



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:56 AM UTC

PDB ID : 7Z88 / pdb_00007z88
EMDB ID : EMD-14546
Title : DNA-PK in the intermediate state
Authors : Liang, S.; Blundell, T.L.
Deposited on : 2022-03-16
Resolution : 3.33 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

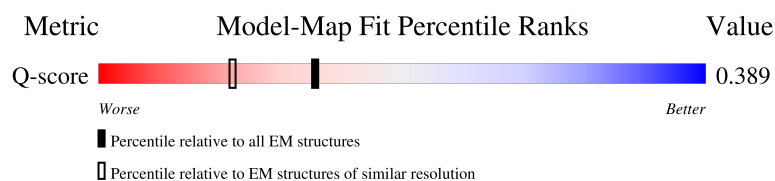
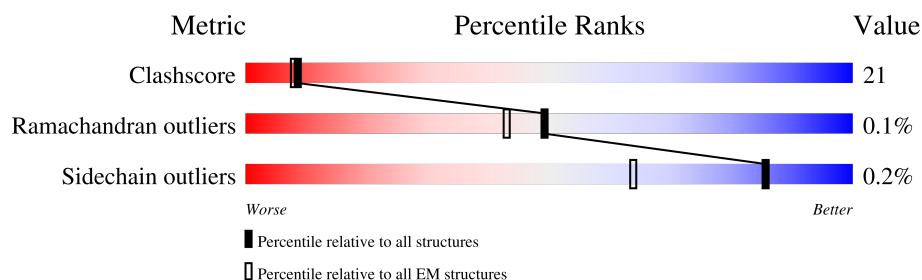
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14484 (2.83 - 3.83)

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	15% 49% 37% 13%
2	B	609	10% 46% 34% 20%
3	C	732	43% 52% 39% 10%
4	D	26	12% 50% 50%

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Mol	Chain	Length	Quality of chain
5	E	26	15%46%54%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38754 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	3599	Total	C	N	O	S	0	0
			28443	18257	4823	5179	184		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3937	2525	667	728	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	661	Total	C	N	O	S	0	0
			5274	3372	882	994	26		

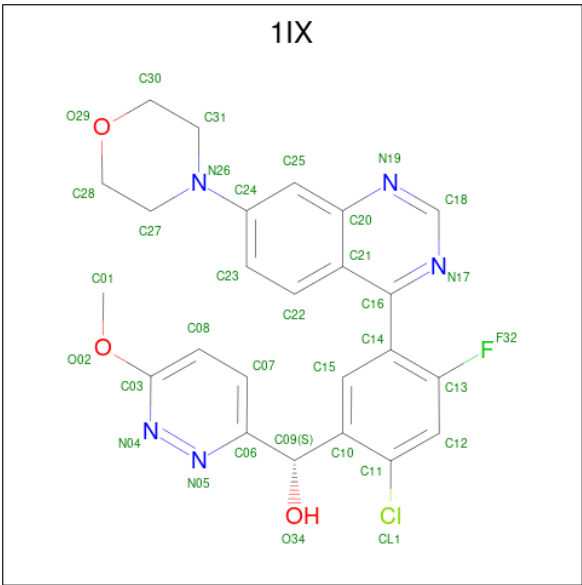
- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	26	Total	C	N	O	P	0	0
			526	250	92	158	26		

- Molecule 5 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	26	Total	C	N	O	P	0	0
			540	254	106	154	26		

- Molecule 6 is ({S})-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl]-(6-methoxypyridazin-3-yl)methanol (CCD ID: 1IX) (formula: C₂₄H₂₁ClFN₅O₃) (labeled as "Ligand of Interest" by depositor).

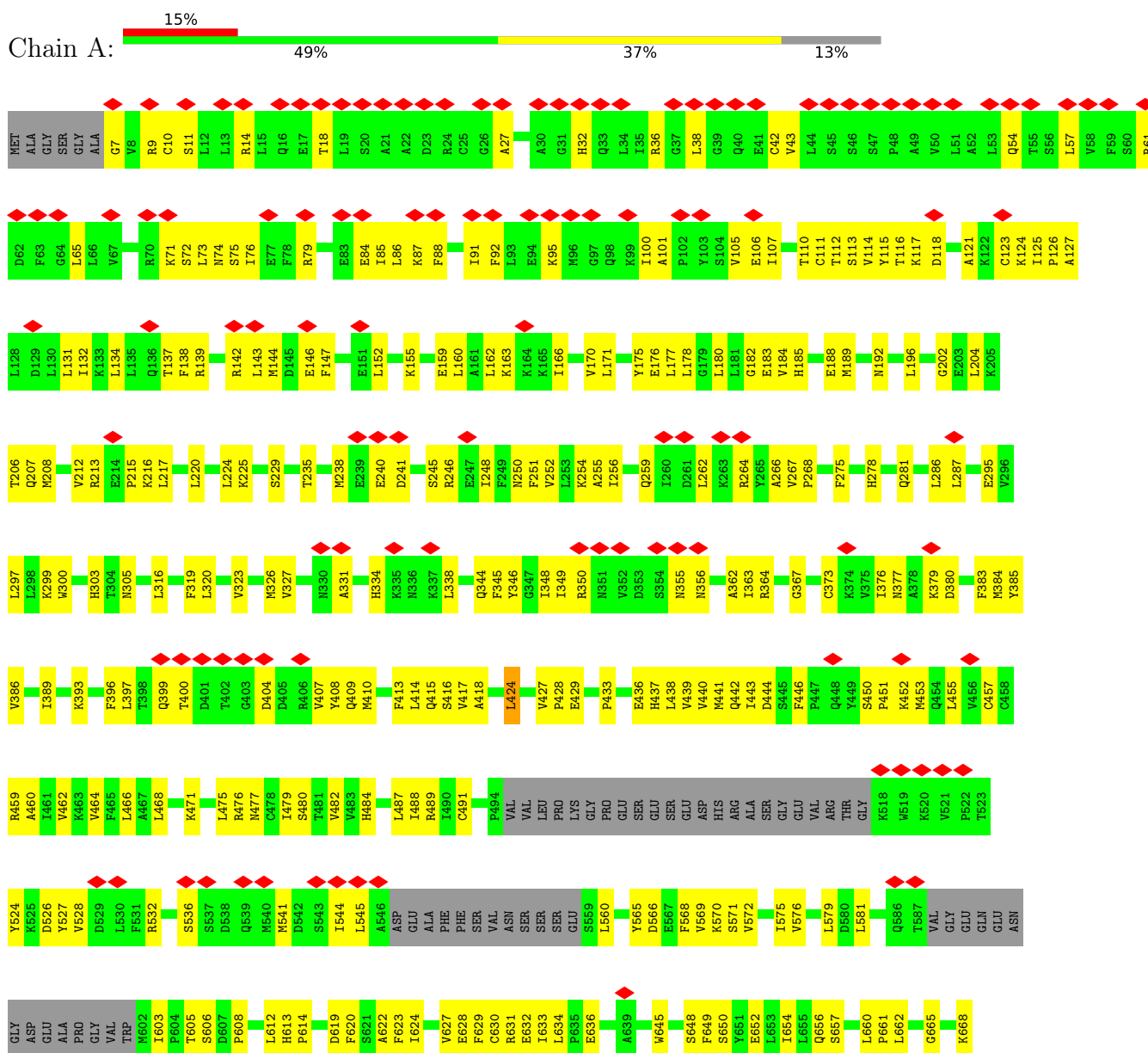


Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	F	N	O	
6	A	1	34	24	1	1	5	3	0

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.

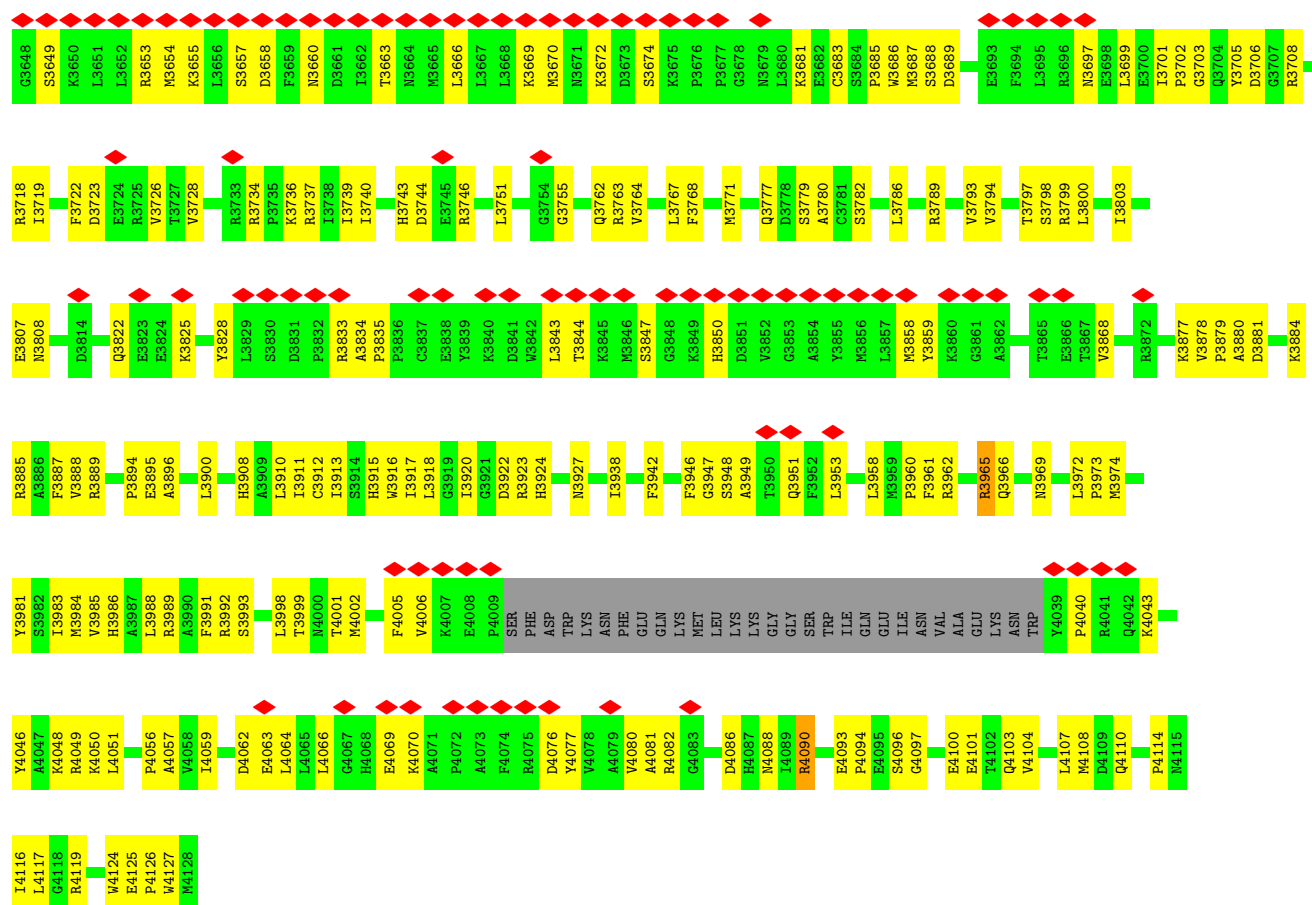
• Molecule 1: DNA-dependent protein kinase catalytic subunit



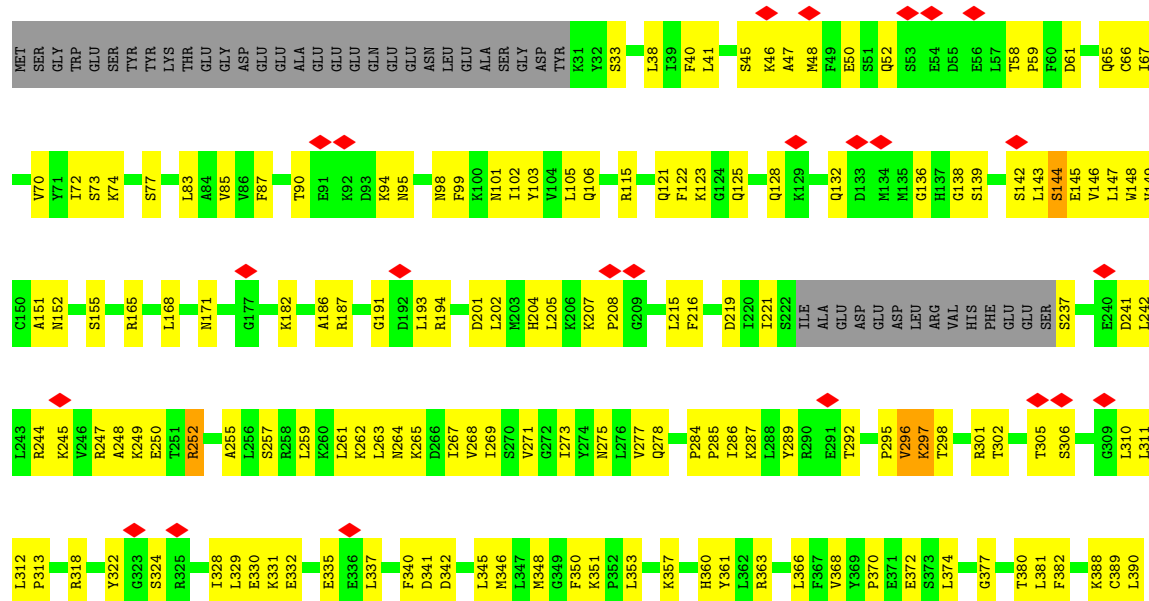


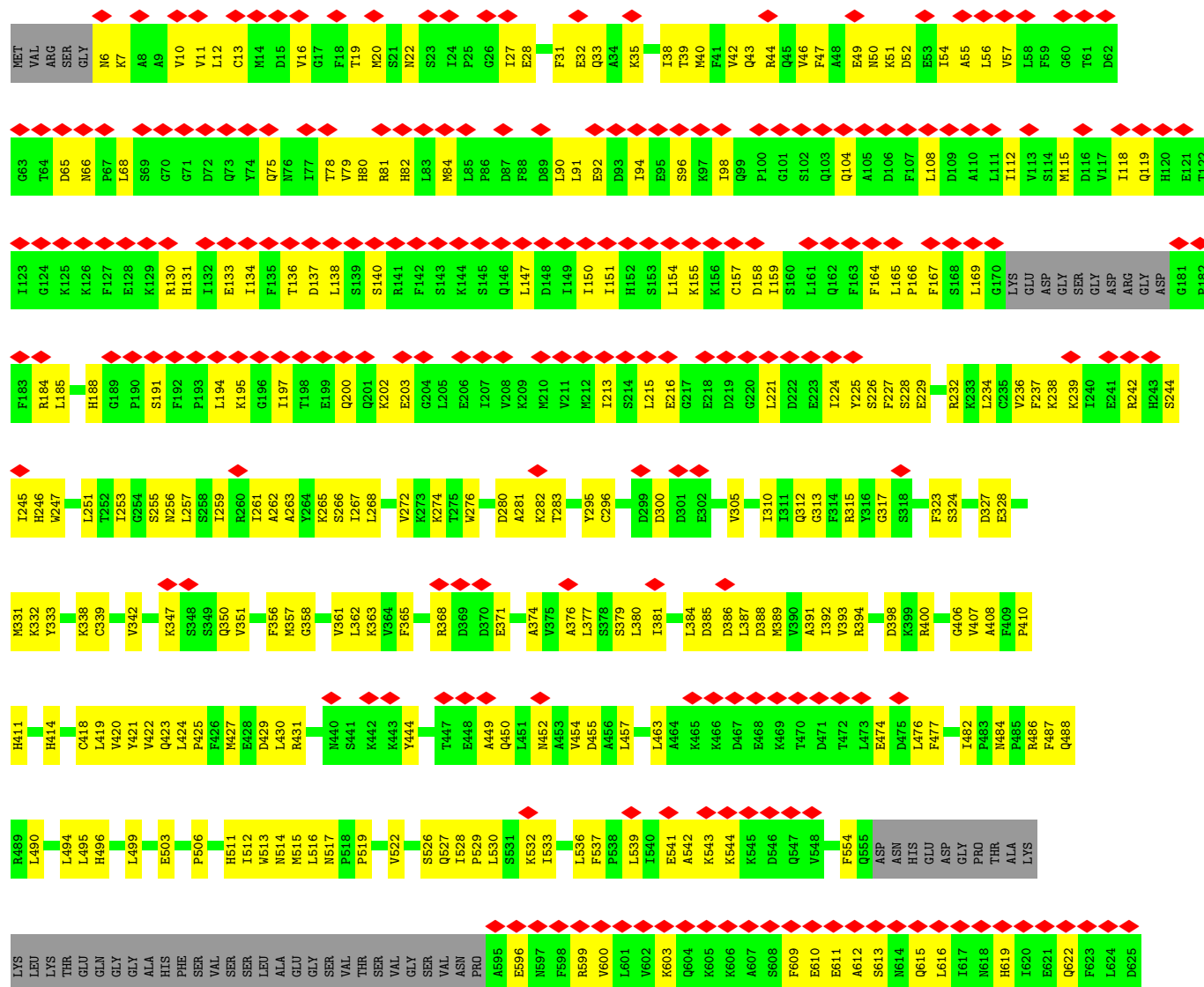


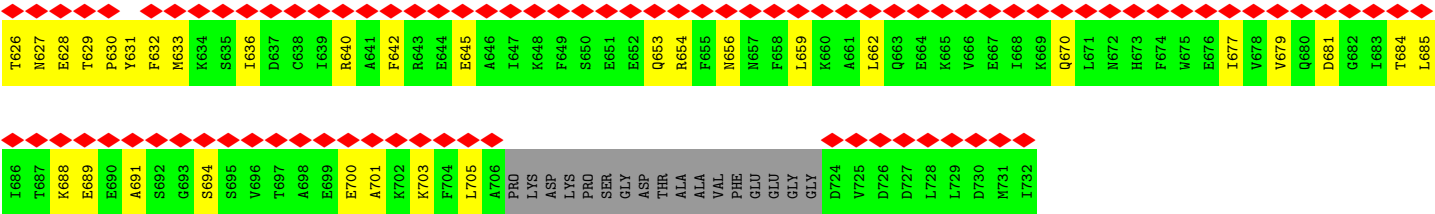
V3588	K3452	Q3326	L3259	F3189	V3119	I3045	L2976	P2887	PHE
S3589	A3453	N3327	L3262	L3190	L3120	R3046	N2977	V2888	NET
N3590	L3454	I3328	H3263	I3193	H3121	S3047	Q2978	K2978	ARG
D3591	K3455	L3329	K3264	E3194	H3122	K3048	Q2979	Q2806	ASP
V3592	A3461	L3330	E3265	E3195	Q3123	L3049	D2980	F2808	GLN
K3593	R3462	G3331	K3266	K3196	L3126	L3053	V2981	S2810	LEU
A3594	F3465	T3332	K3267	L3197	T3127	Q3054	PRO	F2813	LEU
E3595	P3466	T3333	T3268	K3198	K3128	G3055	ALA	F2813	SER
L3596	R3467	R3335	K3269	L3199	L3129	G3056	GLU	E2819	LEU
A3597	S3537	R3336	R3270	PRO	Q3130	P2986	LEU	E2819	MET
K3598	L3468	I3337	D3271	LEU	S3131	T2987	PRO	M2820	TVR
T3599	L3469	A3338	K3272	GLU	V3132	A3057	ALA	F2823	ARG
P3600	Q3470	N3339	K3273	ASP	Q3133	Q3058	LYS	K2824	ARG
V3601	I3472	A3340	V3274	ASN	A3134	E2990	VAL	F2824	GLY
N3602	E3473	L3341	S3275	SER	T3136	L3061	ARG	K2829	VAL
K3603	R3474	E3344	K3276	MET	E3137	L3062	GLY	N2830	ALA
K3604	Y3475	P3345	V3277	ASN	Q3138	Q2991	LYS	N2831	GLU
T3605	P3476	A3346	Q3278	VAL	Q3139	E2993	ALA	L2832	GLN
S3606	E3477	C3347	V3280	GLN	F3141	F2993	ARG	K2835	LYS
T3607	E3478	L3348	C3281	ASP	S3143	W2994	LEU	L2837	LYS
E3607	L3479	A3349	R3282	GLY	E3072	N3003	GLY	F2840	TLE
K3608	L3480	E3350	L3283	ASP	L3073	H3004	GLU	N2841	LYS
K3609	S3481	I3351	S3284	PRO	Q3074	A3006	SER	L2844	GLU
Y3610	T3484	E3352	C3286	ASP	I3077	W3008	LEU	N2845	LYS
E3611	I3487	E3353	R3287	ARG	E3079	K3009	GLY	T2846	GLN
K3612	S3488	D3354	S3290	GLU	Q3148	S3010	LYS	F2851	MET
S3613	E3489	K3355	L3298	GLU	G3149	Y2850	LYS	P2852	LYS
Y3614	V3490	A3356	T3299	VAL	N3150	R2951	GLN	P2853	GLN
A3615	F3495	R3357	V3301	GLN	L3151	S2932	ALA	F2854	ALA
L3616	L3496	R3358	L3302	GLN	S3152	L2939	VAL	C2857	VAL
L3617	S3497	L3359	L3298	GLU	Q3154	I2942	VAL	L2856	VAL
G3618	W3498	L3360	V3300	D3226	V3155	I3019	LEU	Q2859	LEU
D3619	S3500	E3361	L3301	S3227	P3156	L3091	TYR	D2860	TYR
P3620	H3501	SER	K3302	S3228	L3157	Q3093	SER	I2861	ARG
K3621	K3502	GLY	L3306	S3229	K3158	D3094	TYR	Q2864	TYR
A3622	V3503	SER	L3307	I3231	R3159	P3024	ARG	L2868	HIS
P3623	A3504	SER	D3308	S3232	L3160	V3095	GLY	L2871	GLY
L3624	L3505	GLU	E3309	C3234	R3167	R3098	ASP	L2872	ASP
L3625	L3506	SER	N3310	K3235	D3170	A3099	PRO	A2876	PRO
G3626	D3507	SER	N3311	F3236	A3171	K3029	ASP	V2876	ASP
A3627	K3508	GLU	V3312	S3237	K3172	I3030	ILE	Q2784	ILE
F3628	D3509	SER	S3313	M3238	Q3173	Q3031	Q2785	Q2784	Q2784
R3629	Q3510	GLU	S3314	S3239	M3176	S3032	Q2786	Q2785	Q2785
S3630	V3512	I3374	Y3315	M3240	K3179	K3033	K2786	K2786	K2786
K3631	A3513	I3378	L3316	K3241	Q3108	P3035	Z2787	Z2787	Z2787
F3632	V3514	Y3378	L3317	M3242	F3109	F3036	Z2788	Z2788	Z2788
L3633	Q3515	A3381	S3318	I3243	Q3110	Q2972	T2792	T2792	T2792
Q3634	E3519	H3384	N3319	D3244	F3111	E2974	T2793	T2793	T2793
T3635	L3385	L3386	L3320	R3247	Q3112	E2974			
F3636	E3387	E3387	L3321	Q3248	Q3113				
G3637	A3388	A3388	A3322	Q3249	N3113				
K3638	V3389	Q3390	R3324						
E3639									
F3640									
D3641									
K3642									
L3643									
F3644									
G3645									
K3646									
G3647									



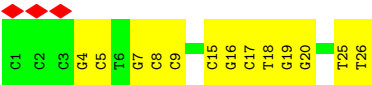
• Molecule 2: X-ray repair cross-complementing protein 6







• Molecule 4: DNA (26-MER)



• Molecule 5: DNA (26-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190498	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 ($e^-/\text{\AA}^2$)	47.22	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.648	Depositor
Minimum map value	-2.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	456.4, 456.4, 456.4	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IIX

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	0.23	0/29016	0.54	5/39251 (0.0%)
2	B	0.24	0/4014	0.56	0/5408
3	C	0.19	0/5374	0.46	0/7246
4	D	0.23	0/587	0.38	0/902
5	E	0.23	0/607	0.35	0/936
All	All	0.23	0/39598	0.53	5/53743 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	2
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2547	SER	CA-C-N	11.82	134.62	119.84
1	A	2547	SER	C-N-CA	11.82	134.62	119.84
1	A	407	VAL	N-CA-C	-6.28	107.38	113.53
1	A	3965	ARG	N-CA-C	6.04	118.64	111.33
1	A	976	VAL	N-CA-C	5.06	115.78	110.62

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	PRO	Peptide
1	A	1175	HIS	Peptide
1	A	3025	PRO	Peptide
1	A	3462	ARG	Peptide
2	B	252	ARG	Peptide
2	B	474	ARG	Peptide

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	28443	0	28622	1225	0
2	B	3937	0	4013	198	0
3	C	5274	0	5275	261	0
4	D	526	0	293	12	0
5	E	540	0	291	14	0
6	A	34	0	0	0	0
All	All	38754	0	38494	1638	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1638) 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:322:TYR:CE2	3:C:274:LYS:HG3	1.64	1.32
3:C:323:PHE:CE1	3:C:328:GLU:HB3	1.82	1.13
2:B:322:TYR:HE2	3:C:274:LYS:CG	1.68	1.05
1:A:2225:HIS:ND1	1:A:2226:PRO:HD2	1.72	1.04
1:A:3190:LEU:HB3	1:A:3235:LYS:HZ2	1.27	0.98
1:A:2458:VAL:HG21	1:A:2476:ILE:HD11	1.49	0.95
1:A:1023:SER:HA	1:A:1026:ARG:HE	1.35	0.92
1:A:1711:ARG:HE	1:A:1757:MET:HB3	1.35	0.91
1:A:2971:GLN:HA	1:A:2974:GLU:HG2	1.54	0.89
1:A:2548:PRO:HG3	1:A:2846:THR:HG22	1.54	0.89
1:A:2280:VAL:HG23	1:A:2285:LEU:HD12	1.54	0.89
2:B:322:TYR:CE2	3:C:274:LYS:NZ	2.43	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2402:LEU:HB2	1:A:2438:ILE:HG22	1.57	0.85
1:A:2421:VAL:HG13	1:A:2457:PRO:HG3	1.58	0.85
1:A:489:ARG:HG3	1:A:2040:MET:HE1	1.56	0.85
1:A:3630:ARG:NH1	1:A:3683:CYS:SG	2.50	0.85
2:B:322:TYR:CD2	3:C:274:LYS:NZ	2.45	0.85
3:C:532:LYS:O	3:C:536:LEU:HB2	1.77	0.85
1:A:3424:LEU:HD21	1:A:3443:PRO:HD3	1.59	0.84
1:A:752:LEU:HD23	1:A:792:ILE:HD11	1.60	0.82
1:A:4064:LEU:HD21	1:A:4077:TYR:HB3	1.61	0.82
1:A:1204:PRO:HB2	1:A:1275:THR:HG23	1.61	0.81
1:A:207:GLN:HE22	1:A:216:LYS:HB2	1.46	0.81
1:A:160:LEU:HD12	2:B:312:LEU:HD11	1.61	0.81
1:A:1892:LYS:HE2	1:A:1905:ILE:HG23	1.62	0.81
1:A:3681:LYS:HE3	1:A:3688:SER:HA	1.62	0.81
1:A:873:VAL:HG13	1:A:874:THR:H	1.46	0.80
1:A:3307:LEU:HD23	1:A:3330:LEU:HD23	1.62	0.80
1:A:3176:MET:SD	1:A:3249:GLN:NE2	2.55	0.79
2:B:144:SER:HB3	2:B:186:ALA:HA	1.63	0.79
1:A:380:ASP:HA	1:A:383:PHE:HB3	1.63	0.79
1:A:3190:LEU:HB3	1:A:3235:LYS:NZ	1.96	0.79
2:B:202:LEU:HD23	2:B:221:ILE:HD12	1.63	0.79
2:B:480:ASN:HD22	2:B:483:LEU:HB2	1.47	0.79
3:C:323:PHE:CE1	3:C:328:GLU:CB	2.66	0.79
2:B:48:MET:HA	2:B:59:PRO:HG2	1.63	0.78
1:A:3173:MET:SD	1:A:3782:SER:OG	2.41	0.78
3:C:56:LEU:H	3:C:81:ARG:HB3	1.49	0.78
1:A:3389:VAL:HG21	1:A:3416:LEU:HD22	1.63	0.78
1:A:1767:CYS:SG	1:A:1823:SER:OG	2.42	0.77
3:C:323:PHE:CD1	3:C:328:GLU:HB3	2.20	0.77
1:A:3718:ARG:H	1:A:3743:HIS:CD2	2.01	0.77
1:A:1876:ILE:HG22	1:A:1880:MET:HE1	1.66	0.77
1:A:2177:ASN:HB3	1:A:2182:ILE:HG23	1.64	0.77
2:B:322:TYR:HE2	3:C:274:LYS:HG3	0.74	0.76
1:A:2459:VAL:HG21	1:A:2501:LEU:HD21	1.67	0.76
2:B:257:SER:HB3	2:B:259:LEU:HD13	1.66	0.76
1:A:1582:LEU:HG	1:A:1593:VAL:HG23	1.66	0.76
1:A:2930:TYR:HE2	1:A:3974:MET:HE3	1.51	0.76
1:A:1437:TYR:HA	1:A:1445:ARG:HH22	1.51	0.75
1:A:1675:TYR:HD1	1:A:1695:LEU:HD22	1.52	0.75
1:A:605:THR:HG21	1:A:1076:LEU:HD21	1.70	0.74
1:A:1769:GLU:O	1:A:1822:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1868:THR:HG22	1:A:1936:ARG:HH21	1.53	0.74
1:A:3231:ILE:HG23	1:A:3235:LYS:HZ3	1.51	0.74
3:C:411:HIS:CB	3:C:418:CYS:H	2.01	0.74
1:A:3718:ARG:HE	1:A:3743:HIS:CD2	2.06	0.73
1:A:1933:LEU:H	1:A:1937:ARG:HH21	1.35	0.73
1:A:3506:LEU:HB2	1:A:3533:PHE:HZ	1.52	0.73
3:C:213:ILE:HD11	3:C:221:LEU:HB2	1.71	0.73
1:A:3951:GLN:HE21	1:A:4063:GLU:HA	1.54	0.73
1:A:3654:MET:HE1	1:A:3657:SER:H	1.54	0.73
1:A:1167:ASP:HA	1:A:1170:LYS:HB2	1.70	0.73
3:C:81:ARG:HH12	3:C:84:MET:H	1.37	0.72
1:A:9:ARG:HE	1:A:57:LEU:HG	1.53	0.72
1:A:396:PHE:HE2	1:A:438:LEU:HD11	1.55	0.72
1:A:1261:LEU:HD13	1:A:1337:VAL:HG12	1.70	0.72
1:A:2784:GLN:HG2	1:A:2785:ILE:HG12	1.71	0.72
1:A:1583:MET:HE1	1:A:1622:ILE:HG22	1.71	0.72
1:A:4090:ARG:NH1	1:A:4110:GLN:HG3	2.05	0.72
1:A:3718:ARG:H	1:A:3743:HIS:HD2	1.36	0.71
2:B:297:LYS:HE3	3:C:296:CYS:SG	2.30	0.71
3:C:323:PHE:HE1	3:C:328:GLU:HB3	1.55	0.71
1:A:762:TYR:HD2	1:A:765:LEU:HB2	1.55	0.71
1:A:2475:ASN:HA	1:A:2478:MET:HE3	1.71	0.71
1:A:2859:GLN:NE2	1:A:2880:CYS:SG	2.63	0.71
1:A:2860:ASP:O	1:A:2864:GLN:NE2	2.23	0.71
1:A:3069:MET:HE1	1:A:3078:LEU:HD11	1.72	0.71
2:B:488:ARG:HG2	2:B:501:GLU:HB2	1.72	0.71
3:C:457:LEU:HD11	3:C:530:LEU:HD23	1.70	0.71
2:B:312:LEU:HG	2:B:313:PRO:HD2	1.72	0.71
2:B:460:GLY:HA2	2:B:463:LYS:HD2	1.73	0.71
1:A:259:GLN:HB3	1:A:262:LEU:HD22	1.71	0.71
1:A:3231:ILE:HG23	1:A:3235:LYS:NZ	2.05	0.71
1:A:3378:TYR:OH	1:A:3426:LYS:NZ	2.24	0.71
1:A:1990:PHE:HD2	1:A:2182:ILE:HG22	1.56	0.71
1:A:2426:HIS:O	1:A:2432:GLN:NE2	2.24	0.71
3:C:65:ASP:H	3:C:78:THR:HG22	1.56	0.70
1:A:2507:ILE:HD11	1:A:2547:SER:CB	2.21	0.70
2:B:410:PHE:HE2	3:C:482:ILE:HD11	1.55	0.70
1:A:36:ARG:HH12	1:A:825:GLY:HA2	1.55	0.70
1:A:876:SER:HB2	1:A:880:MET:HG2	1.72	0.70
2:B:102:ILE:HG21	2:B:149:VAL:HG21	1.73	0.70
1:A:1832:SER:HB2	1:A:1836:LEU:HD22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:533:ILE:HG23	3:C:537:PHE:CD2	2.26	0.70
1:A:1445:ARG:HH21	1:A:1507:CYS:HB3	1.57	0.70
1:A:2953:THR:HG22	1:A:2994:TRP:HE1	1.56	0.70
1:A:1361:LYS:HA	1:A:1364:CYS:HB2	1.73	0.70
2:B:61:ASP:O	2:B:65:GLN:HG2	1.92	0.70
1:A:3531:TYR:CD2	1:A:3532:PRO:HD3	2.27	0.70
1:A:3917:ILE:HG13	1:A:3991:PHE:HD2	1.56	0.70
1:A:144:MET:HE1	1:A:185:HIS:HB2	1.74	0.69
1:A:278:HIS:HB3	1:A:281:GLN:HG3	1.72	0.69
1:A:1198:LEU:HD23	1:A:1200:GLY:H	1.56	0.69
1:A:61:ARG:NH1	1:A:106:GLU:OE2	2.25	0.69
1:A:789:TYR:HA	1:A:792:ILE:HG22	1.74	0.69
1:A:3471:ILE:HA	1:A:3474:ARG:HD3	1.73	0.69
1:A:3763:ARG:NH2	1:A:4005:PHE:O	2.25	0.69
2:B:132:GLN:HA	2:B:136:GLY:HA2	1.73	0.69
3:C:391:ALA:HB3	3:C:408:ALA:HB3	1.73	0.69
1:A:36:ARG:HH22	1:A:825:GLY:H	1.38	0.69
1:A:4050:LYS:HD3	1:A:4059:ILE:HG21	1.74	0.69
3:C:411:HIS:CB	3:C:418:CYS:SG	2.81	0.69
1:A:65:LEU:HD12	1:A:85:ILE:HG23	1.73	0.69
1:A:1108:MET:HE1	1:A:1186:LYS:HB3	1.74	0.68
1:A:880:MET:HA	1:A:883:TYR:HB2	1.76	0.68
1:A:1606:ARG:HG3	1:A:2042:GLN:HG2	1.75	0.68
2:B:388:LYS:HG3	3:C:454:VAL:HG23	1.74	0.68
1:A:1773:VAL:HG13	1:A:1774:MET:HG3	1.74	0.68
1:A:3880:ALA:HB1	1:A:3969:ASN:HD22	1.58	0.68
1:A:2251:ILE:HG12	1:A:2285:LEU:CD1	2.24	0.68
1:A:2510:LEU:O	1:A:2518:GLN:NE2	2.27	0.68
1:A:2952:ILE:HD13	1:A:2975:ALA:HB2	1.74	0.68
1:A:2958:LEU:HD11	1:A:4101:GLU:HG2	1.75	0.68
1:A:1718:ILE:O	1:A:1722:PHE:HB2	1.94	0.68
2:B:322:TYR:HD2	3:C:49:GLU:OE1	1.76	0.68
3:C:357:MET:HE3	3:C:429:ASP:HB3	1.76	0.68
1:A:1783:ARG:HG2	1:A:1830:HIS:CD2	2.29	0.67
1:A:1836:LEU:HB3	1:A:1884:LEU:HD21	1.74	0.67
1:A:3786:LEU:HD22	1:A:3910:LEU:HD23	1.75	0.67
1:A:487:LEU:HD11	1:A:568:PHE:HE1	1.59	0.67
1:A:2224:PHE:HD2	1:A:2272:VAL:CG2	2.07	0.67
1:A:2511:ILE:HD13	1:A:2550:ILE:HG22	1.76	0.67
2:B:264:ASN:OD1	2:B:265:LYS:N	2.25	0.67
2:B:273:ILE:HG12	2:B:368:VAL:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:HIS:CD2	1:A:1165:LEU:HB2	2.30	0.67
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.67	0.67
1:A:3361:GLU:HG3	1:A:3362:LEU:HG	1.76	0.67
1:A:3630:ARG:HB3	1:A:3633:ILE:HG22	1.76	0.67
3:C:10:VAL:HG12	3:C:131:HIS:HB3	1.75	0.67
1:A:1018:VAL:HG11	1:A:1066:LEU:HD11	1.77	0.67
1:A:3410:ILE:O	1:A:3414:MET:HG2	1.95	0.67
3:C:130:ARG:NH2	3:C:157:CYS:O	2.28	0.67
1:A:3495:PHE:HD2	1:A:3502:MET:HE1	1.59	0.66
3:C:185:LEU:HB2	3:C:514:ASN:HD22	1.59	0.66
1:A:1852:LYS:O	1:A:1854:ARG:NH1	2.28	0.66
2:B:40:PHE:HZ	2:B:70:VAL:HG11	1.59	0.66
2:B:248:ALA:O	2:B:249:LYS:NZ	2.22	0.66
3:C:323:PHE:CZ	3:C:331:MET:HE3	2.30	0.66
1:A:1754:GLN:NE2	1:A:1788:ARG:HG2	2.10	0.66
2:B:296:VAL:HG21	3:C:295:TYR:HB3	1.78	0.66
1:A:1301:ILE:HD11	1:A:1334:LYS:HB2	1.78	0.65
1:A:1553:PHE:HE2	1:A:1558:TYR:HB2	1.61	0.65
1:A:984:TYR:HA	1:A:987:LEU:HB2	1.78	0.65
1:A:3577:GLN:HB3	1:A:3630:ARG:HE	1.61	0.65
2:B:409:TYR:HA	2:B:439:PHE:HZ	1.62	0.65
1:A:287:LEU:HB3	1:A:326:MET:HE1	1.78	0.65
1:A:603:ILE:HG21	1:A:1083:ASN:HD22	1.61	0.65
1:A:915:THR:HA	1:A:934:LEU:HD11	1.77	0.65
1:A:3951:GLN:OE1	1:A:4043:LYS:NZ	2.29	0.65
3:C:27:ILE:HG13	3:C:28:GLU:H	1.61	0.65
1:A:1136:ARG:HH11	1:A:1136:ARG:HG3	1.60	0.65
1:A:2859:GLN:HE21	1:A:2876:VAL:HG13	1.59	0.65
1:A:2037:SER:O	1:A:2040:MET:HB2	1.97	0.65
3:C:463:LEU:HD23	3:C:477:PHE:HB3	1.79	0.65
1:A:899:ARG:NH2	1:A:2565:MET:O	2.30	0.65
1:A:918:ALA:O	1:A:927:LYS:NZ	2.29	0.65
1:A:997:ASN:HA	1:A:1043:GLN:HG2	1.78	0.65
1:A:1770:GLN:HA	1:A:1814:PHE:HZ	1.61	0.65
1:A:2957:LEU:HD21	1:A:2993:PHE:HZ	1.62	0.65
2:B:297:LYS:CE	3:C:296:CYS:SG	2.85	0.65
1:A:1004:GLN:HA	1:A:1007:VAL:HG12	1.79	0.64
1:A:2548:PRO:CG	1:A:2846:THR:HG22	2.25	0.64
1:A:3455:LYS:NZ	1:A:3489:SER:OG	2.30	0.64
2:B:451:LYS:NZ	3:C:414:HIS:O	2.27	0.64
2:B:335:GLU:O	2:B:405:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:339:CYS:SG	3:C:394:ARG:NH1	2.70	0.64
1:A:7:GLY:N	1:A:10:CYS:SG	2.70	0.64
1:A:1671:VAL:HG22	1:A:1675:TYR:CE2	2.32	0.64
1:A:1821:ASP:OD1	1:A:1875:LYS:NZ	2.27	0.64
2:B:301:ARG:HE	2:B:310:LEU:HD13	1.62	0.64
1:A:238:MET:HE1	1:A:246:ARG:HG2	1.80	0.64
1:A:628:GLU:HG3	1:A:631:ARG:NH2	2.11	0.64
1:A:1335:CYS:HB3	1:A:1384:PHE:CE1	2.32	0.64
1:A:2887:PRO:HG2	1:A:3895:GLU:HG3	1.79	0.64
3:C:431:ARG:NH2	4:D:17:DC:OP2	2.29	0.64
1:A:264:ARG:HH12	5:E:37:DC:H4'	1.63	0.64
1:A:2126:MET:O	1:A:2130:HIS:HB2	1.98	0.64
1:A:3455:LYS:NZ	1:A:3489:SER:O	2.30	0.64
1:A:4002:MET:O	1:A:4005:PHE:HB3	1.97	0.64
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.26	0.64
1:A:3137:GLU:OE2	1:A:3167:ARG:NH1	2.30	0.64
1:A:3297:VAL:HG23	1:A:3337:ILE:HG23	1.79	0.64
1:A:76:ILE:O	1:A:79:ARG:NH1	2.31	0.64
1:A:1708:GLU:OE1	1:A:1712:ARG:NH1	2.31	0.64
3:C:82:HIS:HB2	3:C:84:MET:HE1	1.78	0.64
3:C:188:HIS:HB2	3:C:519:PRO:HG3	1.78	0.64
1:A:1686:LEU:HD21	1:A:1721:HIS:HB3	1.80	0.63
1:A:3170:ASP:OD2	1:A:3173:MET:HB2	1.97	0.63
3:C:131:HIS:NE2	3:C:133:GLU:OE2	2.29	0.63
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.79	0.63
1:A:396:PHE:CE2	1:A:438:LEU:HD11	2.34	0.63
1:A:1135:CYS:HA	1:A:1138:ILE:HG22	1.80	0.63
1:A:1716:GLN:HA	1:A:1719:VAL:HG12	1.80	0.63
1:A:2251:ILE:CD1	1:A:2285:LEU:HD13	2.28	0.63
1:A:3843:LEU:O	1:A:3847:SER:HB2	1.99	0.63
2:B:45:SER:N	2:B:48:MET:SD	2.64	0.63
2:B:489:ASN:ND2	3:C:331:MET:O	2.30	0.63
1:A:3962:ARG:NH1	1:A:4124:TRP:O	2.31	0.63
2:B:515:ASN:OD1	3:C:255:SER:N	2.32	0.63
1:A:1406:LEU:HD23	1:A:1415:LEU:HD22	1.80	0.63
1:A:1566:THR:HA	1:A:1569:THR:HG22	1.81	0.63
2:B:410:PHE:CE2	3:C:482:ILE:HD11	2.33	0.63
3:C:246:HIS:O	3:C:246:HIS:ND1	2.31	0.63
1:A:2100:LEU:HG	1:A:2104:MET:HE2	1.81	0.62
1:A:2832:ILE:HA	1:A:2835:LYS:HE3	1.81	0.62
3:C:659:LEU:HD12	3:C:662:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:DC:H4'	5:E:35:DG:H5'	1.80	0.62
1:A:631:ARG:HH11	1:A:668:LYS:HB3	1.63	0.62
1:A:665:GLY:HA2	1:A:668:LYS:HB2	1.80	0.62
1:A:2859:GLN:NE2	1:A:2876:VAL:HG13	2.14	0.62
1:A:185:HIS:CE1	1:A:188:GLU:H	2.17	0.62
1:A:3028:ASN:HA	1:A:3031:TRP:HD1	1.64	0.62
1:A:484:HIS:O	1:A:488:ILE:HG12	1.99	0.62
1:A:1572:LEU:HD21	1:A:1604:SER:HB2	1.80	0.62
1:A:2332:GLU:O	1:A:2334:LYS:NZ	2.31	0.62
1:A:3091:LEU:HD12	1:A:3142:ILE:HD12	1.82	0.62
1:A:424:LEU:C	1:A:424:LEU:HD23	2.24	0.62
1:A:3444:ALA:HB1	1:A:3479:THR:HG21	1.81	0.62
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.33	0.62
2:B:330:GLU:HG3	2:B:332:GLU:H	1.64	0.62
1:A:166:ILE:HD11	1:A:171:LEU:HD13	1.82	0.62
1:A:1676:ILE:O	1:A:1680:ALA:HB2	1.98	0.62
1:A:1840:PHE:O	1:A:1844:VAL:HG23	1.99	0.62
1:A:2574:ASN:OD1	1:A:2784:GLN:N	2.33	0.62
1:A:3414:MET:HE1	1:A:3461:ALA:HB2	1.80	0.62
1:A:2216:LEU:HD11	1:A:2220:MET:HE3	1.80	0.62
1:A:2225:HIS:ND1	1:A:2226:PRO:CD	2.58	0.62
1:A:1098:GLN:O	1:A:1152:ARG:NH2	2.33	0.61
3:C:423:GLN:HG2	3:C:424:LEU:H	1.65	0.61
1:A:2962:ARG:O	1:A:2964:ASP:N	2.31	0.61
1:A:3232:ARG:HH11	1:A:3269:ARG:HE	1.45	0.61
1:A:3958:LEU:HD11	1:A:4081:ALA:HB2	1.81	0.61
2:B:41:LEU:HD21	2:B:146:VAL:HG22	1.81	0.61
2:B:426:GLN:NE2	2:B:428:THR:O	2.33	0.61
3:C:40:MET:HA	3:C:43:GLN:HE21	1.65	0.61
1:A:137:THR:HG23	1:A:138:PHE:CD1	2.35	0.61
1:A:2484:TYR:CE2	1:A:2498:ILE:HD11	2.35	0.61
2:B:241:ASP:HA	2:B:245:LYS:HE3	1.80	0.61
2:B:403:ARG:HG2	5:E:29:DG:H5'	1.81	0.61
1:A:349:ILE:HG23	1:A:350:ARG:HD2	1.82	0.61
1:A:1813:SER:HB2	1:A:1868:THR:HG21	1.82	0.61
1:A:3536:SER:HA	1:A:3539:SER:HB3	1.82	0.61
1:A:3755:GLY:HA2	1:A:3799:ARG:HG3	1.82	0.61
1:A:2823:PHE:CD2	1:A:2824:LYS:HG2	2.35	0.61
1:A:3917:ILE:HG13	1:A:3991:PHE:CD2	2.36	0.61
3:C:323:PHE:CE1	3:C:331:MET:HE3	2.36	0.61
1:A:937:MET:O	1:A:941:MET:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2255:LEU:HA	1:A:2258:GLU:HG3	1.81	0.61
1:A:886:TRP:HH2	1:A:915:THR:HG21	1.64	0.61
1:A:2346:ALA:O	1:A:2350:LYS:HG2	2.00	0.61
1:A:2376:ASP:OD1	1:A:2404:ARG:NE	2.24	0.61
3:C:44:ARG:HH12	3:C:234:LEU:HD13	1.66	0.61
1:A:1378:GLU:OE1	1:A:1447:ARG:NH2	2.34	0.60
1:A:1809:ASP:O	1:A:1816:ARG:NH1	2.33	0.60
1:A:2443:MET:HE3	1:A:2479:TRP:CE3	2.36	0.60
1:A:2525:TRP:O	1:A:2531:LEU:HD13	2.01	0.60
3:C:136:THR:HG22	3:C:138:LEU:H	1.65	0.60
1:A:767:GLU:OE2	1:A:854:ARG:NH2	2.34	0.60
1:A:1704:GLY:O	1:A:1708:GLU:HB2	2.01	0.60
1:A:2957:LEU:HD21	1:A:2993:PHE:CZ	2.35	0.60
1:A:3887:PHE:CD2	1:A:3900:LEU:HB3	2.37	0.60
2:B:473:TYR:HB3	3:C:350:GLN:HE21	1.65	0.60
1:A:2464:HIS:ND1	1:A:2469:CYS:SG	2.75	0.60
1:A:524:TYR:HA	1:A:527:TYR:HD2	1.65	0.60
1:A:1579:VAL:O	1:A:1583:MET:HE3	2.01	0.60
1:A:2133:LEU:HD12	1:A:2143:ARG:HG3	1.83	0.60
1:A:2851:PHE:CE2	1:A:2853:PRO:HG2	2.37	0.60
1:A:3915:HIS:HD2	1:A:3920:ILE:HG21	1.67	0.60
2:B:341:ASP:OD1	2:B:342:ASP:N	2.35	0.60
1:A:36:ARG:NH2	1:A:823:GLN:O	2.34	0.60
1:A:1298:LEU:HD11	1:A:1341:ILE:HD13	1.82	0.60
1:A:3885:ARG:O	1:A:3889:ARG:HB2	2.01	0.60
1:A:2302:ALA:O	1:A:2306:ASN:ND2	2.35	0.60
1:A:2440:TYR:CD1	1:A:2476:ILE:HG22	2.37	0.60
1:A:2464:HIS:ND1	1:A:2465:PRO:O	2.30	0.60
1:A:1672:PHE:HA	1:A:1675:TYR:HD2	1.66	0.59
1:A:1014:LEU:O	1:A:1017:ILE:HG22	2.02	0.59
1:A:1364:CYS:HA	1:A:1369:MET:HE1	1.83	0.59
1:A:2417:SER:HB2	2:B:152:ASN:ND2	2.17	0.59
1:A:439:VAL:HG13	1:A:482:VAL:HG21	1.83	0.59
1:A:1491:ILE:HG21	1:A:1562:LEU:HD22	1.85	0.59
1:A:3847:SER:OG	1:A:3858:MET:HE2	2.03	0.59
2:B:95:ASN:OD1	2:B:98:ASN:N	2.35	0.59
1:A:985:GLU:O	1:A:989:MET:HG2	2.03	0.59
1:A:2233:HIS:O	1:A:2237:ILE:HG13	2.02	0.59
1:A:1162:SER:OG	1:A:1164:CYS:SG	2.61	0.59
1:A:886:TRP:CH2	1:A:915:THR:HG21	2.36	0.59
1:A:1186:LYS:O	1:A:1190:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3911:ILE:O	1:A:3915:HIS:ND1	2.34	0.59
1:A:1626:TRP:HE1	1:A:1674:THR:HG21	1.68	0.59
1:A:2150:VAL:HG11	1:A:2168:LEU:HD21	1.84	0.59
1:A:2516:GLY:O	1:A:2520:ILE:HG13	2.03	0.59
1:A:3574:ALA:HB1	1:A:3687:MET:HG3	1.85	0.59
1:A:3833:ARG:HD3	1:A:3877:LYS:HD2	1.84	0.59
3:C:28:GLU:OE2	3:C:32:GLU:HB3	2.02	0.59
1:A:137:THR:HG23	1:A:138:PHE:HD1	1.67	0.59
1:A:1485:SER:O	1:A:1489:LYS:HG2	2.03	0.59
1:A:2480:ILE:O	1:A:2484:TYR:HB2	2.03	0.59
1:A:2507:ILE:CD1	1:A:2547:SER:CB	2.81	0.59
3:C:424:LEU:HD12	3:C:425:PRO:HD2	1.84	0.59
1:A:917:LEU:O	1:A:921:ALA:HB2	2.03	0.59
1:A:3495:PHE:CD2	1:A:3502:MET:HE1	2.38	0.58
1:A:393:LYS:HA	1:A:397:LEU:HD13	1.85	0.58
1:A:424:LEU:O	1:A:471:LYS:NZ	2.36	0.58
1:A:528:VAL:HG11	1:A:632:GLU:CD	2.27	0.58
1:A:1017:ILE:HG23	1:A:1018:VAL:HG13	1.85	0.58
1:A:1089:PHE:CE2	1:A:1100:VAL:HB	2.38	0.58
1:A:2831:ASN:O	1:A:2835:LYS:HG3	2.04	0.58
1:A:2898:LEU:O	1:A:2899:ARG:HD3	2.04	0.58
1:A:1298:LEU:O	1:A:1370:ARG:NH2	2.36	0.58
1:A:1801:VAL:HA	1:A:1804:MET:HE3	1.84	0.58
1:A:1820:VAL:O	1:A:1825:LEU:HG	2.03	0.58
1:A:1261:LEU:HD11	1:A:1340:ARG:HE	1.68	0.58
1:A:1377:CYS:SG	1:A:1422:LYS:NZ	2.72	0.58
1:A:1018:VAL:HG12	1:A:1077:GLY:HA3	1.86	0.58
1:A:1342:MET:HG2	1:A:1402:LEU:HD22	1.86	0.58
1:A:178:LEU:HB3	1:A:196:LEU:HD21	1.86	0.58
1:A:1916:ILE:HD11	1:A:1955:VAL:HG11	1.85	0.58
1:A:862:LEU:HD13	1:A:866:ILE:HG22	1.85	0.58
1:A:3147:LYS:HB3	1:A:3150:ASN:HB2	1.85	0.58
1:A:4090:ARG:HH11	1:A:4110:GLN:HG3	1.67	0.58
2:B:263:LEU:HB2	2:B:267:ILE:HG13	1.86	0.58
3:C:57:VAL:HG12	3:C:79:VAL:HG13	1.86	0.58
3:C:513:TRP:O	3:C:517:ASN:ND2	2.28	0.58
1:A:895:ALA:HB1	1:A:902:LYS:HG2	1.84	0.58
1:A:762:TYR:CE2	1:A:764:PRO:HG2	2.39	0.58
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.86	0.58
2:B:305:THR:HB	2:B:311:LEU:HD21	1.84	0.58
3:C:11:VAL:HG22	3:C:55:ALA:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:385:ASP:OD1	3:C:386:ASP:N	2.37	0.58
1:A:459:ARG:HH21	1:A:544:ILE:HD11	1.67	0.57
1:A:2352:HIS:HB3	1:A:2360:PHE:HB2	1.86	0.57
1:A:899:ARG:NH1	1:A:2565:MET:SD	2.77	0.57
1:A:3949:ALA:HA	1:A:3953:LEU:HD13	1.86	0.57
3:C:347:LYS:HA	3:C:389:MET:HA	1.85	0.57
1:A:1020:PRO:O	1:A:1022:ASP:N	2.37	0.57
1:A:1098:GLN:HB3	1:A:1152:ARG:HB2	1.85	0.57
1:A:3332:THR:HG22	1:A:3335:ARG:HH21	1.70	0.57
3:C:57:VAL:HA	3:C:80:HIS:H	1.69	0.57
3:C:533:ILE:HG23	3:C:537:PHE:HD2	1.67	0.57
1:A:491:CYS:O	1:A:622:ALA:HA	2.04	0.57
1:A:1044:ILE:O	1:A:1049:GLN:NE2	2.37	0.57
1:A:3578:LEU:HD22	1:A:3687:MET:HE1	1.85	0.57
1:A:3880:ALA:HB2	1:A:3965:ARG:NH2	2.20	0.57
2:B:38:LEU:HB2	2:B:83:LEU:HD23	1.84	0.57
3:C:225:TYR:HB3	3:C:229:GLU:HG3	1.87	0.57
3:C:381:ILE:HG22	3:C:419:LEU:HD13	1.87	0.57
1:A:612:LEU:O	1:A:613:HIS:ND1	2.38	0.57
1:A:899:ARG:NH2	1:A:2568:MET:SD	2.71	0.57
1:A:919:LEU:HD21	1:A:968:VAL:HG23	1.86	0.57
1:A:2478:MET:HG2	1:A:2524:PHE:CD1	2.40	0.57
1:A:418:ALA:HB2	1:A:464:VAL:HG22	1.85	0.57
1:A:572:VAL:O	1:A:576:VAL:HG23	2.04	0.57
2:B:33:SER:HB3	5:E:32:DA:H5''	1.87	0.57
1:A:1774:MET:HB3	1:A:1777:LEU:HD12	1.87	0.57
1:A:1938:ARG:NH2	1:A:1981:LEU:O	2.34	0.57
1:A:3887:PHE:HD2	1:A:3900:LEU:HB3	1.68	0.57
1:A:1117:ASP:OD1	1:A:1118:GLU:N	2.33	0.56
1:A:415:GLN:HE21	1:A:460:ALA:HB2	1.70	0.56
1:A:462:VAL:HG21	1:A:541:MET:HE2	1.87	0.56
1:A:855:VAL:O	1:A:859:LEU:HB2	2.05	0.56
1:A:1893:GLU:HB2	1:A:1896:ILE:HG12	1.88	0.56
1:A:1979:GLU:HG2	1:A:1984:LEU:HD11	1.88	0.56
1:A:3108:GLN:O	1:A:3112:GLN:HG3	2.05	0.56
1:A:409:GLN:N	1:A:409:GLN:OE1	2.38	0.56
1:A:532:ARG:O	1:A:536:SER:OG	2.23	0.56
1:A:575:ILE:O	1:A:579:LEU:HG	2.06	0.56
1:A:1711:ARG:NE	1:A:1757:MET:HB3	2.15	0.56
1:A:1963:GLN:N	1:A:1963:GLN:OE1	2.38	0.56
1:A:2093:CYS:HA	1:A:2096:PRO:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3828:TYR:OH	1:A:4125:GLU:OE1	2.21	0.56
4:D:20:DG:N2	5:E:25:DC:O2	2.39	0.56
1:A:113:SER:HA	1:A:116:THR:HG22	1.86	0.56
1:A:2536:LEU:HD11	1:A:2820:MET:HB3	1.86	0.56
1:A:2572:TYR:CE2	1:A:2788:SER:HB3	2.41	0.56
1:A:3285:HIS:CE1	1:A:3329:LEU:HD22	2.41	0.56
2:B:65:GLN:OE1	2:B:123:LYS:HE3	2.06	0.56
1:A:427:VAL:HG12	1:A:429:GLU:H	1.71	0.56
1:A:1195:VAL:HG23	1:A:1196:PRO:HD3	1.88	0.56
1:A:2257:PHE:HA	1:A:2260:PHE:CZ	2.41	0.56
1:A:1157:PHE:HD2	1:A:1163:LEU:HD23	1.71	0.56
1:A:3407:ALA:O	1:A:3411:ASP:N	2.36	0.56
2:B:262:LYS:NZ	2:B:346:MET:HB3	2.21	0.56
3:C:66:ASN:ND2	3:C:68:LEU:O	2.32	0.56
1:A:940:PHE:O	1:A:944:LYS:HG2	2.06	0.56
1:A:1493:PRO:HG3	1:A:1501:PRO:HD3	1.88	0.56
2:B:165:ARG:NH1	2:B:201:ASP:OD2	2.39	0.56
2:B:275:ASN:ND2	2:B:278:GLN:OE1	2.39	0.56
1:A:1029:CYS:O	1:A:1033:ILE:HG13	2.06	0.56
1:A:1733:THR:OG1	1:A:1735:ARG:NH1	2.39	0.56
1:A:3332:THR:HA	1:A:3335:ARG:HD3	1.88	0.56
1:A:3335:ARG:HG2	1:A:3419:PHE:CD2	2.41	0.56
1:A:3723:ASP:HB3	1:A:3739:ILE:HB	1.88	0.56
3:C:327:ASP:O	3:C:331:MET:HG2	2.05	0.56
3:C:384:LEU:HB3	3:C:410:PRO:HG3	1.88	0.56
1:A:1915:LEU:HD12	1:A:1918:LEU:HD11	1.88	0.56
3:C:351:VAL:HG21	3:C:407:VAL:HG21	1.88	0.56
4:D:4:DG:H2''	4:D:5:DC:H5''	1.88	0.56
1:A:185:HIS:HE1	1:A:188:GLU:HB2	1.71	0.55
1:A:1881:TYR:CD2	1:A:1951:VAL:HG12	2.41	0.55
1:A:2228:ARG:HD3	5:E:41:DG:H5'	1.87	0.55
1:A:3764:VAL:HG12	1:A:4005:PHE:HE2	1.70	0.55
1:A:3835:PRO:HD3	1:A:3877:LYS:HD3	1.87	0.55
1:A:931:CYS:O	1:A:984:TYR:OH	2.21	0.55
1:A:962:TYR:HA	1:A:965:THR:HG22	1.88	0.55
1:A:1369:MET:HE3	1:A:1414:ILE:HG21	1.87	0.55
1:A:3577:GLN:O	1:A:3630:ARG:NH2	2.39	0.55
1:A:72:SER:O	1:A:75:SER:OG	2.22	0.55
1:A:1420:ARG:O	1:A:1424:THR:HB	2.06	0.55
1:A:2303:LEU:HA	1:A:2306:ASN:HD21	1.71	0.55
1:A:2331:MET:HG3	1:A:2371:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3244:ASP:O	1:A:3248:LYS:HG2	2.06	0.55
1:A:3807:GLU:OE1	1:A:3808:ASN:ND2	2.39	0.55
3:C:347:LYS:HD2	3:C:388:ASP:HB3	1.88	0.55
1:A:2038:GLU:HG2	1:A:2042:GLN:HE22	1.72	0.55
1:A:2434:VAL:O	1:A:2438:ILE:HG23	2.07	0.55
1:A:2436:LEU:HA	1:A:2439:ILE:HG22	1.89	0.55
1:A:1282:LEU:HD22	1:A:1291:LEU:HD21	1.87	0.55
1:A:1419:LEU:HD13	1:A:1458:LEU:HD11	1.88	0.55
1:A:1649:LEU:HD11	1:A:1675:TYR:OH	2.06	0.55
1:A:2224:PHE:HD2	1:A:2272:VAL:HG21	1.71	0.55
3:C:272:VAL:HG13	3:C:486:ARG:HH12	1.72	0.55
3:C:645:GLU:HG3	3:C:654:ARG:HH22	1.71	0.55
1:A:185:HIS:O	1:A:185:HIS:ND1	2.39	0.55
1:A:865:GLN:HG2	1:A:3170:ASP:HB3	1.88	0.55
1:A:1107:TYR:CZ	1:A:1130:ALA:HB3	2.41	0.55
1:A:3048:LYS:HB3	1:A:3061:LEU:HD22	1.89	0.55
1:A:3472:ILE:HG21	1:A:3480:LEU:HD11	1.88	0.55
1:A:3786:LEU:HD21	1:A:3983:ILE:HD12	1.88	0.55
3:C:6:ASN:O	3:C:242:ARG:NH1	2.39	0.55
1:A:348:ILE:HB	1:A:362:ALA:HB2	1.88	0.55
1:A:2813:PHE:HZ	1:A:2836:LEU:HD22	1.71	0.55
1:A:3989:ARG:NH2	1:A:4100:GLU:OE1	2.36	0.55
2:B:85:VAL:HG23	2:B:105:LEU:HB3	1.89	0.55
1:A:3143:SER:O	1:A:3146:SER:OG	2.24	0.55
1:A:3454:LEU:HD12	1:A:3462:ARG:HA	1.88	0.55
1:A:628:GLU:HG3	1:A:631:ARG:HH22	1.69	0.55
1:A:3045:ILE:HD11	1:A:3082:TYR:CD1	2.41	0.55
1:A:3512:VAL:HA	1:A:3515:GLN:HG3	1.89	0.55
1:A:7:GLY:N	1:A:10:CYS:HG	2.06	0.54
1:A:105:VAL:HA	1:A:147:PHE:CE1	2.42	0.54
1:A:2280:VAL:CG2	1:A:2285:LEU:HD12	2.33	0.54
1:A:3880:ALA:HB1	1:A:3969:ASN:ND2	2.21	0.54
3:C:54:ILE:O	3:C:81:ARG:NH1	2.40	0.54
3:C:259:ILE:HG21	3:C:377:LEU:HB3	1.89	0.54
3:C:363:LYS:HG2	3:C:420:VAL:HG12	1.89	0.54
1:A:43:VAL:HG12	1:A:818:LEU:HD21	1.89	0.54
1:A:636:GLU:HA	1:A:679:LYS:HZ1	1.72	0.54
1:A:756:PHE:HE1	1:A:770:LEU:HD22	1.72	0.54
1:A:909:VAL:HB	1:A:2807:GLN:HE21	1.72	0.54
1:A:3734:ARG:HB2	1:A:3734:ARG:NH1	2.22	0.54
1:A:459:ARG:HD2	1:A:541:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ARG:HG2	1:A:3111:MET:HE3	1.88	0.54
1:A:3031:TRP:HB3	1:A:3074:GLN:HE21	1.73	0.54
1:A:112:THR:HG21	1:A:155:LYS:HE3	1.89	0.54
1:A:414:LEU:HG	1:A:442:GLN:NE2	2.22	0.54
1:A:466:LEU:HB2	1:A:560:LEU:HD22	1.89	0.54
1:A:1028:PHE:HA	1:A:1031:ARG:HD3	1.89	0.54
1:A:1075:ARG:NH2	1:A:1117:ASP:OD2	2.40	0.54
1:A:1649:LEU:O	1:A:1653:LEU:HG	2.07	0.54
1:A:1770:GLN:HA	1:A:1814:PHE:CZ	2.41	0.54
1:A:2358:ASP:OD1	1:A:2359:LYS:N	2.41	0.54
1:A:3422:GLN:NE2	1:A:3423:GLN:OE1	2.40	0.54
1:A:3529:ILE:O	1:A:3532:PRO:HD2	2.07	0.54
3:C:130:ARG:NH2	3:C:158:ASP:OD1	2.39	0.54
3:C:188:HIS:H	3:C:232:ARG:NH1	2.05	0.54
3:C:633:MET:HA	3:C:636:ILE:HG22	1.90	0.54
1:A:672:ILE:O	1:A:676:ASN:ND2	2.35	0.54
1:A:978:GLN:OE1	1:A:981:ARG:NH2	2.32	0.54
1:A:1963:GLN:HG2	1:A:2123:PRO:HG2	1.90	0.54
1:A:2265:PRO:HB3	1:A:2309:PHE:CG	2.42	0.54
1:A:3951:GLN:HE22	1:A:4066:LEU:HD23	1.73	0.54
1:A:1362:ASP:OD1	1:A:1363:LEU:N	2.39	0.54
1:A:1990:PHE:CD2	1:A:2182:ILE:HG22	2.41	0.54
1:A:1992:VAL:HG11	1:A:2225:HIS:HE2	1.72	0.54
1:A:2182:ILE:HB	1:A:2185:MET:HB3	1.87	0.54
1:A:2363:CYS:O	1:A:2367:VAL:HG23	2.07	0.54
2:B:348:MET:HB2	2:B:397:LEU:HD23	1.90	0.54
1:A:933:LEU:HD11	1:A:2794:LEU:HA	1.90	0.54
1:A:2458:VAL:O	1:A:2461:PHE:HB2	2.08	0.54
3:C:659:LEU:HD23	3:C:685:LEU:HD12	1.89	0.54
1:A:450:SER:O	1:A:453:MET:HG2	2.07	0.54
1:A:1515:LEU:HD11	1:A:1566:THR:OG1	2.08	0.54
1:A:1807:LYS:HZ1	1:A:1811:ARG:HH12	1.56	0.54
1:A:2503:LYS:O	1:A:2507:ILE:HG12	2.07	0.54
2:B:403:ARG:HB2	2:B:406:ILE:HG13	1.88	0.54
3:C:28:GLU:OE1	3:C:33:GLN:HG3	2.07	0.54
1:A:73:LEU:HB2	1:A:117:LYS:HD3	1.90	0.54
1:A:1727:ARG:HD3	1:A:1773:VAL:HB	1.90	0.54
1:A:1986:ARG:HE	1:A:1988:TYR:HE1	1.55	0.54
1:A:2379:MET:O	1:A:2382:VAL:HG12	2.08	0.54
1:A:3183:ILE:HD12	1:A:3238:MET:HG2	1.89	0.54
1:A:107:ILE:HA	1:A:110:THR:HG22	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:HG3	1:A:143:LEU:HG	1.89	0.53
1:A:453:MET:O	1:A:457:CYS:N	2.35	0.53
1:A:3357:ARG:O	1:A:3361:GLU:N	2.39	0.53
1:A:2086:ASP:OD1	1:A:2087:GLU:N	2.39	0.53
2:B:143:LEU:O	2:B:145:GLU:N	2.42	0.53
1:A:965:THR:O	1:A:969:LEU:HD23	2.08	0.53
1:A:2506:LEU:HD13	1:A:2524:PHE:CE2	2.44	0.53
1:A:3228:SER:HA	1:A:3231:ILE:HD12	1.90	0.53
3:C:188:HIS:CE1	3:C:232:ARG:HD3	2.44	0.53
1:A:1702:LEU:HD23	1:A:1706:SER:HB2	1.89	0.53
1:A:1969:GLU:N	1:A:1969:GLU:OE1	2.41	0.53
3:C:628:GLU:HB2	3:C:631:TYR:HD2	1.72	0.53
1:A:935:HIS:ND1	1:A:983:LEU:HD11	2.23	0.53
2:B:262:LYS:HB3	2:B:268:VAL:HG12	1.89	0.53
2:B:277:VAL:HB	3:C:357:MET:CE	2.38	0.53
5:E:20:DT:H2"	5:E:21:DG:C8	2.43	0.53
1:A:476:ARG:O	1:A:479:ILE:HG22	2.08	0.53
1:A:2190:VAL:HA	1:A:2193:ILE:HG12	1.90	0.53
1:A:3859:TYR:HE1	1:A:4119:ARG:HG2	1.73	0.53
3:C:91:LEU:HD21	3:C:495:LEU:HD13	1.90	0.53
1:A:3357:ARG:HA	1:A:3360:LEU:HB2	1.90	0.53
1:A:3418:ASP:OD1	1:A:3419:PHE:N	2.41	0.53
1:A:935:HIS:CE1	1:A:987:LEU:HD21	2.44	0.53
1:A:1564:SER:O	1:A:1568:ASN:ND2	2.41	0.53
1:A:3843:LEU:O	1:A:3847:SER:CB	2.56	0.53
1:A:3868:VAL:HG22	1:A:4114:PRO:HB2	1.89	0.53
1:A:4057:ALA:HB1	1:A:4082:ARG:HA	1.90	0.53
1:A:4126:PRO:HD2	1:A:4127:TRP:CE3	2.44	0.53
2:B:143:LEU:HD23	2:B:182:LYS:HD3	1.91	0.53
3:C:386:ASP:OD1	3:C:387:LEU:N	2.42	0.53
1:A:1188:ILE:HD13	1:A:1269:THR:HG21	1.90	0.53
1:A:1414:ILE:O	1:A:1418:HIS:HB2	2.08	0.53
1:A:2426:HIS:CG	1:A:2427:ARG:H	2.27	0.53
1:A:2439:ILE:O	1:A:2443:MET:HB2	2.08	0.53
3:C:81:ARG:NH1	3:C:84:MET:SD	2.82	0.53
1:A:479:ILE:HA	1:A:482:VAL:HG12	1.91	0.53
1:A:571:SER:O	1:A:575:ILE:HG13	2.09	0.53
1:A:581:LEU:HB2	1:A:660:LEU:HD13	1.90	0.53
1:A:749:VAL:HG23	1:A:750:PRO:HD3	1.91	0.53
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.42	0.53
1:A:1297:PHE:CZ	1:A:1337:VAL:HG23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:LYS:NZ	1:A:1382:ILE:O	2.26	0.53
1:A:10:CYS:SG	1:A:14:ARG:NH2	2.82	0.52
1:A:2476:ILE:O	1:A:2480:ILE:HG13	2.09	0.52
1:A:3578:LEU:HG	1:A:3736:LYS:HD2	1.91	0.52
1:A:3961:PHE:HE1	1:A:4107:LEU:HG	1.74	0.52
3:C:232:ARG:HA	3:C:515:MET:SD	2.49	0.52
1:A:1013:ILE:HD11	1:A:1029:CYS:HA	1.90	0.52
1:A:2548:PRO:HG3	1:A:2846:THR:CG2	2.35	0.52
1:A:3988:LEU:O	1:A:3992:ARG:HG2	2.09	0.52
1:A:275:PHE:HE2	1:A:319:PHE:HB2	1.74	0.52
1:A:1335:CYS:HA	1:A:1338:VAL:HG12	1.92	0.52
1:A:3588:TRP:CD1	1:A:3609:MET:HE1	2.44	0.52
2:B:476:ASP:HB3	3:C:427:MET:SD	2.50	0.52
3:C:679:VAL:HG12	3:C:705:LEU:HD21	1.90	0.52
1:A:1302:ALA:HB3	1:A:1370:ARG:HH12	1.74	0.52
1:A:1802:TYR:CZ	1:A:1843:ILE:HD12	2.45	0.52
1:A:1851:LEU:HB3	1:A:1918:LEU:HD13	1.91	0.52
3:C:244:SER:O	3:C:245:ILE:HG13	2.09	0.52
1:A:2357:GLU:HG2	1:A:2385:LEU:HD11	1.91	0.52
1:A:2420:PHE:CE1	1:A:2438:ILE:HD11	2.45	0.52
2:B:480:ASN:O	2:B:484:GLN:HG2	2.10	0.52
1:A:204:LEU:HD23	1:A:251:PHE:CD2	2.44	0.52
1:A:256:ILE:HB	1:A:300:TRP:HZ3	1.74	0.52
1:A:1407:LYS:HG3	1:A:1463:LEU:HD11	1.91	0.52
1:A:3028:ASN:HA	1:A:3031:TRP:CD1	2.45	0.52
1:A:3946:PHE:HE2	1:A:4006:VAL:HB	1.74	0.52
2:B:46:LYS:HD2	2:B:47:ALA:HB2	1.92	0.52
1:A:415:GLN:NE2	1:A:460:ALA:HB2	2.24	0.52
1:A:797:ASP:OD1	1:A:798:GLY:N	2.42	0.52
1:A:2257:PHE:HB2	1:A:2299:TYR:CE2	2.44	0.52
1:A:3147:LYS:HE3	1:A:3149:GLY:H	1.75	0.52
1:A:43:VAL:O	1:A:95:LYS:NZ	2.41	0.52
1:A:433:PRO:HB2	1:A:2047:THR:HG23	1.92	0.52
1:A:1147:LYS:O	1:A:1151:ARG:NH2	2.41	0.52
1:A:1675:TYR:CD1	1:A:1695:LEU:HD22	2.40	0.52
1:A:1847:ALA:HA	1:A:1850:VAL:HG12	1.92	0.52
1:A:2251:ILE:CD1	1:A:2285:LEU:CD1	2.88	0.52
1:A:2933:ILE:HD12	1:A:3121:LEU:HD13	1.91	0.52
3:C:323:PHE:HE1	3:C:328:GLU:CB	2.16	0.52
3:C:328:GLU:O	3:C:332:LYS:HB3	2.10	0.52
3:C:449:ALA:HA	3:C:452:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:522:VAL:O	3:C:526:SER:HB3	2.10	0.52
1:A:295:GLU:O	1:A:299:LYS:HG2	2.10	0.52
1:A:650:SER:O	1:A:654:ILE:HD12	2.09	0.52
1:A:1105:VAL:HG23	1:A:1171:TRP:CZ2	2.44	0.52
1:A:2503:LYS:HD2	1:A:2525:TRP:HH2	1.74	0.52
1:A:3113:ASN:O	1:A:3117:ILE:HD12	2.10	0.52
1:A:3358:ARG:HA	1:A:3361:GLU:HG2	1.92	0.52
2:B:143:LEU:O	2:B:146:VAL:N	2.29	0.52
2:B:372:GLU:OE1	2:B:377:GLY:N	2.43	0.52
1:A:215:PRO:HB2	1:A:217:LEU:HD22	1.92	0.52
1:A:1118:GLU:HB3	1:A:1121:LEU:HB2	1.91	0.52
1:A:2931:ARG:NH2	1:A:3043:TYR:OH	2.42	0.52
1:A:2977:ASN:O	1:A:2979:GLN:NE2	2.42	0.52
1:A:3033:GLU:O	1:A:3035:PHE:N	2.42	0.52
1:A:3502:MET:HB2	1:A:3514:VAL:HG21	1.91	0.52
1:A:3969:ASN:HA	1:A:3972:LEU:HD22	1.91	0.52
1:A:440:VAL:CG1	1:A:482:VAL:HG23	2.40	0.51
1:A:911:LEU:HD21	1:A:961:LEU:HD21	1.92	0.51
1:A:2085:MET:SD	1:A:2090:ARG:HG2	2.51	0.51
1:A:3281:CYS:HB3	1:A:3329:LEU:HD13	1.92	0.51
1:A:3478:GLU:OE1	1:A:3479:THR:OG1	2.16	0.51
3:C:31:PHE:HE2	3:C:98:ILE:HD12	1.75	0.51
1:A:444:ASP:OD2	1:A:489:ARG:NH1	2.43	0.51
1:A:1178:ARG:O	1:A:1184:ARG:NH2	2.41	0.51
1:A:1355:GLY:O	1:A:1358:LEU:HG	2.09	0.51
1:A:2121:ASP:HA	1:A:2160:TYR:HE2	1.75	0.51
1:A:2857:CYS:O	1:A:2861:ILE:HG12	2.10	0.51
1:A:3649:SER:O	1:A:3653:ARG:NH1	2.41	0.51
2:B:261:LEU:HD11	2:B:269:ILE:HD12	1.92	0.51
3:C:185:LEU:HB2	3:C:514:ASN:ND2	2.24	0.51
1:A:146:GLU:OE2	1:A:146:GLU:N	2.43	0.51
1:A:424:LEU:HD23	1:A:424:LEU:O	2.11	0.51
1:A:1418:HIS:O	1:A:1421:GLU:HG2	2.11	0.51
1:A:1872:GLY:O	1:A:1876:ILE:HG13	2.11	0.51
1:A:2823:PHE:HD2	1:A:2824:LYS:HG2	1.73	0.51
1:A:2987:THR:HG22	1:A:2989:ALA:H	1.76	0.51
1:A:3030:ILE:HD12	1:A:3041:LEU:HD13	1.92	0.51
1:A:3443:PRO:HB3	1:A:3471:ILE:HG21	1.92	0.51
2:B:59:PRO:HB2	2:B:205:LEU:HD13	1.91	0.51
2:B:66:CYS:SG	2:B:242:LEU:HD22	2.50	0.51
3:C:266:SER:OG	3:C:267:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:HG22	1:A:281:GLN:HE22	1.75	0.51
1:A:1783:ARG:HG2	1:A:1830:HIS:NE2	2.25	0.51
1:A:3577:GLN:HB3	1:A:3630:ARG:NE	2.25	0.51
1:A:3844:THR:HG22	1:A:3850:HIS:HA	1.91	0.51
3:C:251:LEU:HB2	3:C:259:ILE:HB	1.91	0.51
1:A:32:HIS:NE2	1:A:84:GLU:OE1	2.44	0.51
1:A:437:HIS:HB2	1:A:2047:THR:HG21	1.91	0.51
1:A:526:ASP:OD1	1:A:526:ASP:N	2.44	0.51
1:A:1249:SER:HB3	1:A:1326:GLU:HB3	1.93	0.51
1:A:1841:SER:O	1:A:1898:GLN:NE2	2.43	0.51
1:A:3356:ALA:O	1:A:3360:LEU:N	2.36	0.51
1:A:3923:ARG:O	1:A:4124:TRP:NE1	2.43	0.51
3:C:315:ARG:NH2	3:C:317:GLY:O	2.42	0.51
1:A:1089:PHE:CZ	1:A:1099:PHE:HB2	2.46	0.51
1:A:3619:ASP:N	1:A:3619:ASP:OD1	2.44	0.51
1:A:3767:LEU:HD13	1:A:3918:LEU:HD22	1.92	0.51
1:A:3960:PRO:HB2	1:A:3961:PHE:CD1	2.45	0.51
2:B:204:HIS:HB3	2:B:237:SER:N	2.26	0.51
2:B:277:VAL:HB	3:C:357:MET:HE2	1.92	0.51
1:A:2182:ILE:HG13	1:A:2186:VAL:HG23	1.91	0.51
1:A:2280:VAL:O	1:A:2285:LEU:HB2	2.10	0.51
2:B:463:LYS:O	2:B:467:GLU:HG2	2.10	0.51
1:A:2383:PHE:HE2	1:A:2408:MET:HE1	1.76	0.51
1:A:3992:ARG:HB3	1:A:4051:LEU:O	2.11	0.51
2:B:345:LEU:HD21	2:B:434:LEU:HD21	1.92	0.51
1:A:603:ILE:HG12	1:A:1083:ASN:HB3	1.92	0.51
1:A:1294:VAL:HB	1:A:1341:ILE:CD1	2.41	0.51
1:A:2101:VAL:HG12	1:A:2156:VAL:HG21	1.93	0.51
1:A:2409:THR:HG23	1:A:2410:GLU:OE1	2.11	0.51
1:A:3510:GLN:HE22	1:A:3513:ALA:HB2	1.76	0.51
3:C:39:THR:O	3:C:43:GLN:HG2	2.11	0.51
4:D:18:DT:H2"	4:D:19:DG:C8	2.46	0.51
1:A:1651:LYS:O	1:A:1655:ILE:HG12	2.11	0.51
1:A:1723:PRO:HD2	1:A:1739:TYR:CE1	2.45	0.51
1:A:2424:MET:HE3	1:A:2457:PRO:HG2	1.93	0.51
1:A:2550:ILE:HG13	1:A:2550:ILE:O	2.11	0.51
2:B:318:ARG:HH22	2:B:331:LYS:HE2	1.76	0.51
2:B:350:PHE:HB3	2:B:394:VAL:HG22	1.93	0.51
1:A:1887:ASP:OD1	1:A:1888:ASP:N	2.43	0.50
2:B:298:THR:HB	3:C:295:TYR:CD1	2.46	0.50
2:B:467:GLU:O	2:B:470:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:LYS:NZ	3:C:94:ILE:O	2.44	0.50
3:C:81:ARG:NH1	3:C:84:MET:H	2.08	0.50
1:A:101:ALA:HB1	1:A:143:LEU:HD22	1.94	0.50
1:A:451:PRO:O	1:A:452:LYS:HG2	2.11	0.50
1:A:2155:GLU:CD	1:A:2155:GLU:H	2.19	0.50
1:A:3506:LEU:HA	1:A:3511:ALA:HB1	1.92	0.50
1:A:3670:MET:O	1:A:3674:SER:HB3	2.11	0.50
2:B:301:ARG:NE	2:B:310:LEU:HD13	2.25	0.50
1:A:267:VAL:HG21	3:C:554:PHE:HZ	1.76	0.50
1:A:636:GLU:HA	1:A:679:LYS:NZ	2.27	0.50
1:A:1093:GLU:HA	1:A:1096:VAL:HG22	1.92	0.50
1:A:4080:VAL:HG12	1:A:4116:ILE:HG22	1.92	0.50
2:B:518:LEU:HD23	3:C:256:ASN:HD21	1.76	0.50
3:C:684:THR:HG21	3:C:701:ALA:HA	1.94	0.50
1:A:2571:ASP:C	1:A:2573:PRO:HD3	2.35	0.50
1:A:3768:PHE:HE2	1:A:3942:PHE:CZ	2.29	0.50
2:B:340:PHE:CG	2:B:408:PRO:HD3	2.47	0.50
3:C:19:THR:O	3:C:22:ASN:ND2	2.33	0.50
1:A:662:LEU:HD23	1:A:662:LEU:H	1.77	0.50
1:A:1249:SER:OG	1:A:1326:GLU:OE1	2.23	0.50
1:A:2310:VAL:HG23	1:A:2310:VAL:O	2.12	0.50
1:A:3049:LEU:O	1:A:3053:LEU:HD23	2.12	0.50
3:C:40:MET:HG3	3:C:488:GLN:NE2	2.26	0.50
1:A:111:CYS:SG	1:A:131:LEU:HB2	2.52	0.50
1:A:1139:GLU:HB2	1:A:1197:LEU:HD11	1.93	0.50
1:A:3706:ASP:OD1	1:A:3706:ASP:N	2.43	0.50
2:B:411:VAL:HG21	2:B:434:LEU:HD22	1.94	0.50
3:C:115:MET:O	3:C:119:GLN:HG3	2.12	0.50
1:A:204:LEU:HD12	1:A:220:LEU:HD12	1.92	0.50
1:A:250:ASN:O	1:A:254:LYS:HG3	2.12	0.50
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.84	0.50
1:A:1668:PHE:O	1:A:1672:PHE:HD2	1.94	0.50
1:A:1747:LEU:HD21	1:A:1781:SER:HB3	1.94	0.50
1:A:1875:LYS:O	1:A:1879:VAL:HG23	2.12	0.50
1:A:2872:ASP:HB3	1:A:2875:ALA:HB3	1.94	0.50
1:A:3299:THR:OG1	1:A:3302:LYS:NZ	2.45	0.50
1:A:3355:LYS:O	1:A:3358:ARG:HB2	2.10	0.50
1:A:3596:LEU:HD11	1:A:3606:ILE:HB	1.93	0.50
2:B:255:ALA:HB3	5:E:30:DG:H4'	1.94	0.50
3:C:238:LYS:O	3:C:239:LYS:HG3	2.12	0.50
3:C:376:ALA:O	3:C:379:SER:OG	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2824:LYS:O	1:A:2829:LYS:HG3	2.11	0.50
1:A:3535:ILE:HD13	1:A:3798:SER:HB3	1.94	0.50
1:A:3922:ASP:OD1	1:A:3924:HIS:NE2	2.45	0.50
2:B:286:ILE:O	3:C:313:GLY:N	2.33	0.50
1:A:977:ASP:HB2	1:A:980:THR:HG22	1.93	0.50
1:A:2402:LEU:HB2	1:A:2438:ILE:CG2	2.36	0.50
1:A:3335:ARG:NH1	1:A:3418:ASP:OD1	2.45	0.50
1:A:105:VAL:HA	1:A:147:PHE:HE1	1.75	0.49
1:A:346:TYR:HA	1:A:349:ILE:HG22	1.94	0.49
1:A:1105:VAL:O	1:A:1109:GLU:HG2	2.12	0.49
1:A:1675:TYR:CE1	1:A:1699:PHE:HE1	2.30	0.49
1:A:3233:SER:HA	1:A:3272:TRP:HZ2	1.77	0.49
1:A:3462:ARG:HE	1:A:3708:ARG:NH2	2.10	0.49
2:B:473:TYR:CD1	3:C:392:ILE:HG13	2.46	0.49
3:C:184:ARG:HG2	3:C:185:LEU:N	2.27	0.49
3:C:276:TRP:HZ2	3:C:494:LEU:HD11	1.77	0.49
1:A:859:LEU:HD21	1:A:870:LEU:HD13	1.94	0.49
1:A:2840:PHE:CE2	1:A:2868:LEU:HD21	2.47	0.49
1:A:2841:ASN:O	1:A:2845:ASN:ND2	2.33	0.49
1:A:3834:ALA:HA	1:A:3877:LYS:HD3	1.94	0.49
3:C:527:GLN:HA	3:C:530:LEU:HD12	1.94	0.49
1:A:152:LEU:HA	1:A:155:LYS:HZ3	1.77	0.49
1:A:1014:LEU:O	1:A:1017:ILE:N	2.45	0.49
1:A:1195:VAL:CG2	1:A:1196:PRO:HD3	2.42	0.49
1:A:1342:MET:HE1	1:A:1375:THR:HG21	1.95	0.49
1:A:2268:LYS:HD2	1:A:2314:GLU:OE2	2.11	0.49
1:A:3268:THR:HG23	1:A:3269:ARG:HG3	1.93	0.49
1:A:3726:VAL:HG11	1:A:3736:LYS:HD3	1.94	0.49
1:A:3744:ASP:HB2	1:A:3746:ARG:HE	1.77	0.49
3:C:381:ILE:HG21	3:C:419:LEU:HB2	1.93	0.49
1:A:87:LYS:O	1:A:91:ILE:HG12	2.12	0.49
1:A:355:ASN:OD1	1:A:356:ASN:N	2.42	0.49
1:A:1759:LEU:HD12	1:A:1797:LEU:HD22	1.92	0.49
1:A:2256:ILE:HG22	1:A:2276:LEU:HD13	1.93	0.49
1:A:3062:LEU:HD12	1:A:3062:LEU:H	1.76	0.49
1:A:3334:TYR:HB2	1:A:3381:ALA:HB2	1.95	0.49
1:A:3420:CYS:SG	1:A:3445:LEU:HD22	2.52	0.49
2:B:40:PHE:CZ	2:B:70:VAL:HG11	2.44	0.49
2:B:360:HIS:HA	3:C:267:ILE:HD12	1.93	0.49
2:B:441:ASP:OD2	3:C:44:ARG:NH2	2.46	0.49
3:C:640:ARG:HH21	3:C:681:ASP:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1379:PRO:O	1:A:1384:PHE:HB2	2.12	0.49
1:A:3316:LEU:HD22	1:A:3323:PHE:HD1	1.77	0.49
2:B:392:LYS:NZ	3:C:455:ASP:OD1	2.44	0.49
1:A:86:LEU:HD21	1:A:114:VAL:HG11	1.94	0.49
1:A:202:GLY:O	1:A:206:THR:HG23	2.13	0.49
1:A:208:MET:HE1	1:A:255:ALA:HB2	1.94	0.49
1:A:524:TYR:HA	1:A:527:TYR:CD2	2.47	0.49
1:A:1618:LEU:O	1:A:1622:ILE:HG12	2.13	0.49
1:A:2085:MET:HG3	1:A:2090:ARG:HG2	1.93	0.49
1:A:3118:ASP:OD1	1:A:3119:VAL:N	2.44	0.49
2:B:473:TYR:HB3	3:C:350:GLN:NE2	2.25	0.49
3:C:151:ILE:HD12	3:C:215:LEU:HD13	1.95	0.49
1:A:115:TYR:HB2	1:A:127:ALA:HB1	1.94	0.49
1:A:252:VAL:O	1:A:256:ILE:HG12	2.13	0.49
1:A:606:SER:OG	1:A:608:PRO:O	2.25	0.49
1:A:1736:PHE:O	1:A:1740:VAL:HG23	2.12	0.49
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	1.95	0.49
3:C:90:LEU:O	3:C:94:ILE:HG13	2.12	0.49
1:A:373:CYS:HA	1:A:376:ILE:HG22	1.93	0.49
1:A:1138:ILE:HG13	1:A:1141:LYS:HE3	1.95	0.49
1:A:1970:LYS:HD2	1:A:1970:LYS:O	2.13	0.49
1:A:2205:VAL:HB	1:A:2208:ASP:HB3	1.94	0.49
1:A:3699:LEU:HD12	1:A:3719:ILE:HG21	1.95	0.49
1:A:4046:TYR:CZ	1:A:4062:ASP:HB3	2.47	0.49
3:C:33:GLN:HB3	3:C:227:PHE:HB3	1.94	0.49
3:C:356:PHE:CG	3:C:422:VAL:HG11	2.48	0.49
3:C:457:LEU:HD13	3:C:533:ILE:HD12	1.93	0.49
1:A:1088:GLU:C	1:A:1090:ARG:H	2.21	0.49
1:A:1432:CYS:HB3	1:A:1486:LEU:HD22	1.95	0.49
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.94	0.49
1:A:1613:HIS:O	1:A:1617:LYS:HG3	2.12	0.49
1:A:2239:LYS:HA	1:A:2242:VAL:HG12	1.95	0.49
1:A:3468:LEU:HA	1:A:3471:ILE:HG22	1.93	0.49
1:A:3767:LEU:O	1:A:3771:MET:HG3	2.12	0.49
1:A:4069:GLU:O	1:A:4070:LYS:HG2	2.11	0.49
2:B:262:LYS:HZ3	2:B:346:MET:HB3	1.77	0.49
2:B:348:MET:HE1	3:C:516:LEU:O	2.12	0.49
1:A:450:SER:OG	1:A:453:MET:SD	2.71	0.49
1:A:1932:GLN:H	1:A:1937:ARG:NH2	2.11	0.49
1:A:3499:ILE:O	1:A:3503:VAL:HG22	2.12	0.49
1:A:3798:SER:O	1:A:3799:ARG:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:SER:OG	2:B:249:LYS:HB2	2.12	0.49
2:B:247:ARG:HH21	2:B:488:ARG:HG3	1.77	0.49
1:A:1142:HIS:CE1	1:A:1146:ASN:HA	2.48	0.48
1:A:1820:VAL:HA	1:A:1824:LEU:HG	1.95	0.48
1:A:1881:TYR:CE1	1:A:1889:VAL:HG11	2.48	0.48
1:A:2933:ILE:HG22	1:A:2933:ILE:O	2.13	0.48
3:C:323:PHE:HE1	3:C:328:GLU:CA	2.25	0.48
1:A:410:MET:HE1	1:A:441:MET:HE2	1.95	0.48
1:A:919:LEU:HD11	1:A:968:VAL:HG23	1.95	0.48
1:A:1249:SER:CB	1:A:1326:GLU:HB3	2.43	0.48
1:A:3465:PHE:O	1:A:3469:LEU:HG	2.13	0.48
1:A:3734:ARG:HB2	1:A:3734:ARG:HH11	1.78	0.48
3:C:39:THR:HA	3:C:42:VAL:HG22	1.95	0.48
4:D:16:DG:H2'	4:D:17:DC:C6	2.48	0.48
1:A:759:GLY:C	1:A:761:SER:H	2.20	0.48
1:A:858:MET:HA	1:A:861:SER:HB2	1.95	0.48
1:A:897:PRO:O	1:A:2566:THR:OG1	2.23	0.48
1:A:1271:ILE:HG22	1:A:1276:VAL:HG23	1.96	0.48
1:A:2182:ILE:O	1:A:2186:VAL:HG23	2.13	0.48
1:A:2225:HIS:C	1:A:2227:LYS:H	2.21	0.48
1:A:2414:GLN:O	1:A:2418:LYS:HG2	2.13	0.48
1:A:3141:PHE:CD1	1:A:3189:PHE:HB3	2.48	0.48
1:A:3144:PHE:O	1:A:3150:ASN:ND2	2.45	0.48
2:B:48:MET:SD	2:B:48:MET:N	2.87	0.48
2:B:73:SER:O	2:B:77:SER:HB3	2.12	0.48
2:B:106:GLN:HB3	2:B:115:ARG:NH1	2.28	0.48
1:A:152:LEU:HA	1:A:155:LYS:NZ	2.29	0.48
1:A:235:THR:CG2	1:A:281:GLN:HE22	2.26	0.48
1:A:297:LEU:HB3	1:A:316:LEU:HD12	1.94	0.48
1:A:1389:VAL:HG13	1:A:1390:GLN:N	2.29	0.48
1:A:1470:SER:OG	1:A:1477:HIS:HA	2.14	0.48
1:A:1505:LEU:HD23	1:A:1505:LEU:H	1.77	0.48
1:A:2923:TRP:CH2	1:A:3973:PRO:HB2	2.49	0.48
1:A:2972:TYR:O	1:A:2976:LEU:HB2	2.13	0.48
2:B:241:ASP:OD1	2:B:242:LEU:N	2.46	0.48
2:B:529:VAL:HG23	2:B:530:TYR:HD1	1.78	0.48
1:A:1107:TYR:OH	1:A:1127:CYS:HA	2.13	0.48
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.13	0.48
1:A:3916:TRP:CD1	1:A:3960:PRO:HB3	2.49	0.48
2:B:297:LYS:HE2	3:C:296:CYS:SG	2.53	0.48
2:B:363:ARG:NH2	2:B:363:ARG:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:632:PHE:HB3	3:C:677:ILE:HD13	1.94	0.48
3:C:688:LYS:HE3	3:C:694:SER:H	1.79	0.48
1:A:439:VAL:O	1:A:443:ILE:HG12	2.14	0.48
1:A:1058:SER:HA	1:A:1061:LYS:HG3	1.95	0.48
1:A:1638:PRO:C	1:A:1640:GLU:H	2.22	0.48
1:A:2440:TYR:HD1	1:A:2476:ILE:HG22	1.77	0.48
1:A:3055:GLY:O	1:A:3056:GLU:HG3	2.14	0.48
1:A:3448:GLU:HB3	1:A:3452:LYS:HE2	1.93	0.48
2:B:297:LYS:O	2:B:297:LYS:HG2	2.12	0.48
3:C:338:LYS:HB3	3:C:398:ASP:HA	1.96	0.48
3:C:411:HIS:CB	3:C:418:CYS:N	2.74	0.48
1:A:101:ALA:HB2	1:A:143:LEU:HD13	1.96	0.48
1:A:455:LEU:O	1:A:459:ARG:HG2	2.13	0.48
1:A:1886:LYS:HB2	1:A:1890:HIS:CD2	2.48	0.48
1:A:1920:TYR:O	1:A:1924:THR:OG1	2.23	0.48
3:C:387:LEU:CD2	3:C:389:MET:HG3	2.43	0.48
3:C:511:HIS:O	3:C:515:MET:HG2	2.13	0.48
3:C:528:ILE:HB	3:C:529:PRO:HD3	1.96	0.48
1:A:1649:LEU:HD21	1:A:1675:TYR:CE1	2.48	0.48
1:A:3090:TYR:HD2	1:A:3098:ARG:HB3	1.79	0.48
1:A:629:PHE:O	1:A:633:ILE:HG12	2.14	0.48
1:A:1668:PHE:HB3	1:A:1669:PRO:HD3	1.95	0.48
1:A:1864:ASP:O	1:A:1868:THR:HG23	2.14	0.48
1:A:2398:LEU:HA	1:A:2401:VAL:HG22	1.96	0.48
1:A:3133:GLN:HG2	1:A:3182:ILE:HD11	1.96	0.48
1:A:3550:LYS:O	1:A:3553:GLU:HG3	2.14	0.48
2:B:145:GLU:O	2:B:148:TRP:HB3	2.14	0.48
3:C:155:LYS:NZ	3:C:216:GLU:OE1	2.45	0.48
3:C:653:GLN:HA	3:C:656:ASN:HD21	1.77	0.48
1:A:92:PHE:HA	1:A:95:LYS:HB3	1.95	0.48
1:A:1616:LEU:O	1:A:1620:THR:HG23	2.14	0.48
3:C:44:ARG:HD3	3:C:237:PHE:CZ	2.49	0.48
3:C:194:LEU:O	3:C:195:LYS:HE2	2.14	0.48
1:A:1389:VAL:HG13	1:A:1390:GLN:H	1.79	0.47
1:A:1484:LEU:HD21	1:A:1531:LEU:HD12	1.94	0.47
1:A:1685:ASP:O	1:A:1689:LYS:HG3	2.14	0.47
1:A:3685:PRO:O	1:A:3689:ASP:N	2.44	0.47
1:A:144:MET:CE	1:A:185:HIS:HB2	2.41	0.47
1:A:1772:HIS:H	1:A:1822:ARG:HH22	1.62	0.47
1:A:2412:TYR:HE2	1:A:2454:LEU:HG	1.80	0.47
1:A:3737:ARG:HB3	1:A:3751:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:DC:H1'	5:E:35:DG:C8	2.49	0.47
1:A:377:ASN:C	1:A:379:LYS:H	2.23	0.47
1:A:1301:ILE:HG23	1:A:1302:ALA:H	1.78	0.47
1:A:2286:PRO:HG2	1:A:2288:TYR:CD1	2.49	0.47
1:A:2341:LEU:H	1:A:2341:LEU:HD23	1.79	0.47
1:A:3053:LEU:HD22	1:A:3092:LEU:HD11	1.97	0.47
1:A:3496:ILE:HG21	1:A:3705:TYR:HB3	1.97	0.47
1:A:3654:MET:SD	1:A:3655:LYS:N	2.88	0.47
2:B:368:VAL:CG2	2:B:432:PHE:HB2	2.44	0.47
3:C:253:ILE:HB	3:C:257:LEU:HB3	1.97	0.47
1:A:267:VAL:HG21	3:C:554:PHE:CZ	2.50	0.47
1:A:1893:GLU:O	1:A:1897:ASN:ND2	2.47	0.47
1:A:1919:CYS:SG	1:A:1920:TYR:N	2.87	0.47
1:A:2528:GLU:O	1:A:2529:THR:OG1	2.27	0.47
1:A:3281:CYS:SG	1:A:3307:LEU:HD21	2.54	0.47
1:A:3417:ALA:HB1	1:A:3446:VAL:HG13	1.96	0.47
1:A:3558:ILE:O	1:A:3562:LEU:N	2.44	0.47
2:B:442:ASP:O	3:C:267:ILE:HA	2.14	0.47
3:C:229:GLU:HB3	3:C:232:ARG:HH21	1.79	0.47
3:C:371:GLU:HB3	3:C:374:ALA:HB2	1.97	0.47
1:A:1696:LEU:O	1:A:1700:THR:HG23	2.15	0.47
1:A:2088:LEU:O	1:A:2094:MET:HE3	2.15	0.47
1:A:2546:TYR:CD2	1:A:2548:PRO:HD3	2.49	0.47
1:A:3057:ALA:C	1:A:3059:GLN:H	2.22	0.47
1:A:3172:LYS:HA	1:A:3779:SER:HB2	1.95	0.47
1:A:3534:ILE:HG13	1:A:3535:ILE:HG13	1.96	0.47
2:B:366:LEU:HB2	2:B:434:LEU:HB2	1.96	0.47
3:C:688:LYS:HB3	3:C:694:SER:HB2	1.97	0.47
1:A:765:LEU:HA	1:A:768:VAL:HG12	1.97	0.47
1:A:2572:TYR:N	1:A:2573:PRO:HD3	2.29	0.47
1:A:3086:LEU:HB3	1:A:3102:TYR:CD2	2.50	0.47
1:A:3356:ALA:HA	1:A:3359:ILE:HD12	1.95	0.47
1:A:3728:VAL:HG12	1:A:3736:LYS:HE3	1.96	0.47
1:A:3960:PRO:HB2	1:A:3961:PHE:HD1	1.79	0.47
2:B:289:TYR:HD2	2:B:292:THR:H	1.62	0.47
2:B:466:VAL:HA	2:B:469:LEU:HB2	1.96	0.47
1:A:111:CYS:HA	1:A:114:VAL:HG12	1.96	0.47
1:A:385:TYR:CE1	1:A:389:ILE:HD11	2.49	0.47
1:A:624:ILE:O	1:A:627:VAL:HG22	2.14	0.47
1:A:631:ARG:NH1	1:A:668:LYS:HD3	2.30	0.47
1:A:750:PRO:HA	1:A:753:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:VAL:HG13	1:A:874:THR:N	2.23	0.47
1:A:901:MET:HG3	1:A:903:PRO:HD3	1.96	0.47
1:A:1067:ALA:O	1:A:1075:ARG:HG2	2.14	0.47
1:A:1325:GLN:NE2	1:A:1326:GLU:HG3	2.30	0.47
1:A:1952:ILE:O	1:A:1955:VAL:HG22	2.14	0.47
1:A:2377:ARG:HG3	1:A:2378:PHE:CD1	2.49	0.47
1:A:2433:LYS:NZ	1:A:2437:ASP:OD1	2.47	0.47
1:A:2547:SER:HA	1:A:2548:PRO:HD2	1.52	0.47
1:A:2840:PHE:HE2	1:A:2868:LEU:HD21	1.80	0.47
1:A:3120:LEU:HD13	1:A:3896:ALA:HA	1.96	0.47
1:A:3296:GLN:O	1:A:3300:VAL:HG12	2.14	0.47
1:A:3351:ILE:HG13	1:A:3351:ILE:O	2.14	0.47
1:A:3522:THR:O	1:A:3526:PRO:HB3	2.15	0.47
1:A:3558:ILE:HA	1:A:3561:LYS:HG2	1.96	0.47
2:B:255:ALA:C	2:B:257:SER:H	2.23	0.47
2:B:517:ARG:NH1	2:B:517:ARG:HB2	2.30	0.47
3:C:27:ILE:HG13	3:C:28:GLU:N	2.29	0.47
1:A:475:LEU:HD23	1:A:475:LEU:H	1.80	0.47
1:A:1539:SER:HA	1:A:1552:HIS:HA	1.95	0.47
1:A:1861:SER:O	1:A:1865:THR:HG23	2.15	0.47
1:A:1947:CYS:O	1:A:1951:VAL:HG13	2.14	0.47
1:A:2574:ASN:O	1:A:2576:MET:N	2.47	0.47
1:A:3240:MET:HE2	1:A:3240:MET:HB2	1.80	0.47
1:A:3498:TRP:HH2	1:A:4001:THR:HG23	1.80	0.47
3:C:167:PHE:O	3:C:191:SER:OG	2.29	0.47
3:C:246:HIS:CG	3:C:368:ARG:HH22	2.32	0.47
1:A:399:GLN:HG3	1:A:400:THR:HG23	1.97	0.47
1:A:2563:LEU:O	1:A:2566:THR:HG22	2.15	0.47
1:A:2956:ALA:HB2	1:A:2971:GLN:HG3	1.97	0.47
1:A:3018:SER:OG	1:A:3040:TYR:OH	2.28	0.47
1:A:3469:LEU:HD22	1:A:3510:GLN:NE2	2.29	0.47
1:A:3567:VAL:HG11	1:A:3697:ASN:HB2	1.96	0.47
2:B:125:GLN:OE1	2:B:128:GLN:NE2	2.48	0.47
3:C:96:SER:O	3:C:96:SER:OG	2.28	0.47
4:D:8:DC:H4'	4:D:9:DC:OP1	2.14	0.47
1:A:189:MET:HB2	1:A:192:ASN:OD1	2.15	0.47
1:A:1129:ASP:O	1:A:1132:ASP:HB3	2.15	0.47
1:A:1221:ILE:O	1:A:1225:GLU:HG2	2.13	0.47
1:A:1267:TYR:O	1:A:1271:ILE:HG12	2.15	0.47
1:A:1592:MET:O	1:A:1596:VAL:HG23	2.15	0.47
1:A:1690:GLY:HA2	1:A:1693:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1714:LEU:O	1:A:1718:ILE:HG12	2.15	0.47
1:A:2182:ILE:HG13	1:A:2182:ILE:O	2.14	0.47
1:A:2401:VAL:O	1:A:2405:VAL:HG13	2.15	0.47
1:A:2436:LEU:HD21	1:A:2458:VAL:HG23	1.96	0.47
1:A:2885:GLN:O	1:A:2888:VAL:HG22	2.14	0.47
1:A:2967:GLU:HA	1:A:2970:LYS:HB2	1.97	0.47
1:A:3335:ARG:HG2	1:A:3419:PHE:HD2	1.80	0.47
2:B:513:ALA:O	2:B:516:LYS:HG3	2.14	0.47
1:A:204:LEU:HD11	1:A:224:LEU:HG	1.96	0.46
1:A:1294:VAL:HB	1:A:1341:ILE:HD12	1.97	0.46
1:A:2166:SER:O	1:A:2170:GLN:HG2	2.15	0.46
1:A:2420:PHE:HA	1:A:2423:VAL:HG12	1.97	0.46
1:A:3277:VAL:HG21	1:A:3311:ASN:HD22	1.80	0.46
1:A:3307:LEU:HA	1:A:3311:ASN:HD21	1.80	0.46
1:A:4096:SER:OG	1:A:4097:GLY:N	2.47	0.46
3:C:197:ILE:HD13	3:C:202:LYS:HZ3	1.79	0.46
3:C:689:GLU:HG3	3:C:691:ALA:HB3	1.97	0.46
1:A:266:ALA:N	1:A:268:PRO:HD2	2.31	0.46
1:A:2225:HIS:C	1:A:2227:LYS:N	2.73	0.46
1:A:3006:ALA:HB1	1:A:3008:TRP:CE2	2.50	0.46
1:A:3179:TRP:O	1:A:3183:ILE:HG12	2.15	0.46
1:A:3793:VAL:HG13	1:A:3803:ILE:HG12	1.96	0.46
2:B:269:ILE:CD1	2:B:381:LEU:HD11	2.46	0.46
3:C:92:GLU:OE1	3:C:499:LEU:HD22	2.15	0.46
1:A:862:LEU:HD13	1:A:866:ILE:CG2	2.46	0.46
1:A:901:MET:HE3	1:A:2819:GLU:HB3	1.97	0.46
2:B:361:TYR:OH	3:C:422:VAL:HG13	2.16	0.46
3:C:496:HIS:CG	3:C:506:PRO:HG3	2.50	0.46
5:E:37:DC:H2''	5:E:38:DA:H5''	1.98	0.46
1:A:1353:PRO:HB3	1:A:1408:MET:HE1	1.96	0.46
1:A:2091:HIS:CG	1:A:2091:HIS:O	2.69	0.46
1:A:2786:LYS:HG3	1:A:2787:HIS:H	1.80	0.46
1:A:3134:ALA:O	1:A:3138:ILE:HG12	2.16	0.46
1:A:3822:GLN:HA	1:A:3825:LYS:HG2	1.96	0.46
2:B:330:GLU:HG3	2:B:332:GLU:N	2.30	0.46
1:A:477:ASN:O	1:A:480:SER:OG	2.33	0.46
1:A:1224:PHE:HB3	1:A:1266:CYS:SG	2.55	0.46
1:A:1428:ILE:HD13	1:A:1468:LEU:HD11	1.98	0.46
1:A:2392:VAL:O	1:A:2396:LEU:HG	2.15	0.46
1:A:3532:PRO:O	1:A:3536:SER:N	2.37	0.46
2:B:351:LYS:CG	3:C:463:LEU:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:VAL:O	3:C:389:MET:HE1	2.15	0.46
1:A:11:SER:HB2	1:A:38:LEU:HD21	1.98	0.46
1:A:1604:SER:HB2	1:A:1618:LEU:HD21	1.98	0.46
1:A:3274:VAL:HA	1:A:3277:VAL:HG12	1.97	0.46
1:A:3588:TRP:HD1	1:A:3609:MET:HE1	1.81	0.46
1:A:1922:ALA:C	1:A:1924:THR:H	2.23	0.46
1:A:2268:LYS:HG2	1:A:2312:TYR:CD2	2.51	0.46
1:A:3138:ILE:HD12	1:A:3189:PHE:HZ	1.80	0.46
1:A:3183:ILE:HG13	1:A:3242:MET:HB2	1.98	0.46
3:C:46:VAL:HG13	3:C:47:PHE:HD1	1.81	0.46
3:C:609:PHE:CD2	3:C:610:GLU:HG2	2.51	0.46
1:A:240:GLU:HG2	1:A:241:ASP:H	1.81	0.46
1:A:579:LEU:HD21	1:A:2036:LEU:HD12	1.98	0.46
1:A:935:HIS:O	1:A:939:MET:HG2	2.16	0.46
1:A:1409:SER:HB2	1:A:1410:PRO:HD2	1.98	0.46
1:A:3632:PHE:O	1:A:3636:PHE:CB	2.64	0.46
1:A:9:ARG:NE	1:A:57:LEU:HG	2.26	0.46
1:A:367:GLY:HA3	1:A:416:SER:HA	1.98	0.46
1:A:1210:ASP:O	1:A:1213:LYS:HG3	2.16	0.46
1:A:1590:THR:HA	1:A:1593:VAL:HG12	1.97	0.46
1:A:1726:SER:OG	1:A:1727:ARG:N	2.48	0.46
1:A:2091:HIS:C	1:A:2093:CYS:H	2.23	0.46
1:A:4064:LEU:CD2	1:A:4077:TYR:HB3	2.38	0.46
2:B:302:THR:HG23	2:B:311:LEU:HB2	1.97	0.46
3:C:56:LEU:O	3:C:81:ARG:N	2.44	0.46
3:C:265:LYS:HD3	3:C:268:LEU:HD13	1.98	0.46
1:A:338:LEU:HD21	1:A:373:CYS:SG	2.55	0.46
1:A:569:VAL:HA	1:A:572:VAL:HG12	1.98	0.46
1:A:959:TYR:HD2	1:A:963:LYS:HD2	1.81	0.46
1:A:2038:GLU:O	1:A:2041:SER:N	2.49	0.46
2:B:337:LEU:HD11	3:C:490:LEU:HD12	1.97	0.46
1:A:821:ALA:HB1	1:A:829:VAL:HG23	1.99	0.45
1:A:880:MET:C	1:A:883:TYR:H	2.23	0.45
1:A:973:ALA:O	1:A:981:ARG:HG3	2.16	0.45
1:A:1298:LEU:CD2	1:A:1368:LEU:HA	2.46	0.45
1:A:1689:LYS:O	1:A:1693:VAL:N	2.40	0.45
1:A:1689:LYS:HA	1:A:1692:ALA:HB3	1.98	0.45
1:A:2038:GLU:CG	1:A:2042:GLN:HE22	2.28	0.45
1:A:3045:ILE:HD11	1:A:3082:TYR:CE1	2.50	0.45
1:A:3580:ASN:O	1:A:3583:LEU:HG	2.15	0.45
1:A:3606:ILE:HG21	1:A:3655:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3780:ALA:HB1	1:A:3986:HIS:ND1	2.32	0.45
2:B:187:ARG:HB2	2:B:187:ARG:CZ	2.46	0.45
1:A:166:ILE:HB	1:A:170:VAL:CG2	2.46	0.45
1:A:623:PHE:O	1:A:627:VAL:HG13	2.17	0.45
1:A:645:TRP:CZ3	1:A:1505:LEU:HD13	2.51	0.45
1:A:1297:PHE:HZ	1:A:1337:VAL:HG23	1.80	0.45
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.49	0.45
1:A:1657:SER:OG	1:A:1658:SER:N	2.49	0.45
1:A:1945:TYR:HE1	1:A:1966:LEU:HA	1.81	0.45
1:A:3100:LYS:O	1:A:3103:ILE:HG22	2.16	0.45
1:A:3385:LEU:HD21	1:A:3416:LEU:HA	1.99	0.45
1:A:3699:LEU:HB2	1:A:3719:ILE:CG2	2.47	0.45
1:A:3789:ARG:HB3	1:A:3938:ILE:HG23	1.99	0.45
2:B:219:ASP:N	2:B:219:ASP:OD1	2.48	0.45
2:B:322:TYR:CE2	3:C:274:LYS:CG	2.59	0.45
1:A:873:VAL:CG1	1:A:874:THR:H	2.23	0.45
1:A:1034:ARG:HA	1:A:1085:ILE:HG22	1.98	0.45
1:A:2091:HIS:O	1:A:2091:HIS:ND1	2.50	0.45
1:A:2528:GLU:OE2	1:A:2533:SER:OG	2.26	0.45
1:A:3128:LYS:HA	1:A:3128:LYS:HD2	1.76	0.45
1:A:3409:VAL:HG22	1:A:3413:TYR:CE2	2.52	0.45
1:A:3462:ARG:HD3	1:A:3497:SER:OG	2.15	0.45
1:A:3908:HIS:NE2	1:A:3912:CYS:SG	2.89	0.45
1:A:4126:PRO:HD2	1:A:4127:TRP:CZ3	2.52	0.45
2:B:72:ILE:HD11	2:B:495:LEU:HD21	1.98	0.45
2:B:261:LEU:CD1	2:B:269:ILE:HD12	2.47	0.45
3:C:154:LEU:HD22	3:C:159:ILE:HD11	1.99	0.45
3:C:496:HIS:CE1	3:C:503:GLU:HB2	2.51	0.45
1:A:344:GLN:O	1:A:348:ILE:HG12	2.16	0.45
1:A:439:VAL:CG1	1:A:482:VAL:HG21	2.47	0.45
1:A:565:TYR:OH	1:A:634:LEU:HD22	2.17	0.45
1:A:3091:LEU:HD22	1:A:3188:PHE:CE2	2.51	0.45
1:A:3708:ARG:HA	1:A:3708:ARG:HD3	1.54	0.45
1:A:3880:ALA:HB2	1:A:3965:ARG:HH21	1.79	0.45
1:A:3889:ARG:HG2	1:A:3889:ARG:HH21	1.81	0.45
2:B:94:LYS:H	2:B:103:TYR:HA	1.80	0.45
3:C:362:LEU:HD12	3:C:421:TYR:CD2	2.52	0.45
1:A:176:GLU:HG3	1:A:225:LYS:HG3	1.98	0.45
1:A:320:LEU:HD22	1:A:345:PHE:HZ	1.80	0.45
1:A:2216:LEU:O	1:A:2220:MET:HG3	2.17	0.45
1:A:2844:LEU:HD11	1:A:2871:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3496:ILE:HD12	1:A:3496:ILE:H	1.80	0.45
1:A:3681:LYS:HD2	1:A:3722:PHE:HB3	1.97	0.45
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	1.98	0.45
1:A:4049:ARG:HB3	1:A:4059:ILE:HD11	1.99	0.45
2:B:297:LYS:NZ	2:B:297:LYS:HB3	2.25	0.45
3:C:164:PHE:CE2	3:C:236:VAL:HG12	2.52	0.45
1:A:440:VAL:HG13	1:A:482:VAL:HG23	1.97	0.45
1:A:1178:ARG:HE	1:A:1180:GLN:NE2	2.14	0.45
1:A:1356:TRP:HA	1:A:1359:LEU:HD13	1.97	0.45
1:A:1965:PHE:O	1:A:1966:LEU:HB2	2.16	0.45
1:A:2251:ILE:CG1	1:A:2285:LEU:CD1	2.94	0.45
1:A:2486:ASP:O	1:A:2488:GLU:N	2.49	0.45
1:A:3172:LYS:NZ	1:A:3777:GLN:HG3	2.32	0.45
1:A:3281:CYS:SG	1:A:3285:HIS:CE1	3.10	0.45
1:A:3506:LEU:HB2	1:A:3533:PHE:CZ	2.42	0.45
1:A:4116:ILE:HG13	1:A:4117:LEU:HD12	1.97	0.45
2:B:58:THR:HG23	2:B:61:ASP:H	1.81	0.45
2:B:446:MET:HB2	2:B:448:PHE:CE1	2.51	0.45
3:C:342:VAL:HG22	3:C:393:VAL:HG22	1.99	0.45
1:A:125:ILE:HB	1:A:126:PRO:HD3	1.97	0.45
1:A:459:ARG:HH22	1:A:545:LEU:HD11	1.80	0.45
1:A:1432:CYS:HB3	1:A:1486:LEU:CD2	2.46	0.45
1:A:3011:LEU:HD11	1:A:3043:TYR:HD1	1.82	0.45
2:B:470:ARG:NH2	3:C:347:LYS:HB3	2.31	0.45
3:C:627:ASN:HD22	3:C:632:PHE:HZ	1.64	0.45
4:D:18:DT:H3	5:E:26:DA:H2	1.65	0.45
1:A:737:PRO:C	1:A:739:ASN:H	2.24	0.45
1:A:1804:MET:HA	1:A:1807:LYS:HZ2	1.81	0.45
1:A:2575:PRO:HD3	1:A:2787:HIS:HB2	1.98	0.45
1:A:3407:ALA:HA	1:A:3410:ILE:HG12	1.99	0.45
1:A:3413:TYR:CD1	1:A:3449:LYS:HB3	2.52	0.45
1:A:3496:ILE:O	1:A:3499:ILE:HG22	2.17	0.45
2:B:263:LEU:HD11	2:B:269:ILE:HD11	1.99	0.45
3:C:226:SER:OG	3:C:228:SER:OG	2.30	0.45
3:C:357:MET:CE	3:C:429:ASP:HB3	2.45	0.45
1:A:1090:ARG:HD3	1:A:1137:ILE:HG21	1.98	0.45
2:B:191:GLY:HA2	2:B:194:ARG:HG2	1.98	0.45
1:A:1626:TRP:CH2	1:A:1649:LEU:HD13	2.52	0.45
1:A:1779:GLN:HB3	1:A:1783:ARG:HH12	1.82	0.45
1:A:1983:ASP:OD1	1:A:1986:ARG:N	2.50	0.45
1:A:1988:TYR:CZ	1:A:2088:LEU:HD21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:PHE:CD2	1:A:2272:VAL:HG21	2.52	0.45
1:A:2980:ASP:OD1	1:A:2981:TRP:N	2.43	0.45
1:A:3126:LEU:O	1:A:3130:GLN:HG3	2.17	0.45
1:A:3658:ASP:OD1	1:A:3658:ASP:N	2.49	0.45
3:C:347:LYS:HD3	3:C:387:LEU:HD21	1.99	0.45
3:C:484:ASN:HB3	3:C:487:PHE:CD1	2.51	0.45
1:A:139:ARG:HH12	1:A:183:GLU:CD	2.26	0.44
1:A:1190:LEU:HD12	1:A:1194:PHE:CE2	2.52	0.44
1:A:1433:ALA:H	1:A:1436:LEU:HD21	1.82	0.44
1:A:2920:VAL:O	1:A:2924:VAL:HG23	2.16	0.44
1:A:3455:LYS:HA	1:A:3490:VAL:HG23	1.99	0.44
1:A:3514:VAL:HG23	1:A:3514:VAL:O	2.17	0.44
1:A:3531:TYR:O	1:A:3535:ILE:HD12	2.18	0.44
1:A:3660:ASN:HD22	1:A:3663:THR:HG21	1.82	0.44
1:A:4088:ASN:HB3	1:A:4090:ARG:HG2	1.99	0.44
3:C:200:GLN:O	3:C:203:GLU:HG3	2.17	0.44
3:C:519:PRO:O	3:C:522:VAL:HG22	2.17	0.44
1:A:712:LYS:O	1:A:716:VAL:HG23	2.17	0.44
1:A:1839:PHE:O	1:A:1843:ILE:HG12	2.17	0.44
1:A:2953:THR:O	1:A:2957:LEU:HD23	2.18	0.44
1:A:3026:ASP:N	1:A:3026:ASP:OD1	2.47	0.44
1:A:3911:ILE:HG23	1:A:3915:HIS:CE1	2.52	0.44
1:A:3951:GLN:HG2	1:A:4063:GLU:O	2.18	0.44
2:B:87:PHE:HE2	2:B:105:LEU:HD22	1.82	0.44
2:B:242:LEU:HD23	2:B:242:LEU:O	2.17	0.44
4:D:15:DC:H42	5:E:28:DC:H42	1.65	0.44
1:A:303:HIS:ND1	1:A:305:ASN:HB2	2.31	0.44
1:A:400:THR:HB	1:A:404:ASP:HB3	2.00	0.44
1:A:619:ASP:OD2	1:A:2035:THR:HB	2.17	0.44
1:A:671:SER:HA	1:A:674:VAL:HG12	1.98	0.44
1:A:1589:ASN:HB3	1:A:1592:MET:HB2	1.98	0.44
1:A:1888:ASP:N	1:A:1888:ASP:OD1	2.49	0.44
1:A:2182:ILE:O	1:A:2186:VAL:N	2.41	0.44
1:A:2338:GLU:O	1:A:2342:CYS:HB2	2.17	0.44
1:A:3495:PHE:O	1:A:3499:ILE:N	2.50	0.44
1:A:3569:GLN:HE21	1:A:3573:ASN:CG	2.26	0.44
2:B:351:LYS:HG3	3:C:463:LEU:HB2	1.99	0.44
3:C:147:LEU:O	3:C:150:ILE:HG12	2.17	0.44
4:D:25:DT:H2"	4:D:26:DT:H5"	1.98	0.44
1:A:212:VAL:HG12	1:A:213:ARG:HB2	1.99	0.44
1:A:1605:PHE:HB2	1:A:1655:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2034:SER:N	1:A:2037:SER:HG	2.15	0.44
2:B:390:LEU:HD22	2:B:417:GLU:CD	2.42	0.44
2:B:423:GLN:HG3	2:B:425:ILE:HG23	1.98	0.44
2:B:526:LYS:HA	2:B:530:TYR:CZ	2.53	0.44
3:C:362:LEU:HB2	3:C:421:TYR:HD2	1.82	0.44
1:A:114:VAL:HG13	1:A:127:ALA:HB2	2.00	0.44
1:A:134:LEU:HD21	1:A:147:PHE:CE1	2.52	0.44
1:A:363:ILE:HD12	1:A:413:PHE:CE1	2.52	0.44
1:A:670:LEU:HA	1:A:673:THR:HG22	1.99	0.44
1:A:1504:ASP:N	1:A:1507:CYS:SG	2.88	0.44
1:A:1832:SER:CB	1:A:1836:LEU:HD22	2.45	0.44
1:A:2183:HIS:O	1:A:2187:VAL:HG23	2.16	0.44
1:A:2251:ILE:HD13	1:A:2285:LEU:HD13	2.00	0.44
1:A:2365:ASN:O	1:A:2369:LYS:HG3	2.18	0.44
1:A:3297:VAL:HG21	1:A:3341:LEU:HD11	1.99	0.44
2:B:439:PHE:CD1	3:C:484:ASN:HA	2.52	0.44
3:C:305:VAL:HG21	3:C:310:ILE:HD11	2.00	0.44
1:A:100:ILE:HB	1:A:138:PHE:HZ	1.82	0.44
1:A:1720:ALA:HA	3:C:596:GLU:HG2	1.99	0.44
1:A:1788:ARG:HA	1:A:1788:ARG:HD3	1.63	0.44
1:A:1896:ILE:HG13	1:A:1897:ASN:N	2.32	0.44
1:A:2459:VAL:HG11	1:A:2501:LEU:CD2	2.48	0.44
1:A:2472:GLN:O	1:A:2476:ILE:HG23	2.18	0.44
1:A:2952:ILE:HD11	1:A:2971:GLN:HB2	2.00	0.44
2:B:207:LYS:HB3	2:B:208:PRO:HD3	1.99	0.44
3:C:398:ASP:OD1	3:C:400:ARG:N	2.45	0.44
1:A:793:LEU:N	1:A:794:PRO:HD2	2.33	0.44
1:A:1360:LYS:HE2	1:A:1362:ASP:OD2	2.18	0.44
1:A:1807:LYS:NZ	1:A:1811:ARG:HH12	2.15	0.44
1:A:1991:PRO:O	1:A:2184:TYR:HD1	2.00	0.44
1:A:2274:ILE:HD12	1:A:2318:ALA:HB3	2.00	0.44
2:B:284:PRO:HA	2:B:285:PRO:HD3	1.83	0.44
2:B:350:PHE:HB3	2:B:394:VAL:CG2	2.47	0.44
3:C:13:CYS:SG	3:C:134:ILE:HA	2.58	0.44
3:C:365:PHE:CD1	3:C:418:CYS:HB3	2.53	0.44
3:C:450:GLN:O	3:C:454:VAL:HG22	2.18	0.44
3:C:512:ILE:O	3:C:515:MET:HB2	2.17	0.44
1:A:162:LEU:HD12	1:A:163:LYS:O	2.18	0.44
1:A:657:SER:O	1:A:661:PRO:HA	2.18	0.44
1:A:759:GLY:O	1:A:760:LEU:HB2	2.18	0.44
1:A:1990:PHE:HZ	1:A:2088:LEU:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2958:LEU:HD11	1:A:4101:GLU:CG	2.44	0.44
1:A:3282:ARG:HA	1:A:3285:HIS:ND1	2.33	0.44
1:A:3503:VAL:CG2	1:A:3532:PRO:HG3	2.48	0.44
1:A:3686:TRP:HH2	1:A:3699:LEU:HD11	1.81	0.44
1:A:3916:TRP:HH2	1:A:4103:GLN:HE21	1.66	0.44
2:B:142:SER:C	2:B:143:LEU:HD22	2.43	0.44
3:C:155:LYS:HE3	3:C:215:LEU:CD1	2.48	0.44
1:A:1059:LEU:O	1:A:1062:ARG:HG2	2.18	0.44
1:A:1766:LEU:HB2	1:A:1778:PHE:CE2	2.53	0.44
1:A:1828:LEU:HB3	1:A:1879:VAL:HG11	2.00	0.44
1:A:2987:THR:O	1:A:2991:LYS:HG3	2.18	0.44
1:A:3137:GLU:OE2	1:A:3186:ARG:NH2	2.51	0.44
1:A:3552:LYS:HE3	1:A:3552:LYS:HB2	1.90	0.44
1:A:3567:VAL:HG13	1:A:3568:ILE:N	2.33	0.44
1:A:3981:TYR:HD1	1:A:4108:MET:HE1	1.83	0.44
2:B:121:GLN:HG3	2:B:122:PHE:CE1	2.53	0.44
2:B:244:ARG:HG3	2:B:245:LYS:N	2.33	0.44
2:B:252:ARG:HH11	3:C:431:ARG:HE	1.64	0.44
2:B:409:TYR:HA	2:B:439:PHE:CZ	2.47	0.44
3:C:50:ASN:OD1	3:C:52:ASP:HB2	2.18	0.44
1:A:100:ILE:HB	1:A:138:PHE:CZ	2.52	0.43
1:A:180:LEU:O	1:A:184:VAL:HG22	2.18	0.43
1:A:2105:HIS:CE1	1:A:2156:VAL:HA	2.53	0.43
1:A:3285:HIS:HE1	1:A:3329:LEU:HD22	1.80	0.43
2:B:444:ARG:CZ	3:C:268:LEU:HD21	2.48	0.43
2:B:451:LYS:HD2	2:B:451:LYS:HA	1.83	0.43
3:C:532:LYS:O	3:C:536:LEU:CB	2.58	0.43
1:A:121:ALA:HA	1:A:124:LYS:HB2	1.99	0.43
1:A:1268:ASN:HD21	1:A:1343:GLU:HG3	1.82	0.43
1:A:3309:GLU:HG2	1:A:3310:ASN:N	2.33	0.43
1:A:3595:GLU:O	1:A:3602:ASN:ND2	2.42	0.43
2:B:357:LYS:HG2	2:B:360:HIS:CD2	2.52	0.43
1:A:436:GLU:O	1:A:440:VAL:HG13	2.18	0.43
1:A:913:ARG:HD2	1:A:913:ARG:HA	1.76	0.43
1:A:941:MET:HE3	1:A:958:MET:HE1	1.98	0.43
1:A:941:MET:HE2	1:A:962:TYR:CE1	2.54	0.43
1:A:1488:TYR:CE2	1:A:1531:LEU:HD22	2.54	0.43
1:A:1970:LYS:HA	1:A:1971:PRO:HD3	1.85	0.43
1:A:2277:LEU:HA	1:A:2280:VAL:HG12	2.00	0.43
2:B:360:HIS:ND1	3:C:267:ILE:HD11	2.33	0.43
2:B:515:ASN:ND2	3:C:256:ASN:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:599:ARG:HD3	3:C:599:ARG:HA	1.73	0.43
1:A:238:MET:SD	1:A:245:SER:HB3	2.58	0.43
1:A:323:VAL:O	1:A:327:VAL:HG12	2.18	0.43
1:A:1007:VAL:O	1:A:1011:GLU:HG3	2.19	0.43
1:A:1298:LEU:CD1	1:A:1341:ILE:HD13	2.48	0.43
1:A:1679:LEU:HD23	1:A:1689:LYS:HD3	2.00	0.43
1:A:3353:GLU:HB2	1:A:3355:LYS:NZ	2.33	0.43
2:B:380:THR:HG22	3:C:444:TYR:HA	2.01	0.43
3:C:104:GLN:CD	3:C:140:SER:HB3	2.44	0.43
3:C:165:LEU:HD12	3:C:166:PRO:O	2.18	0.43
3:C:312:GLN:NE2	3:C:324:SER:O	2.51	0.43
3:C:526:SER:O	3:C:529:PRO:HD2	2.19	0.43
1:A:118:ASP:OD1	1:A:123:CYS:HB2	2.19	0.43
1:A:160:LEU:HD22	1:A:175:TYR:HE1	1.84	0.43
1:A:413:PHE:O	1:A:417:VAL:HG23	2.18	0.43
1:A:1965:PHE:C	1:A:1967:PHE:H	2.26	0.43
1:A:1975:LEU:O	1:A:1976:LEU:HD23	2.19	0.43
1:A:2443:MET:HE3	1:A:2479:TRP:CD2	2.53	0.43
1:A:3240:MET:SD	1:A:3279:SER:OG	2.66	0.43
1:A:566:ASP:O	1:A:570:LYS:HG3	2.19	0.43
1:A:1124:ILE:HG13	1:A:1125:GLN:OE1	2.19	0.43
1:A:1488:TYR:CD2	1:A:1531:LEU:HD13	2.53	0.43
1:A:1775:GLU:O	1:A:1779:GLN:HG2	2.19	0.43
1:A:2286:PRO:HG2	1:A:2288:TYR:CE1	2.54	0.43
1:A:2546:TYR:CE1	1:A:2854:PHE:CZ	3.07	0.43
1:A:3410:ILE:HA	1:A:3413:TYR:HB2	2.01	0.43
1:A:3835:PRO:HG2	1:A:3878:VAL:HG13	2.00	0.43
1:A:3913:ILE:HD11	1:A:3988:LEU:HB2	2.00	0.43
2:B:41:LEU:HD12	2:B:41:LEU:HA	1.88	0.43
2:B:138:GLY:O	2:B:139:SER:OG	2.33	0.43
3:C:247:TRP:HE3	3:C:263:ALA:HB3	1.83	0.43
3:C:700:GLU:HA	3:C:703:LYS:HG2	2.00	0.43
1:A:275:PHE:HZ	1:A:286:LEU:HD11	1.83	0.43
1:A:624:ILE:O	1:A:628:GLU:OE1	2.36	0.43
1:A:935:HIS:HE2	1:A:939:MET:HE2	1.82	0.43
1:A:1150:LYS:HA	1:A:1150:LYS:HD2	1.78	0.43
1:A:1153:LEU:HD12	1:A:1154:PRO:HD2	2.01	0.43
1:A:1759:LEU:HD23	1:A:1759:LEU:HA	1.86	0.43
1:A:1868:THR:HG22	1:A:1936:ARG:NH2	2.28	0.43
1:A:2555:LEU:HD13	1:A:2806:LYS:HA	1.99	0.43
1:A:3089:LEU:HA	1:A:3092:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3981:TYR:HB2	1:A:4108:MET:HE1	2.01	0.43
2:B:361:TYR:HE1	3:C:422:VAL:HG22	1.84	0.43
2:B:389:CYS:HA	2:B:394:VAL:HG12	2.01	0.43
2:B:396:ALA:HB3	2:B:413:LEU:HB2	2.01	0.43
2:B:477:SER:O	2:B:477:SER:OG	2.31	0.43
3:C:357:MET:O	3:C:357:MET:HG3	2.18	0.43
1:A:1149:LYS:HZ3	1:A:1151:ARG:HH22	1.67	0.43
1:A:1479:VAL:O	1:A:1482:GLU:HG3	2.18	0.43
1:A:1719:VAL:HG23	3:C:631:TYR:CE1	2.54	0.43
1:A:2372:PRO:O	1:A:2374:LEU:N	2.45	0.43
1:A:2478:MET:HG2	1:A:2524:PHE:CE1	2.53	0.43
1:A:2567:SER:HA	1:A:2572:TYR:OH	2.18	0.43
1:A:2888:VAL:HG12	1:A:3894:PRO:HG2	2.01	0.43
1:A:3441:ALA:HB1	1:A:3444:ALA:HB3	2.00	0.43
1:A:3575:LEU:HB2	1:A:3800:LEU:HD21	2.00	0.43
1:A:3701:ILE:HA	1:A:3702:PRO:HD3	1.83	0.43
3:C:75:GLN:OE1	3:C:75:GLN:N	2.52	0.43
3:C:232:ARG:HA	3:C:515:MET:HE1	2.00	0.43
1:A:18:THR:OG1	1:A:27:ALA:HB1	2.18	0.43
1:A:112:THR:O	1:A:116:THR:N	2.43	0.43
1:A:115:TYR:CE1	1:A:124:LYS:HE3	2.53	0.43
1:A:1290:LEU:O	1:A:1294:VAL:HG13	2.19	0.43
1:A:1626:TRP:NE1	1:A:1674:THR:HG21	2.32	0.43
1:A:1839:PHE:O	1:A:1842:THR:OG1	2.31	0.43
1:A:2317:ALA:HB1	1:A:2366:LYS:NZ	2.34	0.43
1:A:2516:GLY:O	1:A:2520:ILE:N	2.45	0.43
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.73	0.43
2:B:52:GLN:OE1	2:B:207:LYS:HG2	2.19	0.43
2:B:247:ARG:HE	2:B:488:ARG:NH1	2.16	0.43
3:C:276:TRP:CZ2	3:C:494:LEU:HD11	2.53	0.43
1:A:132:ILE:HG13	1:A:177:LEU:HD13	2.00	0.43
1:A:384:MET:C	1:A:386:VAL:H	2.26	0.43
1:A:851:ILE:O	1:A:855:VAL:HG23	2.19	0.43
1:A:909:VAL:C	1:A:2807:GLN:NE2	2.77	0.43
1:A:1223:THR:HG23	1:A:1224:PHE:CD1	2.53	0.43
1:A:1676:ILE:O	1:A:1680:ALA:CB	2.67	0.43
1:A:2207:LYS:O	1:A:2211:LEU:HD23	2.18	0.43
1:A:2386:LEU:O	1:A:2394:LYS:HE3	2.19	0.43
1:A:2967:GLU:O	1:A:2971:GLN:NE2	2.47	0.43
1:A:3155:VAL:HG23	1:A:3156:PRO:HD3	2.01	0.43
1:A:3947:GLY:O	1:A:4043:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ALA:HB2	2:B:193:LEU:HD11	1.99	0.43
1:A:123:CYS:C	1:A:126:PRO:HD2	2.44	0.42
1:A:939:MET:HA	1:A:942:LEU:HG	2.00	0.42
1:A:1291:LEU:HA	1:A:1294:VAL:HG22	2.01	0.42
1:A:1834:ASP:OD1	1:A:1835:ALA:N	2.52	0.42
1:A:1988:TYR:CE2	1:A:2088:LEU:HD11	2.54	0.42
1:A:2503:LYS:HD2	1:A:2525:TRP:CH2	2.52	0.42
3:C:115:MET:HA	3:C:118:ILE:HD12	2.01	0.42
3:C:147:LEU:O	3:C:151:ILE:HG12	2.18	0.42
3:C:463:LEU:HD21	3:C:477:PHE:HD2	1.84	0.42
1:A:54:GLN:HA	1:A:57:LEU:HB3	2.01	0.42
1:A:429:GLU:OE1	1:A:1591:LYS:HD3	2.18	0.42
1:A:614:PRO:HG3	1:A:620:PHE:CD2	2.54	0.42
1:A:876:SER:HB2	1:A:880:MET:CG	2.45	0.42
1:A:935:HIS:NE2	1:A:939:MET:HE2	2.34	0.42
1:A:1553:PHE:CD2	1:A:1554:SER:N	2.88	0.42
1:A:1597:LEU:HD11	1:A:1622:ILE:HG21	2.01	0.42
1:A:1775:GLU:OE2	1:A:1779:GLN:NE2	2.51	0.42
1:A:2331:MET:HG3	1:A:2371:PHE:HE1	1.82	0.42
1:A:3122:HIS:O	1:A:3123:GLN:HB3	2.19	0.42
1:A:3666:LEU:HD12	1:A:3666:LEU:HA	1.91	0.42
1:A:3916:TRP:O	1:A:4050:LYS:HE3	2.19	0.42
3:C:543:LYS:C	3:C:544:LYS:HD3	2.44	0.42
4:D:7:DG:H1	5:E:37:DC:H42	1.65	0.42
1:A:9:ARG:HB2	1:A:57:LEU:HD11	2.01	0.42
1:A:648:SER:O	1:A:652:GLU:OE1	2.38	0.42
1:A:943:GLY:O	1:A:2576:MET:HE3	2.19	0.42
1:A:1667:SER:O	1:A:1671:VAL:HG12	2.19	0.42
1:A:3151:LEU:HD21	1:A:3196:LYS:HD3	2.02	0.42
2:B:328:ILE:O	2:B:329:LEU:HD12	2.19	0.42
3:C:380:LEU:O	3:C:384:LEU:HD23	2.19	0.42
3:C:474:GLU:N	3:C:474:GLU:OE1	2.52	0.42
3:C:610:GLU:HA	3:C:613:SER:HB3	2.01	0.42
1:A:766:ALA:O	1:A:770:LEU:HD23	2.18	0.42
1:A:835:LYS:HA	1:A:835:LYS:HD2	1.75	0.42
1:A:1136:ARG:HG3	1:A:1136:ARG:NH1	2.32	0.42
1:A:1880:MET:HB3	1:A:1884:LEU:HD12	2.00	0.42
1:A:2251:ILE:HD11	1:A:2285:LEU:CD1	2.49	0.42
1:A:2257:PHE:CZ	1:A:2294:ILE:HD13	2.55	0.42
1:A:2326:ILE:O	1:A:2330:VAL:HG22	2.19	0.42
1:A:2426:HIS:CG	1:A:2427:ARG:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2436:LEU:HA	1:A:2436:LEU:HD23	1.90	0.42
1:A:3946:PHE:O	1:A:3948:SER:N	2.52	0.42
1:A:4093:GLU:OE1	1:A:4094:PRO:HD2	2.19	0.42
3:C:44:ARG:HD3	3:C:237:PHE:CE2	2.54	0.42
3:C:356:PHE:O	3:C:358:GLY:N	2.53	0.42
3:C:365:PHE:O	3:C:377:LEU:HD11	2.20	0.42
3:C:653:GLN:HG2	3:C:654:ARG:N	2.35	0.42
1:A:248:ILE:O	1:A:252:VAL:HG23	2.19	0.42
1:A:793:LEU:HB3	1:A:870:LEU:HA	2.01	0.42
1:A:1212:LEU:HD12	1:A:1212:LEU:HA	1.89	0.42
1:A:1779:GLN:O	1:A:1783:ARG:HG3	2.20	0.42
3:C:280:ASP:OD2	3:C:283:THR:OG1	2.30	0.42
1:A:182:GLY:HA2	1:A:189:MET:SD	2.60	0.42
1:A:259:GLN:HG2	1:A:262:LEU:HB3	2.00	0.42
1:A:1057:LYS:O	1:A:1061:LYS:HG3	2.19	0.42
1:A:1538:LEU:O	1:A:1552:HIS:HA	2.19	0.42
1:A:1563:PHE:O	1:A:1565:GLU:N	2.52	0.42
1:A:1582:LEU:HD23	1:A:1597:LEU:HD13	2.02	0.42
1:A:1933:LEU:H	1:A:1937:ARG:NH2	2.11	0.42
1:A:3139:GLN:O	1:A:3142:ILE:HG22	2.19	0.42
1:A:3669:LYS:HA	1:A:3672:LYS:HG2	2.01	0.42
2:B:152:ASN:HA	2:B:155:SER:HB3	2.01	0.42
2:B:400:TYR:CZ	2:B:402:PRO:HB3	2.55	0.42
2:B:446:MET:HE3	2:B:448:PHE:HE1	1.85	0.42
1:A:327:VAL:HG23	1:A:334:HIS:HB3	2.01	0.42
1:A:424:LEU:HD21	1:A:428:PRO:HD3	2.01	0.42
1:A:446:PHE:HD1	1:A:457:CYS:HG	1.68	0.42
1:A:1431:LEU:HD13	1:A:1451:VAL:HG11	2.02	0.42
1:A:1591:LYS:HE3	1:A:1591:LYS:HB2	1.88	0.42
1:A:1668:PHE:CD1	1:A:1672:PHE:CE2	3.08	0.42
1:A:2318:ALA:O	1:A:2322:VAL:HG12	2.20	0.42
1:A:2879:GLY:O	1:A:2883:SER:HB3	2.20	0.42
1:A:3443:PRO:HB3	1:A:3471:ILE:CG2	2.50	0.42
3:C:281:ALA:O	3:C:282:LYS:HG2	2.20	0.42
3:C:463:LEU:O	3:C:476:LEU:HB3	2.20	0.42
3:C:616:LEU:HD13	3:C:642:PHE:CE2	2.53	0.42
3:C:619:HIS:O	3:C:622:GLN:HG2	2.20	0.42
1:A:73:LEU:HD12	1:A:74:ASN:N	2.34	0.42
1:A:166:ILE:HB	1:A:170:VAL:HG23	2.00	0.42
1:A:183:GLU:HB2	1:A:229:SER:O	2.20	0.42
1:A:656:GLN:O	1:A:660:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:VAL:O	1:A:903:PRO:HD2	2.20	0.42
1:A:915:THR:OG1	1:A:968:VAL:HG21	2.20	0.42
1:A:1339:VAL:HG13	1:A:1398:VAL:HG11	2.02	0.42
1:A:1369:MET:HE3	1:A:1414:ILE:CG2	2.50	0.42
1:A:1622:ILE:HD11	1:A:1652:ILE:HG12	2.02	0.42
1:A:1672:PHE:CE1	1:A:1702:LEU:HD21	2.54	0.42
1:A:2143:ARG:HG2	1:A:2171:LEU:HD13	2.02	0.42
1:A:3344:GLU:HB2	1:A:3348:LEU:HD23	2.02	0.42
1:A:3484:THR:HA	1:A:3487:ILE:HG22	2.00	0.42
1:A:3703:GLY:HA2	1:A:3794:VAL:HG21	2.02	0.42
2:B:249:LYS:O	2:B:250:GLU:HG3	2.20	0.42
3:C:12:LEU:HD13	3:C:38:ILE:HG13	2.01	0.42
3:C:600:VAL:HA	3:C:603:LYS:HE2	2.02	0.42
4:D:25:DT:H2''	4:D:26:DT:C5'	2.50	0.42
1:A:648:SER:O	1:A:649:PHE:C	2.62	0.42
1:A:1301:ILE:HG23	1:A:1302:ALA:N	2.35	0.42
1:A:1458:LEU:HD12	1:A:1463:LEU:O	2.19	0.42
1:A:1675:TYR:CZ	1:A:1699:PHE:CE1	3.08	0.42
1:A:1750:LEU:HG	1:A:1785:ILE:HD11	2.00	0.42
1:A:2150:VAL:HG23	1:A:2157:PHE:CE1	2.55	0.42
1:A:2203:THR:HG21	1:A:2247:ASP:HB2	2.02	0.42
1:A:3232:ARG:HG2	1:A:3272:TRP:HH2	1.85	0.42
1:A:3568:ILE:O	1:A:3572:ILE:HG13	2.20	0.42
1:A:3762:GLN:HG3	1:A:3793:VAL:O	2.20	0.42
1:A:3998:LEU:O	1:A:4002:MET:HG3	2.19	0.42
2:B:215:LEU:HD22	2:B:216:PHE:HD1	1.84	0.42
2:B:252:ARG:HD2	3:C:431:ARG:NE	2.35	0.42
2:B:271:VAL:CG2	2:B:368:VAL:HB	2.50	0.42
2:B:353:LEU:HD21	2:B:414:VAL:HG13	2.02	0.42
3:C:406:GLY:HA2	3:C:424:LEU:HB2	2.02	0.42
1:A:789:TYR:CD2	1:A:866:ILE:HG23	2.55	0.42
1:A:1382:ILE:HD11	1:A:1384:PHE:CE2	2.55	0.42
1:A:1695:LEU:HD13	1:A:1699:PHE:HD1	1.85	0.42
1:A:1814:PHE:O	1:A:1817:GLN:HG3	2.20	0.42
1:A:2476:ILE:HG21	1:A:2476:ILE:HD13	1.85	0.42
1:A:2575:PRO:HD2	1:A:2785:ILE:O	2.19	0.42
1:A:2786:LYS:HG3	1:A:2787:HIS:N	2.35	0.42
1:A:2978:LYS:HE2	1:A:2981:TRP:CE3	2.55	0.42
1:A:3005:LEU:HG	1:A:3007:GLU:OE1	2.20	0.42
1:A:3236:PHE:CE1	1:A:3262:LEU:HD21	2.55	0.42
1:A:3913:ILE:HB	1:A:3984:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3985:VAL:CG2	1:A:4104:VAL:HG11	2.50	0.42
2:B:41:LEU:HB3	2:B:168:LEU:HD12	2.01	0.42
1:A:792:ILE:HG23	1:A:793:LEU:HD22	2.02	0.41
1:A:1299:GLU:HA	1:A:1367:HIS:HD2	1.84	0.41
1:A:2547:SER:O	1:A:2549:LYS:N	2.53	0.41
1:A:3535:ILE:HD11	1:A:3797:THR:OG1	2.20	0.41
1:A:3879:PRO:O	1:A:3966:GLN:NE2	2.50	0.41
2:B:77:SER:O	2:B:250:GLU:HA	2.20	0.41
2:B:363:ARG:NH1	4:D:18:DT:OP1	2.53	0.41
3:C:261:ILE:HD13	3:C:377:LEU:CD2	2.50	0.41
3:C:300:ASP:OD1	3:C:300:ASP:N	2.53	0.41
1:A:1018:VAL:CG1	1:A:1077:GLY:HA3	2.50	0.41
1:A:1448:LEU:HA	1:A:1451:VAL:HG12	2.01	0.41
1:A:1487:VAL:HG11	1:A:1515:LEU:HD23	2.01	0.41
1:A:1641:THR:O	1:A:1645:VAL:HG12	2.20	0.41
1:A:1787:ARG:HA	1:A:1831:CYS:SG	2.59	0.41
1:A:2534:ASN:C	1:A:2536:LEU:H	2.28	0.41
1:A:2788:SER:O	1:A:2792:THR:HG22	2.21	0.41
1:A:3316:LEU:HD13	1:A:3323:PHE:HE1	1.85	0.41
1:A:3999:THR:HB	1:A:4048:LYS:NZ	2.34	0.41
2:B:473:TYR:HD1	3:C:392:ILE:HG13	1.84	0.41
3:C:81:ARG:HH12	3:C:84:MET:N	2.13	0.41
3:C:165:LEU:HD23	3:C:224:ILE:HD11	2.02	0.41
1:A:2281:MET:O	1:A:2283:ASN:O	2.38	0.41
1:A:2327:LEU:HD11	1:A:2345:VAL:HG11	2.02	0.41
1:A:3006:ALA:HB1	1:A:3008:TRP:CZ2	2.56	0.41
1:A:3113:ASN:O	1:A:3116:SER:OG	2.35	0.41
1:A:3332:THR:O	1:A:3336:ILE:HG13	2.20	0.41
2:B:74:LYS:HD3	2:B:83:LEU:HD11	2.01	0.41
2:B:143:LEU:HG	2:B:182:LYS:HB3	2.02	0.41
3:C:629:THR:OG1	3:C:630:PRO:HD3	2.20	0.41
1:A:42:CYS:SG	1:A:88:PHE:HE1	2.44	0.41
1:A:1165:LEU:HD23	1:A:1165:LEU:O	2.20	0.41
1:A:2093:CYS:O	1:A:2097:LEU:HB2	2.20	0.41
1:A:2307:MET:SD	1:A:2345:VAL:HG23	2.60	0.41
1:A:2368:THR:HA	1:A:2371:PHE:O	2.21	0.41
1:A:3244:ASP:OD1	1:A:3247:ARG:NH2	2.49	0.41
1:A:3283:LEU:O	1:A:3287:ARG:HG2	2.20	0.41
1:A:3502:MET:HE2	1:A:3502:MET:HB3	1.92	0.41
1:A:4056:PRO:HG3	1:A:4107:LEU:HD13	2.02	0.41
2:B:67:ILE:HD13	2:B:85:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:VAL:HG12	3:C:31:PHE:HE1	1.86	0.41
1:A:630:CYS:O	1:A:634:LEU:N	2.50	0.41
1:A:1366:THR:HG23	1:A:1418:HIS:NE2	2.36	0.41
1:A:1760:GLU:OE2	1:A:1800:SER:HB2	2.21	0.41
1:A:2220:MET:SD	1:A:2252:PRO:HG2	2.60	0.41
1:A:2358:ASP:O	1:A:2362:VAL:HG23	2.21	0.41
1:A:2837:LEU:HD12	1:A:2868:LEU:HA	2.02	0.41
1:A:3061:LEU:H	1:A:3061:LEU:HD23	1.85	0.41
1:A:3110:PHE:HD1	1:A:3128:LYS:HE3	1.85	0.41
1:A:3575:LEU:HB3	1:A:3800:LEU:HD11	2.02	0.41
1:A:3699:LEU:HD23	1:A:3699:LEU:HA	1.94	0.41
3:C:20:MET:SD	3:C:137:ASP:HB2	2.61	0.41
1:A:1031:ARG:O	1:A:1034:ARG:HG2	2.19	0.41
1:A:1344:PHE:HA	1:A:1347:THR:HG22	2.02	0.41
1:A:2398:LEU:O	1:A:2401:VAL:HG22	2.19	0.41
1:A:2884:LEU:HD13	1:A:3116:SER:OG	2.20	0.41
1:A:3132:VAL:HA	1:A:3135:LEU:HG	2.03	0.41
1:A:3859:TYR:HB3	1:A:4076:ASP:CB	2.50	0.41
2:B:146:VAL:HG13	2:B:147:LEU:N	2.35	0.41
2:B:287:LYS:O	2:B:295:PRO:HA	2.20	0.41
2:B:473:TYR:CE2	2:B:474:ARG:HG3	2.55	0.41
2:B:505:ASP:OD1	2:B:508:LEU:N	2.54	0.41
3:C:457:LEU:HD22	3:C:533:ILE:CD1	2.51	0.41
1:A:816:SER:N	1:A:819:SER:OG	2.53	0.41
1:A:1064:TYR:OH	1:A:1099:PHE:O	2.23	0.41
1:A:1198:LEU:HG	1:A:1199:PRO:HD2	2.02	0.41
1:A:1538:LEU:HG	1:A:1555:HIS:CB	2.51	0.41
1:A:1776:GLU:H	1:A:1776:GLU:CD	2.28	0.41
1:A:1911:LEU:HA	1:A:1914:THR:OG1	2.19	0.41
1:A:2252:PRO:HB2	1:A:2255:LEU:HD21	2.02	0.41
1:A:2327:LEU:O	1:A:2331:MET:HG2	2.20	0.41
1:A:3259:LEU:HB3	1:A:3276:TRP:CZ2	2.56	0.41
1:A:3354:ASP:O	1:A:3357:ARG:HG2	2.20	0.41
2:B:48:MET:HE3	2:B:171:ASN:OD1	2.21	0.41
2:B:267:ILE:HG13	2:B:267:ILE:O	2.20	0.41
2:B:322:TYR:CD2	3:C:49:GLU:OE1	2.66	0.41
2:B:324:SER:O	2:B:324:SER:OG	2.36	0.41
2:B:329:LEU:HD22	3:C:276:TRP:CH2	2.56	0.41
2:B:374:LEU:O	3:C:542:ALA:HB3	2.21	0.41
3:C:261:ILE:HD12	3:C:262:ALA:H	1.85	0.41
1:A:131:LEU:HD22	1:A:177:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:VAL:O	1:A:787:PRO:HD2	2.21	0.41
1:A:1018:VAL:HG23	1:A:1018:VAL:O	2.21	0.41
1:A:1441:ALA:HA	1:A:1445:ARG:HD2	2.02	0.41
1:A:2534:ASN:O	1:A:2535:THR:OG1	2.31	0.41
1:A:3227:ILE:O	1:A:3231:ILE:HG13	2.21	0.41
1:A:3384:HIS:O	1:A:3387:GLU:HG2	2.21	0.41
1:A:3881:ASP:OD1	1:A:3884:LYS:HB3	2.20	0.41
1:A:3951:GLN:NE2	1:A:4066:LEU:HD23	2.36	0.41
2:B:361:TYR:CE1	3:C:361:VAL:HG22	2.55	0.41
1:A:71:LYS:HE2	1:A:71:LYS:HB3	1.82	0.41
1:A:115:TYR:HE2	1:A:159:GLU:OE2	2.03	0.41
1:A:863:GLY:O	1:A:867:ASN:HB2	2.21	0.41
1:A:911:LEU:CD2	1:A:961:LEU:HD21	2.50	0.41
1:A:924:ARG:O	1:A:928:VAL:HG23	2.21	0.41
1:A:1184:ARG:HH11	1:A:1265:GLU:CD	2.29	0.41
1:A:1257:LEU:HD22	1:A:1337:VAL:HG21	2.02	0.41
1:A:1330:TYR:CE2	1:A:1334:LYS:HD3	2.56	0.41
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	2.03	0.41
1:A:1423:ILE:HD11	1:A:1467:ILE:HG21	2.02	0.41
1:A:1611:GLN:C	1:A:1613:HIS:H	2.28	0.41
1:A:2402:LEU:HA	1:A:2405:VAL:HG13	2.03	0.41
1:A:2454:LEU:HD23	1:A:2454:LEU:HA	1.83	0.41
1:A:2546:TYR:CE1	1:A:2854:PHE:CE2	3.09	0.41
1:A:2810:SER:OG	1:A:2857:CYS:SG	2.61	0.41
1:A:2880:CYS:HB3	1:A:2886:GLN:HA	2.02	0.41
1:A:2931:ARG:HD2	1:A:2939:LEU:HD21	2.03	0.41
1:A:3722:PHE:CE2	1:A:3740:ILE:HG22	2.56	0.41
1:A:3951:GLN:NE2	1:A:4063:GLU:OE1	2.53	0.41
2:B:95:ASN:HD21	2:B:99:PHE:H	1.68	0.41
2:B:244:ARG:CZ	2:B:245:LYS:HE2	2.50	0.41
2:B:370:PRO:HD3	2:B:382:PHE:CE1	2.56	0.41
2:B:497:LEU:O	2:B:497:LEU:HD12	2.20	0.41
3:C:430:LEU:HD23	3:C:430:LEU:H	1.86	0.41
3:C:526:SER:O	3:C:527:GLN:C	2.63	0.41
1:A:424:LEU:C	1:A:424:LEU:CD2	2.92	0.41
1:A:488:ILE:HG23	1:A:2036:LEU:HG	2.02	0.41
1:A:1436:LEU:O	1:A:1445:ARG:NH1	2.53	0.41
1:A:1723:PRO:HG3	1:A:1729:PHE:CE2	2.56	0.41
2:B:50:GLU:HG3	2:B:52:GLN:H	1.86	0.41
2:B:305:THR:O	2:B:306:SER:OG	2.37	0.41
2:B:477:SER:N	3:C:427:MET:SD	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:539:LEU:HD23	3:C:539:LEU:H	1.86	0.41
1:A:852:ARG:HG2	1:A:3111:MET:CE	2.51	0.40
1:A:1068:LEU:HD13	1:A:1155:ARG:NH2	2.36	0.40
1:A:1672:PHE:O	1:A:1673:THR:C	2.63	0.40
1:A:2224:PHE:CD1	1:A:2224:PHE:C	2.99	0.40
1:A:2978:LYS:NZ	1:A:2986:PRO:HD3	2.36	0.40
1:A:2990:GLU:HA	1:A:2993:PHE:HB3	2.03	0.40
1:A:3642:LYS:HE3	1:A:3643:HIS:CE1	2.56	0.40
1:A:4086:ASP:OD1	1:A:4086:ASP:N	2.54	0.40
2:B:90:THR:O	2:B:101:ASN:HA	2.21	0.40
2:B:252:ARG:CZ	3:C:431:ARG:HH21	2.34	0.40
3:C:43:GLN:HA	3:C:46:VAL:HG12	2.03	0.40
3:C:408:ALA:HB1	3:C:419:LEU:HG	2.03	0.40
3:C:611:GLU:HG3	3:C:612:ALA:N	2.36	0.40
3:C:612:ALA:O	3:C:615:GLN:HG2	2.21	0.40
3:C:626:THR:OG1	3:C:628:GLU:OE1	2.26	0.40
1:A:207:GLN:NE2	1:A:216:LYS:HE2	2.36	0.40
1:A:331:ALA:HA	1:A:334:HIS:HB2	2.04	0.40
1:A:1717:LEU:HD23	1:A:1746:PHE:HZ	1.85	0.40
1:A:2953:THR:HG22	1:A:2994:TRP:NE1	2.31	0.40
1:A:3003:ASN:OD1	1:A:3046:ARG:NH1	2.54	0.40
1:A:3147:LYS:HG3	1:A:3150:ASN:H	1.85	0.40
1:A:3552:LYS:HA	1:A:3555:VAL:HG22	2.03	0.40
1:A:3568:ILE:HD13	1:A:3699:LEU:HD23	2.04	0.40
1:A:3570:ASP:OD1	1:A:3686:TRP:NE1	2.54	0.40
2:B:348:MET:HE2	2:B:410:PHE:HE1	1.86	0.40
2:B:505:ASP:OD2	3:C:333:TYR:OH	2.20	0.40
3:C:169:LEU:HD21	3:C:226:SER:HB3	2.03	0.40
3:C:184:ARG:HG2	3:C:185:LEU:H	1.85	0.40
3:C:188:HIS:ND1	3:C:232:ARG:HD3	2.37	0.40
1:A:9:ARG:HH11	1:A:57:LEU:HA	1.86	0.40
1:A:185:HIS:HE1	1:A:188:GLU:CB	2.33	0.40
1:A:464:VAL:O	1:A:468:LEU:HG	2.22	0.40
1:A:1141:LYS:HE3	1:A:1142:HIS:HB2	2.03	0.40
1:A:1915:LEU:HA	1:A:1918:LEU:HG	2.03	0.40
1:A:2315:VAL:HG13	1:A:2316:TYR:N	2.35	0.40
2:B:264:ASN:HB3	3:C:530:LEU:HD22	2.02	0.40
3:C:7:LYS:HB2	3:C:51:LYS:O	2.21	0.40
3:C:108:LEU:O	3:C:112:ILE:HG12	2.20	0.40
3:C:422:VAL:HG12	3:C:423:GLN:O	2.20	0.40
3:C:539:LEU:HG	3:C:541:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:NH2	1:A:415:GLN:OE1	2.54	0.40
1:A:723:ASP:OD1	1:A:723:ASP:N	2.52	0.40
1:A:959:TYR:CD2	1:A:963:LYS:HD2	2.57	0.40
1:A:1089:PHE:HE1	1:A:1099:PHE:HD2	1.70	0.40
1:A:1597:LEU:HA	1:A:1597:LEU:HD12	1.87	0.40
1:A:1876:ILE:HG22	1:A:1880:MET:CE	2.44	0.40
1:A:1920:TYR:CE2	1:A:1965:PHE:HA	2.56	0.40
1:A:2098:THR:O	1:A:2102:LYS:HG3	2.22	0.40
1:A:2447:LYS:HB2	1:A:2450:GLU:OE1	2.21	0.40
1:A:2927:ALA:HB2	1:A:2942:ILE:HD11	2.04	0.40
1:A:2970:LYS:HA	1:A:2970:LYS:HD2	1.92	0.40
1:A:3104:GLN:O	1:A:3108:GLN:OE1	2.39	0.40
1:A:3628:PHE:CD1	1:A:3685:PRO:HD2	2.56	0.40
1:A:3993:SER:O	1:A:3993:SER:OG	2.30	0.40
1:A:4006:VAL:HG22	1:A:4040:PRO:HB3	2.03	0.40
5:E:33:DT:H2''	5:E:34:DC:H5'	2.03	0.40
1:A:408:TYR:CE2	1:A:453:MET:HE1	2.57	0.40
1:A:1433:ALA:N	1:A:1436:LEU:HD21	2.37	0.40
1:A:1448:LEU:HA	1:A:1448:LEU:HD23	1.94	0.40
1:A:1725:GLN:NE2	1:A:1728:GLU:OE2	2.55	0.40
1:A:1945:TYR:CE2	1:A:1949:ILE:HD11	2.57	0.40
1:A:1951:VAL:O	1:A:1955:VAL:N	2.55	0.40
1:A:2417:SER:HB2	2:B:152:ASN:HD22	1.87	0.40
1:A:2563:LEU:HD11	1:A:2808:LEU:HD21	2.04	0.40
1:A:3259:LEU:HD11	1:A:3279:SER:HB2	2.04	0.40
1:A:3762:GLN:HA	1:A:3793:VAL:HB	2.04	0.40
3:C:155:LYS:HE2	3:C:155:LYS:HA	2.02	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	3555/4128 (86%)	3157 (89%)	395 (11%)	3 (0%)	48	76
2	B	486/609 (80%)	418 (86%)	67 (14%)	1 (0%)	43	71
3	C	653/732 (89%)	585 (90%)	68 (10%)	0	100	100
All	All	4694/5469 (86%)	4160 (89%)	530 (11%)	4 (0%)	49	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2548	PRO
1	A	1021	VAL
2	B	144	SER
1	A	1020	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3121/3671 (85%)	3116 (100%)	5 (0%)	87	87
2	B	439/548 (80%)	437 (100%)	2 (0%)	81	82
3	C	585/649 (90%)	584 (100%)	1 (0%)	87	87
All	All	4145/4868 (85%)	4137 (100%)	8 (0%)	85	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	LEU
1	A	976	VAL
1	A	1771	GLN
1	A	2285	LEU
1	A	4090	ARG
2	B	296	VAL
2	B	297	LYS
3	C	670	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	322	GLN
1	A	390	GLN
1	A	656	GLN
1	A	720	GLN
1	A	771	ASN
1	A	823	GLN
1	A	827	ASN
1	A	1043	GLN
1	A	1083	ASN
1	A	1175	HIS
1	A	1477	HIS
1	A	1738	ASN
1	A	1830	HIS
1	A	2177	ASN
1	A	2266	ASN
1	A	2306	ASN
1	A	2365	ASN
1	A	2414	GLN
1	A	2432	GLN
1	A	2518	GLN
1	A	2807	GLN
1	A	2859	GLN
1	A	2864	GLN
1	A	3510	GLN
1	A	3524	ASN
1	A	3551	ASN
1	A	3569	GLN
1	A	3660	ASN
1	A	3743	HIS
1	A	3777	GLN
1	A	3903	HIS
1	A	3969	ASN
1	A	4103	GLN
2	B	101	ASN
2	B	106	GLN
2	B	128	GLN
2	B	174	ASN
2	B	480	ASN
3	C	43	GLN
3	C	350	GLN

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Mol	Chain	Res	Type
3	C	360	GLN
3	C	382	HIS
3	C	452	ASN
3	C	488	GLN
3	C	511	HIS
3	C	656	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	1IX	A	4201	-	38,38,38	2.25	10 (26%)	53,54,54	2.12	20 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1IX	A	4201	-	-	0/18/26/26	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4201	1IX	C14-C16	6.32	1.56	1.49
6	A	4201	1IX	C12-C13	5.72	1.47	1.37
6	A	4201	1IX	C11-CL1	4.27	1.83	1.73
6	A	4201	1IX	C21-C20	-3.67	1.36	1.42
6	A	4201	1IX	C24-N26	3.33	1.48	1.38
6	A	4201	1IX	C25-C20	3.18	1.46	1.41
6	A	4201	1IX	C15-C14	2.45	1.43	1.39
6	A	4201	1IX	C10-C09	2.43	1.56	1.52
6	A	4201	1IX	C20-N19	-2.36	1.33	1.37
6	A	4201	1IX	C15-C10	2.22	1.43	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4201	1IX	C18-N19-C20	5.43	121.60	115.43
6	A	4201	1IX	C21-C16-N17	-5.33	119.52	123.04
6	A	4201	1IX	N19-C18-N17	-4.84	122.10	128.67
6	A	4201	1IX	C21-C20-N19	-4.22	118.34	122.82
6	A	4201	1IX	C10-C09-C06	-3.85	107.55	111.20
6	A	4201	1IX	C15-C10-C11	3.32	120.30	117.14
6	A	4201	1IX	C03-N04-N05	3.29	122.76	118.42
6	A	4201	1IX	C16-C21-C20	3.01	118.47	115.90
6	A	4201	1IX	C12-C11-C10	-2.96	119.27	122.46
6	A	4201	1IX	C25-C20-N19	2.83	121.26	118.01
6	A	4201	1IX	C15-C14-C13	2.54	118.99	115.98
6	A	4201	1IX	C27-N26-C24	2.37	124.58	118.11
6	A	4201	1IX	C11-C12-C13	2.33	120.18	118.42
6	A	4201	1IX	C01-O02-C03	-2.33	113.87	117.33
6	A	4201	1IX	C30-C31-N26	2.29	114.26	109.93
6	A	4201	1IX	C23-C24-N26	-2.25	118.27	121.39
6	A	4201	1IX	C14-C16-N17	2.16	119.01	115.17
6	A	4201	1IX	C12-C13-C14	-2.09	120.24	123.59
6	A	4201	1IX	C07-C06-N05	-2.03	120.52	122.36
6	A	4201	1IX	C28-C27-N26	2.01	113.74	109.93

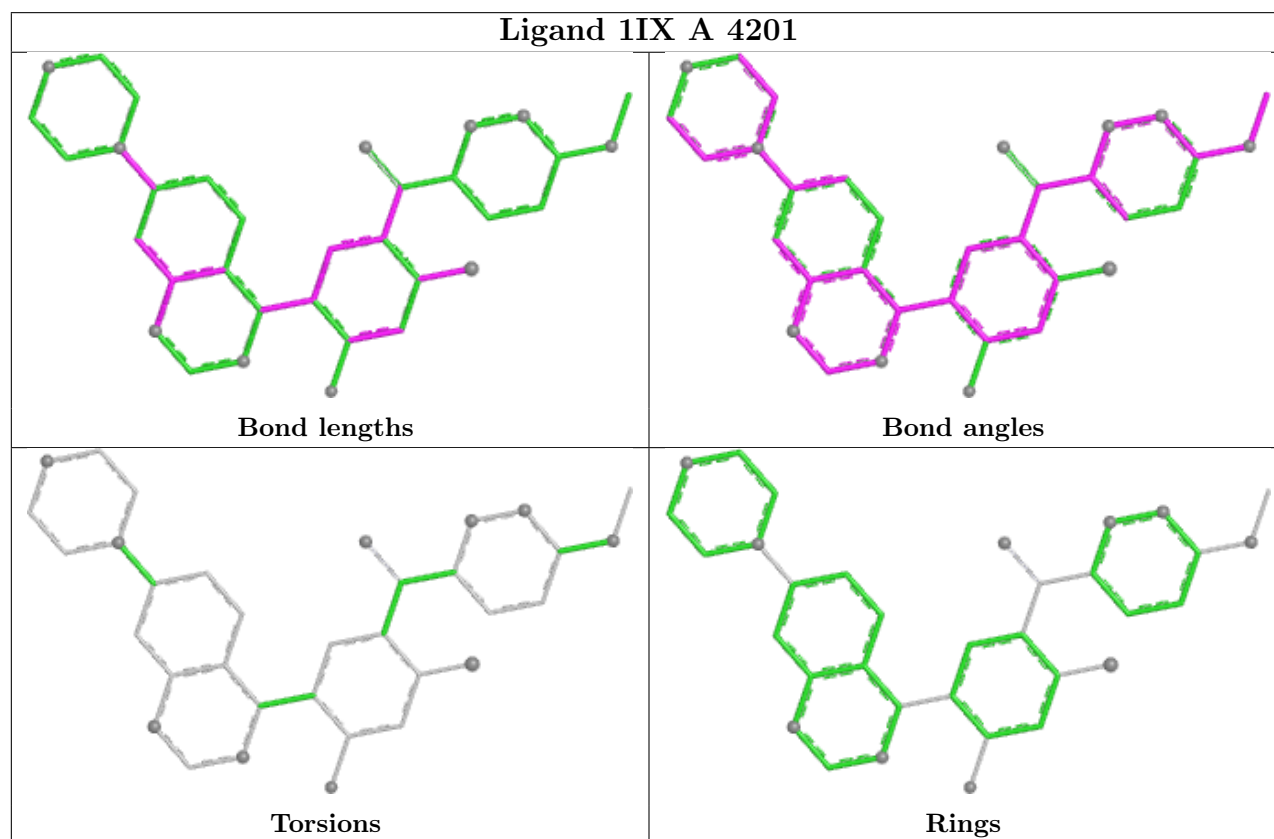
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

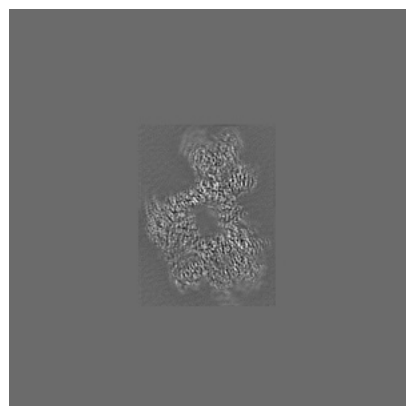
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14546. 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

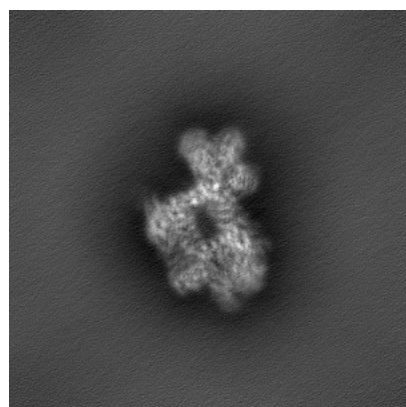


Y

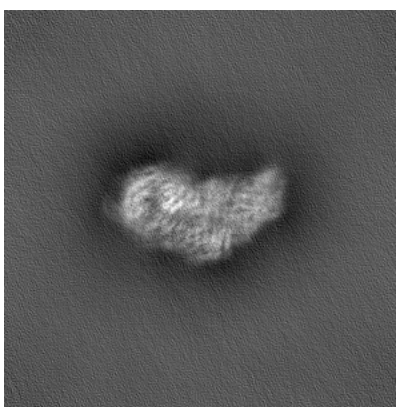


Z

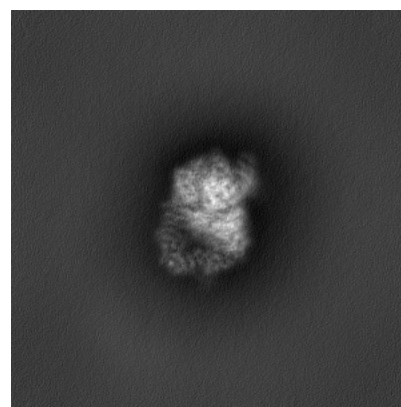
6.1.2 Raw map



X



Y

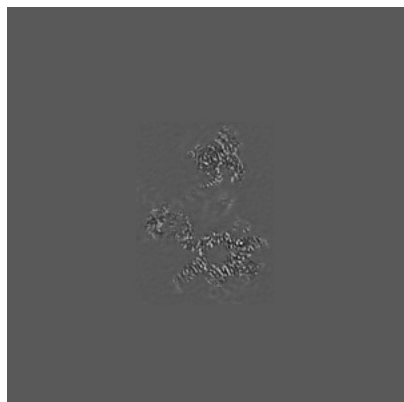


Z

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

6.2 Central slices [i](#)

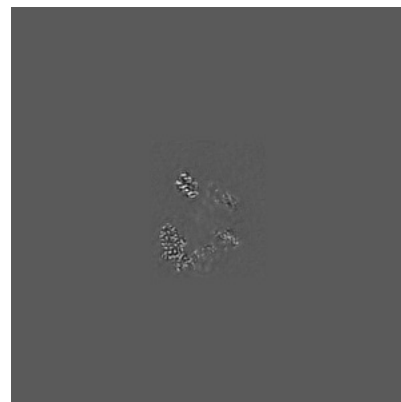
6.2.1 Primary map



X Index: 175

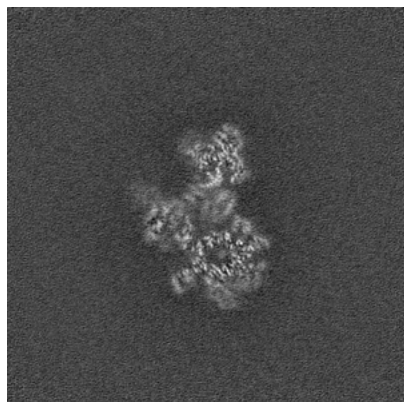


Y Index: 175

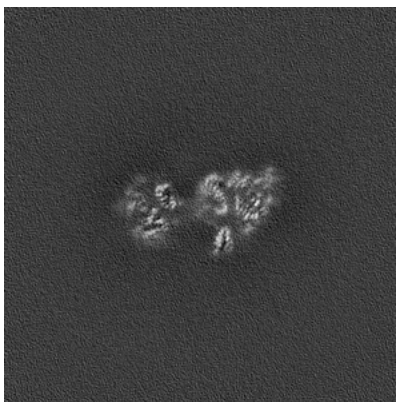


Z Index: 175

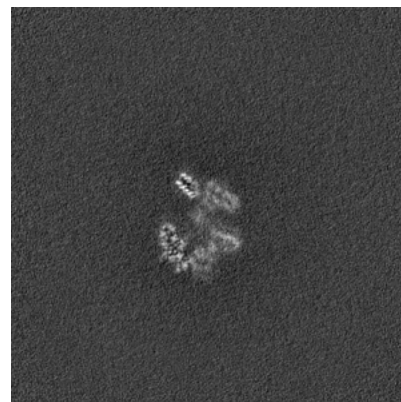
6.2.2 Raw map



X Index: 175



Y Index: 175

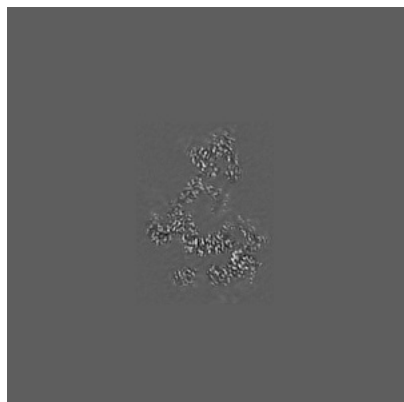


Z Index: 175

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

6.3 Largest variance slices [i](#)

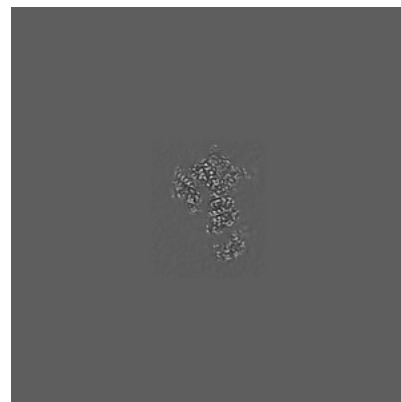
6.3.1 Primary map



X Index: 182

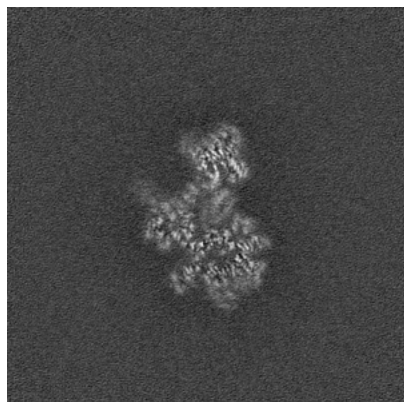


Y Index: 194

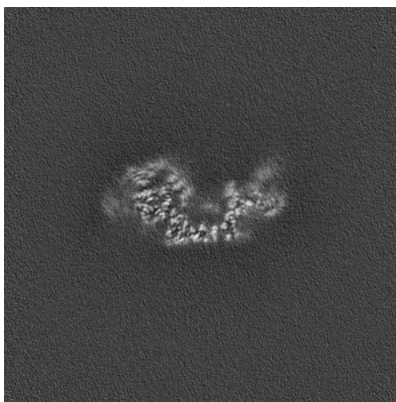


Z Index: 143

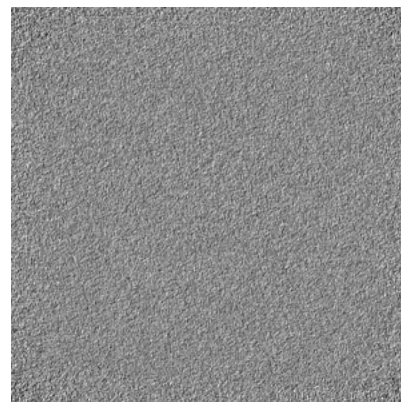
6.3.2 Raw map



X Index: 177



Y Index: 197

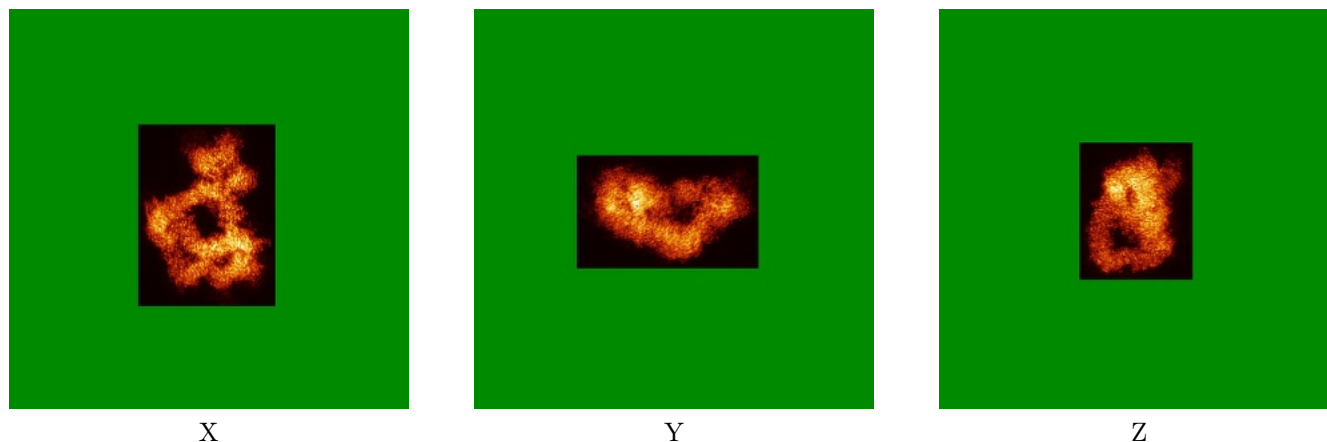


Z Index: 0

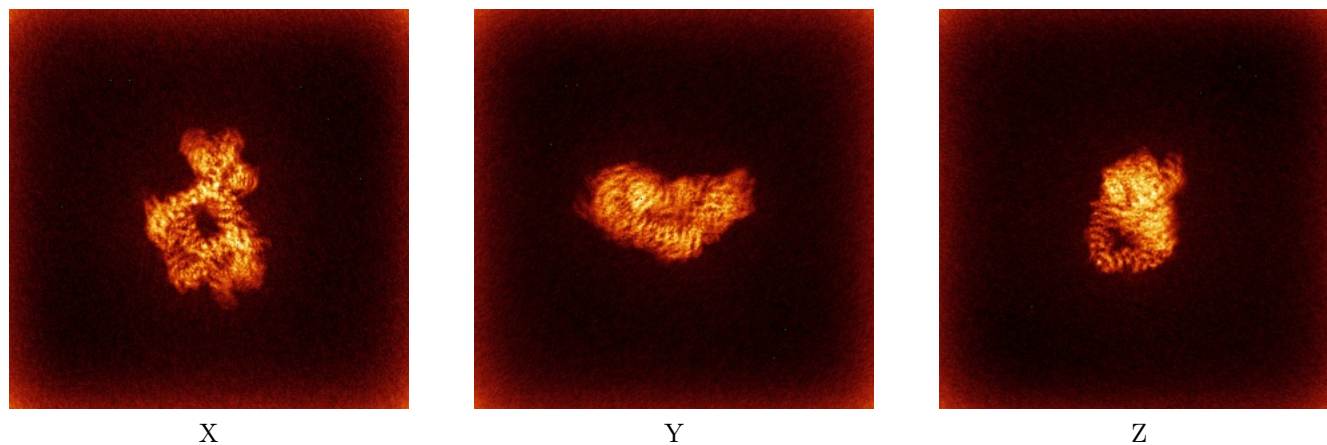
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

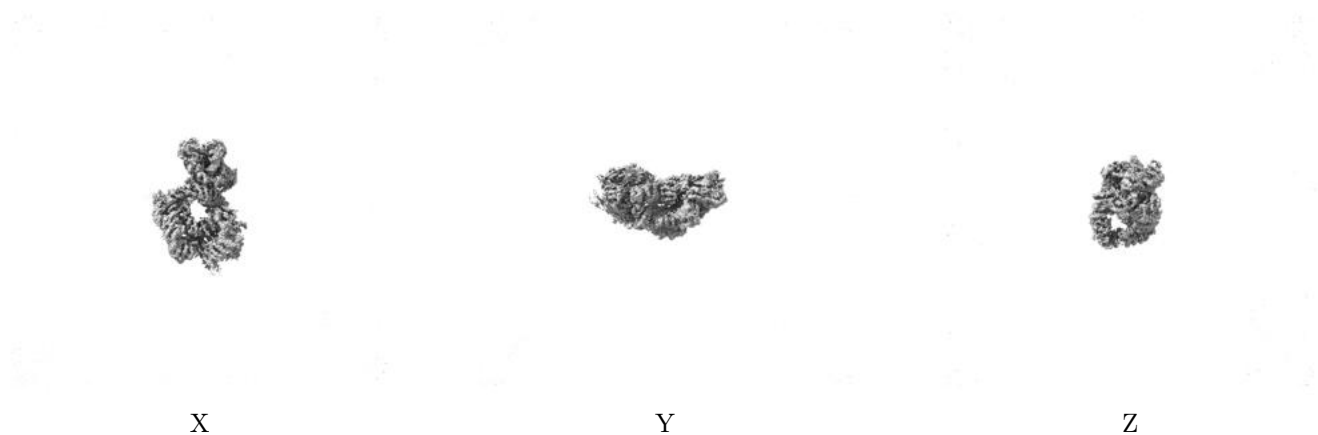
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

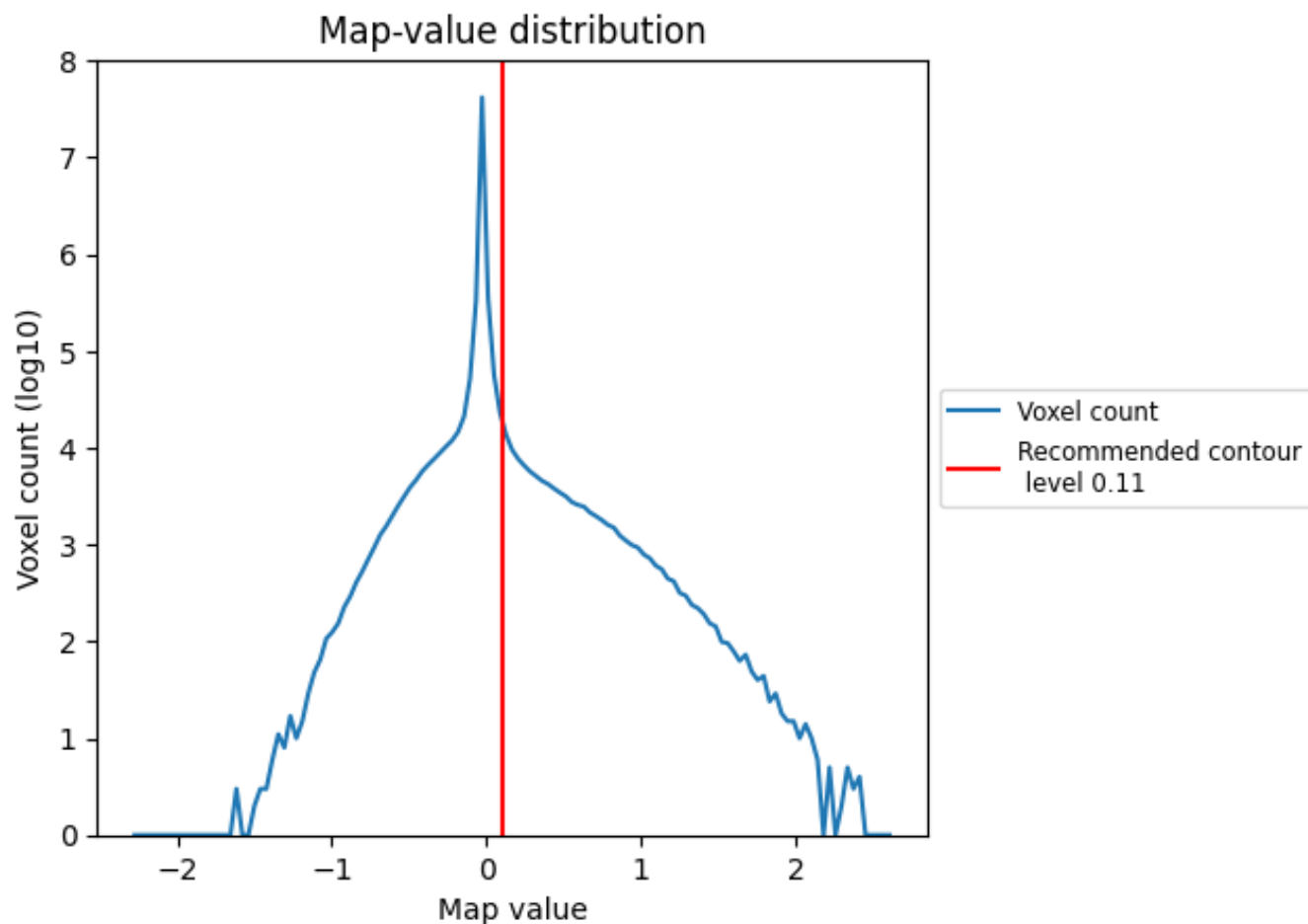
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

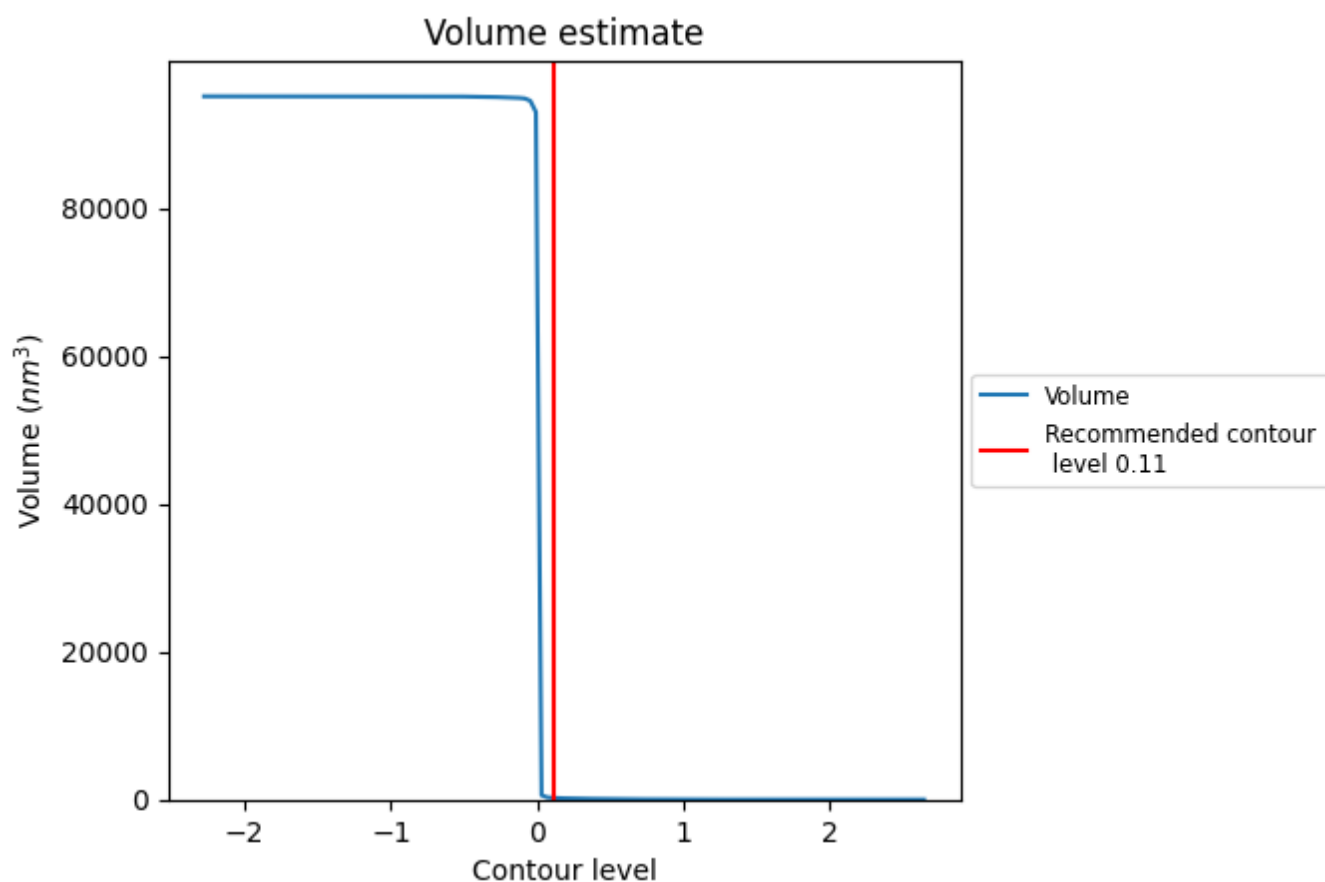
This section contains the results of statistical analysis of the map.

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.

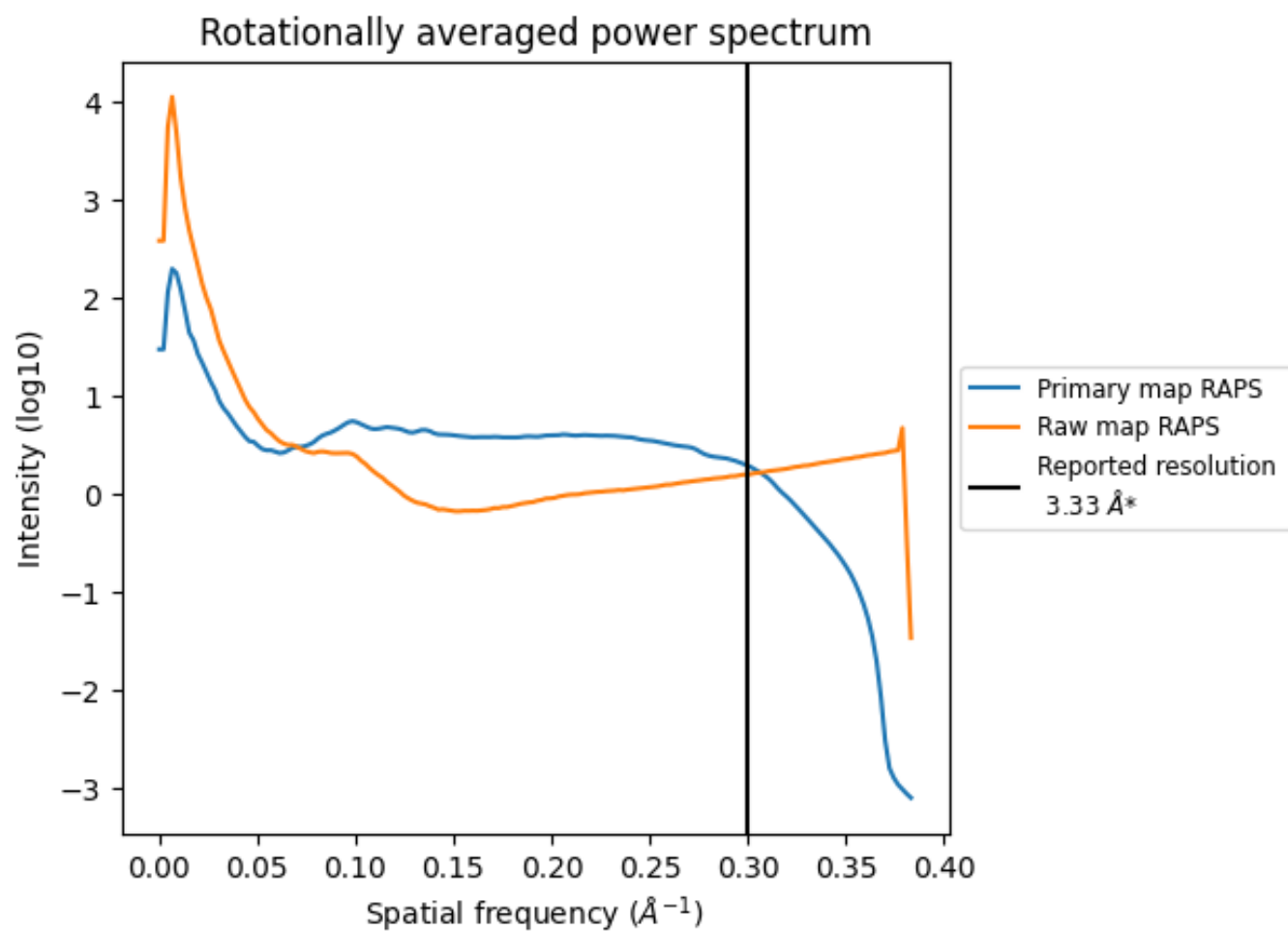
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm³; this corresponds to an approximate mass of 207 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 ⓘ

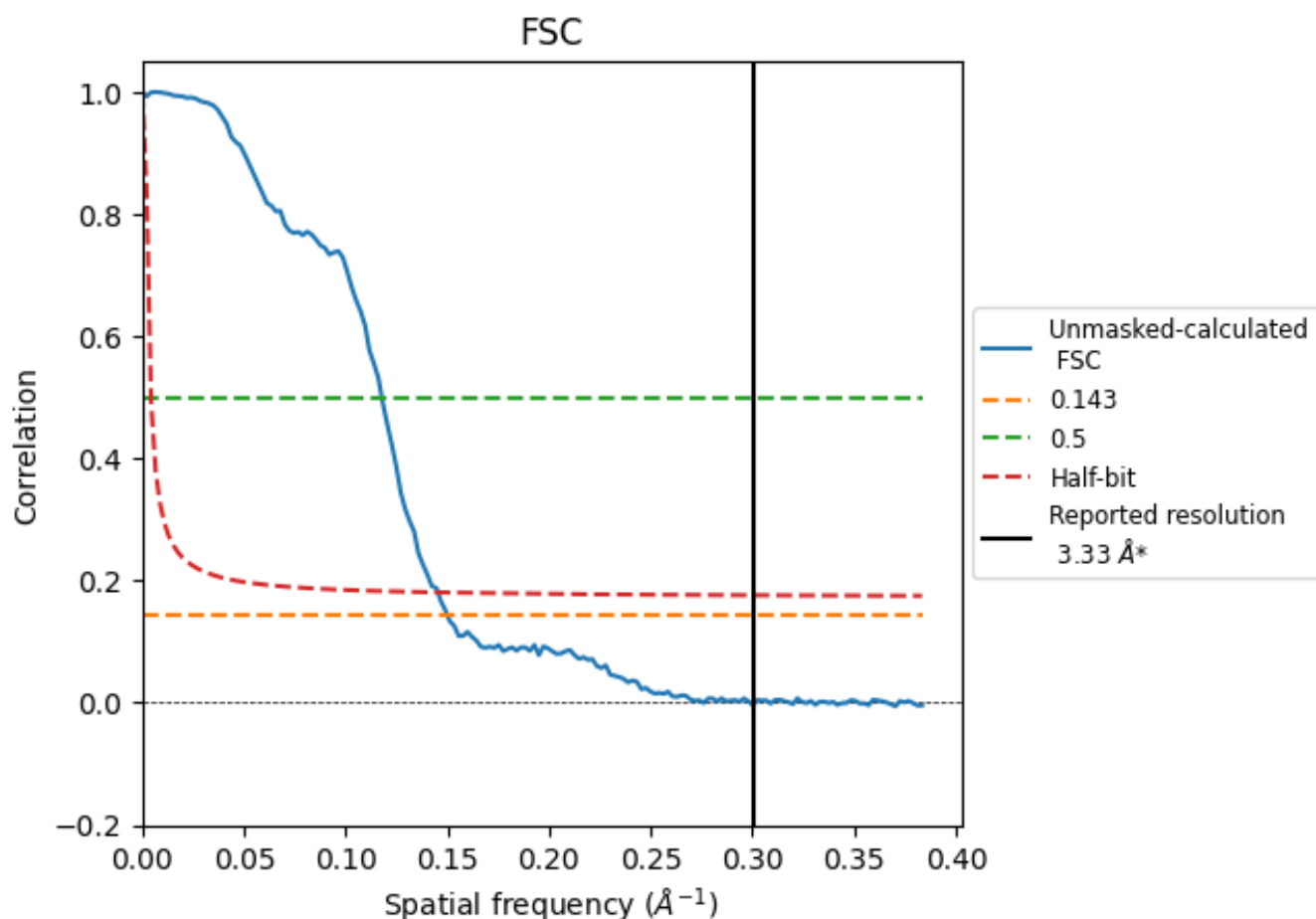


*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.300 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

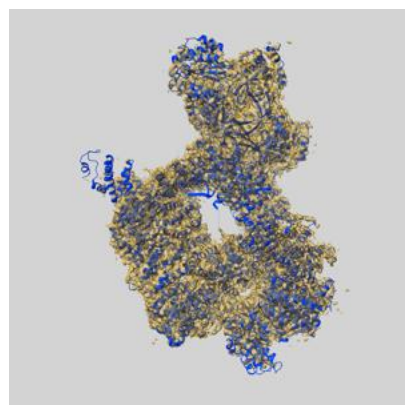
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.67	8.49	6.88

*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 6.67 differs from the reported value 3.33 by more than 10 %

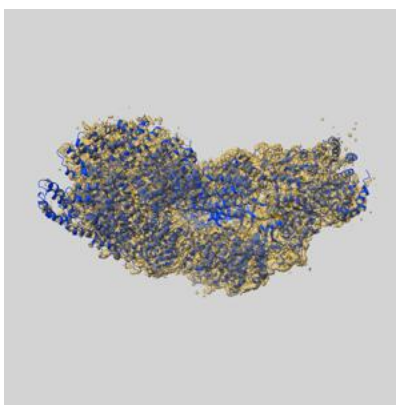
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14546 and PDB model 7Z88. Per-residue inclusion information can be found in section 3 on page 6.

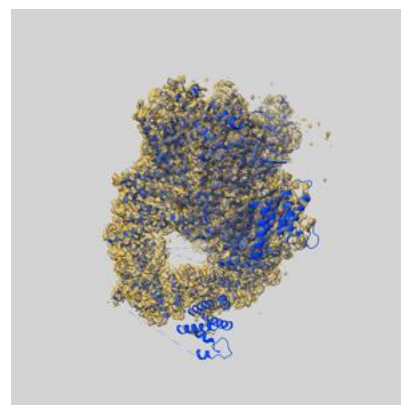
9.1 Map-model overlay [i](#)



X



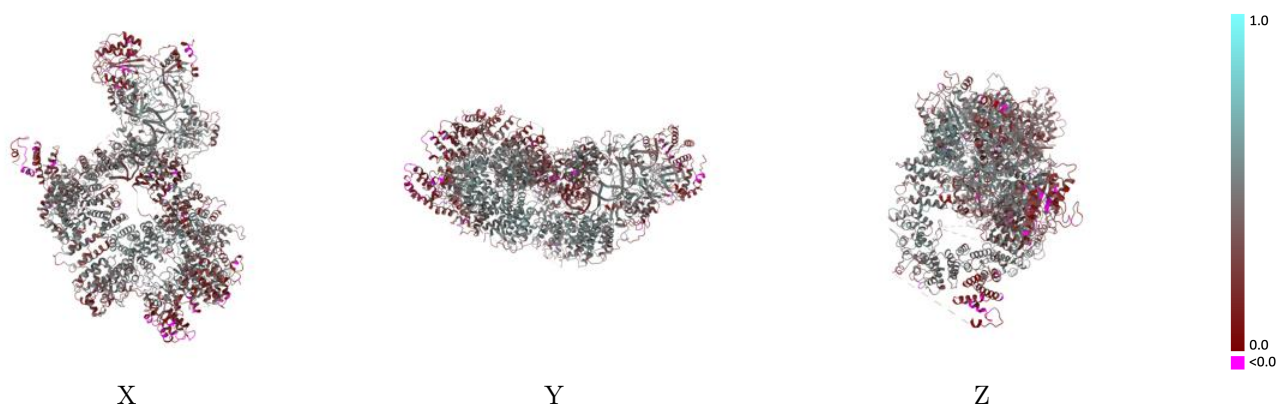
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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](#)

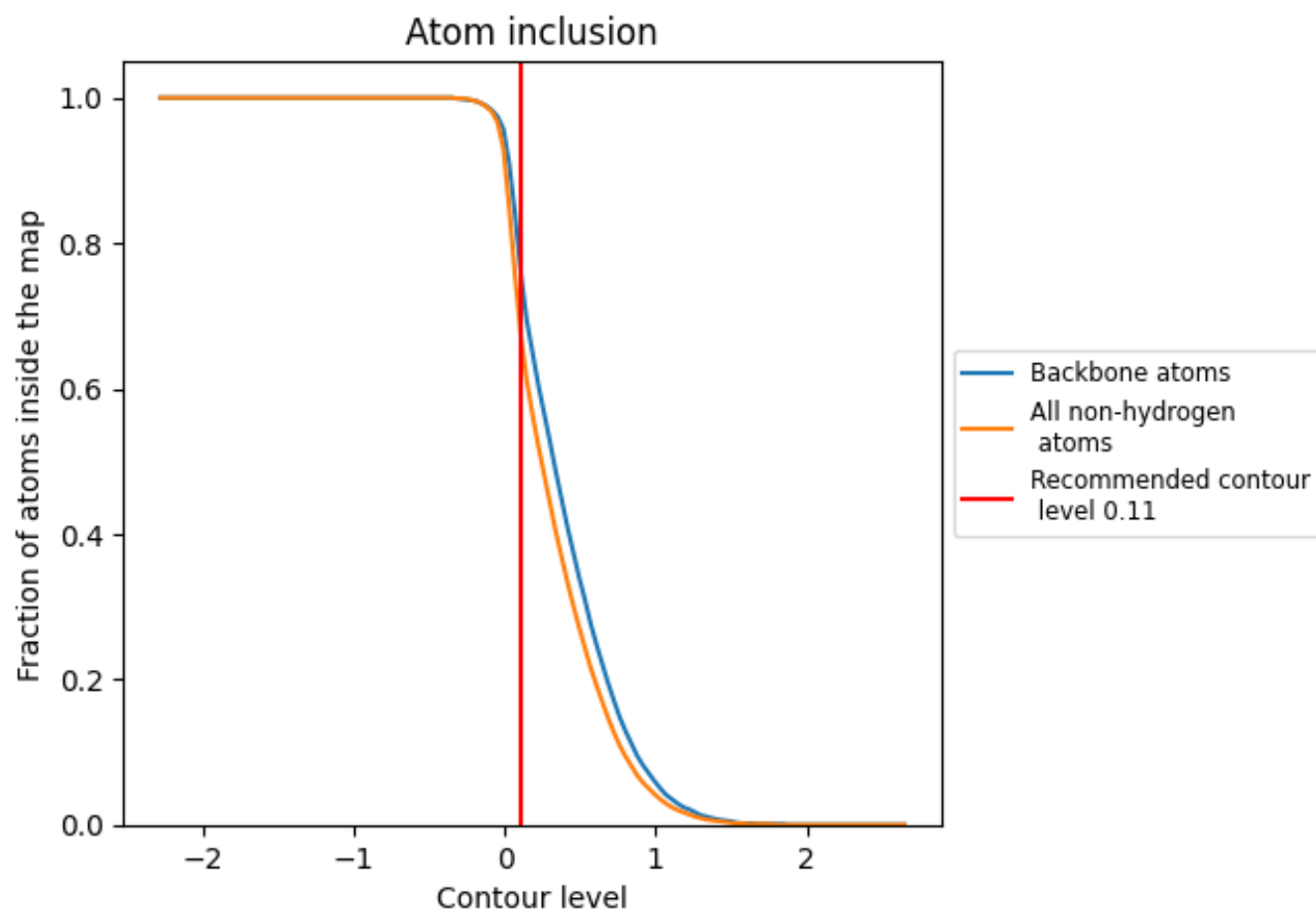


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6700	0.3890
A	0.7000	0.4010
B	0.7340	0.4110
C	0.4540	0.3040
D	0.7450	0.4420
E	0.6940	0.3990

