PHE:HA	1.93	0.51
3:C:247:TRP:HE3	3:C:263:ALA:HB3	1.76	0.51
3:C:529:PRO:HA	3:C:532:LYS:HG2	1.93	0.51
1:A:1310:GLU:O	1:A:1311:LYS:HG2	2.12	0.50
1:A:1379:PRO:HB2	1:A:1383:GLY:O	2.10	0.50
1:A:1396:PRO:HA	1:A:1457:GLN:HE22	1.74	0.50
1:A:2887:PRO:HG2	1:A:3895:GLU:HB3	1.93	0.50
2:B:425:ILE:O	2:B:426:GLN:C	2.55	0.50
1:A:736:LEU:HD12	1:A:740:ILE:HB	1.92	0.50
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	1.94	0.50
1:A:2876:VAL:HG21	1:A:2892:LEU:HD23	1.91	0.50
2:B:76:ILE:HD12	2:B:248:ALA:N	2.26	0.50
2:B:412:ALA:HB2	2:B:437:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HA	1:A:190:ILE:HB	1.91	0.50
1:A:346:TYR:HA	1:A:349:ILE:HG12	1.92	0.50
1:A:709:LYS:HA	1:A:712:LYS:HG2	1.94	0.50
1:A:1154:PRO:HD2	1:A:1157:PHE:HB2	1.92	0.50
1:A:1339:VAL:HG12	1:A:1395:LEU:HD21	1.94	0.50
1:A:2129:LEU:HA	1:A:2132:LYS:HB3	1.93	0.50
1:A:2838:GLN:NE2	1:A:2839:ASP:OD1	2.44	0.50
2:B:276:LEU:HD21	3:C:354:ARG:NH1	2.26	0.50
1:A:1257:LEU:HA	1:A:1260:LEU:HD12	1.93	0.50
1:A:3759:ARG:N	1:A:3795:PRO:HG3	2.26	0.50
1:A:3955:VAL:HG21	1:A:4121:TRP:CG	2.46	0.50
3:C:165:LEU:N	3:C:226:SER:HA	2.26	0.50
3:C:633:MET:HA	3:C:636:ILE:HG12	1.92	0.50
1:A:2217:ASN:HA	1:A:2220:MET:HG2	1.92	0.50
1:A:2835:LYS:O	1:A:2838:GLN:HG3	2.11	0.50
1:A:3464:LYS:HE3	1:A:3997:LEU:HD23	1.93	0.50
1:A:3485:LYS:O	1:A:3488:SER:OG	2.20	0.50
2:B:40:PHE:CD1	2:B:167:MET:HG2	2.47	0.50
2:B:183:ALA:HB1	2:B:187:ARG:HH12	1.76	0.50
2:B:276:LEU:HD22	2:B:367:PHE:HB2	1.93	0.50
3:C:332:LYS:HG2	3:C:334:LYS:HZ3	1.76	0.50
1:A:800:LEU:O	1:A:3115:SER:OG	2.26	0.50
1:A:1208:LEU:HA	1:A:1211:VAL:HG22	1.94	0.50
1:A:1519:PHE:HB3	1:A:1573:LYS:HE3	1.94	0.50
1:A:2120:ARG:NH1	1:A:2159:PRO:O	2.45	0.50
1:A:2581:LEU:HD12	1:A:2781:PRO:HD2	1.94	0.50
1:A:3337:ILE:HG23	1:A:3377:LEU:HD21	1.94	0.50
1:A:3924:HIS:HB3	1:A:4125:GLU:CD	2.37	0.50
2:B:145:GLU:O	2:B:149:VAL:HG13	2.12	0.50
2:B:492:ALA:HA	2:B:497:LEU:HB2	1.94	0.50
3:C:251:LEU:HD23	3:C:261:ILE:HD13	1.93	0.50
4:F:82:HIS:HA	4:F:108:GLN:H	1.77	0.50
1:A:348:ILE:HG13	1:A:362:ALA:HB2	1.92	0.50
1:A:1597:LEU:HD21	1:A:1648:LEU:HD22	1.92	0.50
1:A:1605:PHE:O	1:A:1608:ARG:NH1	2.38	0.50
1:A:1767:CYS:SG	1:A:1819:PHE:HA	2.51	0.50
1:A:2470:ARG:HA	1:A:2473:MET:HE2	1.94	0.50
1:A:3301:LEU:O	1:A:3305:SER:HB3	2.12	0.50
2:B:64:ILE:O	2:B:67:ILE:HG22	2.12	0.50
2:B:276:LEU:HD23	2:B:276:LEU:H	1.76	0.50
2:B:402:PRO:HD2	2:B:406:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:ARG:NH1	6:D:32:DA:OP2	2.45	0.50
2:B:468:LYS:HB2	2:B:518:LEU:HG	1.93	0.50
1:A:554:ASN:ND2	1:A:556:SER:O	2.45	0.50
1:A:683:PHE:HZ	1:A:707:PHE:CD2	2.25	0.50
1:A:4007:LYS:NZ	1:A:4040:PRO:HB2	2.26	0.50
2:B:282:LYS:NZ	2:B:283:PRO:O	2.38	0.50
2:B:310:LEU:HD11	3:C:292:GLU:HB3	1.93	0.50
4:F:111:LYS:HA	4:F:132:ILE:HD11	1.94	0.50
1:A:801:LYS:HD3	1:A:3115:SER:HA	1.94	0.50
1:A:3009:LYS:HA	1:A:3012:GLU:OE2	2.12	0.50
1:A:3049:LEU:HA	1:A:3052:LEU:HD12	1.94	0.50
1:A:3671:ASN:OD1	1:A:3672:LYS:N	2.43	0.50
1:A:965:THR:O	1:A:968:VAL:HG12	2.12	0.49
1:A:1448:LEU:O	1:A:1452:VAL:HG13	2.12	0.49
1:A:1956:PHE:HE2	1:A:1961:PHE:HA	1.76	0.49
1:A:3117:ILE:HD11	1:A:3124:SER:HB2	1.94	0.49
1:A:3714:GLU:O	1:A:3718:ARG:NH2	2.42	0.49
2:B:345:LEU:HB3	2:B:400:TYR:CD1	2.39	0.49
3:C:165:LEU:O	3:C:227:PHE:N	2.38	0.49
3:C:357:MET:HG2	3:C:425:PRO:HB3	1.93	0.49
3:C:457:LEU:HD23	3:C:529:PRO:HB2	1.92	0.49
6:D:43:DT:H3	7:E:15:DA:H4'	1.76	0.49
1:A:240:GLU:OE2	1:A:246:ARG:NH1	2.44	0.49
1:A:381:VAL:HA	1:A:384:MET:HG3	1.93	0.49
1:A:3262:LEU:HD23	1:A:3276:TRP:HD1	1.76	0.49
2:B:397:LEU:HD21	3:C:477:PHE:HD2	1.76	0.49
3:C:17:GLY:O	3:C:101:GLY:N	2.45	0.49
1:A:210:SER:O	3:C:549:THR:N	2.31	0.49
1:A:430:VAL:O	1:A:433:PRO:HD2	2.11	0.49
1:A:1391:VAL:HG23	1:A:1392:MET:SD	2.52	0.49
1:A:1476:HIS:HB3	1:A:1479:VAL:HG12	1.94	0.49
1:A:2494:ASP:O	1:A:2497:GLU:HG2	2.12	0.49
2:B:69:SER:O	2:B:244:ARG:NH1	2.46	0.49
2:B:290:ARG:NH2	3:C:311:ILE:HD13	2.25	0.49
2:B:311:LEU:HD21	3:C:288:ASP:O	2.13	0.49
3:C:45:GLN:O	3:C:49:GLU:N	2.45	0.49
3:C:679:VAL:HG13	3:C:683:ILE:HD11	1.94	0.49
1:A:175:TYR:O	1:A:227:LEU:HD13	2.13	0.49
1:A:545:LEU:HA	1:A:548:GLU:HG2	1.93	0.49
1:A:620:PHE:O	1:A:624:ILE:HG12	2.12	0.49
1:A:1225:GLU:HB3	1:A:1231:GLN:HE22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1645:VAL:HA	1:A:1648:LEU:HG	1.93	0.49
1:A:1725:GLN:OE1	1:A:1726:SER:N	2.45	0.49
1:A:2357:GLU:HG3	1:A:2358:ASP:H	1.77	0.49
1:A:3114:TYR:O	1:A:3117:ILE:HG22	2.12	0.49
1:A:396:PHE:HE1	1:A:406:ARG:HB2	1.76	0.49
1:A:1335:CYS:O	1:A:1339:VAL:HG13	2.12	0.49
1:A:1714:LEU:O	1:A:1718:ILE:HG12	2.13	0.49
1:A:3033:GLU:HB2	1:A:3034:PRO:HD3	1.92	0.49
1:A:3775:LEU:HD13	1:A:3786:LEU:HB3	1.92	0.49
1:A:4047:ALA:O	1:A:4050:LYS:HG2	2.12	0.49
1:A:385:TYR:CE2	1:A:427:VAL:HG23	2.47	0.49
1:A:876:SER:HB2	1:A:879:MET:HB2	1.95	0.49
1:A:1166:LEU:HB3	1:A:1170:LYS:NZ	2.27	0.49
1:A:1458:LEU:O	1:A:1462:GLY:N	2.42	0.49
1:A:2270:ASN:HD22	1:A:2309:PHE:HE2	1.61	0.49
1:A:4012:ASP:H	1:A:4015:ASN:HB2	1.78	0.49
2:B:355:LEU:HB2	3:C:473:LEU:HD13	1.95	0.49
3:C:136:THR:HG22	3:C:138:LEU:H	1.77	0.49
3:C:622:GLN:NE2	3:C:623:PHE:HB2	2.28	0.49
4:F:86:ASP:HB2	4:F:89:MET:HG2	1.95	0.49
1:A:966:PHE:HB2	1:A:1011:GLU:CD	2.38	0.49
1:A:1115:HIS:CD2	1:A:1181:THR:HG22	2.46	0.49
1:A:1817:GLN:HA	1:A:1820:VAL:HG22	1.93	0.49
1:A:1949:ILE:HG12	1:A:2100:LEU:HD11	1.95	0.49
1:A:2429:ASP:O	1:A:2432:GLN:HG2	2.13	0.49
1:A:4020:MET:SD	1:A:4027:TRP:HB3	2.52	0.49
3:C:394:ARG:HE	3:C:403:PRO:HB3	1.78	0.49
1:A:487:LEU:O	1:A:490:ILE:HG22	2.12	0.49
1:A:603:ILE:HD11	1:A:1031:ARG:HD2	1.95	0.49
1:A:683:PHE:HE2	1:A:740:ILE:HD11	1.77	0.49
1:A:974:CYS:SG	1:A:1025:LEU:HB2	2.52	0.49
1:A:1582:LEU:HD11	1:A:1593:VAL:HG22	1.94	0.49
1:A:2266:ASN:HA	1:A:2311:ARG:HG2	1.94	0.49
1:A:2573:PRO:HA	1:A:2786:LYS:HD3	1.94	0.49
1:A:2976:LEU:O	1:A:2979:GLN:NE2	2.45	0.49
1:A:4088:ASN:HD21	1:A:4113:ASP:HB2	1.77	0.49
2:B:90:THR:HG21	2:B:103:TYR:HB2	1.95	0.49
3:C:265:LYS:HB3	3:C:268:LEU:HD11	1.94	0.49
4:F:121:GLU:O	4:F:123:ARG:NH1	2.46	0.49
6:D:36:DA:H2'	6:D:37:DT:H1'	1.94	0.49
6:D:43:DT:C4	7:E:16:DA:C5	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASN:O	1:A:409:GLN:NE2	2.45	0.49
1:A:914:VAL:HA	1:A:917:LEU:HG	1.93	0.49
1:A:1493:PRO:HB3	1:A:1500:LEU:H	1.78	0.49
1:A:2254:ARG:HH21	1:A:2293:GLY:N	2.09	0.49
2:B:369:TYR:CD1	2:B:370:PRO:HD2	2.48	0.49
4:F:54:GLY:H	4:F:57:ARG:NE	2.10	0.49
1:A:31:GLY:O	1:A:35:ILE:HG12	2.13	0.49
1:A:150:GLY:HA2	1:A:188:GLU:OE2	2.13	0.49
1:A:2135:ASN:O	1:A:2138:VAL:HG22	2.13	0.49
1:A:2135:ASN:O	1:A:2143:ARG:NH1	2.45	0.49
1:A:2559:THR:OG1	1:A:2795:GLN:NE2	2.46	0.49
1:A:3144:PHE:HA	1:A:3150:ASN:HD22	1.77	0.49
1:A:3588:TRP:NE1	1:A:3613:MET:HE3	2.28	0.49
1:A:756:PHE:O	1:A:799:TYR:OH	2.26	0.48
1:A:1887:ASP:OD1	1:A:1888:ASP:N	2.44	0.48
1:A:2157:PHE:HB3	1:A:2164:TRP:CD1	2.48	0.48
1:A:2318:ALA:O	1:A:2322:VAL:HG13	2.13	0.48
1:A:2376:ASP:OD1	1:A:2404:ARG:HD3	2.13	0.48
2:B:297:LYS:HE3	3:C:296:CYS:SG	2.53	0.48
3:C:280:ASP:OD2	3:C:282:LYS:NZ	2.46	0.48
3:C:649:PHE:CE2	3:C:651:GLU:HB2	2.48	0.48
4:F:91:TYR:HB2	4:F:134:ILE:HA	1.95	0.48
1:A:111:CYS:O	1:A:114:VAL:HG22	2.13	0.48
1:A:200:PHE:CZ	1:A:227:LEU:HD21	2.48	0.48
1:A:205:LYS:HA	1:A:208:MET:HB3	1.95	0.48
1:A:210:SER:OG	2:B:339:ARG:NH1	2.28	0.48
1:A:1057:LYS:HB3	1:A:1061:LYS:HZ1	1.78	0.48
2:B:446:MET:HE2	3:C:363:LYS:HB2	1.94	0.48
6:D:36:DA:H2'	6:D:37:DT:C1'	2.43	0.48
1:A:360:SER:HA	1:A:363:ILE:HG12	1.95	0.48
1:A:734:LEU:HD22	1:A:768:VAL:HG13	1.95	0.48
1:A:2269:ASP:N	1:A:2269:ASP:OD1	2.46	0.48
1:A:4114:PRO:HA	1:A:4117:LEU:HD12	1.94	0.48
7:E:26:DT:H2'	7:E:27:DT:H73	1.96	0.48
1:A:171:LEU:HD23	1:A:171:LEU:H	1.79	0.48
1:A:1986:ARG:HD2	1:A:2184:TYR:HA	1.94	0.48
1:A:2338:GLU:OE2	1:A:2340:SER:OG	2.32	0.48
1:A:3424:LEU:O	1:A:3428:GLU:N	2.36	0.48
1:A:1093:GLU:OE1	1:A:1093:GLU:N	2.46	0.48
1:A:1333:SER:O	1:A:1337:VAL:HG13	2.13	0.48
1:A:2397:CYS:HA	1:A:2400:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2421:VAL:O	1:A:2425:ARG:HG3	2.14	0.48
1:A:3809:THR:OG1	1:A:3929:MET:SD	2.64	0.48
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.96	0.48
2:B:490:LEU:HB3	3:C:316:TYR:CE2	2.44	0.48
3:C:94:ILE:HG23	3:C:98:ILE:HG13	1.95	0.48
4:F:44:LEU:HG	4:F:82:HIS:CD2	2.48	0.48
1:A:12:LEU:HD23	1:A:15:LEU:HD12	1.95	0.48
1:A:208:MET:HG2	1:A:249:PHE:HD1	1.77	0.48
1:A:898:PHE:CD1	1:A:2535:THR:HG21	2.49	0.48
1:A:1575:LEU:HD12	1:A:1576:ASP:N	2.28	0.48
1:A:1816:ARG:HA	1:A:1819:PHE:HD2	1.78	0.48
1:A:1966:LEU:H	1:A:1969:GLU:CD	2.20	0.48
1:A:2158:ARG:NH2	1:A:2195:SER:O	2.46	0.48
1:A:2205:VAL:HG12	1:A:2207:LYS:N	2.29	0.48
1:A:2262:GLY:HA3	1:A:2270:ASN:ND2	2.27	0.48
1:A:2420:PHE:CE1	1:A:2424:MET:HB3	2.49	0.48
1:A:3261:GLU:OE1	1:A:3261:GLU:N	2.32	0.48
1:A:3702:PRO:HB2	1:A:3794:VAL:HG11	1.96	0.48
2:B:130:ARG:HA	2:B:133:ASP:OD2	2.14	0.48
3:C:526:SER:O	3:C:530:LEU:N	2.39	0.48
3:C:610:GLU:OE2	3:C:654:ARG:NE	2.36	0.48
1:A:461:ILE:HA	1:A:464:VAL:HG22	1.95	0.48
1:A:1244:LEU:HD11	1:A:1310:GLU:HB2	1.96	0.48
1:A:1740:VAL:HA	1:A:1743:MET:HG2	1.95	0.48
1:A:1791:CYS:SG	1:A:1792:VAL:N	2.87	0.48
1:A:1894:SER:HB3	1:A:1910:GLU:N	2.29	0.48
1:A:2365:ASN:HB2	1:A:2396:LEU:HD23	1.94	0.48
1:A:2891:ARG:HA	1:A:2894:GLU:HG2	1.96	0.48
2:B:112:GLY:H	2:B:115:ARG:HG3	1.77	0.48
4:F:71:GLN:HE22	4:F:73:CYS:HB3	1.78	0.48
6:D:31:DA:H2"	6:D:32:DA:C8	2.48	0.48
1:A:151:GLU:HA	4:F:133:PHE:CE2	2.49	0.48
1:A:451:PRO:HA	1:A:454:GLN:HB2	1.96	0.48
1:A:734:LEU:HD23	1:A:734:LEU:O	2.13	0.48
1:A:1037:LEU:O	1:A:1040:SER:OG	2.29	0.48
1:A:1399:CYS:SG	1:A:1403:MET:HE1	2.54	0.48
1:A:1804:MET:O	1:A:1811:ARG:NH2	2.47	0.48
1:A:2561:PHE:HB3	1:A:2565:MET:HE1	1.96	0.48
1:A:3086:LEU:HD23	1:A:3089:LEU:HD21	1.96	0.48
1:A:3511:ALA:O	1:A:3515:GLN:N	2.42	0.48
2:B:103:TYR:CD1	2:B:135:MET:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:VAL:HG12	2:B:436:PHE:HD1	1.79	0.48
2:B:492:ALA:HB2	2:B:499:GLU:HA	1.96	0.48
3:C:11:VAL:HG21	3:C:114:SER:HB2	1.95	0.48
1:A:562:HIS:HB2	1:A:641:PHE:CE1	2.48	0.48
1:A:1565:GLU:H	1:A:1565:GLU:CD	2.21	0.48
1:A:2104:MET:O	1:A:2108:LEU:HG	2.13	0.48
1:A:2122:LEU:HB3	1:A:2127:LYS:HD3	1.95	0.48
1:A:2345:VAL:HA	1:A:2348:GLN:HG3	1.95	0.48
1:A:2358:ASP:N	1:A:2358:ASP:OD1	2.45	0.48
1:A:3467:ARG:O	1:A:3470:GLN:HG2	2.14	0.48
1:A:3911:ILE:HD12	1:A:3928:PHE:CE1	2.49	0.48
3:C:377:LEU:O	3:C:381:ILE:HG23	2.14	0.48
1:A:910:PHE:CE1	1:A:2807:GLN:HG3	2.49	0.48
1:A:1527:ARG:O	1:A:1531:LEU:HG	2.14	0.48
1:A:2044:ASP:O	1:A:2048:GLY:N	2.47	0.48
1:A:2576:MET:SD	1:A:2576:MET:N	2.87	0.48
1:A:3493:TRP:HA	1:A:3521:ILE:HD11	1.96	0.48
1:A:3531:TYR:HB3	1:A:3796:MET:HA	1.95	0.48
2:B:41:LEU:HD13	2:B:86:VAL:HG13	1.96	0.48
2:B:375:VAL:HG13	2:B:378:SER:OG	2.13	0.48
3:C:263:ALA:HB1	3:C:362:LEU:HD11	1.95	0.48
3:C:457:LEU:CD1	3:C:533:ILE:HG13	2.44	0.48
2:B:143:LEU:H	2:B:182:LYS:HD3	1.79	0.47
2:B:388:LYS:HB3	2:B:390:LEU:HD23	1.95	0.47
1:A:1718:ILE:HA	1:A:1722:PHE:HD1	1.79	0.47
1:A:1762:MET:HE1	1:A:1782:PHE:HE1	1.78	0.47
1:A:1809:ASP:O	1:A:1811:ARG:N	2.44	0.47
1:A:2576:MET:HE1	1:A:2785:ILE:HG13	1.96	0.47
1:A:3008:TRP:CE2	1:A:3050:LYS:HG3	2.49	0.47
1:A:3577:GLN:OE1	1:A:3629:ARG:NE	2.43	0.47
1:A:3750:PHE:HA	1:A:3804:GLU:HA	1.96	0.47
1:A:3772:ASN:OD1	1:A:3787:GLN:HB2	2.14	0.47
1:A:3806:LEU:O	1:A:3807:GLU:HG3	2.14	0.47
1:A:4057:ALA:HB2	1:A:4090:ARG:HD2	1.96	0.47
2:B:341:ASP:CG	2:B:346:MET:HE3	2.39	0.47
4:F:40:TRP:HZ2	4:F:119:LEU:CA	2.25	0.47
6:D:43:DT:N3	7:E:15:DA:H4'	2.29	0.47
1:A:897:PRO:HB2	1:A:2569:SER:OG	2.14	0.47
1:A:3083:SER:O	1:A:3102:TYR:HB3	2.14	0.47
1:A:3923:ARG:HD3	1:A:3928:PHE:CZ	2.48	0.47
2:B:375:VAL:HA	3:C:540:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:20:DT:O2	7:E:36:DA:H5''	2.14	0.47
1:A:531:PHE:HD1	1:A:534:LEU:HD12	1.76	0.47
1:A:1468:LEU:HD13	1:A:1521:PHE:HE2	1.80	0.47
1:A:2519:LEU:HD11	1:A:2522:ARG:HH21	1.79	0.47
1:A:3549:HIS:HA	1:A:3552:LYS:HB2	1.94	0.47
1:A:3718:ARG:H	1:A:3743:HIS:CE1	2.31	0.47
1:A:3828:TYR:HH	1:A:4127:TRP:CD1	2.33	0.47
2:B:345:LEU:HB2	2:B:398:CYS:SG	2.54	0.47
2:B:355:LEU:HD13	3:C:473:LEU:HB2	1.95	0.47
2:B:442:ASP:OD1	3:C:269:GLN:HG2	2.15	0.47
3:C:33:GLN:HA	3:C:36:LYS:HG2	1.97	0.47
3:C:148:ASP:O	3:C:151:ILE:HG22	2.14	0.47
1:A:237:SER:HB2	1:A:283:SER:OG	2.14	0.47
1:A:1175:HIS:CG	1:A:1229:CYS:HA	2.49	0.47
1:A:1395:LEU:O	1:A:1399:CYS:HB2	2.15	0.47
1:A:1825:LEU:HD12	1:A:1826:THR:N	2.30	0.47
1:A:1828:LEU:HD11	1:A:1879:VAL:HG13	1.96	0.47
1:A:3050:LYS:HD3	1:A:3053:LEU:HD21	1.95	0.47
1:A:3168:TYR:CE1	1:A:3241:LYS:HE2	2.50	0.47
1:A:3190:LEU:HD22	1:A:3231:ILE:HG12	1.96	0.47
1:A:3479:THR:O	1:A:3480:LEU:HD22	2.14	0.47
1:A:3839:TYR:HE2	1:A:4122:GLU:HB2	1.80	0.47
1:A:3951:GLN:HE21	1:A:4063:GLU:HB3	1.78	0.47
1:A:4013:TRP:CD1	1:A:4035:GLU:HB3	2.49	0.47
2:B:203:MET:HG2	2:B:239:LEU:HB3	1.96	0.47
3:C:106:ASP:OD1	3:C:107:PHE:N	2.46	0.47
1:A:320:LEU:HA	1:A:323:VAL:HG22	1.95	0.47
1:A:1029:CYS:HA	1:A:1032:CYS:SG	2.53	0.47
1:A:1178:ARG:HD3	1:A:1180:GLN:HB2	1.95	0.47
1:A:2415:LEU:HB3	1:A:2420:PHE:HB2	1.95	0.47
1:A:2555:LEU:HD12	1:A:2555:LEU:HA	1.76	0.47
2:B:488:ARG:NH1	2:B:503:ALA:O	2.48	0.47
1:A:848:LEU:O	1:A:851:ILE:HB	2.14	0.47
1:A:921:ALA:HB3	1:A:927:LYS:HG3	1.96	0.47
1:A:1076:LEU:HD23	1:A:1121:LEU:HD21	1.97	0.47
1:A:1235:ILE:HG22	1:A:1256:TRP:NE1	2.30	0.47
1:A:1513:GLY:O	1:A:1516:GLU:HG3	2.14	0.47
1:A:3759:ARG:O	1:A:3762:GLN:HG3	2.15	0.47
1:A:3820:MET:HB3	1:A:3882:LEU:HD11	1.96	0.47
2:B:105:LEU:HD21	2:B:131:PHE:HE1	1.79	0.47
2:B:275:ASN:O	3:C:431:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:PRO:HG2	3:C:259:ILE:HD12	1.97	0.47
3:C:7:LYS:NZ	3:C:121:GLU:O	2.46	0.47
3:C:413:LYS:HG3	3:C:415:ASN:H	1.80	0.47
3:C:496:HIS:O	3:C:500:HIS:N	2.29	0.47
1:A:286:LEU:HD12	1:A:319:PHE:CD1	2.47	0.47
1:A:1948:ALA:HA	1:A:1951:VAL:HG12	1.96	0.47
1:A:2964:ASP:O	1:A:2967:GLU:N	2.48	0.47
1:A:3567:VAL:O	1:A:3571:PHE:HB2	2.14	0.47
3:C:457:LEU:HD11	3:C:533:ILE:HG13	1.96	0.47
1:A:349:ILE:HG13	1:A:350:ARG:N	2.29	0.47
1:A:374:LYS:NZ	1:A:425:ASP:OD1	2.47	0.47
1:A:632:GLU:OE1	1:A:632:GLU:N	2.48	0.47
1:A:1031:ARG:NH1	1:A:1084:ASN:OD1	2.48	0.47
1:A:1601:LEU:HG	1:A:1655:ILE:HD12	1.96	0.47
1:A:1959:LEU:HG	1:A:1960:LYS:H	1.80	0.47
1:A:2576:MET:HG3	1:A:2787:HIS:CD2	2.49	0.47
1:A:3466:PRO:HA	1:A:3469:LEU:HB3	1.97	0.47
1:A:3571:PHE:CE2	1:A:3575:LEU:HD11	2.50	0.47
1:A:3965:ARG:HA	1:A:3968:ILE:HG12	1.97	0.47
2:B:276:LEU:O	3:C:431:ARG:N	2.44	0.47
2:B:344:GLY:O	2:B:401:THR:N	2.39	0.47
2:B:370:PRO:HB3	2:B:382:PHE:HB3	1.97	0.47
2:B:458:GLN:HB2	3:C:379:SER:OG	2.15	0.47
1:A:248:ILE:O	1:A:252:VAL:HG23	2.15	0.47
1:A:1105:VAL:O	1:A:1108:MET:HG3	2.15	0.47
1:A:2517:LEU:O	1:A:2521:ILE:HG12	2.14	0.47
1:A:3052:LEU:HD23	1:A:3057:ALA:HA	1.96	0.47
1:A:3072:GLU:OE2	1:A:3075:LYS:NZ	2.47	0.47
1:A:3868:VAL:HG13	1:A:4114:PRO:HB2	1.97	0.47
1:A:128:LEU:O	1:A:131:LEU:HG	2.15	0.46
1:A:1714:LEU:HD11	1:A:1761:LEU:HD22	1.97	0.46
1:A:2365:ASN:HD22	1:A:2399:GLU:CD	2.23	0.46
1:A:2854:PHE:CE2	1:A:2858:ILE:HD11	2.49	0.46
1:A:3981:TYR:HA	1:A:3984:MET:HE2	1.97	0.46
2:B:345:LEU:HA	2:B:400:TYR:HA	1.97	0.46
2:B:468:LYS:O	2:B:517:ARG:NH1	2.44	0.46
3:C:250:ARG:HG2	3:C:260:ARG:HA	1.97	0.46
3:C:389:MET:HE2	3:C:389:MET:HA	1.97	0.46
3:C:598:PHE:CZ	3:C:616:LEU:HB3	2.50	0.46
4:F:54:GLY:N	4:F:57:ARG:HE	2.12	0.46
6:D:24:DA:H1'	6:D:25:DA:H5'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ALA:HB1	1:A:642:PHE:HB3	1.96	0.46
1:A:1761:LEU:HD23	1:A:1764:GLU:OE2	2.15	0.46
1:A:2133:LEU:O	1:A:2143:ARG:NH2	2.49	0.46
1:A:2891:ARG:HG3	1:A:3894:PRO:HB3	1.97	0.46
1:A:3692:VAL:HA	1:A:3696:ARG:HH21	1.80	0.46
1:A:3842:TRP:HA	1:A:3845:LYS:HG2	1.98	0.46
1:A:3988:LEU:HD23	1:A:4100:GLU:HB2	1.97	0.46
2:B:203:MET:HE2	2:B:237:SER:HB2	1.97	0.46
2:B:206:LYS:HB3	2:B:212:ASP:OD2	2.15	0.46
3:C:261:ILE:HG22	3:C:366:ALA:HA	1.96	0.46
1:A:36:ARG:HE	1:A:40:GLN:HG2	1.80	0.46
1:A:527:TYR:HB2	1:A:629:PHE:CE1	2.51	0.46
1:A:1856:THR:OG1	1:A:1857:LYS:N	2.48	0.46
1:A:2782:ASP:O	1:A:2785:ILE:HG23	2.15	0.46
4:F:111:LYS:N	4:F:130:PHE:O	2.43	0.46
1:A:447:PRO:HB3	1:A:526:ASP:HB3	1.97	0.46
1:A:762:TYR:HD2	1:A:765:LEU:HG	1.81	0.46
1:A:786:GLN:N	1:A:787:PRO:HD2	2.30	0.46
1:A:1339:VAL:HA	1:A:1342:MET:HG3	1.96	0.46
1:A:1400:VAL:HG23	1:A:1457:GLN:NE2	2.30	0.46
1:A:2265:PRO:HB3	1:A:2309:PHE:HA	1.96	0.46
1:A:2320:ALA:HB2	1:A:2363:CYS:HA	1.98	0.46
1:A:2372:PRO:HB2	1:A:2404:ARG:NH1	2.31	0.46
1:A:2413:PHE:CB	2:B:148:TRP:HH2	2.28	0.46
1:A:2978:LYS:O	1:A:2981:TRP:NE1	2.48	0.46
1:A:3236:PHE:CD2	1:A:3262:LEU:HD11	2.49	0.46
1:A:3266:SER:OG	1:A:3273:LEU:HA	2.16	0.46
1:A:3646:LYS:HB3	1:A:3651:LEU:HD23	1.98	0.46
2:B:352:PRO:HD2	3:C:464:ALA:H	1.81	0.46
3:C:249:CYS:SG	3:C:250:ARG:N	2.88	0.46
3:C:368:ARG:HG3	3:C:369:ASP:H	1.79	0.46
1:A:989:MET:O	1:A:993:HIS:ND1	2.49	0.46
1:A:1122:GLY:O	1:A:1126:GLN:HG2	2.16	0.46
1:A:1161:ALA:O	1:A:1163:LEU:HD22	2.16	0.46
1:A:1640:GLU:HA	1:A:1643:MET:HE2	1.97	0.46
1:A:3029:LYS:HB3	1:A:3033:GLU:HG3	1.98	0.46
1:A:3256:MET:HE3	1:A:3287:ARG:NH1	2.31	0.46
1:A:3460:GLU:O	1:A:3464:LYS:HG2	2.16	0.46
1:A:3666:LEU:HD23	1:A:3669:LYS:HD3	1.98	0.46
1:A:3736:LYS:O	1:A:3751:LEU:HD12	2.15	0.46
3:C:89:ASP:O	3:C:92:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:MET:HA	3:C:130:ARG:HH12	1.80	0.46
6:D:20:DT:C5	7:E:35:DT:H72	2.51	0.46
1:A:876:SER:O	1:A:880:MET:HE3	2.16	0.46
1:A:1015:ASP:OD1	1:A:1016:GLY:N	2.49	0.46
1:A:2234:ASN:HA	1:A:2237:ILE:HG12	1.97	0.46
1:A:2386:LEU:HB2	1:A:2387:PRO:HD3	1.98	0.46
1:A:2533:SER:HA	1:A:2538:ARG:HH21	1.81	0.46
1:A:2554:PHE:O	1:A:2557:LEU:HG	2.16	0.46
1:A:2803:ILE:HA	1:A:2806:LYS:HD3	1.97	0.46
1:A:3384:HIS:O	1:A:3387:GLU:HG2	2.16	0.46
2:B:362:LEU:HD23	2:B:363:ARG:NH1	2.31	0.46
2:B:387:ILE:HG13	2:B:388:LYS:HG3	1.97	0.46
3:C:265:LYS:NZ	3:C:360:GLN:HG3	2.30	0.46
1:A:1952:ILE:HD11	1:A:1956:PHE:HD2	1.80	0.46
1:A:2364:LEU:CD1	1:A:2400:VAL:HG11	2.45	0.46
1:A:2439:ILE:HA	1:A:2442:MET:HG3	1.98	0.46
1:A:3356:ALA:HB1	1:A:3360:LEU:HB2	1.97	0.46
1:A:3413:TYR:HB2	1:A:3453:ALA:HB2	1.98	0.46
1:A:4046:TYR:CZ	1:A:4066:LEU:HD11	2.51	0.46
2:B:452:ILE:HG12	3:C:375:VAL:HG12	1.97	0.46
3:C:512:ILE:HA	3:C:515:MET:HE2	1.97	0.46
1:A:1428:ILE:H	1:A:1428:ILE:HD12	1.81	0.46
1:A:1569:THR:HA	1:A:1572:LEU:HD12	1.97	0.46
1:A:1649:LEU:HA	1:A:1652:ILE:HG22	1.98	0.46
1:A:2122:LEU:HD21	1:A:2163:HIS:CD2	2.51	0.46
1:A:2422:GLN:HB2	1:A:2425:ARG:HH21	1.81	0.46
1:A:2776:ARG:NH2	1:A:2782:ASP:OD2	2.49	0.46
1:A:3133:GLN:O	1:A:3137:GLU:HG3	2.16	0.46
1:A:3179:TRP:CE3	1:A:3242:MET:HE1	2.51	0.46
1:A:3294:SER:HA	1:A:3297:VAL:HG22	1.97	0.46
1:A:3881:ASP:O	1:A:3885:ARG:HG3	2.16	0.46
1:A:4089:ILE:H	1:A:4089:ILE:HD12	1.81	0.46
2:B:36:ASP:HA	2:B:163:HIS:O	2.16	0.46
2:B:38:LEU:HD12	2:B:167:MET:CE	2.46	0.46
1:A:656:GLN:HG3	1:A:666:PHE:CZ	2.51	0.46
1:A:931:CYS:HA	1:A:934:LEU:HG	1.98	0.46
1:A:1756:PRO:O	1:A:1760:GLU:HG2	2.16	0.46
1:A:1762:MET:HA	1:A:1765:VAL:HG22	1.98	0.46
1:A:2410:GLU:OE2	1:A:2412:TYR:N	2.49	0.46
1:A:2817:LEU:HD12	1:A:2865:HIS:CE1	2.51	0.46
1:A:3012:GLU:OE2	1:A:3051:LEU:HD11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3493:TRP:CZ3	1:A:3525:TYR:HB2	2.50	0.46
2:B:338:LYS:NZ	2:B:405:ASN:O	2.48	0.46
2:B:447:PRO:HD3	3:C:243:HIS:CE1	2.50	0.46
3:C:53:GLU:HG2	3:C:85:LEU:HD22	1.98	0.46
3:C:356:PHE:O	3:C:357:MET:HE2	2.16	0.46
4:F:41:LEU:H	4:F:68:HIS:HB3	1.81	0.46
1:A:525:LYS:O	1:A:528:VAL:HG22	2.16	0.46
1:A:1758:LEU:HA	1:A:1761:LEU:HD12	1.97	0.46
1:A:1976:LEU:HB3	1:A:2145:PHE:CE2	2.51	0.46
1:A:2128:PHE:O	1:A:2132:LYS:N	2.28	0.46
1:A:3515:GLN:O	1:A:3518:VAL:HG12	2.16	0.46
2:B:493:LEU:HD22	3:C:323:PHE:HD2	1.81	0.46
4:F:114:TRP:HB2	4:F:130:PHE:CG	2.50	0.46
7:E:32:DT:H2''	7:E:33:DA:N7	2.31	0.46
1:A:435:LEU:HA	1:A:438:LEU:HD12	1.97	0.45
1:A:903:PRO:HB3	1:A:2815:GLY:C	2.41	0.45
1:A:922:SER:C	1:A:924:ARG:H	2.23	0.45
1:A:996:THR:HB	1:A:1036:PHE:CE1	2.51	0.45
1:A:1487:VAL:HB	1:A:1559:PHE:CE1	2.51	0.45
1:A:2300:PHE:HA	1:A:2303:LEU:HD12	1.97	0.45
1:A:2371:PHE:HD2	1:A:2374:LEU:HG	1.81	0.45
1:A:2470:ARG:HA	1:A:2473:MET:HG2	1.98	0.45
1:A:3291:GLN:OE1	1:A:3343:SER:OG	2.32	0.45
1:A:3567:VAL:O	1:A:3571:PHE:CB	2.64	0.45
3:C:62:ASP:OD1	3:C:62:ASP:N	2.45	0.45
7:E:27:DT:H2''	7:E:28:DA:H5'	1.99	0.45
1:A:196:LEU:HB3	1:A:200:PHE:CZ	2.51	0.45
1:A:497:LEU:HD23	1:A:497:LEU:H	1.80	0.45
1:A:1308:ALA:H	1:A:1319:GLY:N	2.15	0.45
1:A:1369:MET:HE2	1:A:1418:HIS:ND1	2.31	0.45
1:A:1696:LEU:HG	1:A:1749:ALA:HB1	1.97	0.45
1:A:3164:TRP:HA	1:A:3167:ARG:HG2	1.97	0.45
2:B:350:PHE:HA	2:B:396:ALA:HA	1.97	0.45
2:B:452:ILE:HG23	3:C:378:SER:HB3	1.97	0.45
6:D:21:DA:H1'	7:E:36:DA:C4	2.51	0.45
1:A:194:GLU:HG2	1:A:195:ASN:N	2.31	0.45
1:A:283:SER:C	1:A:285:CYS:H	2.25	0.45
1:A:895:ALA:HA	1:A:903:PRO:O	2.15	0.45
1:A:913:ARG:O	1:A:917:LEU:HG	2.15	0.45
1:A:1135:CYS:O	1:A:1138:ILE:N	2.49	0.45
1:A:1157:PHE:HZ	1:A:1167:ASP:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:CYS:HA	1:A:1368:LEU:HB3	1.98	0.45
1:A:1653:LEU:HG	1:A:1698:PHE:HD2	1.82	0.45
1:A:1664:SER:HA	1:A:1668:PHE:CD2	2.51	0.45
1:A:2526:SER:O	1:A:2538:ARG:NH2	2.48	0.45
1:A:3493:TRP:HB2	1:A:3524:ASN:ND2	2.31	0.45
2:B:41:LEU:HD12	2:B:88:TYR:HD1	1.81	0.45
2:B:480:ASN:HB2	3:C:428:GLU:OE2	2.16	0.45
1:A:71:LYS:HG2	1:A:78:PHE:CG	2.51	0.45
1:A:111:CYS:O	1:A:115:TYR:HD1	1.98	0.45
1:A:236:LYS:N	1:A:281:GLN:OE1	2.36	0.45
1:A:238:MET:SD	1:A:243:GLN:NE2	2.89	0.45
1:A:1493:PRO:HB3	1:A:1500:LEU:HD22	1.99	0.45
1:A:1579:VAL:O	1:A:1583:MET:HG3	2.16	0.45
1:A:2218:PHE:HA	1:A:2221:LYS:NZ	2.32	0.45
1:A:3961:PHE:CE2	1:A:3963:LEU:HB2	2.52	0.45
2:B:515:ASN:OD1	2:B:516:LYS:N	2.49	0.45
3:C:147:LEU:HA	3:C:150:ILE:HG12	1.98	0.45
4:F:47:HIS:HB2	4:F:73:CYS:O	2.16	0.45
1:A:61:ARG:HH22	1:A:102:PRO:HB2	1.81	0.45
1:A:152:LEU:HB3	1:A:156:PHE:HE2	1.81	0.45
1:A:654:ILE:HD11	1:A:707:PHE:HE1	1.82	0.45
1:A:801:LYS:HE3	1:A:3119:VAL:HG12	1.98	0.45
1:A:878:GLU:HA	1:A:881:LYS:HE2	1.97	0.45
1:A:1538:LEU:HD11	1:A:1555:HIS:CG	2.52	0.45
1:A:1803:GLU:O	1:A:1806:ARG:NH1	2.49	0.45
1:A:2273:GLY:O	1:A:2276:LEU:HG	2.17	0.45
1:A:2330:VAL:O	1:A:2332:GLU:N	2.46	0.45
1:A:2382:VAL:HB	1:A:2397:CYS:SG	2.56	0.45
1:A:2888:VAL:HB	1:A:3894:PRO:HG2	1.98	0.45
1:A:3178:ILE:H	1:A:3178:ILE:HD12	1.81	0.45
1:A:3411:ASP:HA	1:A:3414:MET:HG2	1.99	0.45
1:A:3549:HIS:HA	1:A:3552:LYS:HD3	1.98	0.45
1:A:3749:PRO:O	1:A:3805:TRP:N	2.50	0.45
1:A:3813:LYS:N	1:A:3925:LEU:HB3	2.32	0.45
2:B:444:ARG:HD3	3:C:265:LYS:O	2.16	0.45
2:B:458:GLN:HE22	2:B:527:GLU:HB2	1.81	0.45
3:C:138:LEU:HD22	3:C:204:GLY:HA3	1.98	0.45
3:C:225:TYR:CD2	3:C:236:VAL:HG12	2.52	0.45
3:C:336:GLU:O	3:C:399:LYS:HD3	2.17	0.45
1:A:78:PHE:O	1:A:81:CYS:HB2	2.17	0.45
1:A:124:LYS:HA	1:A:169:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:VAL:HA	1:A:579:LEU:HG	1.98	0.45
1:A:863:GLY:H	1:A:866:ILE:HD12	1.80	0.45
1:A:886:TRP:HE1	1:A:912:PRO:HG3	1.81	0.45
1:A:1135:CYS:SG	1:A:1136:ARG:N	2.90	0.45
1:A:1202:ARG:HB2	1:A:1207:TRP:HB2	1.99	0.45
1:A:2257:PHE:HA	1:A:2260:PHE:HE1	1.80	0.45
1:A:3107:ILE:HD11	1:A:3139:GLN:NE2	2.31	0.45
1:A:3864:ARG:O	1:A:3868:VAL:HG23	2.17	0.45
6:D:33:DA:H2''	6:D:34:DC:C5	2.52	0.45
1:A:903:PRO:HB2	1:A:905:ILE:HD11	1.97	0.45
1:A:1313:PHE:CZ	1:A:1321:ARG:HD2	2.52	0.45
1:A:1672:PHE:O	1:A:1676:ILE:HG12	2.17	0.45
1:A:2364:LEU:O	1:A:2368:THR:HG22	2.17	0.45
1:A:2422:GLN:HA	1:A:2425:ARG:NE	2.32	0.45
1:A:3240:MET:HE3	1:A:3262:LEU:CD2	2.44	0.45
1:A:4080:VAL:HG13	1:A:4116:ILE:HG13	1.98	0.45
3:C:28:GLU:OE1	3:C:36:LYS:NZ	2.49	0.45
1:A:289:ASN:OD1	1:A:292:SER:HB3	2.17	0.45
1:A:776:TRP:O	1:A:780:ILE:N	2.45	0.45
1:A:890:LYS:HB3	1:A:906:PHE:CG	2.51	0.45
1:A:1416:GLU:HG3	1:A:1420:ARG:HH22	1.81	0.45
1:A:1583:MET:CE	1:A:1628:LYS:HB2	2.44	0.45
1:A:2122:LEU:HD13	1:A:2127:LYS:HD3	1.98	0.45
1:A:2265:PRO:HA	1:A:2309:PHE:CG	2.52	0.45
1:A:2880:CYS:SG	1:A:2889:GLY:HA3	2.57	0.45
1:A:2884:LEU:HD13	1:A:3117:ILE:HA	1.97	0.45
1:A:3113:ASN:HB3	1:A:3128:LYS:NZ	2.32	0.45
1:A:3372:LYS:HA	1:A:3375:ALA:HB3	1.98	0.45
2:B:390:LEU:HD23	2:B:390:LEU:H	1.82	0.45
3:C:43:GLN:HA	3:C:46:VAL:HG22	1.98	0.45
1:A:493:LYS:O	1:A:625:ASN:ND2	2.50	0.45
1:A:913:ARG:HD2	1:A:916:GLU:OE2	2.17	0.45
3:C:88:PHE:HA	3:C:91:LEU:HG	1.99	0.45
3:C:600:VAL:HA	3:C:603:LYS:HG2	1.99	0.45
1:A:92:PHE:O	1:A:133:LYS:NZ	2.50	0.45
1:A:885:ALA:HB3	1:A:888:ARG:HA	1.99	0.45
1:A:2193:ILE:HA	1:A:2196:TRP:NE1	2.32	0.45
1:A:3419:PHE:O	1:A:3422:GLN:HG2	2.18	0.45
1:A:3622:ALA:O	1:A:3625:LEU:HD22	2.17	0.45
1:A:3638:LYS:O	1:A:3642:LYS:N	2.44	0.45
1:A:3976:GLU:CD	1:A:3977:THR:HG23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4104:VAL:HA	1:A:4107:LEU:HD12	1.98	0.45
2:B:282:LYS:HD2	2:B:283:PRO:HD2	1.99	0.45
2:B:526:LYS:C	2:B:528:LEU:H	2.25	0.45
3:C:306:LEU:HG	3:C:308:GLU:H	1.81	0.45
1:A:289:ASN:HD21	1:A:292:SER:HB3	1.81	0.44
1:A:450:SER:OG	1:A:453:MET:HG3	2.17	0.44
1:A:969:LEU:HB3	1:A:984:TYR:OH	2.17	0.44
1:A:1070:PRO:HD2	1:A:3741:ARG:HD2	1.99	0.44
1:A:3335:ARG:HH22	1:A:3418:ASP:HB3	1.82	0.44
2:B:44:ALA:HB3	2:B:89:GLY:O	2.17	0.44
2:B:193:LEU:HB2	2:B:198:ILE:CG2	2.48	0.44
1:A:851:ILE:O	1:A:855:VAL:HG23	2.17	0.44
1:A:1021:VAL:O	1:A:1026:ARG:NH1	2.50	0.44
1:A:1216:GLY:HA2	1:A:1219:PHE:HB3	1.97	0.44
1:A:1492:ALA:HB2	1:A:1555:HIS:HE1	1.81	0.44
1:A:1714:LEU:HA	1:A:1717:LEU:HD12	1.99	0.44
1:A:1776:GLU:HA	1:A:1779:GLN:HG2	1.99	0.44
1:A:2214:ARG:HH22	1:A:2221:LYS:HZ3	1.65	0.44
1:A:3479:THR:C	1:A:3480:LEU:HD22	2.41	0.44
1:A:3530:VAL:HA	1:A:3533:PHE:HB3	2.00	0.44
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	2.00	0.44
2:B:54:GLU:HB3	2:B:56:GLU:HG2	1.99	0.44
3:C:413:LYS:HG3	3:C:415:ASN:N	2.32	0.44
1:A:264:ARG:HD3	1:A:305:ASN:HB2	2.00	0.44
1:A:493:LYS:HA	1:A:493:LYS:HD3	1.78	0.44
1:A:535:LEU:HD13	1:A:637:LYS:HB2	1.99	0.44
1:A:1248:PHE:HB3	1:A:1319:GLY:HA2	1.98	0.44
1:A:1496:GLU:HG3	1:A:1498:GLN:HB2	1.99	0.44
1:A:2493:ASN:OD1	1:A:2494:ASP:N	2.51	0.44
1:A:3526:PRO:C	1:A:3528:ALA:H	2.24	0.44
2:B:464:ALA:O	2:B:468:LYS:HG3	2.17	0.44
4:F:114:TRP:HE1	4:F:125:VAL:C	2.26	0.44
1:A:850:GLU:HA	1:A:853:ILE:HG12	1.99	0.44
1:A:2430:GLU:N	1:A:2430:GLU:OE1	2.48	0.44
1:A:3296:GLN:O	1:A:3300:VAL:HG23	2.18	0.44
1:A:3350:GLU:OE1	1:A:3350:GLU:N	2.43	0.44
1:A:3730:ALA:HA	1:A:3734:ARG:HA	1.98	0.44
2:B:364:PRO:HG3	3:C:357:MET:HA	1.99	0.44
4:F:53:ILE:N	4:F:86:ASP:OD1	2.51	0.44
1:A:432:THR:O	1:A:435:LEU:HG	2.17	0.44
1:A:1661:PHE:HA	1:A:1665:HIS:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1777:LEU:O	1:A:1780:SER:OG	2.29	0.44
1:A:1786:ALA:HB1	1:A:1831:CYS:HA	1.99	0.44
1:A:1811:ARG:HG3	1:A:1816:ARG:HH21	1.82	0.44
1:A:2220:MET:SD	1:A:2252:PRO:HG3	2.58	0.44
1:A:2559:THR:HG22	1:A:2808:LEU:HD11	2.00	0.44
1:A:2563:LEU:HD13	1:A:2795:GLN:CB	2.47	0.44
1:A:3839:TYR:OH	1:A:4120:THR:O	2.30	0.44
3:C:44:ARG:NH2	3:C:234:LEU:HD13	2.32	0.44
3:C:86:PRO:HA	3:C:90:LEU:HD21	1.99	0.44
3:C:363:LYS:NZ	3:C:418:CYS:SG	2.75	0.44
3:C:665:LYS:HD2	3:C:665:LYS:HA	1.85	0.44
4:F:45:ARG:H	4:F:81:THR:HB	1.83	0.44
6:D:27:DC:H1'	6:D:28:DT:C2	2.53	0.44
6:D:30:DA:C4	6:D:31:DA:C6	3.06	0.44
6:D:39:DA:C2	7:E:19:DA:C5	3.05	0.44
1:A:1017:ILE:HA	1:A:1026:ARG:HG2	1.98	0.44
1:A:1097:GLU:O	1:A:1151:ARG:HD3	2.17	0.44
1:A:1185:HIS:HA	1:A:1188:ILE:HG12	1.99	0.44
1:A:1267:TYR:HA	1:A:1270:PHE:HB2	1.99	0.44
1:A:1306:ILE:O	1:A:1320:ASN:HB2	2.17	0.44
1:A:1375:THR:HA	1:A:1379:PRO:HA	1.99	0.44
1:A:1945:TYR:HE2	1:A:2097:LEU:HD11	1.82	0.44
1:A:3478:GLU:HG2	1:A:3483:MET:HE3	2.00	0.44
1:A:3660:ASN:O	1:A:3664:ASN:N	2.45	0.44
1:A:3856:MET:HG2	1:A:4077:TYR:OH	2.17	0.44
2:B:376:ILE:HG12	3:C:540:ILE:HG12	2.00	0.44
1:A:63:PHE:O	1:A:67:VAL:HG23	2.18	0.44
1:A:208:MET:SD	1:A:253:LEU:HG	2.58	0.44
1:A:210:SER:HB2	3:C:548:VAL:HG23	2.00	0.44
1:A:865:GLN:HA	1:A:868:LYS:HG2	2.00	0.44
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.18	0.44
1:A:1424:THR:HG1	1:A:1427:SER:H	1.65	0.44
1:A:2326:ILE:C	1:A:2328:ARG:H	2.25	0.44
1:A:2899:ARG:HD2	1:A:2900:LEU:N	2.33	0.44
1:A:3079:GLU:HG2	1:A:3080:LEU:N	2.33	0.44
1:A:3320:ILE:HG21	1:A:3394:GLU:OE1	2.18	0.44
2:B:50:GLU:HG3	2:B:52:GLN:H	1.81	0.44
2:B:131:PHE:HA	2:B:134:MET:HG3	1.99	0.44
1:A:101:ALA:HB3	1:A:102:PRO:CD	2.48	0.44
1:A:364:ARG:HA	1:A:415:GLN:HE22	1.83	0.44
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ARG:HH22	1:A:1389:VAL:HA	1.83	0.44
1:A:1326:GLU:O	1:A:1330:TYR:N	2.49	0.44
1:A:2490:GLU:O	1:A:2495:SER:OG	2.31	0.44
1:A:3059:GLN:HE22	1:A:3062:LEU:HD23	1.82	0.44
1:A:3555:VAL:HA	1:A:3558:ILE:HG22	1.99	0.44
1:A:3726:VAL:HG23	1:A:3738:ILE:HG13	2.00	0.44
1:A:3809:THR:HG21	1:A:3938:ILE:HD13	2.00	0.44
2:B:174:ASN:CB	2:B:216:PHE:HB3	2.48	0.44
2:B:190:ALA:HA	2:B:193:LEU:HG	1.99	0.44
2:B:317:LYS:HD3	2:B:330:GLU:OE1	2.18	0.44
2:B:335:GLU:OE2	2:B:405:ASN:ND2	2.50	0.44
2:B:422:ASP:C	2:B:424:LYS:N	2.75	0.44
2:B:478:PHE:C	3:C:427:MET:HE1	2.43	0.44
3:C:67:PRO:HD3	3:C:79:VAL:HG11	2.00	0.44
7:E:19:DA:H2'	7:E:20:DT:O4'	2.17	0.44
1:A:484:HIS:CE1	1:A:574:LYS:HG3	2.53	0.44
1:A:793:LEU:HD21	1:A:867:ASN:HA	1.99	0.44
1:A:989:MET:HG3	1:A:993:HIS:HE1	1.80	0.44
1:A:1712:ARG:HE	1:A:1712:ARG:HB2	1.56	0.44
1:A:1713:VAL:O	1:A:1716:GLN:HG3	2.18	0.44
1:A:1718:ILE:HA	1:A:1722:PHE:CD1	2.53	0.44
1:A:2872:ASP:OD1	1:A:2872:ASP:N	2.51	0.44
1:A:3631:LYS:O	1:A:3635:THR:HG22	2.17	0.44
2:B:353:LEU:H	2:B:394:VAL:HA	1.82	0.44
1:A:411:PRO:HB3	1:A:456:VAL:HG12	2.00	0.43
1:A:1073:PHE:O	1:A:1076:LEU:HG	2.17	0.43
1:A:2095:ALA:HB3	1:A:2096:PRO:HD3	2.00	0.43
1:A:3413:TYR:CD1	1:A:3449:LYS:HB2	2.53	0.43
1:A:3735:PRO:HB3	1:A:3751:LEU:HD11	1.98	0.43
1:A:3847:SER:HA	1:A:3858:MET:HE1	2.00	0.43
1:A:3986:HIS:O	1:A:3989:ARG:NH1	2.51	0.43
2:B:97:VAL:HG11	2:B:149:VAL:HG12	2.00	0.43
2:B:358:LYS:HA	3:C:353:ARG:HH22	1.82	0.43
2:B:480:ASN:HB3	2:B:483:LEU:HB2	1.99	0.43
3:C:115:MET:SD	3:C:130:ARG:NH2	2.91	0.43
3:C:130:ARG:HG2	3:C:159:ILE:HG23	2.00	0.43
3:C:599:ARG:HH11	3:C:641:ALA:HB3	1.83	0.43
4:F:119:LEU:O	4:F:122:ARG:HD2	2.18	0.43
1:A:478:CYS:O	1:A:482:VAL:HG13	2.19	0.43
1:A:1941:HIS:HB2	1:A:1974:ASN:O	2.19	0.43
1:A:2099:ALA:HA	1:A:2102:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2574:ASN:O	1:A:2787:HIS:ND1	2.52	0.43
1:A:2938:VAL:O	1:A:2942:ILE:HG12	2.18	0.43
1:A:3321:LEU:O	1:A:3324:ARG:HG2	2.18	0.43
1:A:3765:GLU:OE2	1:A:3791:TYR:N	2.34	0.43
1:A:3815:LEU:HA	1:A:3818:ASN:HD21	1.83	0.43
2:B:34:GLY:HA3	2:B:162:SER:HB3	2.01	0.43
2:B:85:VAL:HB	2:B:106:GLN:HB2	1.99	0.43
2:B:246:VAL:O	2:B:249:LYS:NZ	2.49	0.43
2:B:484:GLN:HA	2:B:487:PHE:HD2	1.82	0.43
3:C:250:ARG:HE	3:C:260:ARG:HG2	1.83	0.43
1:A:159:GLU:O	1:A:165:LYS:HG3	2.18	0.43
1:A:172:GLU:O	1:A:175:TYR:HB2	2.18	0.43
1:A:583:LEU:HD22	1:A:612:LEU:HB3	2.00	0.43
1:A:889:GLU:HG3	1:A:891:ARG:HG2	1.99	0.43
1:A:943:GLY:HA3	1:A:2577:PHE:CE2	2.54	0.43
1:A:1344:PHE:CE2	1:A:1348:LEU:HD11	2.53	0.43
1:A:1363:LEU:HB3	1:A:1367:HIS:CE1	2.47	0.43
1:A:1400:VAL:O	1:A:1404:LYS:HG2	2.19	0.43
1:A:1740:VAL:HA	1:A:1743:MET:HE3	2.01	0.43
1:A:1780:SER:HA	1:A:1783:ARG:HG2	2.00	0.43
1:A:1857:LYS:O	1:A:1858:LEU:HD22	2.19	0.43
1:A:2098:THR:HG22	1:A:2153:THR:HG23	2.01	0.43
1:A:2418:LYS:NZ	2:B:152:ASN:HA	2.33	0.43
1:A:2809:PHE:HA	1:A:2812:LEU:HG	2.01	0.43
1:A:2972:TYR:HB2	1:A:2998:SER:HB2	2.00	0.43
1:A:2986:PRO:HG3	1:A:2994:TRP:CH2	2.53	0.43
1:A:3113:ASN:HB3	1:A:3128:LYS:HZ1	1.83	0.43
1:A:3681:LYS:HE3	1:A:3723:ASP:O	2.17	0.43
1:A:3806:LEU:HG	1:A:3938:ILE:HG21	1.99	0.43
1:A:3833:ARG:CZ	1:A:3877:LYS:HZ1	2.30	0.43
1:A:4058:VAL:HG21	1:A:4095:GLU:HB3	2.00	0.43
3:C:135:PHE:HD1	3:C:227:PHE:HE1	1.67	0.43
1:A:133:LYS:O	1:A:137:THR:HG23	2.18	0.43
1:A:415:GLN:NE2	1:A:416:SER:OG	2.51	0.43
1:A:531:PHE:HA	1:A:534:LEU:HB2	2.00	0.43
1:A:643:GLU:HA	1:A:646:VAL:HG13	1.98	0.43
1:A:898:PHE:H	1:A:902:LYS:HE3	1.83	0.43
1:A:1186:LYS:O	1:A:1190:LEU:HB2	2.19	0.43
1:A:2424:MET:SD	1:A:2457:PRO:HB2	2.58	0.43
1:A:2519:LEU:HD12	1:A:2522:ARG:HE	1.84	0.43
1:A:2933:ILE:HG23	1:A:3121:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3410:ILE:HG22	1:A:3453:ALA:HA	1.99	0.43
1:A:3531:TYR:HB2	1:A:3532:PRO:HD3	1.99	0.43
1:A:3737:ARG:HD2	1:A:3805:TRP:CG	2.53	0.43
2:B:318:ARG:HH21	2:B:331:LYS:HD2	1.84	0.43
2:B:442:ASP:HB3	3:C:267:ILE:HG23	2.00	0.43
2:B:496:ASP:OD1	2:B:497:LEU:HD22	2.18	0.43
1:A:624:ILE:O	1:A:627:VAL:HG22	2.18	0.43
1:A:860:GLY:HA2	1:A:3132:VAL:HG13	2.00	0.43
1:A:885:ALA:HB3	1:A:888:ARG:HE	1.82	0.43
1:A:930:ALA:O	1:A:933:LEU:HG	2.18	0.43
1:A:1050:GLU:OE2	1:A:1057:LYS:NZ	2.49	0.43
1:A:1696:LEU:O	1:A:1700:THR:HG23	2.18	0.43
1:A:1813:SER:HB3	1:A:1936:ARG:HH21	1.82	0.43
1:A:3727:THR:O	1:A:3736:LYS:HA	2.19	0.43
1:A:4020:MET:HE2	1:A:4027:TRP:HD1	1.84	0.43
2:B:41:LEU:HD12	2:B:88:TYR:CD1	2.53	0.43
2:B:451:LYS:HE3	2:B:451:LYS:HB2	1.81	0.43
2:B:479:GLU:HA	3:C:427:MET:SD	2.58	0.43
3:C:74:TYR:CD1	3:C:109:ASP:HB3	2.54	0.43
3:C:394:ARG:HA	3:C:405:VAL:HG12	1.99	0.43
3:C:512:ILE:O	3:C:516:LEU:HG	2.18	0.43
3:C:594:PRO:HB2	3:C:619:HIS:CE1	2.53	0.43
4:F:73:CYS:SG	4:F:80:VAL:HG22	2.59	0.43
6:D:20:DT:H6	6:D:20:DT:H2'	1.71	0.43
6:D:35:DT:C2	7:E:22:DG:N2	2.86	0.43
1:A:374:LYS:HD3	1:A:381:VAL:HG21	2.01	0.43
1:A:870:LEU:HD21	1:A:3129:LEU:HD11	2.00	0.43
1:A:1423:ILE:HD11	1:A:1428:ILE:HD11	2.00	0.43
1:A:1657:SER:O	1:A:1660:SER:OG	2.34	0.43
1:A:2126:MET:CE	1:A:2130:HIS:HE1	2.30	0.43
1:A:2239:LYS:NZ	1:A:2282:ALA:HB3	2.32	0.43
1:A:2305:ASN:O	1:A:2308:SER:OG	2.23	0.43
1:A:2382:VAL:O	1:A:2386:LEU:HG	2.18	0.43
1:A:2447:LYS:O	1:A:2451:LEU:HG	2.19	0.43
1:A:2515:PRO:HA	1:A:2518:GLN:HE21	1.84	0.43
1:A:3046:ARG:O	1:A:3050:LYS:HG2	2.19	0.43
1:A:3320:ILE:HG22	1:A:3324:ARG:HH21	1.83	0.43
1:A:3568:ILE:H	1:A:3568:ILE:HD12	1.84	0.43
1:A:3762:GLN:NE2	1:A:3763:ARG:HD2	2.34	0.43
1:A:4090:ARG:NH1	1:A:4110:GLN:HA	2.34	0.43
3:C:677:ILE:O	3:C:680:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:PRO:HA	1:A:970:LEU:HG	2.00	0.43
1:A:1322:THR:HG22	1:A:1324:PRO:HD2	2.01	0.43
1:A:1618:LEU:O	1:A:1622:ILE:HG12	2.19	0.43
1:A:2143:ARG:HH21	1:A:2171:LEU:HB3	1.83	0.43
1:A:2349:LEU:HB3	1:A:2360:PHE:CE1	2.53	0.43
1:A:2563:LEU:HD11	1:A:2792:THR:HA	2.00	0.43
1:A:3179:TRP:O	1:A:3183:ILE:HG12	2.18	0.43
2:B:240:GLU:HA	2:B:243:LEU:HD12	2.01	0.43
2:B:264:ASN:HD21	2:B:266:ASP:HB2	1.84	0.43
2:B:376:ILE:HG23	3:C:540:ILE:HG12	2.01	0.43
3:C:7:LYS:HB2	3:C:125:LYS:HG3	1.99	0.43
3:C:261:ILE:HA	3:C:366:ALA:HA	2.00	0.43
1:A:922:SER:OG	1:A:923:ASP:N	2.49	0.43
1:A:2403:CYS:SG	1:A:2404:ARG:N	2.92	0.43
1:A:3500:SER:HB3	1:A:3532:PRO:HB3	1.99	0.43
1:A:3663:THR:O	1:A:3667:LEU:N	2.41	0.43
1:A:3759:ARG:O	1:A:3763:ARG:HD3	2.18	0.43
1:A:3828:TYR:O	1:A:3834:ALA:HB1	2.18	0.43
1:A:3913:ILE:O	1:A:3917:ILE:HG12	2.19	0.43
2:B:182:LYS:HA	2:B:185:ARG:HG2	2.01	0.43
1:A:52:ALA:O	1:A:55:THR:OG1	2.35	0.43
1:A:293:LEU:HD12	1:A:294:PHE:N	2.34	0.43
1:A:452:LYS:HG3	1:A:453:MET:H	1.83	0.43
1:A:479:ILE:HG21	1:A:567:GLU:OE1	2.17	0.43
1:A:624:ILE:O	1:A:625:ASN:C	2.61	0.43
1:A:1471:GLN:HA	1:A:1477:HIS:NE2	2.34	0.43
1:A:1986:ARG:HB2	1:A:2183:HIS:C	2.43	0.43
1:A:2824:LYS:HB3	1:A:2824:LYS:HE2	1.76	0.43
1:A:3974:MET:HG2	1:A:3978:GLY:HA3	2.01	0.43
1:A:3980:MET:SD	1:A:3980:MET:N	2.90	0.43
2:B:187:ARG:HH11	2:B:187:ARG:HG3	1.84	0.43
3:C:209:LYS:HA	3:C:212:MET:HE2	2.00	0.43
3:C:596:GLU:HB3	3:C:599:ARG:HH21	1.84	0.43
1:A:351:ASN:OD1	1:A:352:VAL:N	2.51	0.43
1:A:1299:GLU:HG3	1:A:1304:HIS:CD2	2.54	0.43
1:A:1558:TYR:O	1:A:1562:LEU:HG	2.19	0.43
1:A:1592:MET:SD	1:A:1592:MET:N	2.92	0.43
1:A:1632:TRP:CD1	1:A:1645:VAL:HB	2.53	0.43
1:A:2950:LYS:HE3	1:A:2986:PRO:HB3	2.01	0.43
1:A:3266:SER:OG	1:A:3273:LEU:HD12	2.19	0.43
1:A:3737:ARG:NH1	1:A:3751:LEU:HD13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:TYR:CE1	3:C:435:PHE:HB3	2.54	0.43
2:B:476:ASP:HA	3:C:427:MET:HE3	2.01	0.43
1:A:151:GLU:HG3	1:A:152:LEU:HD22	2.00	0.42
1:A:326:MET:HA	1:A:329:LYS:HE2	1.99	0.42
1:A:339:GLN:HA	1:A:342:MET:HE3	2.00	0.42
1:A:1248:PHE:CE1	1:A:1321:ARG:HD3	2.54	0.42
1:A:1298:LEU:HA	1:A:1367:HIS:CG	2.54	0.42
1:A:1339:VAL:O	1:A:1342:MET:HG3	2.19	0.42
1:A:1372:LEU:HA	1:A:1375:THR:HG22	2.00	0.42
1:A:1438:GLY:O	1:A:1445:ARG:NH2	2.51	0.42
1:A:1444:ASP:N	1:A:1444:ASP:OD1	2.51	0.42
1:A:1491:ILE:HD12	1:A:1558:TYR:HD2	1.84	0.42
1:A:1629:CYS:HB3	1:A:1633:TRP:HE1	1.84	0.42
1:A:2950:LYS:NZ	1:A:2983:ASP:O	2.47	0.42
1:A:3810:VAL:HG12	1:A:3932:MET:HE3	2.00	0.42
3:C:265:LYS:HD2	3:C:362:LEU:HD13	2.01	0.42
6:D:40:DT:C4	7:E:17:DT:O4	2.72	0.42
6:D:43:DT:C4	7:E:16:DA:C6	3.07	0.42
1:A:275:PHE:HD2	1:A:315:ALA:HB1	1.83	0.42
1:A:465:PHE:CE2	1:A:564:LEU:HD21	2.52	0.42
1:A:1098:GLN:O	1:A:1152:ARG:HB2	2.19	0.42
1:A:1157:PHE:HE2	1:A:1168:LEU:HD13	1.84	0.42
1:A:1571:LEU:HD23	1:A:1600:MET:HE3	2.00	0.42
1:A:1614:GLN:O	1:A:1618:LEU:HG	2.19	0.42
1:A:2295:GLN:OE1	1:A:2298:GLU:N	2.50	0.42
1:A:2440:TYR:O	1:A:2443:MET:HG3	2.19	0.42
1:A:2931:ARG:HG2	1:A:2936:TYR:CE1	2.54	0.42
1:A:3189:PHE:O	1:A:3193:ILE:HG12	2.19	0.42
1:A:4064:LEU:HD23	1:A:4068:HIS:CE1	2.54	0.42
3:C:205:LEU:O	3:C:209:LYS:HB2	2.19	0.42
4:F:50:ARG:HH21	4:F:55:ARG:HA	1.85	0.42
6:D:34:DC:C6	6:D:35:DT:C4	3.07	0.42
1:A:465:PHE:HA	1:A:468:LEU:HG	2.02	0.42
1:A:1175:HIS:HB3	1:A:1178:ARG:NH1	2.34	0.42
1:A:2093:CYS:C	1:A:2096:PRO:HD2	2.45	0.42
1:A:2563:LEU:HD13	1:A:2795:GLN:HB3	2.02	0.42
1:A:2804:ILE:HG22	1:A:2808:LEU:HD23	2.01	0.42
1:A:3175:PRO:HA	1:A:3249:GLN:HE22	1.84	0.42
1:A:3862:ALA:O	1:A:4119:ARG:NH2	2.38	0.42
2:B:48:MET:N	2:B:48:MET:SD	2.91	0.42
2:B:420:LEU:HA	2:B:426:GLN:HA	0.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:GLU:HG3	4:F:54:GLY:HA3	2.01	0.42
1:A:896:VAL:HG12	1:A:903:PRO:HG2	2.02	0.42
1:A:933:LEU:HD12	1:A:934:LEU:N	2.34	0.42
1:A:1149:LYS:N	1:A:1163:LEU:O	2.52	0.42
1:A:1565:GLU:OE1	1:A:1565:GLU:N	2.40	0.42
1:A:3067:LYS:HB2	1:A:3067:LYS:HE2	1.80	0.42
1:A:3442:TYR:N	1:A:3443:PRO:HD2	2.34	0.42
1:A:3581:PRO:HD3	1:A:3629:ARG:HH11	1.85	0.42
1:A:3696:ARG:NH1	1:A:3698:GLU:HA	2.34	0.42
1:A:3924:HIS:H	1:A:3927:ASN:HD22	1.67	0.42
2:B:361:TYR:C	2:B:362:LEU:HD12	2.44	0.42
3:C:33:GLN:NE2	3:C:231:LEU:HD22	2.34	0.42
1:A:656:GLN:HG3	1:A:666:PHE:HZ	1.84	0.42
1:A:901:MET:HA	1:A:2819:GLU:HG2	2.01	0.42
1:A:1264:LEU:HD11	1:A:1341:ILE:HB	2.02	0.42
1:A:1632:TRP:HB3	1:A:1645:VAL:HG11	2.01	0.42
1:A:2200:ALA:O	1:A:2245:TRP:NE1	2.48	0.42
1:A:2852:PRO:HB2	1:A:2853:PRO:HD3	2.01	0.42
1:A:3063:THR:HA	1:A:3066:ASP:OD2	2.19	0.42
1:A:3066:ASP:HA	1:A:3069:MET:HE1	2.01	0.42
1:A:3171:ALA:HA	1:A:3179:TRP:HE1	1.84	0.42
1:A:3755:GLY:HA2	1:A:3800:LEU:HA	2.00	0.42
1:A:3950:THR:HG22	1:A:3957:GLU:O	2.19	0.42
3:C:593:ASN:HB2	3:C:594:PRO:HD3	2.01	0.42
1:A:172:GLU:HG3	1:A:220:LEU:CA	2.50	0.42
1:A:1066:LEU:O	1:A:1074:LYS:HB3	2.19	0.42
1:A:1897:ASN:O	1:A:1902:GLY:N	2.41	0.42
1:A:1952:ILE:HD12	1:A:1956:PHE:HB3	2.01	0.42
1:A:2092:GLU:OE1	1:A:2092:GLU:N	2.53	0.42
1:A:3816:LEU:O	1:A:3820:MET:HG3	2.19	0.42
1:A:3953:LEU:HD22	1:A:4026:SER:HB3	2.01	0.42
1:A:4014:LYS:NZ	1:A:4032:ASN:O	2.52	0.42
2:B:124:GLY:O	2:B:128:GLN:HB2	2.20	0.42
6:D:43:DT:H3	7:E:15:DA:C4'	2.32	0.42
1:A:289:ASN:ND2	1:A:292:SER:HB3	2.34	0.42
1:A:1794:GLN:O	1:A:1798:LEU:HG	2.20	0.42
1:A:2316:TYR:CZ	1:A:2359:LYS:HG2	2.55	0.42
1:A:2320:ALA:CB	1:A:2363:CYS:HA	2.49	0.42
1:A:3006:ALA:HB3	1:A:3257:LYS:HD2	2.02	0.42
1:A:3959:MET:HE2	1:A:4124:TRP:CE3	2.54	0.42
1:A:3964:THR:HG22	1:A:4128:MET:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ASN:OD1	2:B:95:ASN:N	2.53	0.42
2:B:301:ARG:HH22	2:B:313:PRO:HD3	1.85	0.42
2:B:401:THR:HG23	2:B:406:ILE:HB	2.02	0.42
3:C:434:MET:SD	3:C:435:PHE:N	2.93	0.42
3:C:635:SER:O	3:C:639:ILE:HG12	2.19	0.42
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.89	0.42
1:A:269:SER:HB2	1:A:308:LEU:HD23	2.02	0.42
1:A:357:LYS:O	1:A:361:ILE:HG12	2.18	0.42
1:A:905:ILE:HG23	1:A:2811:SER:HB2	2.01	0.42
1:A:1154:PRO:HG2	1:A:1157:PHE:HD2	1.84	0.42
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.92	0.42
1:A:1715:GLU:O	1:A:1719:VAL:HG13	2.20	0.42
1:A:2304:VAL:HA	1:A:2307:MET:HG3	2.02	0.42
1:A:2481:HIS:O	1:A:2485:ARG:HB3	2.20	0.42
1:A:2918:PRO:HA	1:A:2921:LEU:HB3	2.01	0.42
1:A:3154:GLN:HA	1:A:3157:LEU:HD12	2.02	0.42
1:A:3669:LYS:HE2	1:A:3669:LYS:HB3	1.77	0.42
1:A:3875:GLU:CB	1:A:3965:ARG:HD2	2.49	0.42
1:A:4042:GLN:OE1	1:A:4042:GLN:N	2.53	0.42
3:C:57:VAL:HA	3:C:79:VAL:HA	2.02	0.42
3:C:346:CYS:SG	3:C:390:VAL:HG23	2.59	0.42
3:C:510:GLN:HA	3:C:513:TRP:HD1	1.84	0.42
3:C:644:GLU:O	3:C:648:LYS:HG3	2.19	0.42
6:D:37:DT:H2'	6:D:38:DT:N1	2.33	0.42
1:A:89:LEU:HB3	1:A:133:LYS:HE2	2.02	0.42
1:A:386:VAL:HG12	1:A:431:TYR:HE2	1.83	0.42
1:A:414:LEU:HA	1:A:417:VAL:HG12	2.00	0.42
1:A:764:PRO:O	1:A:768:VAL:HG12	2.20	0.42
1:A:1326:GLU:HA	1:A:1329:ARG:HB2	2.02	0.42
1:A:1565:GLU:HG2	1:A:1566:THR:H	1.85	0.42
1:A:2394:LYS:O	1:A:2398:LEU:HG	2.20	0.42
1:A:3820:MET:HE1	1:A:3824:GLU:C	2.45	0.42
1:A:3843:LEU:HD13	1:A:3855:TYR:CE1	2.55	0.42
2:B:95:ASN:ND2	2:B:102:ILE:HB	2.34	0.42
3:C:66:ASN:OD1	3:C:66:ASN:N	2.53	0.42
4:F:93:ARG:HE	4:F:97:LEU:HG	1.85	0.42
1:A:565:TYR:O	1:A:569:VAL:HG23	2.20	0.42
1:A:1769:GLU:HB3	1:A:1772:HIS:CG	2.55	0.42
1:A:2126:MET:O	1:A:2130:HIS:ND1	2.49	0.42
1:A:2240:THR:O	1:A:2243:GLU:HG3	2.20	0.42
1:A:2891:ARG:O	1:A:2892:LEU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3169:PRO:HD2	1:A:3179:TRP:CZ3	2.55	0.42
1:A:3409:VAL:HG22	1:A:3413:TYR:CE2	2.54	0.42
1:A:3574:ALA:HB1	1:A:3686:TRP:HB3	2.01	0.42
1:A:3971:MET:HE2	1:A:3980:MET:HE2	2.02	0.42
1:A:4055:ASN:HB2	1:A:4095:GLU:HA	2.02	0.42
3:C:16:VAL:HG12	3:C:59:PHE:O	2.20	0.42
1:A:323:VAL:HA	1:A:326:MET:CG	2.49	0.41
1:A:722:LYS:HD3	1:A:722:LYS:HA	1.78	0.41
1:A:907:LEU:HA	1:A:910:PHE:CE2	2.55	0.41
1:A:1477:HIS:O	1:A:1481:THR:OG1	2.24	0.41
1:A:1803:GLU:OE2	1:A:1804:MET:HE3	2.20	0.41
1:A:1945:TYR:CE2	1:A:1949:ILE:HD11	2.54	0.41
1:A:3537:SER:HA	1:A:3540:TYR:CG	2.55	0.41
1:A:3574:ALA:HB3	1:A:3687:MET:HE3	2.02	0.41
1:A:3959:MET:HG3	1:A:4124:TRP:CH2	2.55	0.41
1:A:4089:ILE:O	1:A:4093:GLU:N	2.53	0.41
1:A:4115:ASN:OD1	1:A:4119:ARG:NH2	2.53	0.41
2:B:89:GLY:HA2	2:B:140:ASP:O	2.20	0.41
3:C:209:LYS:O	3:C:213:ILE:HG23	2.20	0.41
1:A:136:GLN:O	1:A:140:SER:N	2.53	0.41
1:A:156:PHE:HA	1:A:159:GLU:OE1	2.20	0.41
1:A:202:GLY:O	1:A:206:THR:HG23	2.20	0.41
1:A:389:ILE:HG22	1:A:393:LYS:HZ1	1.83	0.41
1:A:411:PRO:HG3	1:A:457:CYS:SG	2.60	0.41
1:A:1188:ILE:HG13	1:A:1189:GLU:N	2.35	0.41
1:A:1407:LYS:HA	1:A:1412:LYS:HD3	2.01	0.41
1:A:1436:LEU:HG	1:A:1437:TYR:H	1.84	0.41
1:A:2260:PHE:HA	1:A:2273:GLY:HA3	2.01	0.41
1:A:2274:ILE:HG23	1:A:2306:ASN:ND2	2.36	0.41
1:A:2281:MET:HE2	1:A:2326:ILE:CD1	2.50	0.41
1:A:2813:PHE:CE2	1:A:2868:LEU:HD11	2.51	0.41
1:A:2927:ALA:HB1	1:A:2931:ARG:HH12	1.84	0.41
1:A:3631:LYS:HB3	1:A:3631:LYS:HE3	1.87	0.41
1:A:3704:GLN:CD	1:A:3716:HIS:HB3	2.45	0.41
1:A:3806:LEU:C	1:A:3807:GLU:HG3	2.45	0.41
1:A:3967:PHE:O	1:A:3970:LEU:N	2.54	0.41
1:A:4114:PRO:HA	1:A:4117:LEU:HB2	2.01	0.41
2:B:64:ILE:HG21	2:B:123:LYS:HB3	2.02	0.41
2:B:86:VAL:HA	2:B:104:VAL:HA	2.00	0.41
3:C:632:PHE:O	3:C:636:ILE:HG23	2.20	0.41
4:F:50:ARG:NH2	4:F:58:ALA:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:O	1:A:120:ALA:HA	2.20	0.41
1:A:333:MET:HG3	1:A:334:HIS:N	2.35	0.41
1:A:1297:PHE:HA	1:A:1300:SER:OG	2.20	0.41
1:A:2244:CYS:SG	1:A:2245:TRP:N	2.93	0.41
1:A:2551:GLU:HA	1:A:2554:PHE:HD2	1.83	0.41
1:A:2953:THR:OG1	1:A:2994:TRP:NE1	2.47	0.41
1:A:2978:LYS:HG2	1:A:2981:TRP:CE2	2.55	0.41
1:A:3840:LYS:HD2	1:A:3840:LYS:HA	1.92	0.41
2:B:113:ALA:O	2:B:117:LEU:HG	2.19	0.41
2:B:262:LYS:HA	2:B:268:VAL:HG12	2.01	0.41
2:B:347:LEU:HA	2:B:398:CYS:SG	2.60	0.41
2:B:356:LEU:HG	2:B:358:LYS:NZ	2.35	0.41
2:B:404:ARG:CZ	6:D:31:DA:H3'	2.50	0.41
2:B:484:GLN:HG2	2:B:488:ARG:CZ	2.50	0.41
3:C:338:LYS:HG3	3:C:398:ASP:HA	2.02	0.41
3:C:609:PHE:O	3:C:612:ALA:N	2.42	0.41
1:A:416:SER:O	1:A:420:VAL:HG13	2.20	0.41
1:A:3147:LYS:NZ	1:A:3149:GLY:H	2.19	0.41
1:A:3192:LYS:HA	1:A:3192:LYS:HD2	1.87	0.41
1:A:3570:ASP:N	1:A:3570:ASP:OD1	2.53	0.41
2:B:482:VAL:HG22	3:C:333:TYR:CD2	2.55	0.41
2:B:515:ASN:O	2:B:519:GLY:N	2.54	0.41
3:C:56:LEU:HD23	3:C:80:HIS:ND1	2.35	0.41
3:C:342:VAL:HG22	3:C:393:VAL:HG22	2.02	0.41
3:C:528:ILE:HB	3:C:529:PRO:HD3	2.03	0.41
4:F:80:VAL:HG11	4:F:83:ILE:HG13	2.02	0.41
1:A:42:CYS:HB2	1:A:88:PHE:CG	2.55	0.41
1:A:51:LEU:O	1:A:54:GLN:NE2	2.48	0.41
1:A:70:ARG:HB2	1:A:78:PHE:HD2	1.86	0.41
1:A:294:PHE:CE2	1:A:298:LEU:HD11	2.55	0.41
1:A:581:LEU:HD22	1:A:620:PHE:HD1	1.85	0.41
1:A:766:ALA:HB3	1:A:851:ILE:HD12	2.02	0.41
1:A:876:SER:C	1:A:880:MET:HE3	2.46	0.41
1:A:1983:ASP:H	1:A:2090:ARG:CZ	2.34	0.41
1:A:2218:PHE:HA	1:A:2221:LYS:HZ3	1.86	0.41
1:A:2411:LEU:O	1:A:2415:LEU:HG	2.21	0.41
1:A:2436:LEU:HD12	1:A:2469:CYS:HB2	2.03	0.41
1:A:3036:TYR:O	1:A:3039:THR:OG1	2.32	0.41
1:A:3298:LEU:HD23	1:A:3337:ILE:HB	2.03	0.41
1:A:3388:ALA:O	1:A:3392:ALA:N	2.45	0.41
1:A:3681:LYS:C	1:A:3688:SER:HB3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3749:PRO:HB3	1:A:3805:TRP:HD1	1.86	0.41
2:B:65:GLN:HA	2:B:68:GLN:NE2	2.36	0.41
2:B:90:THR:OG1	2:B:136:GLY:HA3	2.20	0.41
2:B:290:ARG:HG2	3:C:309:ASP:C	2.45	0.41
6:D:39:DA:H2'	6:D:40:DT:C5	2.55	0.41
7:E:33:DA:C4	7:E:34:DT:C4	3.09	0.41
1:A:1724:MET:HG2	1:A:1768:ARG:HD3	2.03	0.41
1:A:1864:ASP:HA	1:A:1867:ILE:HG22	2.01	0.41
1:A:3028:ASN:O	1:A:3029:LYS:HD2	2.20	0.41
1:A:3340:ALA:O	1:A:3343:SER:OG	2.38	0.41
1:A:3705:TYR:OH	1:A:3714:GLU:OE1	2.38	0.41
1:A:3762:GLN:HB3	1:A:3793:VAL:HG23	2.02	0.41
1:A:3821:SER:OG	1:A:3823:GLU:OE1	2.31	0.41
1:A:3875:GLU:HB3	1:A:3965:ARG:HD2	2.02	0.41
1:A:4056:PRO:HA	1:A:4059:ILE:HG12	2.02	0.41
2:B:340:PHE:HE2	3:C:485:PRO:HB2	1.86	0.41
3:C:251:LEU:O	3:C:258:SER:HA	2.20	0.41
3:C:546:ASP:OD1	3:C:547:GLN:N	2.54	0.41
1:A:95:LYS:NZ	1:A:140:SER:OG	2.28	0.41
1:A:268:PRO:HG2	1:A:308:LEU:HD21	2.03	0.41
1:A:985:GLU:N	1:A:986:PRO:HD2	2.36	0.41
1:A:1483:LEU:HD11	1:A:1518:ALA:HB1	2.01	0.41
1:A:1653:LEU:HD23	1:A:1695:LEU:HD12	2.02	0.41
1:A:1791:CYS:HB2	1:A:1835:ALA:HB2	2.02	0.41
1:A:2927:ALA:HB1	1:A:2931:ARG:NH1	2.36	0.41
1:A:3667:LEU:HA	1:A:3670:MET:HG3	2.02	0.41
1:A:4040:PRO:HA	1:A:4043:LYS:HD2	2.02	0.41
1:A:4048:LYS:HE2	1:A:4048:LYS:HA	2.01	0.41
1:A:4101:GLU:O	1:A:4105:LYS:HG2	2.20	0.41
2:B:446:MET:HE1	3:C:264:TYR:CG	2.56	0.41
3:C:11:VAL:HG21	3:C:114:SER:CB	2.51	0.41
4:F:111:LYS:HG3	4:F:132:ILE:HD13	2.03	0.41
1:A:20:SER:HA	1:A:23:ASP:CB	2.51	0.41
1:A:196:LEU:HB3	1:A:200:PHE:CE2	2.56	0.41
1:A:581:LEU:HD22	1:A:620:PHE:CD1	2.55	0.41
1:A:583:LEU:HA	1:A:614:PRO:HA	2.03	0.41
1:A:726:LEU:O	1:A:730:LEU:HG	2.21	0.41
1:A:871:LEU:HD21	1:A:3122:HIS:HB2	2.03	0.41
1:A:1235:ILE:HD12	1:A:1289:SER:HB2	2.03	0.41
1:A:2452:ARG:HD3	1:A:2494:ASP:HA	2.02	0.41
1:A:3164:TRP:HB3	1:A:3186:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4073:ALA:O	1:A:4077:TYR:N	2.42	0.41
2:B:38:LEU:HD13	2:B:165:ARG:O	2.21	0.41
2:B:269:ILE:HG13	2:B:270:SER:H	1.85	0.41
2:B:429:PRO:HB3	3:C:435:PHE:CD2	2.56	0.41
3:C:301:ASP:OD1	3:C:301:ASP:N	2.52	0.41
3:C:643:ARG:HH21	3:C:647:ILE:HG13	1.86	0.41
6:D:29:DA:N1	7:E:28:DA:C2	2.89	0.41
1:A:10:CYS:N	1:A:13:LEU:HD12	2.36	0.41
1:A:149:ILE:HG21	1:A:183:GLU:HB2	2.02	0.41
1:A:165:LYS:HA	1:A:165:LYS:HD3	1.82	0.41
1:A:734:LEU:HD21	1:A:769:GLY:N	2.36	0.41
1:A:925:GLN:HA	1:A:928:VAL:HG22	2.03	0.41
1:A:960:GLN:CD	1:A:960:GLN:H	2.28	0.41
1:A:1070:PRO:HA	1:A:1075:ARG:NH2	2.36	0.41
1:A:1076:LEU:HD22	1:A:1121:LEU:HD11	2.03	0.41
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.41
1:A:1191:PHE:O	1:A:1195:VAL:HG23	2.21	0.41
1:A:1430:GLU:O	1:A:1434:VAL:HG13	2.21	0.41
1:A:1748:ASP:OD1	1:A:1749:ALA:N	2.54	0.41
1:A:1836:LEU:HB3	1:A:1840:PHE:CZ	2.56	0.41
1:A:1888:ASP:HB2	1:A:1896:ILE:HG12	2.02	0.41
1:A:1986:ARG:H	1:A:2183:HIS:HA	1.86	0.41
1:A:2126:MET:HB2	1:A:2164:TRP:CZ2	2.56	0.41
1:A:2281:MET:SD	1:A:2287:PRO:HA	2.61	0.41
1:A:2379:MET:HA	1:A:2382:VAL:HG22	2.03	0.41
1:A:2571:ASP:HA	1:A:2574:ASN:HB2	2.03	0.41
1:A:2795:GLN:HA	1:A:2798:ALA:HB3	2.03	0.41
1:A:2831:ASN:HD22	1:A:2834:GLN:NE2	2.18	0.41
1:A:2891:ARG:HH21	1:A:3897:PHE:HD2	1.69	0.41
1:A:3315:TYR:HD1	1:A:3318:LYS:HE3	1.86	0.41
1:A:3320:ILE:CG2	1:A:3324:ARG:HH21	2.34	0.41
1:A:3763:ARG:O	1:A:3766:GLN:HG3	2.20	0.41
1:A:3840:LYS:O	1:A:3844:THR:HG23	2.20	0.41
1:A:3972:LEU:N	1:A:3973:PRO:HD2	2.36	0.41
1:A:4021:LEU:HA	1:A:4028:ILE:HG22	2.02	0.41
2:B:302:THR:HA	3:C:291:LYS:HA	2.03	0.41
2:B:465:ILE:O	2:B:518:LEU:HD11	2.21	0.41
3:C:65:ASP:N	3:C:78:THR:HG22	2.35	0.41
3:C:82:HIS:CE1	3:C:84:MET:HG2	2.56	0.41
3:C:368:ARG:HG3	3:C:369:ASP:N	2.36	0.41
3:C:622:GLN:NE2	3:C:631:TYR:HD2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:65:ILE:HG23	4:F:70:GLY:HA3	2.02	0.41
6:D:20:DT:H2"	6:D:21:DA:OP2	2.21	0.41
7:E:19:DA:C6	7:E:20:DT:C2	3.09	0.41
1:A:178:LEU:HB2	1:A:227:LEU:HD13	2.03	0.41
1:A:458:CYS:HA	1:A:461:ILE:HG12	2.02	0.41
1:A:1336:THR:O	1:A:1339:VAL:HG22	2.21	0.41
1:A:2102:LYS:O	1:A:2106:ARG:HD3	2.21	0.41
1:A:2414:GLN:O	1:A:2418:LYS:HG2	2.21	0.41
1:A:2421:VAL:HG23	1:A:2457:PRO:HG3	2.03	0.41
1:A:3410:ILE:HG21	1:A:3456:LEU:HB2	2.02	0.41
1:A:3493:TRP:H	1:A:3521:ILE:HD11	1.85	0.41
1:A:3771:MET:HE1	1:A:3998:LEU:HD21	2.02	0.41
1:A:3821:SER:O	1:A:3825:LYS:N	2.48	0.41
1:A:3839:TYR:CE2	1:A:4122:GLU:HB2	2.56	0.41
2:B:127:GLY:HA2	2:B:130:ARG:HG2	2.03	0.41
3:C:153:SER:HA	3:C:156:LYS:HE2	2.03	0.41
3:C:553:ILE:HD13	3:C:553:ILE:HA	1.90	0.41
1:A:453:MET:HA	1:A:456:VAL:HB	2.03	0.40
1:A:554:ASN:OD1	1:A:555:SER:N	2.54	0.40
1:A:1109:GLU:O	1:A:1113:LEU:HG	2.21	0.40
1:A:1133:HIS:O	1:A:1136:ARG:HG2	2.21	0.40
1:A:1140:LYS:HB3	1:A:1140:LYS:HE2	1.89	0.40
1:A:1554:SER:OG	1:A:1555:HIS:N	2.54	0.40
1:A:1935:GLU:OE1	1:A:1935:GLU:N	2.51	0.40
1:A:2298:GLU:HA	1:A:2301:GLN:HB3	2.02	0.40
1:A:2454:LEU:C	1:A:2457:PRO:HD2	2.47	0.40
1:A:3280:TYR:CE1	1:A:3304:VAL:HG21	2.56	0.40
2:B:203:MET:SD	2:B:238:LYS:HB2	2.61	0.40
3:C:59:PHE:HA	3:C:76:ASN:O	2.20	0.40
4:F:109:LEU:CG	4:F:132:ILE:HB	2.51	0.40
1:A:670:LEU:HA	1:A:673:THR:HB	2.03	0.40
1:A:772:ALA:O	1:A:776:TRP:CD1	2.75	0.40
1:A:1244:LEU:HD21	1:A:1310:GLU:HB2	2.02	0.40
1:A:1537:VAL:CG2	1:A:1552:HIS:HB3	2.51	0.40
1:A:1596:VAL:O	1:A:1600:MET:HG2	2.21	0.40
1:A:1916:ILE:HD12	1:A:1916:ILE:H	1.85	0.40
1:A:2091:HIS:CG	1:A:2092:GLU:H	2.39	0.40
1:A:2364:LEU:HD13	1:A:2400:VAL:HG11	2.03	0.40
1:A:2930:TYR:O	1:A:2934:GLY:N	2.54	0.40
1:A:3273:LEU:HD21	1:A:3307:LEU:HD21	2.03	0.40
1:A:3822:GLN:HA	1:A:3825:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ARG:O	2:B:118:GLU:HG2	2.21	0.40
3:C:326:VAL:O	3:C:329:GLU:HG2	2.22	0.40
3:C:427:MET:SD	3:C:427:MET:N	2.92	0.40
4:F:111:LYS:HG3	4:F:132:ILE:CD1	2.51	0.40
1:A:333:MET:HG3	1:A:334:HIS:H	1.86	0.40
1:A:452:LYS:HG3	1:A:453:MET:N	2.35	0.40
1:A:1009:LEU:O	1:A:1013:ILE:HG12	2.22	0.40
1:A:1127:CYS:O	1:A:1131:ILE:HG12	2.21	0.40
1:A:2187:VAL:HA	1:A:2190:VAL:HG22	2.02	0.40
1:A:2787:HIS:O	1:A:2790:LEU:HG	2.21	0.40
1:A:2806:LYS:HD2	1:A:2853:PRO:O	2.22	0.40
1:A:3685:PRO:O	1:A:3688:SER:OG	2.31	0.40
1:A:3840:LYS:HG2	1:A:4122:GLU:OE2	2.21	0.40
1:A:4040:PRO:HD2	1:A:4041:ARG:NH1	2.36	0.40
1:A:4093:GLU:HG3	1:A:4098:LEU:HD22	2.04	0.40
2:B:148:TRP:O	2:B:152:ASN:ND2	2.55	0.40
2:B:276:LEU:HD11	3:C:354:ARG:HD3	2.03	0.40
2:B:331:LYS:N	2:B:331:LYS:HD3	2.35	0.40
2:B:446:MET:HE2	3:C:363:LYS:CB	2.52	0.40
3:C:356:PHE:CG	3:C:422:VAL:HG21	2.56	0.40
4:F:91:TYR:CD2	4:F:136:SER:HB2	2.56	0.40
1:A:209:THR:O	1:A:210:SER:C	2.64	0.40
1:A:439:VAL:HG23	1:A:440:VAL:HG13	2.03	0.40
1:A:762:TYR:CZ	1:A:764:PRO:HG2	2.57	0.40
1:A:1184:ARG:O	1:A:1188:ILE:HG12	2.21	0.40
1:A:1279:LEU:HA	1:A:1282:LEU:HG	2.03	0.40
1:A:1392:MET:HA	1:A:1395:LEU:HD12	2.04	0.40
1:A:2480:ILE:HG23	1:A:2484:TYR:HD2	1.87	0.40
1:A:2996:LEU:HA	1:A:2999:LEU:HD12	2.02	0.40
1:A:3417:ALA:HA	1:A:3446:VAL:HG21	2.03	0.40
1:A:3558:ILE:HD12	1:A:3558:ILE:HA	1.93	0.40
1:A:3682:GLU:HA	1:A:3685:PRO:HA	2.04	0.40
1:A:3827:ALA:HA	1:A:3831:ASP:HB2	2.03	0.40
1:A:4121:TRP:O	1:A:4126:PRO:HD3	2.22	0.40
2:B:58:THR:OG1	2:B:61:ASP:N	2.43	0.40
3:C:38:ILE:HD12	3:C:38:ILE:HA	1.96	0.40
3:C:62:ASP:HA	3:C:103:GLN:HE22	1.86	0.40
3:C:398:ASP:H	3:C:401:ALA:HB3	1.85	0.40
1:A:283:SER:O	1:A:284:THR:OG1	2.39	0.40
1:A:341:PHE:HD1	1:A:344:GLN:NE2	2.20	0.40
1:A:377:ASN:HB3	1:A:380:ASP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:NH1	1:A:1734:PRO:HA	2.36	0.40
1:A:670:LEU:HB3	1:A:732:PHE:HE1	1.87	0.40
1:A:1589:ASN:OD1	1:A:1592:MET:HE1	2.22	0.40
1:A:1876:ILE:O	1:A:1879:VAL:HG12	2.22	0.40
1:A:2254:ARG:HE	1:A:2292:CYS:HG	1.66	0.40
1:A:2376:ASP:HB2	1:A:2377:ARG:HD3	2.04	0.40
1:A:3443:PRO:HA	1:A:3446:VAL:CG1	2.49	0.40
1:A:4002:MET:O	1:A:4006:VAL:HG12	2.22	0.40
6:D:33:DA:C8	6:D:34:DC:N3	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3652/4128 (88%)	3389 (93%)	258 (7%)	5 (0%)	48	83
2	B	484/609 (80%)	434 (90%)	44 (9%)	6 (1%)	11	44
3	C	639/732 (87%)	586 (92%)	52 (8%)	1 (0%)	44	78
4	F	96/575 (17%)	91 (95%)	5 (5%)	0	100	100
5	M	21/204 (10%)	21 (100%)	0	0	100	100
All	All	4892/6248 (78%)	4521 (92%)	359 (7%)	12 (0%)	45	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	426	GLN
2	B	418	GLU
2	B	420	LEU
2	B	425	ILE
2	B	429	PRO

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Mol	Chain	Res	Type
1	A	101	ALA
1	A	125	ILE
1	A	2330	VAL
1	A	2331	MET
2	B	423	GLN
3	C	509	GLN
1	A	3832	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3158/3671 (86%)	3157 (100%)	1 (0%)	100	100
2	B	414/548 (76%)	412 (100%)	2 (0%)	86	89
3	C	559/649 (86%)	559 (100%)	0	100	100
4	F	78/480 (16%)	78 (100%)	0	100	100
5	M	15/160 (9%)	15 (100%)	0	100	100
All	All	4224/5508 (77%)	4221 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	855	VAL
2	B	421	ASP
2	B	423	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	250	ASN
1	A	278	HIS
1	A	322	GLN

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Mol	Chain	Res	Type
1	A	330	ASN
1	A	415	GLN
1	A	448	GLN
1	A	738	HIS
1	A	739	ASN
1	A	753	GLN
1	A	990	GLN
1	A	1048	GLN
1	A	1125	GLN
1	A	1238	GLN
1	A	1304	HIS
1	A	1320	ASN
1	A	1367	HIS
1	A	1390	GLN
1	A	1457	GLN
1	A	1603	GLN
1	A	1610	ASN
1	A	1687	HIS
1	A	1738	ASN
1	A	1771	GLN
1	A	1941	HIS
1	A	1957	ASN
1	A	2176	ASN
1	A	2213	ASN
1	A	2270	ASN
1	A	2306	ASN
1	A	2351	GLN
1	A	2352	HIS
1	A	2432	GLN
1	A	2475	ASN
1	A	2496	GLN
1	A	2518	GLN
1	A	2768	GLN
1	A	2807	GLN
1	A	2830	ASN
1	A	2831	ASN
1	A	2838	GLN
1	A	2977	ASN
1	A	3108	GLN
1	A	3150	ASN
1	A	3250	ASN
1	A	3311	ASN

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Mol	Chain	Res	Type
1	A	3524	ASN
1	A	3580	ASN
1	A	3643	HIS
1	A	3660	ASN
1	A	3697	ASN
1	A	3772	ASN
1	A	3818	ASN
1	A	3927	ASN
1	A	3951	GLN
1	A	4037	ASN
2	B	65	GLN
2	B	68	GLN
2	B	132	GLN
2	B	458	GLN
2	B	485	GLN
2	B	489	ASN
3	C	50	ASN
3	C	131	HIS
3	C	352	GLN
3	C	359	ASN
3	C	411	HIS
3	C	547	GLN
3	C	622	GLN
4	F	108	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

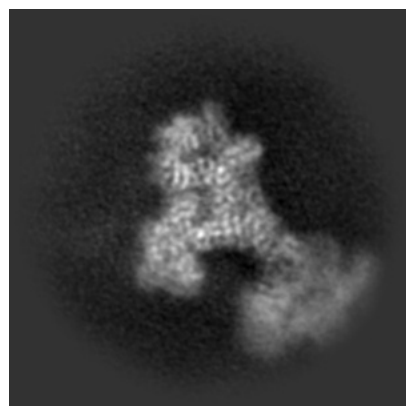
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51156. These allow visual inspection of the internal detail of the map and identification of artifacts.

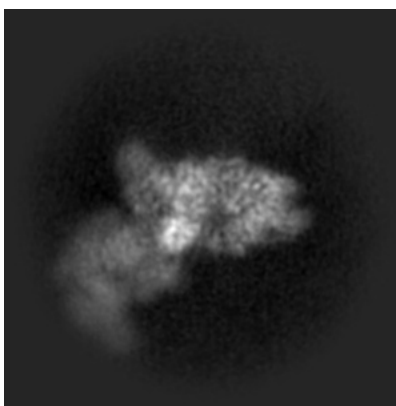
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

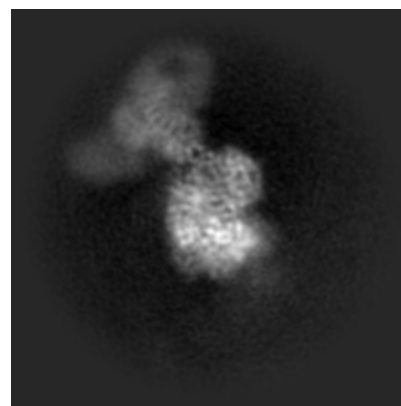
6.1.1 Primary map



X

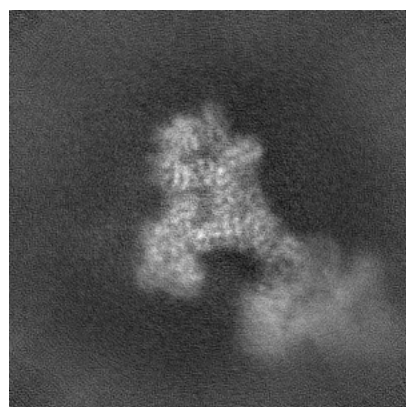


Y

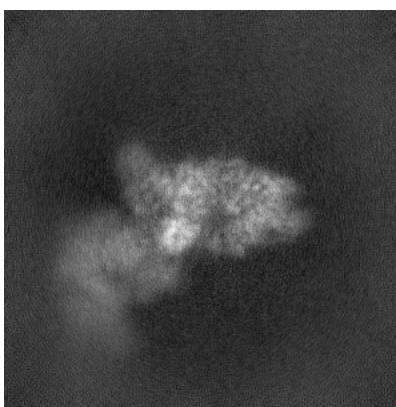


Z

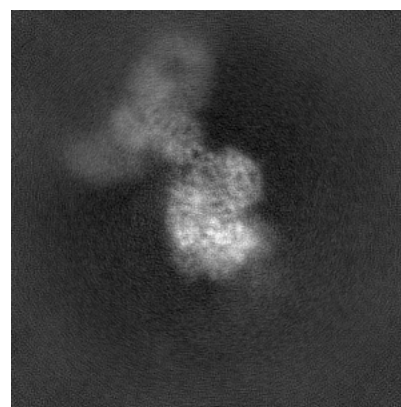
6.1.2 Raw map



X



Y

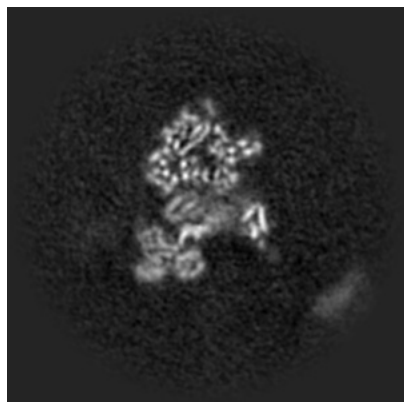


Z

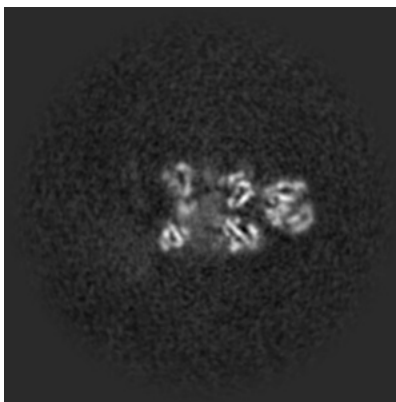
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

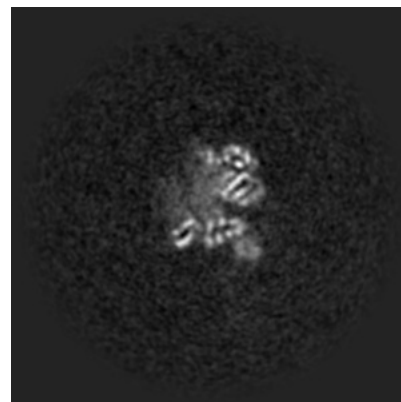
6.2.1 Primary map



X Index: 160

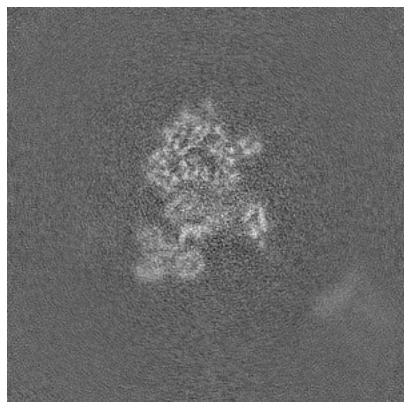


Y Index: 160

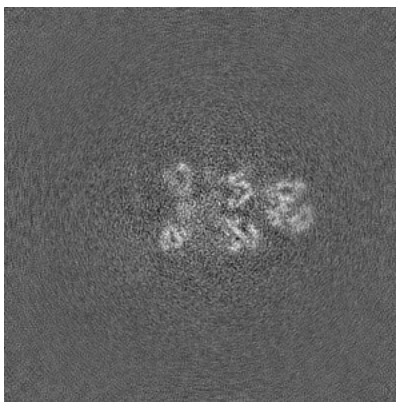


Z Index: 160

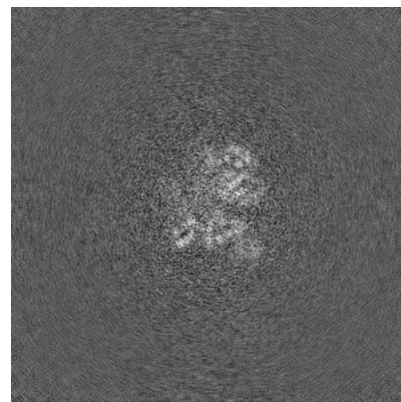
6.2.2 Raw map



X Index: 160



Y Index: 160

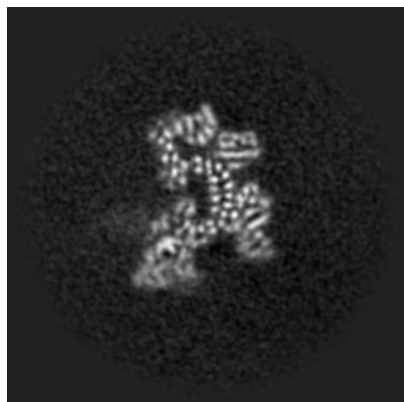


Z Index: 160

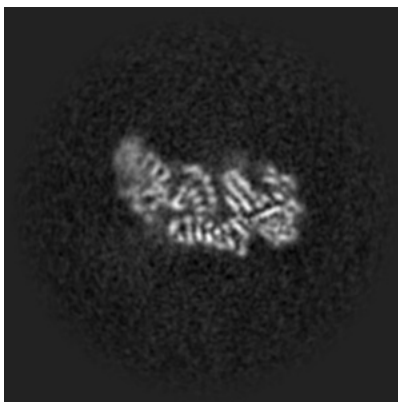
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

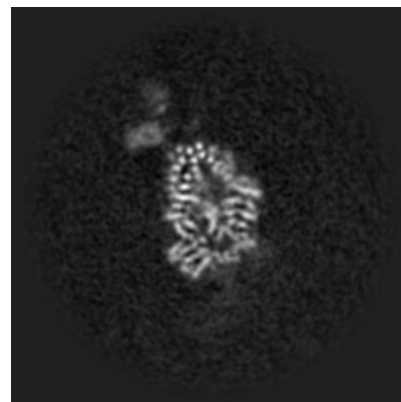
6.3.1 Primary map



X Index: 176

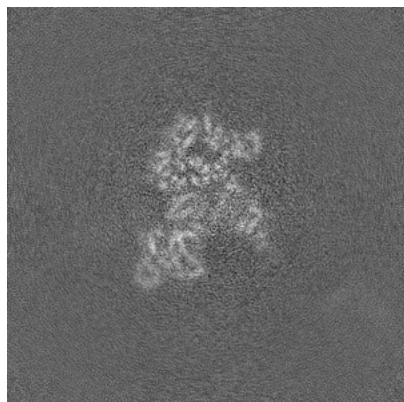


Y Index: 141

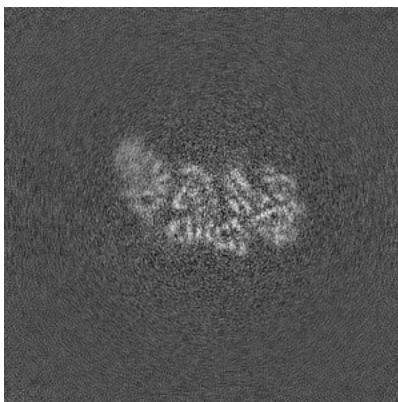


Z Index: 141

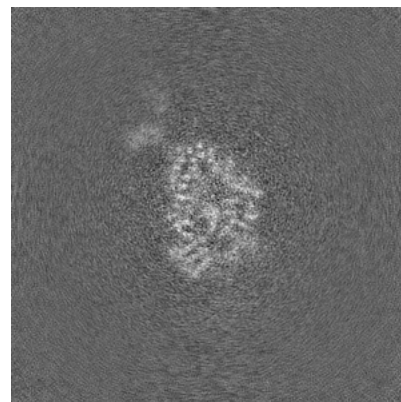
6.3.2 Raw map



X Index: 165



Y Index: 142

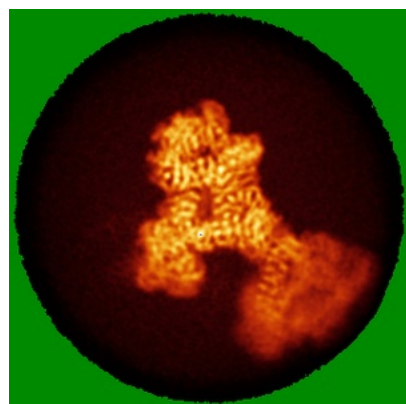


Z Index: 142

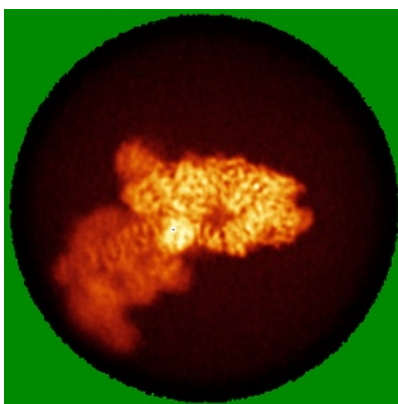
The images above show the largest variance slices of the map in three orthogonal directions.

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

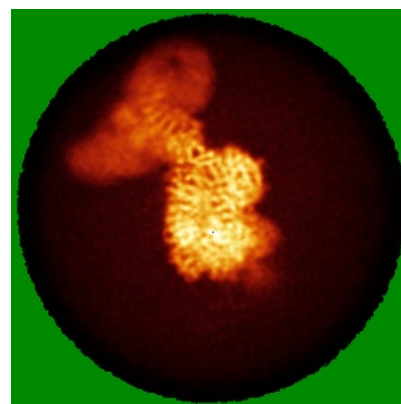
6.4.1 Primary map



X

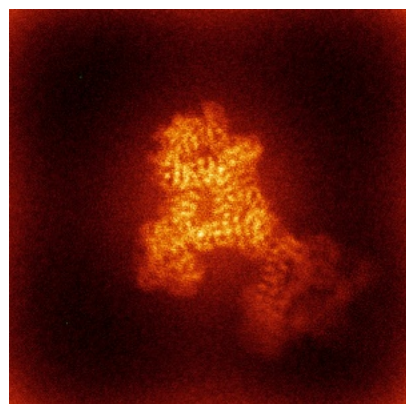


Y

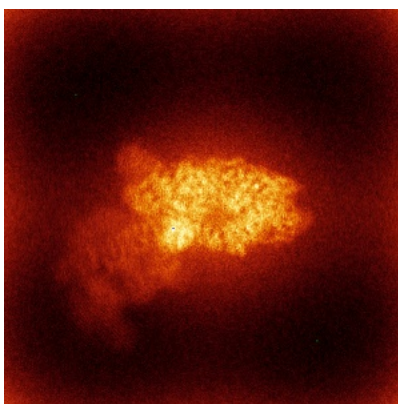


Z

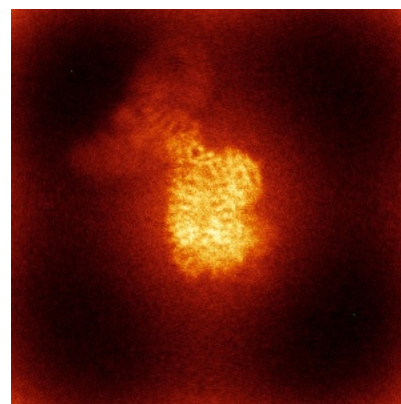
6.4.2 Raw map



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.

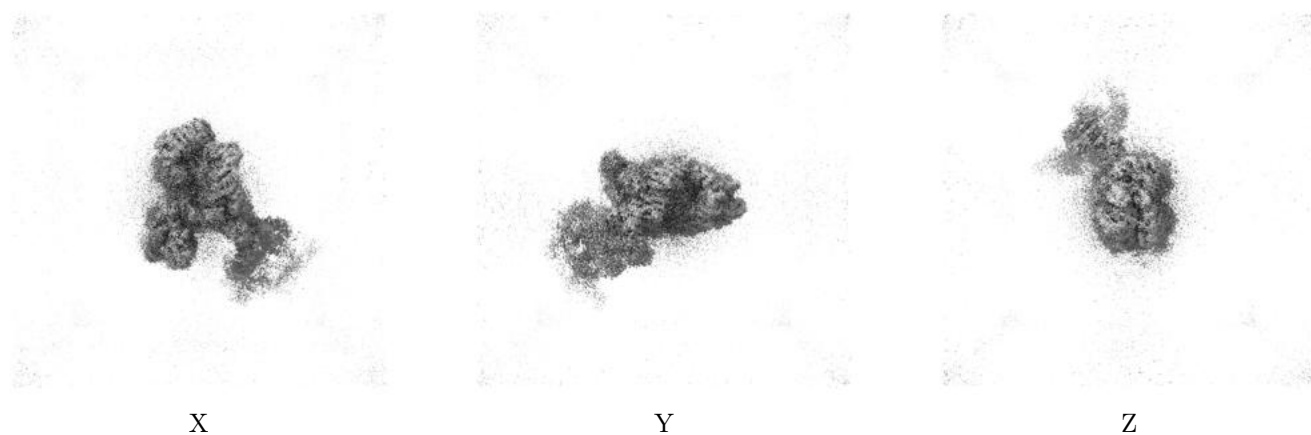
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

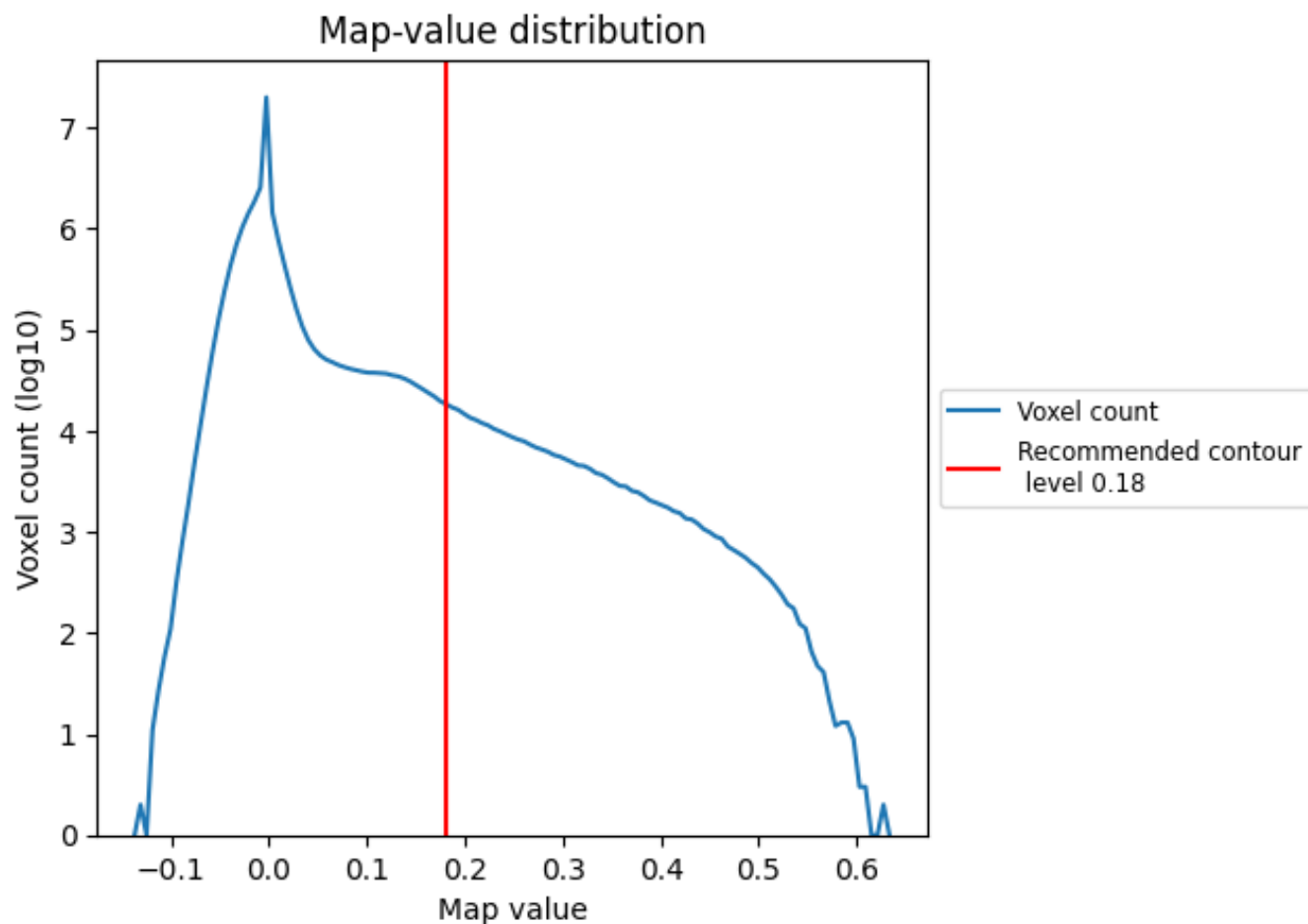
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

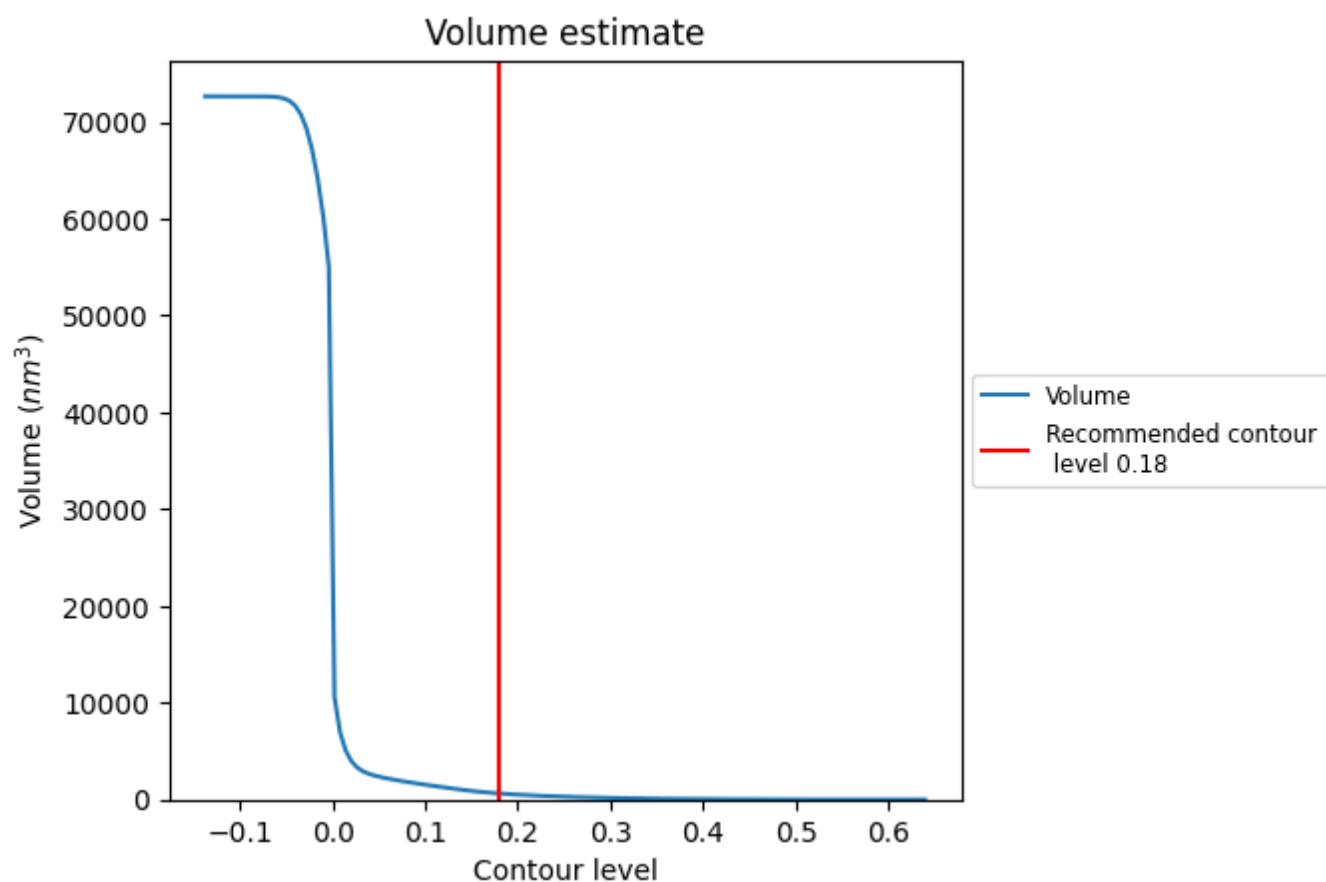
This section contains the results of statistical analysis of the map.

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.

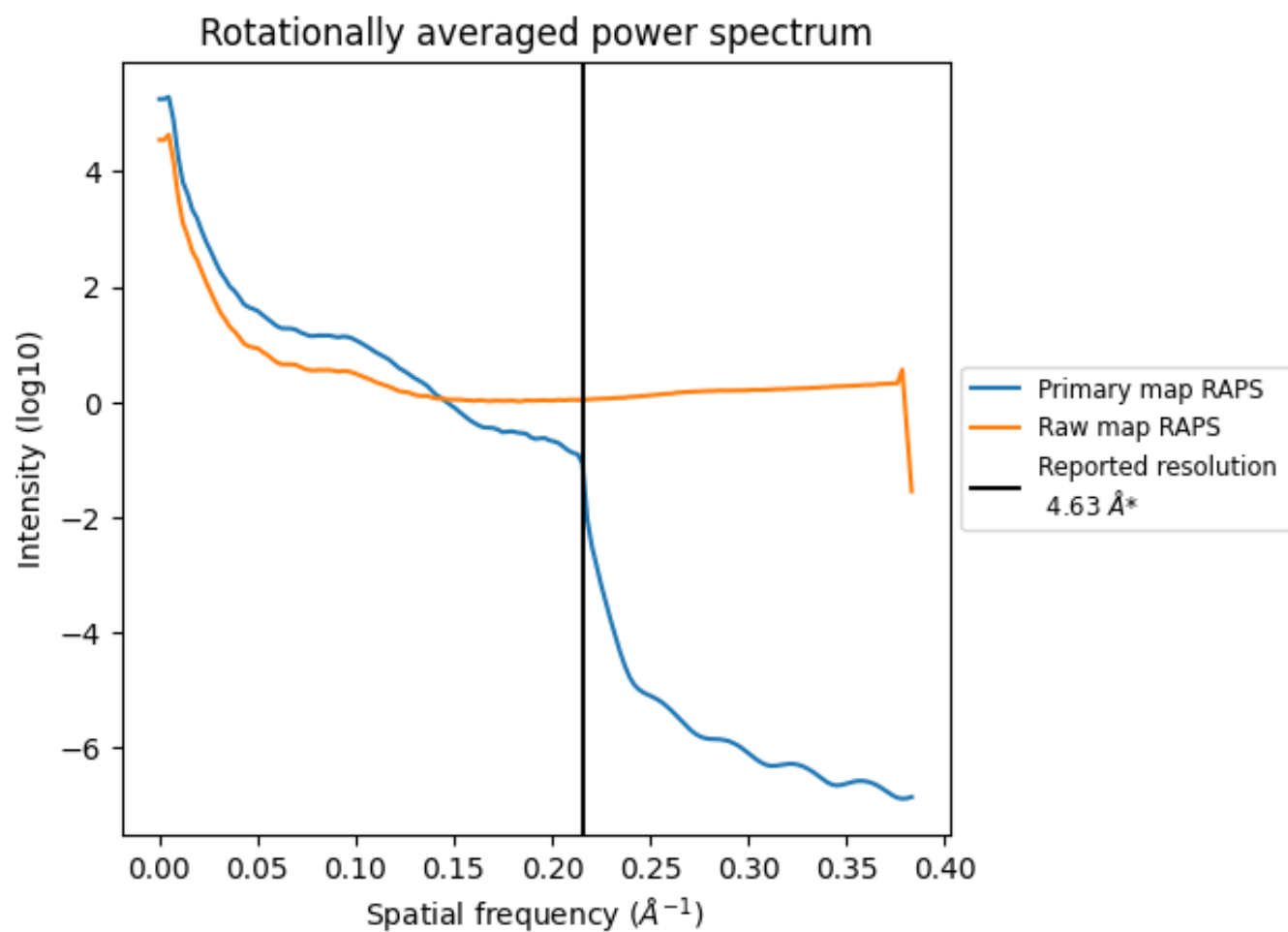
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 632 nm³; this corresponds to an approximate mass of 570 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 ⓘ

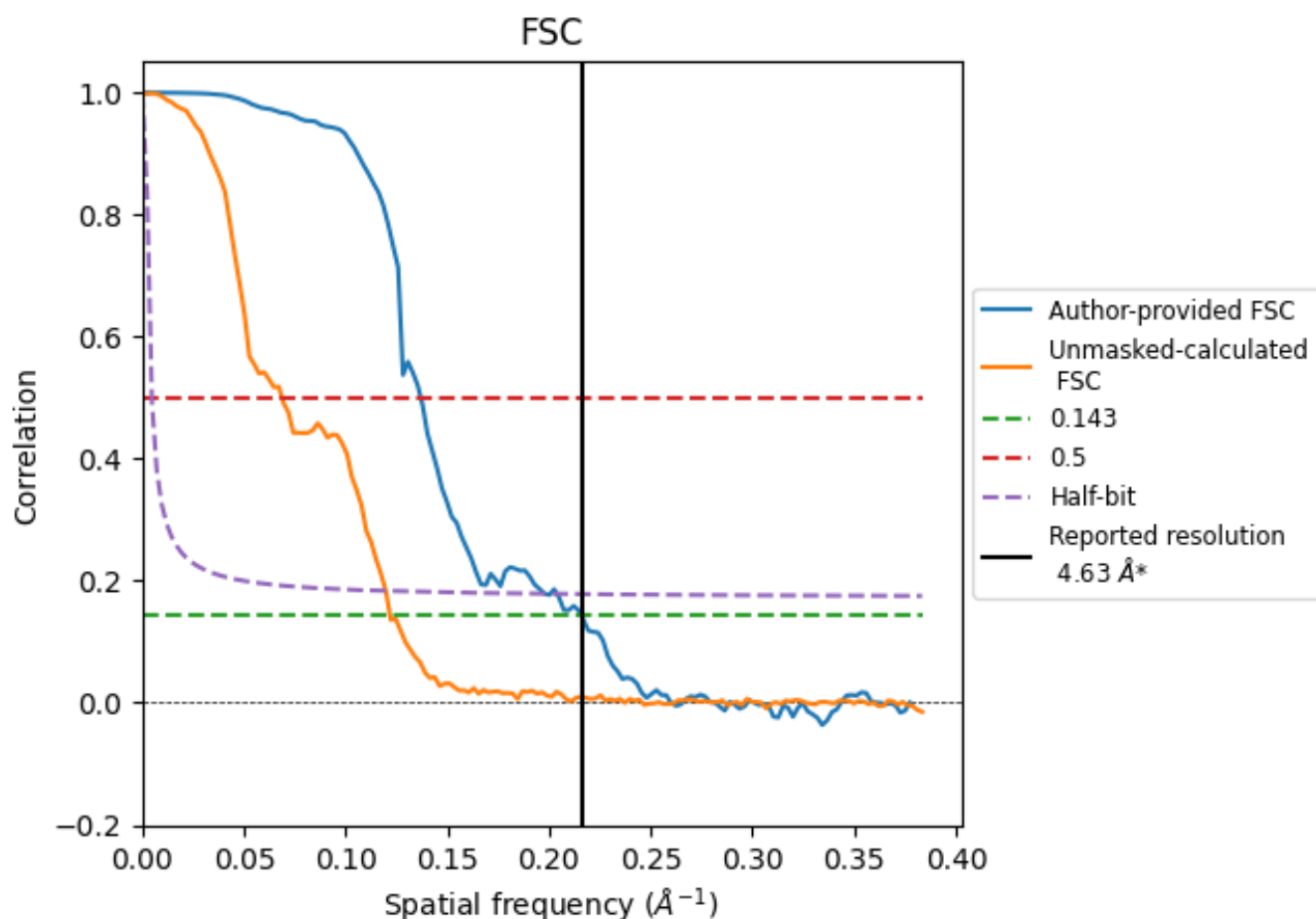


*Reported resolution corresponds to spatial frequency of 0.216 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

8.2 Resolution estimates [i](#)

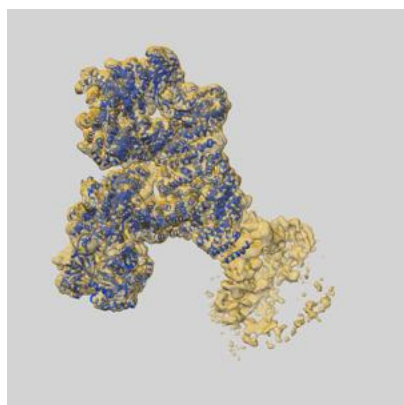
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	7.30	5.05
Unmasked-calculated*	8.20	14.56	8.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.20 differs from the reported value 4.63 by more than 10 %

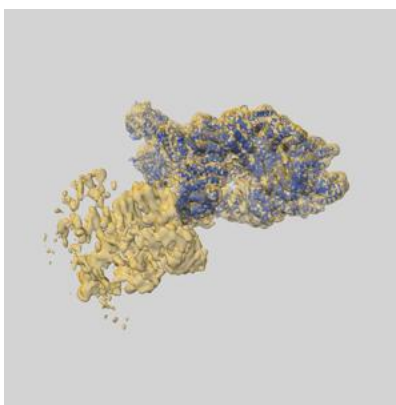
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51156 and PDB model 9G9L. Per-residue inclusion information can be found in section [3](#) on page [5](#).

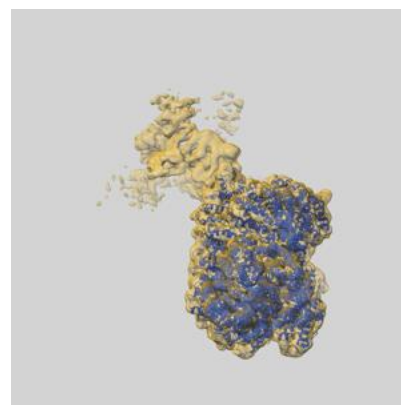
9.1 Map-model overlay [i](#)



X



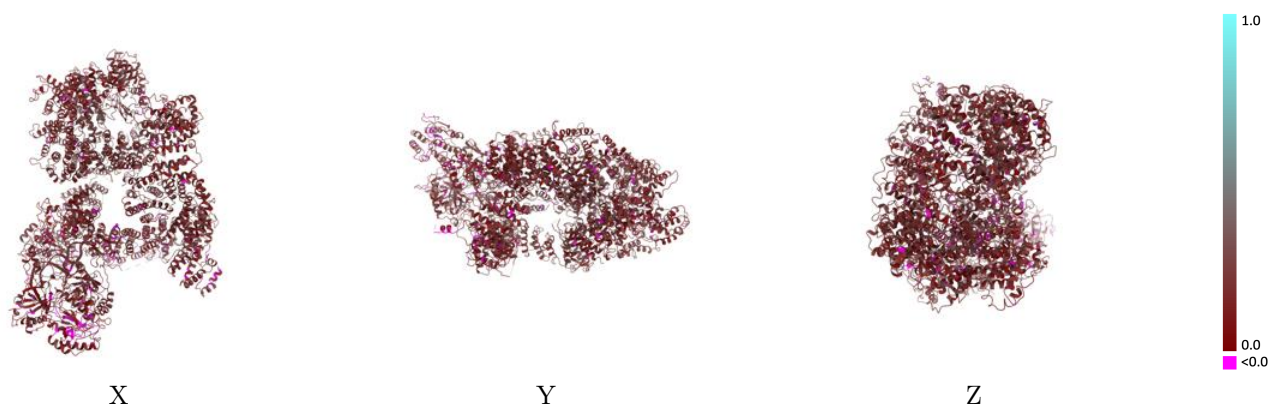
Y



Z

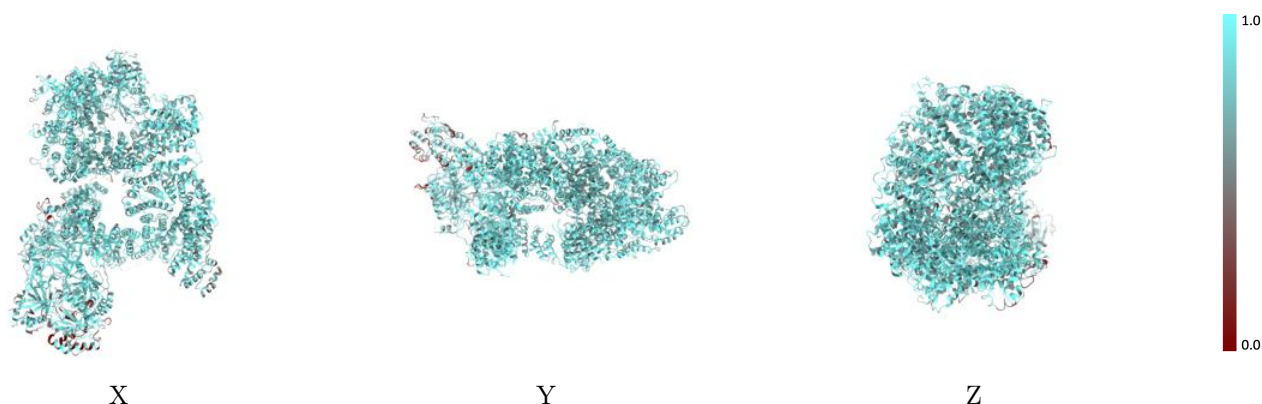
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



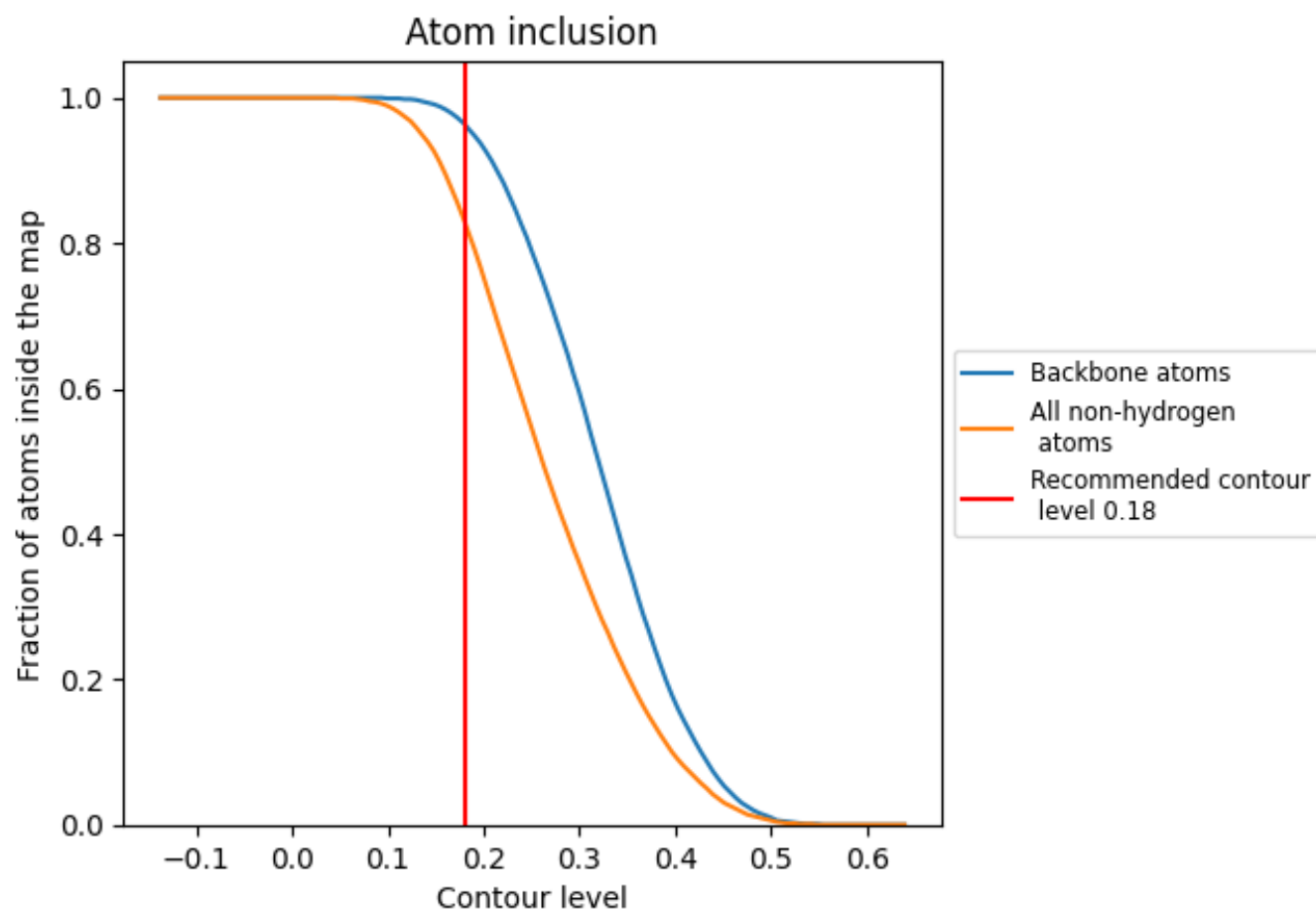
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 83% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8300</div>	<div><div></div>0.1880</div>
A	<div><div></div>0.8470</div>	<div><div></div>0.1930</div>
B	<div><div></div>0.8470</div>	<div><div></div>0.1870</div>
C	<div><div></div>0.7270</div>	<div><div></div>0.1580</div>
D	<div><div></div>0.9570</div>	<div><div></div>0.2320</div>
E	<div><div></div>0.9410</div>	<div><div></div>0.2140</div>
F	<div><div></div>0.6190</div>	<div><div></div>0.1540</div>
M	<div><div></div>0.8520</div>	<div><div></div>0.2220</div>

1.0

0.0

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