



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:05 AM UTC

PDB ID : 6WOU / pdb_00006wou
EMDB ID : EMD-21861
Title : Cryo-EM structure of recombinant mouse Ryanodine Receptor type 2 mutant R176Q in complex with FKBP12.6 in nanodisc
Authors : Iyer, K.A.; Hu, Y.; Kurebayashi, N.; Murayama, T.; Samso, M.
Deposited on : 2020-04-25
Resolution : 3.27 Å(reported)
Based on initial model : 5L1D

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

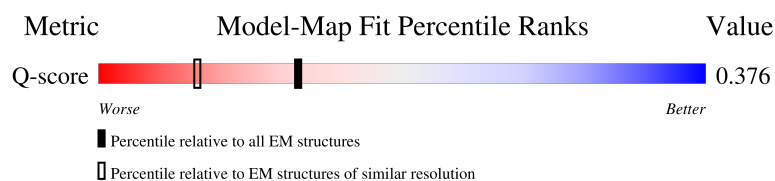
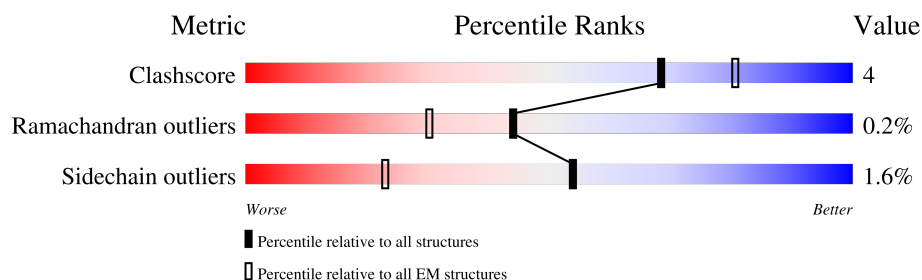
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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	14508 (2.77 - 3.77)

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	4966	
1	B	4966	
1	C	4966	
1	D	4966	

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Mol	Chain	Length	Quality of chain
2	E	107	95%
2	F	107	95%
2	G	107	95%
2	H	107	95%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 245683 atoms, of which 120439 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	3921	Total	C	H	N	O	S	0	0
			59779	19348	29287	5250	5702	192		
1	B	3921	Total	C	H	N	O	S	0	0
			59778	19348	29286	5250	5702	192		
1	C	3921	Total	C	H	N	O	S	0	0
			59778	19348	29286	5250	5702	192		
1	D	3921	Total	C	H	N	O	S	0	0
			59776	19348	29284	5250	5702	192		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	GLN	ARG	engineered mutation	UNP E9Q401
B	176	GLN	ARG	engineered mutation	UNP E9Q401
C	176	GLN	ARG	engineered mutation	UNP E9Q401
D	176	GLN	ARG	engineered mutation	UNP E9Q401

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		
2	F	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		
2	G	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		
2	H	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		

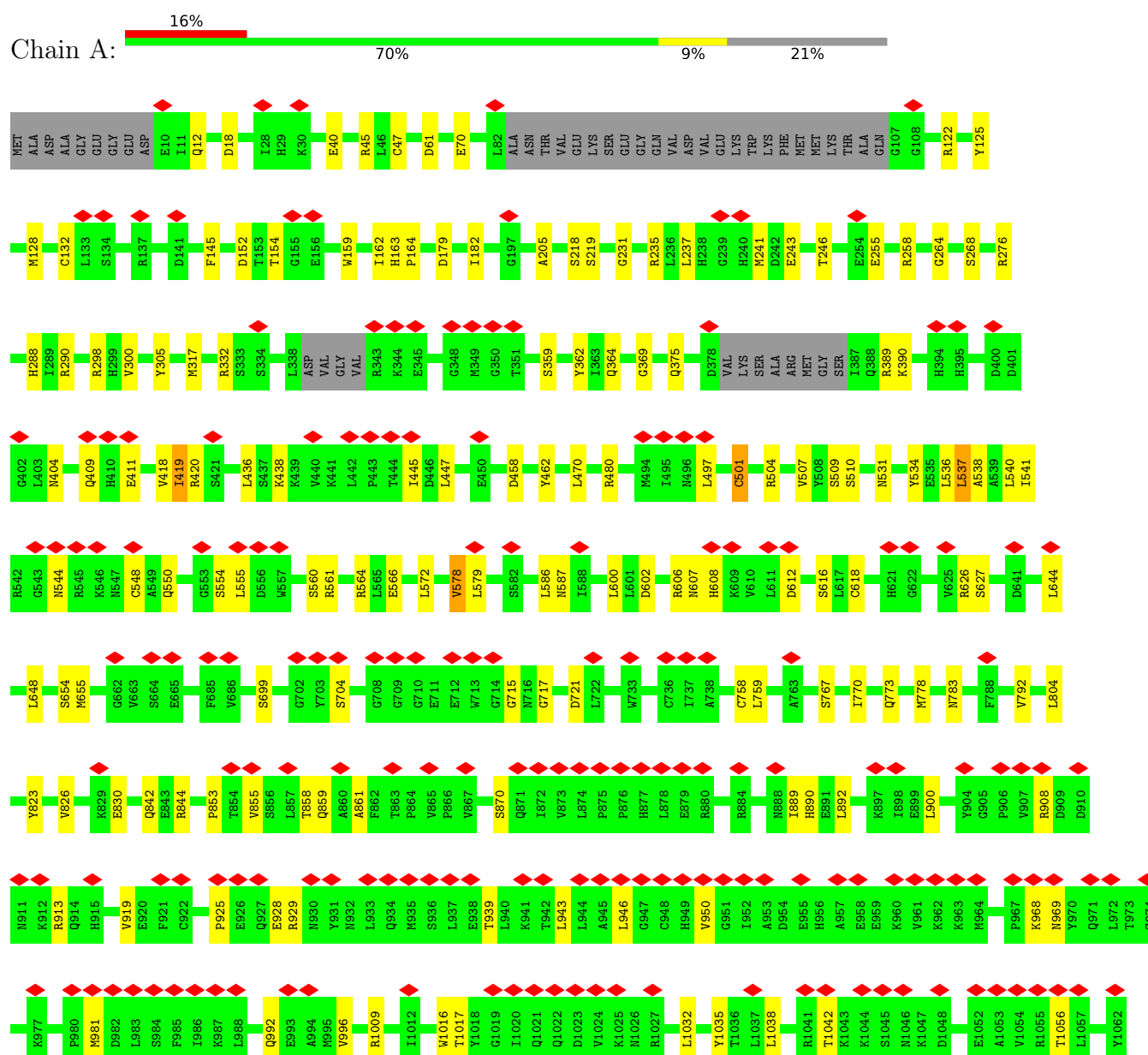
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

3 Residue-property plots

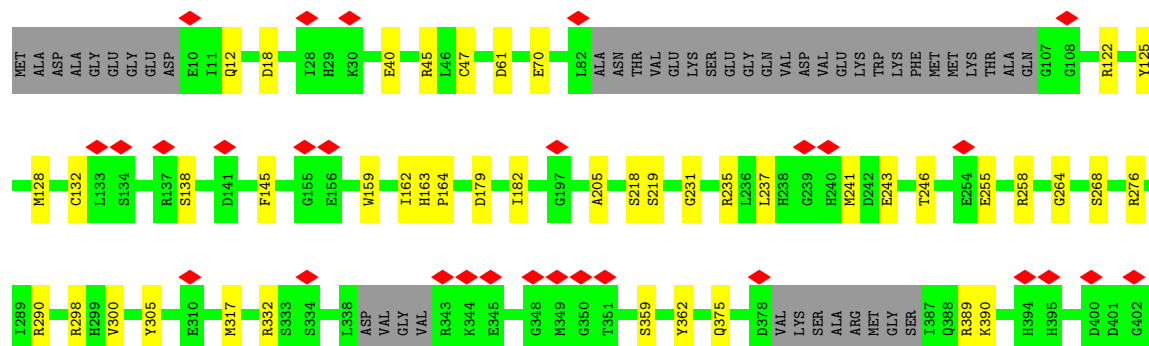
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 2





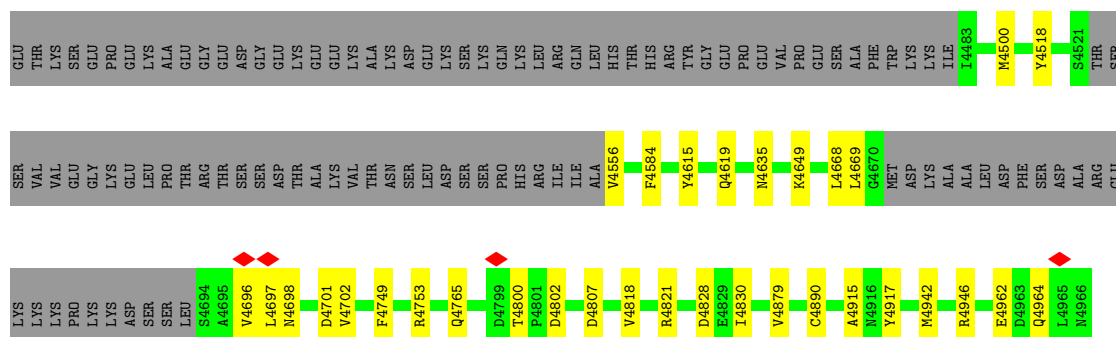
K3470	R3471	L3472	L3473	P3474	L3475	G3476	L3477	N3478	F3419	V3420	Q3421	N3422	E3423	I3424	N3425	N3426	N3427	S3428	F3429	L3430	I3431	T3432	D3433	T3434	K3435	S3436	L3437	N3438	D3439	L3490	A3491	K3492	N3493	R3494	F3495	S3496	L3497	K3498	D3499	T3500	E3501	E3502	E3503	V3504	R3505	D3506	I3507	I3508	ARG	SER	ASN	ILE	LEU	GLN	GLY	LYS	LEU	GLU	ASP	PRO	ALA	ILE	ARG	TRP	GLN	MET	ALA	LEU		
N3410	F3411	K3412	R3413	E3414	E3415	Q3416	N3417	F3418	V3419	V3420	Q3421	N3422	E3423	I3424	N3425	N3426	N3427	S3428	F3429	L3430	I3431	T3432	D3433	T3434	K3435	S3436	L3437	N3438	D3439	L3490	A3491	K3492	N3493	R3494	F3495	S3496	L3497	K3498	D3499	T3500	E3501	E3502	E3503	V3504	R3505	D3506	I3507	I3508	ARG	SER	ASN	ILE	LEU	GLN	GLY	LYS	LEU	GLU	ASP	PRO	ALA	ILE	ARG	TRP	GLN	MET	ALA	LEU		
E3349	A3350	E3351	L3352	L3353	L3354	L3355	D3356	T3359	T3360	L3361	A3362	R3363	D3364	L3365	Y3366	A3367	F3368	Y3369	P3370	L3371	L3372	L3373	R3374	F3375	V3376	D3377	Y3378	N3379	R3380	A3381	K3382	W3383	F3384	L3385	Y3386	P3387	N3388	P3389	GLU	ALA	GLU	GLU	LEU	LEU	ARG	ARG	MET	VAL	ALA	GLU	VAL	PHE	ILE	Y3404	W3405	S3406	K3407	S3408	H3409											
I3282	I3283	Y3284	N3285	N3286	L3287	G3288	I3289	D3290	E3291	G3292	ALA	TRP	MET	LYS	ARG	LEU	ALA	F3301	S3302	Q3303	P3304	I3305	I3306	N3307	K3308	V3309	K3310	P3311	Q3312	L3313	T3316	H3317	F3318	L3319	P3320	L3321	K3324	K3327	K3328	A3329	A3330	M3331	V3332	V3333	E3336	K3340	A3343	R3344	G3345	D3346	M3347	S3348																		
N3206	I3207	P3208	S3209	L3210	T3215	E3219	L3220	A3221	E3222	T3226	Q3229	M3230	P3231	Y3232	M3233	M3234	E3235	V3236	V3237	L3238	P3239	M3240	L3241	C3242	S3243	Y3244	T3245	S3246	R3247	W3248	Q3249	E3250	H3251	G3252	P3253	E3254	N3255	H3256	P3257	E3258	R3259	A3260	E3261	H3270	H3271	M3272	N3273	L3274	LEU	GLY	ASN	LEU	LEU	K3281																
A3064	E3065	E3068	K3069	T3070	M3071	E3072	Q3076	G3077	F3078	T3080	H3081	T3082	Q3085	P3086	I3092	V3098	A3099	H3015	H3016	ARG	ILE	SER	LEU	PHE	ALA	GLY	LEU	GLU	THR	HIS	L3174	D3175	K3176	H3177	N3178	V3179	T3182	R3186	S3187	S3188	R3191	A3192	K3198	D3202	V3203	C3204	P3205																							
GLN	TYR	PHE	ASN	ASN	HIS	ARG	LEU	TYR	PHE	L2982	S2983	R2987	P2988	L2989	A2995	S2996	T3004	G3011	R3015	H3016	ARG	ILE	SER	LEU	PHE	ALA	GLY	LEU	GLU	THR	SER	ILE	VAL	ASN	CYS	LEU	HIS	L3035	A3041	V3044	G3048	S3054	A3055	L3056	R3057	A3058	D3061																							
ASP	THR	PRO	SER	GLU	LYS	PHE	ALA	TYR	SER	L2982	S2983	R2987	P2988	L2989	A2995	S2996	T3004	G3011	R3015	H3016	ARG	ILE	SER	LEU	PHE	ALA	GLY	LEU	GLU	THR	SER	ILE	VAL	ASN	CYS	LEU	HIS	L3035	A3041	V3044	G3048	S3054	A3055	L3056	R3057	A3058	D3061																							
I2850	W2851	A2852	K2853	K2854	K2855	K2856	L2857	E2858	L2859	E2860	K2862	G2863	H2867	P2868	L2869	L2870	V2871	T2872	T2873	L2874	T2875	L2876	T2877	A2878	K2879	E2880	K2881	A2882	K2883	D2884	K2885	E2886	K2887	A2888	Q2889	D2890	L2891	F2892	K2893	F2894	VAL	VAL	LEU	PRO	LEU	LEU	ASP																							
ASP	THR	PRO	SER	GLU	LYS	PHE	ALA	TYR	SER	L2982	S2983	R2987	P2988	L2989	A2995	S2996	T3004	G3011	R3015	H3016	ARG	ILE	SER	LEU	PHE	ALA	GLY	LEU	GLU	THR	SER	ILE	VAL	ASN	CYS	LEU	HIS	L3035	A3041	V3044	G3048	S3054	A3055	L3056	R3057	A3058	D3061																							
K2730	W2731	S2732	M2733	D2734	K2735	L2736	A2737	N2738	G2739	W2740	I2741	Y2742	G2743	E2744	I2745	Y2746	S2747	D2748	S2749	V2750	K2751	I2752	Q2753	P2754	L2755	M2756	K2757	P2758	Y2759	K2760	L2761	L2762	S2763	A2816	A2817	H2818	G2819	Y2820	S2821	P2822	R2823	A2824	L2825	D2826	M2827	K2828	S2829	V2830	T2831	L2832	S2833	R2834	D2835	L2836	H2837	A2838	M2839	A2840	E2841	M2842	M2843	A2844	E2845	N2846	Y2847	H2848	W2796	L2787	L2788	E2789
I2647	L2651	K2654	Y2655	Y2656	E2657	Q2658	Y2659	L2660	F2661	P2666	P2677	D2678	Y2679	M2687	Q2691	S2692	S2693	W2694	ASP	SER	GLU	GLY	ASN	PHE	ASN	PRO	GLN	PRO	W2705	D2706	T2707	S2708	W2709	L2710	L2711	L2712	P2713	E2714	L2715	L2716	E2717	Y2718	L2719	L2720	W2721	L2722	Y2723	A2724	E2725	L2726	H2728	S2729																		



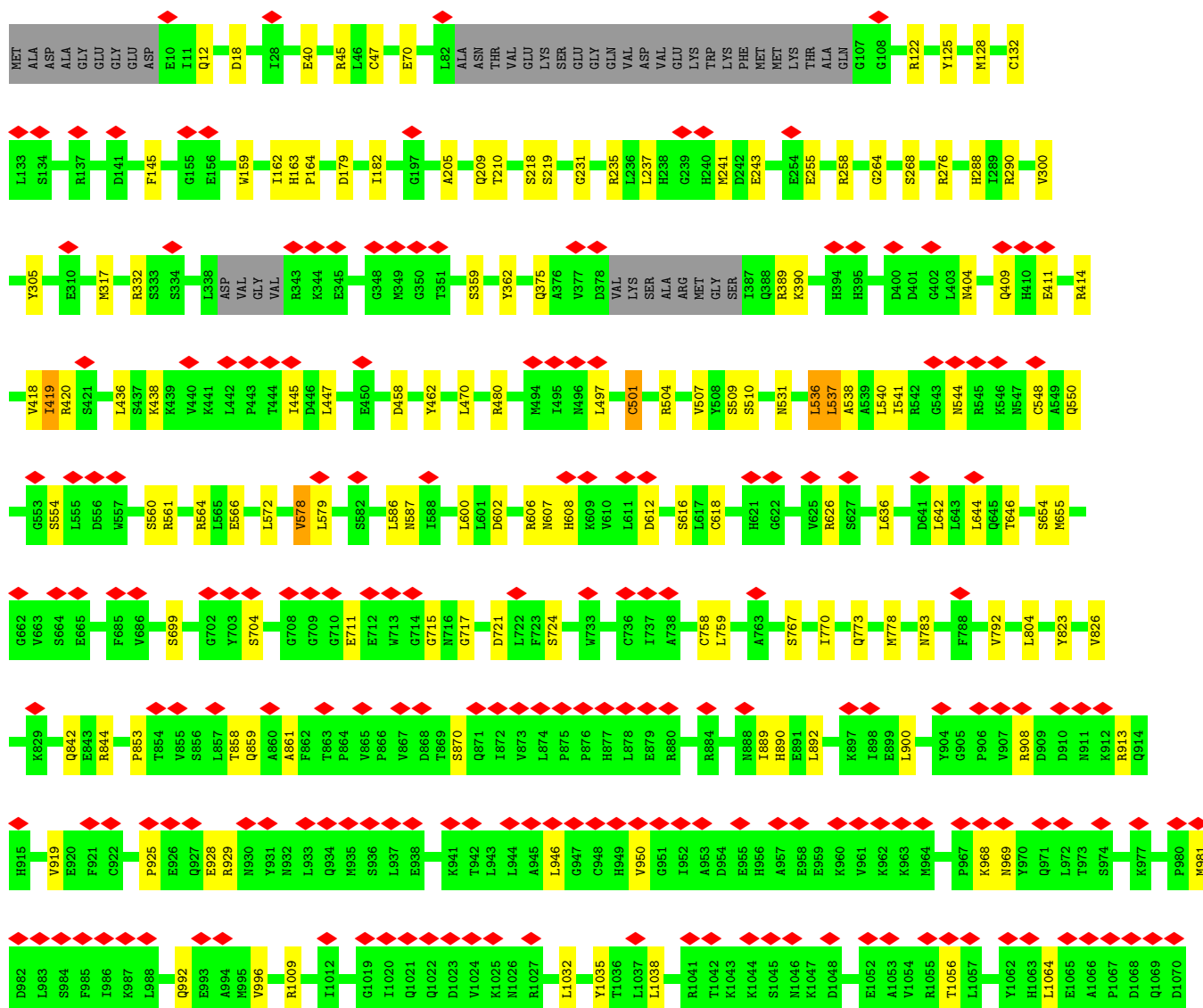






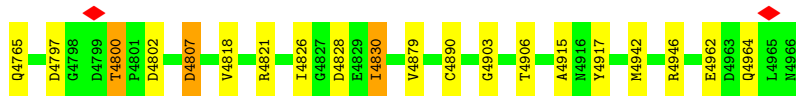


• Molecule 1: Ryanodine receptor 2

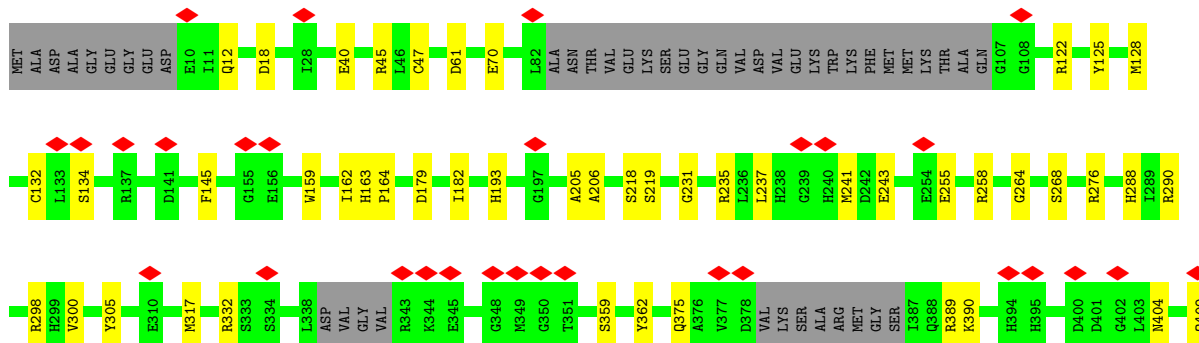


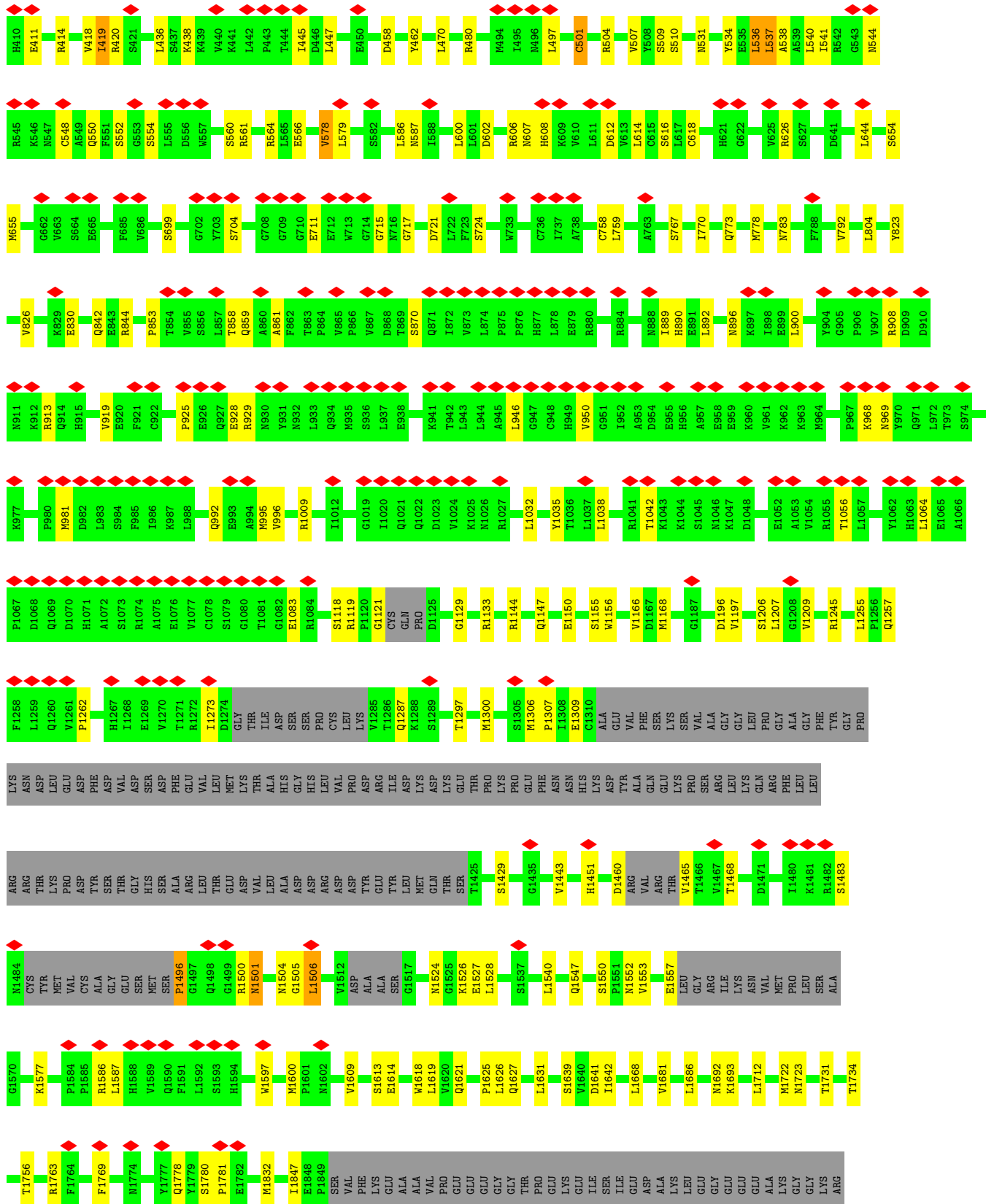






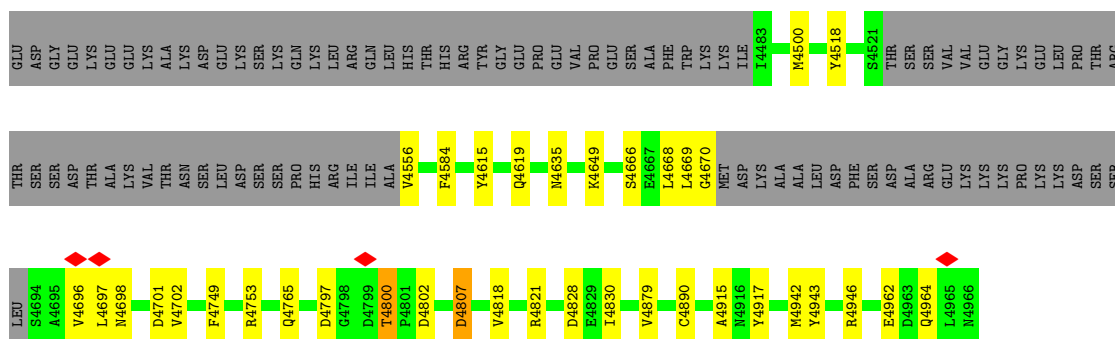
Chain D:





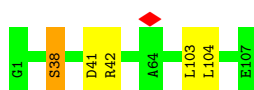






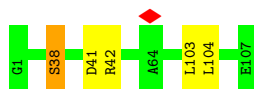
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 95%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 95%



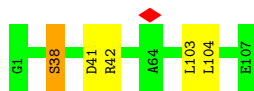
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 95%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 95%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	282778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50, 50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.715	Depositor
Minimum map value	-0.955	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.132	Depositor
Map size ($\text{\AA}$)	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/31107	0.54	5/42056 (0.0%)
1	B	0.32	0/31107	0.54	2/42056 (0.0%)
1	C	0.32	0/31107	0.54	1/42056 (0.0%)
1	D	0.32	0/31107	0.54	5/42056 (0.0%)
2	E	0.21	0/834	0.46	0/1123
2	F	0.21	0/834	0.46	0/1123
2	G	0.21	0/834	0.46	0/1123
2	H	0.21	0/834	0.46	0/1123
All	All	0.32	0/127764	0.54	13/172716 (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	9
1	B	0	9
1	C	0	9
1	D	0	7
All	All	0	34

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1500	ARG	N-CA-C	12.40	126.99	108.14
1	A	1500	ARG	N-CA-C	7.22	126.17	110.80
1	C	1496	PRO	N-CA-CB	6.99	110.69	103.00
1	D	1496	PRO	N-CA-CB	6.98	110.68	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1496	PRO	N-CA-CB	6.94	110.63	103.00
1	A	1496	PRO	N-CA-CB	6.79	110.47	103.00
1	B	1499	GLY	N-CA-C	5.56	117.50	110.38
1	D	1500	ARG	CA-C-N	5.44	131.92	121.54
1	D	1500	ARG	C-N-CA	5.44	131.92	121.54
1	D	2658	GLN	N-CA-C	5.35	122.19	110.80
1	A	2679	TYR	CA-CB-CG	5.19	123.24	113.90
1	A	2678	ASP	CA-C-N	5.15	131.38	121.54
1	A	2678	ASP	C-N-CA	5.15	131.38	121.54

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1552	ASN	Peptide
1	A	159	TRP	Peptide
1	A	1769	PHE	Peptide
1	A	1780	SER	Peptide
1	A	2038	LEU	Peptide
1	A	2131	VAL	Peptide
1	A	2525	PRO	Peptide
1	A	2655	LYS	Peptide
1	A	618	CYS	Peptide
1	B	1552	ASN	Peptide
1	B	159	TRP	Peptide
1	B	1769	PHE	Peptide
1	B	1780	SER	Peptide
1	B	2130	SER	Peptide
1	B	2525	PRO	Peptide
1	B	2655	LYS	Peptide
1	B	2677	PRO	Peptide
1	B	618	CYS	Peptide
1	C	1552	ASN	Peptide
1	C	159	TRP	Peptide
1	C	1769	PHE	Peptide
1	C	1780	SER	Peptide
1	C	2038	LEU	Peptide
1	C	2133	MET	Peptide
1	C	2525	PRO	Peptide
1	C	2657	GLU	Peptide
1	C	618	CYS	Peptide
1	D	1552	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	D	159	TRP	Peptide
1	D	1769	PHE	Peptide
1	D	1780	SER	Peptide
1	D	2038	LEU	Peptide
1	D	2525	PRO	Peptide
1	D	618	CYS	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	30492	29287	29275	220	0
1	B	30492	29286	29275	225	0
1	C	30492	29286	29275	223	0
1	D	30492	29284	29275	232	0
2	E	818	824	824	3	0
2	F	818	824	824	3	0
2	G	818	824	824	3	0
2	H	818	824	824	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	125244	120439	120396	908	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 4.

All (908) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:ASP:O	1:D:616:SER:OG	2.07	0.72
1:C:612:ASP:O	1:C:616:SER:OG	2.07	0.70
1:B:612:ASP:O	1:B:616:SER:OG	2.07	0.70
1:A:612:ASP:O	1:A:616:SER:OG	2.07	0.69
1:C:2278:MET:SD	1:C:2284:TYR:OH	2.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2278:MET:SD	1:A:2284:TYR:OH	2.51	0.69
1:D:2278:MET:SD	1:D:2284:TYR:OH	2.51	0.69
1:B:2278:MET:SD	1:B:2284:TYR:OH	2.51	0.69
1:D:1586:ARG:NH2	1:D:1587:LEU:O	2.27	0.68
1:A:235:ARG:NE	1:A:268:SER:O	2.27	0.68
1:A:900:LEU:O	1:A:913:ARG:NH2	2.26	0.68
1:B:1586:ARG:NH2	1:B:1587:LEU:O	2.27	0.68
1:D:900:LEU:O	1:D:913:ARG:NH2	2.26	0.68
1:A:1586:ARG:NH2	1:A:1587:LEU:O	2.27	0.68
1:B:235:ARG:NE	1:B:268:SER:O	2.27	0.68
1:C:235:ARG:NE	1:C:268:SER:O	2.27	0.68
1:C:699:SER:OG	1:C:721:ASP:OD2	2.12	0.68
1:B:900:LEU:O	1:B:913:ARG:NH2	2.26	0.67
1:C:1586:ARG:NH2	1:C:1587:LEU:O	2.27	0.67
1:C:900:LEU:O	1:C:913:ARG:NH2	2.26	0.67
1:B:1756:THR:OG1	1:B:1922:GLU:OE2	2.12	0.67
1:C:1756:THR:OG1	1:C:1922:GLU:OE2	2.13	0.67
1:D:1990:GLU:OE1	1:D:1992:ARG:NH1	2.28	0.67
1:A:1245:ARG:NH1	1:A:1693:LYS:O	2.28	0.67
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.28	0.67
1:B:699:SER:OG	1:B:721:ASP:OD2	2.13	0.67
1:D:4106:GLU:OE2	1:D:4146:ARG:NH1	2.28	0.67
1:B:1245:ARG:NH1	1:B:1693:LYS:O	2.28	0.67
1:D:235:ARG:NE	1:D:268:SER:O	2.27	0.67
1:D:699:SER:OG	1:D:721:ASP:OD2	2.13	0.67
1:B:1990:GLU:OE1	1:B:1992:ARG:NH1	2.28	0.67
1:B:3078:GLN:O	1:B:3082:THR:OG1	2.13	0.67
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.28	0.67
1:A:1756:THR:OG1	1:A:1922:GLU:OE2	2.13	0.66
1:C:1990:GLU:OE1	1:C:1992:ARG:NH1	2.28	0.66
1:C:4106:GLU:OE2	1:C:4146:ARG:NH1	2.28	0.66
1:D:3891:TYR:OH	1:D:3898:ASP:OD1	2.13	0.66
1:B:4106:GLU:OE2	1:B:4146:ARG:NH1	2.28	0.66
1:D:870:SER:OG	1:D:1009:ARG:NH1	2.28	0.66
1:D:1245:ARG:NH1	1:D:1693:LYS:O	2.28	0.66
1:D:1756:THR:OG1	1:D:1922:GLU:OE2	2.13	0.66
1:A:4106:GLU:OE2	1:A:4146:ARG:NH1	2.28	0.66
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.13	0.66
1:C:721:ASP:O	1:C:724:SER:OG	2.12	0.66
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.28	0.66
1:C:778:MET:O	1:C:1468:THR:OG1	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:SER:OG	1:C:1009:ARG:NH1	2.28	0.66
1:C:1245:ARG:NH1	1:C:1693:LYS:O	2.28	0.66
1:A:699:SER:OG	1:A:721:ASP:OD2	2.13	0.66
1:A:778:MET:O	1:A:1468:THR:OG1	2.14	0.66
1:B:300:VAL:HG21	1:B:419:ILE:HD12	1.77	0.66
1:B:870:SER:OG	1:B:1009:ARG:NH1	2.28	0.66
1:B:1119:ARG:NH2	1:B:1196:ASP:O	2.28	0.66
1:B:969:ASN:ND2	1:B:981:MET:SD	2.69	0.66
1:A:1990:GLU:OE1	1:A:1992:ARG:NH1	2.28	0.66
1:A:3078:GLN:O	1:A:3082:THR:OG1	2.13	0.66
1:C:3891:TYR:OH	1:C:3898:ASP:OD1	2.13	0.66
1:A:560:SER:OG	1:A:561:ARG:NH2	2.29	0.66
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.29	0.66
1:B:497:LEU:O	1:B:501:CYS:N	2.29	0.66
1:D:969:ASN:ND2	1:D:981:MET:SD	2.69	0.66
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.29	0.66
1:B:778:MET:O	1:B:1468:THR:OG1	2.14	0.65
1:C:497:LEU:O	1:C:501:CYS:N	2.29	0.65
1:C:560:SER:OG	1:C:561:ARG:NH2	2.29	0.65
1:A:870:SER:OG	1:A:1009:ARG:NH1	2.28	0.65
1:A:1309:GLU:OE1	1:A:1577:LYS:N	2.30	0.65
1:C:969:ASN:ND2	1:C:981:MET:SD	2.69	0.65
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.29	0.65
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.29	0.65
1:C:1443:VAL:O	1:C:1496:PRO:N	2.29	0.65
1:A:969:ASN:ND2	1:A:981:MET:SD	2.69	0.65
1:C:1309:GLU:OE1	1:C:1577:LYS:N	2.30	0.65
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.30	0.65
1:A:627:SER:OG	1:A:2134:GLY:N	2.30	0.65
1:C:300:VAL:HG21	1:C:419:ILE:HD12	1.77	0.65
1:A:300:VAL:HG21	1:A:419:ILE:HD12	1.77	0.65
1:A:3891:TYR:OH	1:A:3898:ASP:OD1	2.14	0.65
1:B:560:SER:OG	1:B:561:ARG:NH2	2.29	0.65
1:B:721:ASP:O	1:B:724:SER:OG	2.12	0.65
1:D:300:VAL:HG21	1:D:419:ILE:HD12	1.77	0.65
1:D:3078:GLN:O	1:D:3082:THR:OG1	2.13	0.65
1:B:1309:GLU:OE1	1:B:1577:LYS:N	2.30	0.65
1:B:1443:VAL:O	1:B:1496:PRO:N	2.31	0.65
1:C:2018:GLY:O	1:C:2025:ARG:NH2	2.30	0.65
1:D:1309:GLU:OE1	1:D:1577:LYS:N	2.30	0.65
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:778:MET:O	1:D:1468:THR:OG1	2.14	0.64
1:D:4635:ASN:ND2	1:D:4668:LEU:O	2.30	0.64
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.30	0.64
1:D:497:LEU:O	1:D:501:CYS:N	2.30	0.64
1:A:4749:PHE:O	1:A:4753:ARG:NH1	2.30	0.64
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.31	0.64
1:C:4635:ASN:ND2	1:C:4668:LEU:O	2.30	0.64
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.30	0.64
1:D:4749:PHE:O	1:D:4753:ARG:NH1	2.30	0.64
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.30	0.64
1:C:4749:PHE:O	1:C:4753:ARG:NH1	2.30	0.64
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.30	0.64
1:B:4749:PHE:O	1:B:4753:ARG:NH1	2.30	0.64
1:A:2018:GLY:O	1:A:2025:ARG:NH2	2.31	0.64
1:B:4635:ASN:ND2	1:B:4668:LEU:O	2.30	0.64
1:D:2018:GLY:O	1:D:2025:ARG:NH2	2.31	0.64
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.30	0.64
1:B:2018:GLY:O	1:B:2025:ARG:NH2	2.31	0.64
1:C:626:ARG:NH1	1:C:1668:LEU:O	2.31	0.64
1:A:497:LEU:O	1:A:501:CYS:N	2.30	0.63
1:A:4635:ASN:ND2	1:A:4668:LEU:O	2.30	0.63
1:B:332:ARG:N	1:B:362:TYR:O	2.32	0.63
1:A:890:HIS:NE2	1:A:919:VAL:O	2.32	0.63
1:A:626:ARG:NH1	1:A:1668:LEU:O	2.32	0.63
1:D:332:ARG:N	1:D:362:TYR:O	2.32	0.63
1:A:2106:THR:OG1	1:A:3612:ARG:O	2.16	0.62
1:D:890:HIS:NE2	1:D:919:VAL:O	2.32	0.62
1:A:842:GLN:OE1	1:A:844:ARG:NH2	2.32	0.62
1:A:2358:ARG:NH1	1:A:2365:SER:O	2.31	0.62
1:B:3360:THR:O	1:B:3404:TYR:OH	2.17	0.62
1:C:3078:GLN:O	1:C:3082:THR:OG1	2.13	0.62
1:A:332:ARG:N	1:A:362:TYR:O	2.32	0.62
1:B:40:GLU:OE1	1:B:420:ARG:NH1	2.32	0.62
1:B:890:HIS:NE2	1:B:919:VAL:O	2.32	0.62
1:D:842:GLN:OE1	1:D:844:ARG:NH2	2.32	0.62
1:B:2358:ARG:NH1	1:B:2365:SER:O	2.32	0.62
1:A:4136:GLU:O	1:A:4917:TYR:OH	2.18	0.62
1:C:332:ARG:N	1:C:362:TYR:O	2.32	0.62
1:C:2358:ARG:NH1	1:C:2365:SER:O	2.32	0.62
1:D:4014:LYS:NZ	1:D:4060:SER:O	2.33	0.62
1:B:4014:LYS:NZ	1:B:4060:SER:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:890:HIS:NE2	1:C:919:VAL:O	2.32	0.62
1:D:40:GLU:OE1	1:D:420:ARG:NH1	2.32	0.62
1:D:1501:ASN:O	1:D:1505:GLY:N	2.32	0.62
1:C:842:GLN:OE1	1:C:844:ARG:NH2	2.32	0.62
1:D:1443:VAL:O	1:D:1496:PRO:N	2.33	0.62
1:A:2215:ASP:O	1:A:2218:SER:OG	2.15	0.62
1:A:2580:ARG:NH1	1:A:2614:GLU:OE1	2.33	0.62
1:A:4014:LYS:NZ	1:A:4060:SER:O	2.33	0.62
1:C:40:GLU:OE1	1:C:420:ARG:NH1	2.32	0.62
1:C:4014:LYS:NZ	1:C:4060:SER:O	2.33	0.62
1:B:842:GLN:OE1	1:B:844:ARG:NH2	2.32	0.61
1:A:40:GLU:OE1	1:A:420:ARG:NH1	2.32	0.61
1:C:480:ARG:NH1	1:C:3677:GLU:OE2	2.33	0.61
1:D:480:ARG:NH1	1:D:3677:GLU:OE2	2.33	0.61
1:D:2215:ASP:O	1:D:2218:SER:OG	2.15	0.61
1:D:2358:ARG:NH1	1:D:2365:SER:O	2.32	0.61
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.18	0.61
1:B:480:ARG:NH1	1:B:3677:GLU:OE2	2.33	0.61
1:C:1614:GLU:O	1:C:1619:LEU:N	2.34	0.61
1:D:560:SER:OG	1:D:561:ARG:NH2	2.34	0.61
1:A:1614:GLU:O	1:A:1619:LEU:N	2.34	0.61
1:A:480:ARG:NH1	1:A:3677:GLU:OE2	2.33	0.61
1:D:1614:GLU:O	1:D:1619:LEU:N	2.34	0.60
1:D:2580:ARG:NH1	1:D:2614:GLU:OE1	2.34	0.60
1:C:859:GLN:NE2	1:C:859:GLN:O	2.34	0.60
1:B:626:ARG:NH1	1:B:1668:LEU:O	2.34	0.60
1:B:1614:GLU:O	1:B:1619:LEU:N	2.34	0.60
1:B:859:GLN:O	1:B:859:GLN:NE2	2.34	0.60
1:B:4136:GLU:O	1:B:4917:TYR:OH	2.18	0.60
1:C:2215:ASP:O	1:C:2218:SER:OG	2.14	0.60
1:A:1631:LEU:HD13	1:A:1642:ILE:HD11	1.83	0.60
1:D:859:GLN:O	1:D:859:GLN:NE2	2.34	0.60
1:A:859:GLN:O	1:A:859:GLN:NE2	2.34	0.60
2:F:38:SER:OG	2:F:41:ASP:OD1	2.20	0.60
2:E:38:SER:OG	2:E:41:ASP:OD1	2.20	0.60
1:C:1631:LEU:HD13	1:C:1642:ILE:HD11	1.82	0.60
2:H:38:SER:OG	2:H:41:ASP:OD1	2.20	0.60
1:A:1465:VAL:O	1:A:1483:SER:N	2.35	0.59
1:C:2580:ARG:NH1	1:C:2614:GLU:OE1	2.34	0.59
1:A:858:THR:OG1	1:A:861:ALA:O	2.17	0.59
2:G:38:SER:OG	2:G:41:ASP:OD1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1631:LEU:HD13	1:B:1642:ILE:HD11	1.83	0.59
1:B:2580:ARG:NH1	1:B:2614:GLU:OE1	2.36	0.59
1:A:1144:ARG:N	1:A:1150:GLU:O	2.36	0.59
1:B:1465:VAL:O	1:B:1483:SER:N	2.35	0.59
1:B:1501:ASN:N	1:B:1505:GLY:O	2.36	0.59
1:B:2106:THR:OG1	1:B:3612:ARG:O	2.16	0.59
1:D:1465:VAL:O	1:D:1483:SER:N	2.35	0.59
1:D:1631:LEU:HD13	1:D:1642:ILE:HD11	1.82	0.59
1:C:3360:THR:O	1:C:3404:TYR:OH	2.17	0.58
1:C:4136:GLU:O	1:C:4917:TYR:OH	2.18	0.58
1:B:1144:ARG:N	1:B:1150:GLU:O	2.36	0.58
1:C:1144:ARG:N	1:C:1150:GLU:O	2.36	0.58
1:D:45:ARG:NH1	1:D:128:MET:HE2	2.18	0.58
1:D:1144:ARG:N	1:D:1150:GLU:O	2.36	0.58
1:A:255:GLU:OE2	1:A:258:ARG:NH1	2.37	0.58
1:A:3385:LYS:O	1:A:3453:ARG:NH1	2.36	0.58
1:C:1465:VAL:O	1:C:1483:SER:N	2.35	0.58
1:C:2576:CYS:O	1:C:2618:LYS:NZ	2.36	0.58
1:D:2576:CYS:O	1:D:2618:LYS:NZ	2.36	0.58
1:B:770:ILE:O	1:B:773:GLN:NE2	2.36	0.58
1:C:255:GLU:OE2	1:C:258:ARG:NH1	2.37	0.58
1:C:770:ILE:O	1:C:773:GLN:NE2	2.36	0.58
1:C:858:THR:OG1	1:C:861:ALA:O	2.16	0.58
1:D:770:ILE:O	1:D:773:GLN:NE2	2.37	0.58
1:A:770:ILE:O	1:A:773:GLN:NE2	2.36	0.58
1:C:45:ARG:NH1	1:C:128:MET:HE2	2.18	0.58
1:D:3385:LYS:O	1:D:3453:ARG:NH1	2.37	0.58
1:D:3076:GLN:O	1:D:3080:THR:HG23	2.04	0.58
1:B:255:GLU:OE2	1:B:258:ARG:NH1	2.37	0.58
1:B:3385:LYS:O	1:B:3453:ARG:NH1	2.37	0.58
1:B:2576:CYS:O	1:B:2618:LYS:NZ	2.37	0.57
1:C:2154:PHE:HB2	1:C:2161:MET:HE3	1.86	0.57
1:C:3385:LYS:O	1:C:3453:ARG:NH1	2.37	0.57
1:D:255:GLU:OE2	1:D:258:ARG:NH1	2.37	0.57
1:A:45:ARG:NH1	1:A:128:MET:HE2	2.19	0.57
1:B:1504:ASN:O	1:B:1524:ASN:ND2	2.38	0.57
1:A:1763:ARG:O	1:A:1778:GLN:N	2.37	0.57
1:B:45:ARG:NH1	1:B:128:MET:HE2	2.18	0.57
1:C:1763:ARG:O	1:C:1778:GLN:N	2.37	0.57
1:D:889:ILE:HD12	1:D:892:LEU:HD12	1.86	0.57
1:B:889:ILE:HD12	1:B:892:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:889:ILE:HD12	1:C:892:LEU:HD12	1.86	0.57
1:D:2154:PHE:HB2	1:D:2161:MET:HE3	1.86	0.57
1:A:2223:ASN:O	1:A:2225:SER:OG	2.22	0.57
1:C:925:PRO:O	1:C:929:ARG:N	2.38	0.57
1:C:3076:GLN:O	1:C:3080:THR:HG23	2.04	0.57
1:D:3360:THR:O	1:D:3404:TYR:OH	2.17	0.57
1:A:3076:GLN:O	1:A:3080:THR:HG23	2.04	0.57
1:D:858:THR:OG1	1:D:861:ALA:O	2.16	0.57
1:A:889:ILE:HD12	1:A:892:LEU:HD12	1.86	0.56
1:A:1550:SER:O	1:A:1550:SER:OG	2.22	0.56
1:A:2036:THR:HG21	1:A:3628:ILE:HG23	1.87	0.56
1:B:2154:PHE:HB2	1:B:2161:MET:HE3	1.86	0.56
1:B:3076:GLN:O	1:B:3080:THR:HG23	2.04	0.56
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.38	0.56
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.38	0.56
1:B:2636:GLU:OE1	1:B:2679:TYR:OH	2.16	0.56
1:B:4696:VAL:HG13	1:B:4697:LEU:HG	1.87	0.56
1:C:2396:ASP:OD1	1:C:2400:ARG:NE	2.39	0.56
1:C:2106:THR:OG1	1:C:3612:ARG:O	2.17	0.56
1:B:925:PRO:O	1:B:929:ARG:N	2.38	0.56
1:B:2036:THR:HG21	1:B:3628:ILE:HG23	1.88	0.56
1:B:2215:ASP:O	1:B:2218:SER:OG	2.15	0.56
1:D:2106:THR:OG1	1:D:3612:ARG:O	2.16	0.56
1:A:3360:THR:O	1:A:3404:TYR:OH	2.20	0.56
1:C:564:ARG:O	1:C:1586:ARG:NH2	2.39	0.56
1:A:2154:PHE:HB2	1:A:2161:MET:HE3	1.86	0.56
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.38	0.56
1:B:858:THR:OG1	1:B:861:ALA:O	2.16	0.56
1:C:2430:ASP:O	1:C:2434:VAL:HG13	2.05	0.56
1:B:2430:ASP:O	1:B:2434:VAL:HG13	2.05	0.56
1:D:218:SER:OG	1:D:219:SER:N	2.39	0.56
1:D:2430:ASP:O	1:D:2434:VAL:HG13	2.05	0.56
1:A:2430:ASP:O	1:A:2434:VAL:HG13	2.05	0.55
1:D:4696:VAL:HG13	1:D:4697:LEU:HG	1.87	0.55
1:A:1144:ARG:NH1	1:A:1150:GLU:OE2	2.40	0.55
1:A:4696:VAL:HG13	1:A:4697:LEU:HG	1.87	0.55
1:B:564:ARG:O	1:B:1586:ARG:NH2	2.39	0.55
1:C:2036:THR:HG21	1:C:3628:ILE:HG23	1.88	0.55
1:A:925:PRO:O	1:A:929:ARG:N	2.38	0.55
1:D:3458:TYR:O	1:D:3463:SER:N	2.39	0.55
1:A:2576:CYS:O	1:A:2618:LYS:NZ	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2396:ASP:OD1	1:B:2400:ARG:NE	2.39	0.55
1:B:3191:ARG:NE	1:B:3191:ARG:O	2.40	0.55
1:C:2223:ASN:O	1:C:2225:SER:OG	2.22	0.55
1:D:70:GLU:OE1	1:D:122:ARG:NH1	2.40	0.55
1:D:1144:ARG:NH1	1:D:1150:GLU:OE2	2.40	0.55
1:C:4696:VAL:HG13	1:C:4697:LEU:HG	1.88	0.55
1:D:925:PRO:O	1:D:929:ARG:N	2.38	0.55
1:D:3191:ARG:O	1:D:3191:ARG:NE	2.40	0.55
1:A:2077:PRO:HA	1:A:2080:VAL:HG12	1.88	0.55
1:B:218:SER:OG	1:B:219:SER:N	2.39	0.55
1:B:1763:ARG:O	1:B:1778:GLN:N	2.38	0.55
1:A:3191:ARG:O	1:A:3191:ARG:NE	2.39	0.55
1:B:1144:ARG:NH1	1:B:1150:GLU:OE2	2.39	0.55
1:C:3191:ARG:O	1:C:3191:ARG:NE	2.39	0.55
1:A:218:SER:OG	1:A:219:SER:N	2.39	0.55
1:A:1306:MET:HE3	1:A:1307:PRO:O	2.07	0.55
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.38	0.55
1:B:1306:MET:HE3	1:B:1307:PRO:O	2.07	0.55
1:B:3458:TYR:O	1:B:3463:SER:N	2.40	0.55
1:C:1913:CYS:SG	1:C:2090:GLN:NE2	2.80	0.55
1:C:2077:PRO:HA	1:C:2080:VAL:HG12	1.88	0.55
1:C:3458:TYR:O	1:C:3463:SER:N	2.40	0.55
1:D:2396:ASP:OD1	1:D:2400:ARG:NE	2.39	0.55
1:A:70:GLU:OE1	1:A:122:ARG:NH1	2.40	0.54
1:C:237:LEU:O	1:C:404:ASN:N	2.40	0.54
1:C:1306:MET:HE3	1:C:1307:PRO:O	2.07	0.54
1:D:1306:MET:HE3	1:D:1307:PRO:O	2.07	0.54
1:D:1763:ARG:O	1:D:1778:GLN:N	2.37	0.54
1:B:2077:PRO:HA	1:B:2080:VAL:HG12	1.88	0.54
1:C:70:GLU:OE1	1:C:122:ARG:NH1	2.40	0.54
1:B:606:ARG:O	1:B:608:HIS:ND1	2.41	0.54
1:B:783:ASN:ND2	1:B:1460:ASP:O	2.41	0.54
1:C:1144:ARG:NH1	1:C:1150:GLU:OE2	2.40	0.54
1:D:2036:THR:HG21	1:D:3628:ILE:HG23	1.88	0.54
1:C:892:LEU:HD13	1:C:1056:THR:HG21	1.89	0.54
1:A:564:ARG:O	1:A:1586:ARG:NH2	2.39	0.54
1:A:606:ARG:O	1:A:608:HIS:ND1	2.41	0.54
1:A:2396:ASP:OD1	1:A:2400:ARG:NE	2.39	0.54
1:B:892:LEU:HD13	1:B:1056:THR:HG21	1.89	0.54
1:C:218:SER:OG	1:C:219:SER:N	2.40	0.54
1:C:305:TYR:O	1:C:317:MET:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:892:LEU:HD13	1:D:1056:THR:HG21	1.89	0.54
1:B:2223:ASN:O	1:B:2225:SER:OG	2.22	0.54
1:B:70:GLU:OE1	1:B:122:ARG:NH1	2.40	0.54
1:B:237:LEU:O	1:B:404:ASN:N	2.40	0.54
1:D:2077:PRO:HA	1:D:2080:VAL:HG12	1.88	0.54
1:A:305:TYR:O	1:A:317:MET:N	2.40	0.54
1:D:1913:CYS:SG	1:D:2090:GLN:NE2	2.80	0.54
1:A:602:ASP:HB3	1:A:1306:MET:HE1	1.90	0.53
1:A:783:ASN:ND2	1:A:1460:ASP:O	2.41	0.53
1:A:3458:TYR:O	1:A:3463:SER:N	2.40	0.53
1:C:359:SER:O	1:C:404:ASN:ND2	2.41	0.53
1:C:602:ASP:HB3	1:C:1306:MET:HE1	1.90	0.53
1:C:2588:LEU:O	1:C:2592:VAL:HG23	2.08	0.53
1:C:4797:ASP:O	1:C:4800:THR:OG1	2.22	0.53
1:B:602:ASP:HB3	1:B:1306:MET:HE1	1.90	0.53
1:B:1550:SER:O	1:B:1550:SER:OG	2.24	0.53
1:A:2588:LEU:O	1:A:2592:VAL:HG23	2.08	0.53
1:D:564:ARG:O	1:D:1586:ARG:NH2	2.39	0.53
1:D:602:ASP:HB3	1:D:1306:MET:HE1	1.90	0.53
1:D:1129:GLY:O	1:D:1147:GLN:N	2.42	0.53
1:A:359:SER:O	1:A:404:ASN:ND2	2.41	0.53
1:A:1129:GLY:O	1:A:1147:GLN:N	2.42	0.53
1:C:1550:SER:O	1:C:1550:SER:OG	2.25	0.53
1:D:1712:LEU:HD22	1:D:1832:MET:SD	2.49	0.53
1:A:892:LEU:HD13	1:A:1056:THR:HG21	1.89	0.53
1:C:606:ARG:O	1:C:608:HIS:ND1	2.41	0.53
1:D:606:ARG:O	1:D:608:HIS:ND1	2.42	0.53
1:D:783:ASN:ND2	1:D:1460:ASP:O	2.41	0.53
1:A:654:SER:OG	1:A:655:MET:N	2.42	0.53
1:B:359:SER:O	1:B:404:ASN:ND2	2.41	0.53
1:C:783:ASN:ND2	1:C:1460:ASP:O	2.41	0.53
1:C:1712:LEU:HD22	1:C:1832:MET:SD	2.49	0.53
1:D:2588:LEU:O	1:D:2592:VAL:HG23	2.08	0.53
1:A:237:LEU:O	1:A:404:ASN:N	2.41	0.52
1:A:4797:ASP:O	1:A:4800:THR:OG1	2.23	0.52
1:B:305:TYR:O	1:B:317:MET:N	2.40	0.52
1:B:2588:LEU:O	1:B:2592:VAL:HG23	2.08	0.52
1:D:305:TYR:O	1:D:317:MET:N	2.40	0.52
1:D:359:SER:O	1:D:404:ASN:ND2	2.41	0.52
1:C:12:GLN:N	1:C:12:GLN:OE1	2.41	0.52
1:C:1692:ASN:OD1	1:C:1693:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2112:VAL:O	1:D:2116:ILE:HD12	2.10	0.52
1:C:654:SER:OG	1:C:655:MET:N	2.42	0.52
1:A:572:LEU:HD13	1:A:612:ASP:CB	2.40	0.52
1:A:2112:VAL:O	1:A:2116:ILE:HD12	2.10	0.52
1:C:1129:GLY:O	1:C:1147:GLN:N	2.42	0.52
1:C:2112:VAL:O	1:C:2116:ILE:HD12	2.10	0.52
1:A:1691:GLU:OE1	1:A:1791:LYS:NZ	2.33	0.52
1:B:1712:LEU:HD22	1:B:1832:MET:SD	2.49	0.52
1:C:1930:ASP:OD1	1:C:2027:ARG:NH2	2.43	0.52
1:A:1712:LEU:HD22	1:A:1832:MET:SD	2.49	0.52
1:C:1847:ILE:HG22	1:C:1892:LEU:HB3	1.92	0.52
1:D:1692:ASN:OD1	1:D:1693:LYS:N	2.43	0.52
1:D:1847:ILE:HG22	1:D:1892:LEU:HB3	1.92	0.52
1:D:1930:ASP:OD1	1:D:2027:ARG:NH2	2.43	0.52
1:A:1297:THR:O	1:A:1547:GLN:NE2	2.43	0.52
1:B:1692:ASN:OD1	1:B:1693:LYS:N	2.43	0.52
1:B:2112:VAL:O	1:B:2116:ILE:HD12	2.10	0.52
1:D:1297:THR:O	1:D:1547:GLN:NE2	2.43	0.52
1:B:12:GLN:N	1:B:12:GLN:OE1	2.43	0.52
1:B:1297:THR:O	1:B:1547:GLN:NE2	2.43	0.52
1:B:2334:LEU:N	1:B:2338:GLY:O	2.43	0.52
1:C:1691:GLU:OE1	1:C:1791:LYS:NZ	2.33	0.52
1:D:237:LEU:O	1:D:404:ASN:N	2.41	0.52
1:D:1527:GLU:O	1:D:1528:LEU:HD23	2.10	0.52
1:A:12:GLN:OE1	1:A:12:GLN:N	2.43	0.51
1:A:1930:ASP:OD1	1:A:2027:ARG:NH2	2.43	0.51
1:B:654:SER:OG	1:B:655:MET:N	2.42	0.51
1:C:550:GLN:O	1:C:554:SER:N	2.44	0.51
1:D:162:ILE:O	1:D:163:HIS:ND1	2.44	0.51
1:A:162:ILE:O	1:A:163:HIS:ND1	2.44	0.51
1:A:409:GLN:NE2	1:A:3864:ASN:OD1	2.43	0.51
1:C:1297:THR:O	1:C:1547:GLN:NE2	2.43	0.51
1:C:3356:ASP:O	1:C:3360:THR:OG1	2.18	0.51
1:A:418:VAL:HG12	1:A:462:TYR:HE2	1.76	0.51
1:B:162:ILE:O	1:B:163:HIS:ND1	2.44	0.51
1:C:162:ILE:O	1:C:163:HIS:ND1	2.44	0.51
1:A:1692:ASN:OD1	1:A:1693:LYS:N	2.43	0.51
1:B:1847:ILE:HG22	1:B:1892:LEU:HB3	1.92	0.51
1:D:12:GLN:N	1:D:12:GLN:OE1	2.43	0.51
1:D:946:LEU:HD23	1:D:1064:LEU:HD11	1.93	0.51
1:A:1526:LYS:HG3	1:A:1528:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2334:LEU:N	1:A:2338:GLY:O	2.43	0.51
1:B:992:GLN:O	1:B:996:VAL:HG23	2.11	0.51
1:B:2334:LEU:HD21	1:B:2344:ALA:CB	2.41	0.51
1:D:1035:TYR:CD1	1:D:1038:LEU:HD12	2.46	0.51
1:A:1035:TYR:CD1	1:A:1038:LEU:HD12	2.46	0.51
1:A:2334:LEU:HD21	1:A:2344:ALA:CB	2.41	0.51
1:B:418:VAL:HG12	1:B:462:TYR:HE2	1.76	0.51
1:D:418:VAL:HG12	1:D:462:TYR:HE2	1.76	0.51
1:D:1501:ASN:O	1:D:1504:ASN:N	2.44	0.51
1:A:992:GLN:O	1:A:996:VAL:HG23	2.11	0.51
1:D:992:GLN:O	1:D:996:VAL:HG23	2.11	0.51
1:D:2334:LEU:HD21	1:D:2344:ALA:CB	2.41	0.51
1:B:1625:PRO:O	1:B:1626:LEU:HD12	2.11	0.51
1:B:2422:LEU:O	1:B:2431:LEU:HD11	2.11	0.51
1:C:436:LEU:HD13	1:C:447:LEU:HB2	1.92	0.51
1:C:992:GLN:O	1:C:996:VAL:HG23	2.11	0.51
1:C:2334:LEU:N	1:C:2338:GLY:O	2.43	0.51
1:B:1035:TYR:CD1	1:B:1038:LEU:HD12	2.46	0.50
1:C:2422:LEU:O	1:C:2431:LEU:HD11	2.11	0.50
1:D:626:ARG:NH1	1:D:1668:LEU:O	2.43	0.50
1:A:946:LEU:HD23	1:A:1064:LEU:HD11	1.94	0.50
1:A:1625:PRO:O	1:A:1626:LEU:HD12	2.12	0.50
1:B:436:LEU:HD13	1:B:447:LEU:HB2	1.92	0.50
1:B:1930:ASP:OD1	1:B:2027:ARG:NH2	2.43	0.50
1:C:418:VAL:HG12	1:C:462:TYR:HE2	1.76	0.50
1:C:2334:LEU:HD21	1:C:2344:ALA:CB	2.41	0.50
1:A:1847:ILE:HG22	1:A:1892:LEU:HB3	1.92	0.50
1:B:1129:GLY:O	1:B:1147:GLN:N	2.42	0.50
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.12	0.50
1:D:2223:ASN:O	1:D:2225:SER:OG	2.22	0.50
1:D:2334:LEU:N	1:D:2338:GLY:O	2.43	0.50
1:C:1722:MET:SD	1:C:2126:ARG:NH1	2.84	0.50
1:D:550:GLN:O	1:D:554:SER:N	2.43	0.50
1:A:804:LEU:HD12	1:A:1618:TRP:CZ3	2.47	0.50
1:B:946:LEU:HD23	1:B:1064:LEU:HD11	1.94	0.50
1:C:946:LEU:HD23	1:C:1064:LEU:HD11	1.94	0.50
1:D:1625:PRO:O	1:D:1626:LEU:HD12	2.12	0.50
1:D:2422:LEU:O	1:D:2431:LEU:HD11	2.11	0.50
1:A:436:LEU:HD13	1:A:447:LEU:HB2	1.92	0.50
1:C:1526:LYS:HG3	1:C:1528:LEU:HD21	1.93	0.50
1:D:4152:SER:OG	1:D:4153:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4701:ASP:OD1	1:C:4702:VAL:N	2.44	0.50
1:D:436:LEU:HD13	1:D:447:LEU:HB2	1.92	0.50
1:D:654:SER:OG	1:D:655:MET:N	2.42	0.50
1:D:4030:THR:HG21	1:D:4051:MET:SD	2.52	0.50
1:C:804:LEU:HD12	1:C:1618:TRP:CZ3	2.47	0.50
1:C:908:ARG:NH1	1:C:928:GLU:OE2	2.45	0.50
1:D:2996:SER:OG	1:D:3070:THR:HG21	2.12	0.50
1:A:908:ARG:NH1	1:A:928:GLU:OE2	2.45	0.49
1:B:908:ARG:NH1	1:B:928:GLU:OE2	2.45	0.49
1:C:288:HIS:O	1:C:290:ARG:NH1	2.45	0.49
1:C:1035:TYR:CD1	1:C:1038:LEU:HD12	2.46	0.49
1:C:1625:PRO:O	1:C:1626:LEU:HD12	2.12	0.49
1:D:804:LEU:HD12	1:D:1618:TRP:CZ3	2.47	0.49
1:C:2996:SER:OG	1:C:3070:THR:HG21	2.12	0.49
1:A:2422:LEU:O	1:A:2431:LEU:HD11	2.12	0.49
1:A:4152:SER:OG	1:A:4153:GLU:N	2.45	0.49
1:D:243:GLU:OE1	1:D:264:GLY:N	2.46	0.49
1:D:3916:PHE:O	1:D:3920:THR:HG23	2.12	0.49
1:A:2275:SER:HB2	1:A:2383:MET:HE3	1.94	0.49
1:D:4701:ASP:OD1	1:D:4702:VAL:N	2.45	0.49
1:A:4159:TRP:CZ2	1:A:4915:ALA:HB2	2.48	0.49
1:B:804:LEU:HD12	1:B:1618:TRP:CZ3	2.47	0.49
1:B:1526:LYS:HG3	1:B:1528:LEU:HD21	1.93	0.49
1:B:4030:THR:HG21	1:B:4051:MET:SD	2.52	0.49
1:D:288:HIS:O	1:D:290:ARG:NH1	2.46	0.49
1:B:4152:SER:OG	1:B:4153:GLU:N	2.45	0.49
1:B:4701:ASP:OD1	1:B:4702:VAL:N	2.45	0.49
1:C:145:PHE:O	1:C:205:ALA:N	2.43	0.49
1:D:1273:ILE:O	1:D:1287:GLN:N	2.46	0.49
1:A:243:GLU:OE1	1:A:264:GLY:N	2.46	0.49
1:A:550:GLN:O	1:A:554:SER:N	2.44	0.49
1:A:1631:LEU:HD13	1:A:1642:ILE:CD1	2.43	0.49
1:A:2996:SER:OG	1:A:3070:THR:HG21	2.12	0.49
1:A:4030:THR:HG21	1:A:4051:MET:SD	2.52	0.49
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.12	0.49
1:C:243:GLU:OE1	1:C:264:GLY:N	2.45	0.49
1:B:1631:LEU:HD13	1:B:1642:ILE:CD1	2.43	0.49
1:D:2779:LYS:NZ	1:D:2846:ASN:OD1	2.46	0.49
1:D:3687:TYR:OH	1:D:3757:THR:OG1	2.19	0.49
2:E:38:SER:O	2:E:42:ARG:NH2	2.46	0.49
2:F:38:SER:O	2:F:42:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4701:ASP:OD1	1:A:4702:VAL:N	2.45	0.49
1:B:2275:SER:HB2	1:B:2383:MET:HE3	1.94	0.49
1:D:908:ARG:NH1	1:D:928:GLU:OE2	2.45	0.49
1:A:1273:ILE:O	1:A:1287:GLN:N	2.46	0.48
1:A:2008:ILE:HG23	1:A:2012:GLU:HB2	1.95	0.48
1:B:243:GLU:OE1	1:B:264:GLY:N	2.46	0.48
1:B:4159:TRP:CZ2	1:B:4915:ALA:HB2	2.48	0.48
1:D:4159:TRP:CZ2	1:D:4915:ALA:HB2	2.48	0.48
1:A:2582:SER:HB2	1:A:2875:THR:HG22	1.94	0.48
1:B:550:GLN:O	1:B:554:SER:N	2.44	0.48
1:C:4030:THR:HG21	1:C:4051:MET:SD	2.52	0.48
1:D:1631:LEU:HD13	1:D:1642:ILE:CD1	2.43	0.48
1:D:2275:SER:HB2	1:D:2383:MET:HE3	1.94	0.48
1:B:288:HIS:O	1:B:290:ARG:NH1	2.46	0.48
1:B:2582:SER:HB2	1:B:2875:THR:HG22	1.94	0.48
1:C:2275:SER:HB2	1:C:2383:MET:HE3	1.95	0.48
1:D:1526:LYS:HG3	1:D:1528:LEU:HD21	1.95	0.48
1:A:288:HIS:O	1:A:290:ARG:NH1	2.46	0.48
1:A:537:LEU:HD13	1:A:538:ALA:N	2.29	0.48
1:A:1722:MET:SD	1:A:2126:ARG:NH1	2.87	0.48
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.12	0.48
1:B:1500:ARG:HA	1:B:1505:GLY:C	2.39	0.48
1:B:1527:GLU:O	1:B:1528:LEU:HD23	2.14	0.48
1:B:2996:SER:OG	1:B:3070:THR:HG21	2.12	0.48
1:C:2582:SER:HB2	1:C:2875:THR:HG22	1.95	0.48
1:C:4152:SER:OG	1:C:4153:GLU:N	2.45	0.48
1:D:537:LEU:HD13	1:D:538:ALA:N	2.28	0.48
1:A:2779:LYS:NZ	1:A:2846:ASN:OD1	2.46	0.48
1:B:2228:LEU:HD12	1:B:2237:THR:HB	1.96	0.48
1:C:1527:GLU:O	1:C:1528:LEU:HD23	2.12	0.48
1:C:2228:LEU:HD12	1:C:2237:THR:HB	1.96	0.48
1:C:2779:LYS:NZ	1:C:2846:ASN:OD1	2.45	0.48
1:A:145:PHE:O	1:A:205:ALA:N	2.44	0.48
2:G:38:SER:O	2:G:42:ARG:NH2	2.46	0.48
1:A:2228:LEU:HD12	1:A:2237:THR:HB	1.96	0.48
1:B:2779:LYS:NZ	1:B:2846:ASN:OD1	2.46	0.48
1:C:1273:ILE:O	1:C:1287:GLN:N	2.46	0.48
1:C:4159:TRP:CZ2	1:C:4915:ALA:HB2	2.48	0.48
1:C:4649:LYS:HG2	1:C:4669:LEU:HD23	1.96	0.48
1:D:305:TYR:N	1:D:317:MET:O	2.46	0.48
1:D:1550:SER:O	1:D:1550:SER:OG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1722:MET:SD	1:D:2126:ARG:NH1	2.87	0.48
1:D:2582:SER:HB2	1:D:2875:THR:HG22	1.94	0.48
1:D:4649:LYS:HG2	1:D:4669:LEU:HD23	1.96	0.48
1:C:1206:SER:O	1:C:1207:LEU:HD23	2.14	0.48
1:B:537:LEU:HD13	1:B:538:ALA:N	2.28	0.48
2:H:38:SER:O	2:H:42:ARG:NH2	2.46	0.48
1:D:2228:LEU:HD12	1:D:2237:THR:HB	1.96	0.47
1:D:4807:ASP:OD1	1:D:4807:ASP:N	2.47	0.47
1:B:1691:GLU:OE1	1:B:1791:LYS:NZ	2.33	0.47
1:B:2008:ILE:HG23	1:B:2012:GLU:HB2	1.95	0.47
1:D:4797:ASP:O	1:D:4800:THR:OG1	2.22	0.47
1:A:4802:ASP:OD1	1:A:4802:ASP:N	2.48	0.47
1:C:537:LEU:HD13	1:C:538:ALA:N	2.28	0.47
1:D:2008:ILE:HG23	1:D:2012:GLU:HB2	1.95	0.47
1:A:1206:SER:O	1:A:1207:LEU:HD23	2.14	0.47
1:B:409:GLN:NE2	1:B:3864:ASN:OD1	2.48	0.47
1:C:3914:GLN:O	1:C:3918:THR:HG23	2.14	0.47
2:G:103:LEU:HD23	2:G:104:LEU:N	2.30	0.47
1:A:853:PRO:HB2	1:A:1209:VAL:HG22	1.96	0.47
1:A:1527:GLU:O	1:A:1528:LEU:HD23	2.15	0.47
1:A:4042:ILE:HD12	1:A:4043:SER:O	2.14	0.47
1:B:1273:ILE:O	1:B:1287:GLN:N	2.46	0.47
1:D:853:PRO:HB2	1:D:1209:VAL:HG22	1.97	0.47
1:D:1206:SER:O	1:D:1207:LEU:HD23	2.14	0.47
1:C:1631:LEU:HD13	1:C:1642:ILE:CD1	2.43	0.47
1:A:2275:SER:CB	1:A:2383:MET:HE3	2.45	0.47
1:A:4193:GLU:OE2	1:A:4943:TYR:OH	2.28	0.47
1:A:4649:LYS:HG2	1:A:4669:LEU:HD23	1.96	0.47
2:H:103:LEU:HD23	2:H:104:LEU:N	2.29	0.47
1:B:4042:ILE:HD12	1:B:4043:SER:O	2.15	0.47
1:C:305:TYR:N	1:C:317:MET:O	2.46	0.47
1:C:853:PRO:HB2	1:C:1209:VAL:HG22	1.97	0.47
1:D:655:MET:N	1:D:792:VAL:O	2.48	0.47
1:D:4042:ILE:HD12	1:D:4043:SER:O	2.15	0.47
1:D:4193:GLU:OE2	1:D:4943:TYR:OH	2.28	0.47
1:B:1722:MET:SD	1:B:2126:ARG:NH1	2.87	0.47
1:C:2008:ILE:HG23	1:C:2012:GLU:HB2	1.95	0.47
1:C:2275:SER:CB	1:C:2383:MET:HE3	2.45	0.47
2:F:103:LEU:HD23	2:F:104:LEU:N	2.30	0.47
1:B:1206:SER:O	1:B:1207:LEU:HD23	2.14	0.47
1:B:4649:LYS:HG2	1:B:4669:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ASP:N	1:D:18:ASP:OD1	2.47	0.47
1:D:145:PHE:O	1:D:205:ALA:N	2.44	0.47
1:A:4807:ASP:OD1	1:A:4807:ASP:N	2.48	0.46
1:B:241:MET:HE1	1:B:389:ARG:HG3	1.98	0.46
1:B:305:TYR:N	1:B:317:MET:O	2.46	0.46
1:B:2275:SER:CB	1:B:2383:MET:HE3	2.45	0.46
1:C:4042:ILE:HD12	1:C:4043:SER:O	2.14	0.46
1:D:409:GLN:NE2	1:D:3864:ASN:OD1	2.48	0.46
1:D:1257:GLN:O	1:D:1597:TRP:N	2.48	0.46
2:E:103:LEU:HD23	2:E:104:LEU:N	2.29	0.46
1:C:4802:ASP:N	1:C:4802:ASP:OD1	2.47	0.46
1:D:2790:ARG:NH1	1:D:2791:THR:O	2.48	0.46
1:B:3864:ASN:OD1	1:B:3865:THR:OG1	2.15	0.46
1:B:3914:GLN:O	1:B:3918:THR:HG23	2.16	0.46
1:A:241:MET:HE1	1:A:389:ARG:HG3	1.98	0.46
1:A:2586:HIS:NE2	1:A:2875:THR:HG21	2.31	0.46
1:B:18:ASP:N	1:B:18:ASP:OD1	2.47	0.46
1:B:853:PRO:HB2	1:B:1209:VAL:HG22	1.96	0.46
1:B:1257:GLN:O	1:B:1597:TRP:N	2.49	0.46
1:C:241:MET:HE1	1:C:389:ARG:HG3	1.97	0.46
1:C:655:MET:N	1:C:792:VAL:O	2.48	0.46
1:C:2586:HIS:NE2	1:C:2875:THR:HG21	2.31	0.46
1:A:438:LYS:NZ	1:A:507:VAL:HG11	2.31	0.46
1:A:3914:GLN:O	1:A:3918:THR:HG23	2.15	0.46
1:B:612:ASP:O	1:B:616:SER:CB	2.64	0.46
1:B:655:MET:N	1:B:792:VAL:O	2.48	0.46
1:D:4802:ASP:OD1	1:D:4802:ASP:N	2.48	0.46
1:A:830:GLU:OE2	1:A:830:GLU:N	2.49	0.46
1:A:1257:GLN:O	1:A:1597:TRP:N	2.49	0.46
1:B:438:LYS:NZ	1:B:507:VAL:HG11	2.31	0.46
1:B:2586:HIS:NE2	1:B:2875:THR:HG21	2.31	0.46
1:A:231:GLY:O	1:A:276:ARG:NH1	2.48	0.46
1:D:2586:HIS:NE2	1:D:2875:THR:HG21	2.31	0.46
1:D:3914:GLN:O	1:D:3918:THR:HG23	2.15	0.46
1:B:231:GLY:O	1:B:276:ARG:NH1	2.49	0.46
1:C:950:VAL:CG1	1:C:1064:LEU:HD13	2.46	0.46
1:D:241:MET:HE1	1:D:389:ARG:HG3	1.98	0.46
1:D:438:LYS:NZ	1:D:507:VAL:HG11	2.31	0.46
1:D:950:VAL:CG1	1:D:1064:LEU:HD13	2.46	0.46
1:A:655:MET:N	1:A:792:VAL:O	2.48	0.46
1:B:2175:VAL:HG11	1:B:2219:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2133:MET:SD	1:A:2186:ILE:HD13	2.55	0.46
1:C:1257:GLN:O	1:C:1597:TRP:N	2.49	0.46
1:C:1257:GLN:HB2	1:C:1600:MET:HE2	1.97	0.46
1:A:612:ASP:O	1:A:616:SER:CB	2.65	0.45
1:B:572:LEU:HD13	1:B:612:ASP:CB	2.46	0.45
1:B:1257:GLN:HB2	1:B:1600:MET:HE2	1.98	0.45
1:C:3678:LYS:NZ	1:C:3682:GLU:OE1	2.48	0.45
1:A:950:VAL:CG1	1:A:1064:LEU:HD13	2.46	0.45
1:C:4942:MET:O	1:C:4946:ARG:N	2.49	0.45
1:D:2275:SER:CB	1:D:2383:MET:HE3	2.45	0.45
1:A:1155:SER:OG	1:A:1156:TRP:N	2.50	0.45
1:D:231:GLY:O	1:D:276:ARG:NH1	2.48	0.45
1:A:411:GLU:OE1	1:A:411:GLU:N	2.50	0.45
1:A:1097:LYS:NZ	1:A:1198:GLY:O	2.33	0.45
1:A:2154:PHE:CB	1:A:2161:MET:HE3	2.47	0.45
1:C:231:GLY:O	1:C:276:ARG:NH1	2.48	0.45
1:C:548:CYS:SG	1:C:578:VAL:HG22	2.56	0.45
1:C:4807:ASP:OD1	1:C:4807:ASP:N	2.47	0.45
1:D:3678:LYS:NZ	1:D:3682:GLU:OE1	2.48	0.45
1:A:548:CYS:SG	1:A:578:VAL:HG22	2.57	0.45
1:A:1172:THR:O	1:A:1172:THR:OG1	2.34	0.45
1:B:830:GLU:N	1:B:830:GLU:OE1	2.49	0.45
1:C:572:LEU:HD13	1:C:612:ASP:CB	2.47	0.45
1:C:612:ASP:O	1:C:616:SER:CB	2.64	0.45
1:C:1155:SER:OG	1:C:1156:TRP:N	2.50	0.45
1:C:1172:THR:O	1:C:1172:THR:OG1	2.28	0.45
1:D:3923:ILE:HD13	1:D:3984:MET:SD	2.57	0.45
1:A:305:TYR:N	1:A:317:MET:O	2.46	0.45
1:C:438:LYS:NZ	1:C:507:VAL:HG11	2.31	0.45
1:B:1155:SER:OG	1:B:1156:TRP:N	2.49	0.45
1:B:3923:ILE:HD13	1:B:3984:MET:SD	2.57	0.45
1:B:4942:MET:O	1:B:4946:ARG:N	2.49	0.45
1:D:548:CYS:SG	1:D:578:VAL:HG22	2.57	0.45
1:D:1257:GLN:HB2	1:D:1600:MET:HE2	1.97	0.45
1:A:18:ASP:OD1	1:A:18:ASP:N	2.47	0.45
1:A:1257:GLN:HB2	1:A:1600:MET:HE2	1.98	0.45
1:A:1550:SER:HA	1:A:1553:VAL:HG12	1.99	0.45
1:B:2154:PHE:CB	1:B:2161:MET:HE3	2.47	0.45
1:B:4807:ASP:N	1:B:4807:ASP:OD1	2.47	0.45
1:D:1155:SER:OG	1:D:1156:TRP:N	2.50	0.45
1:A:4942:MET:O	1:A:4946:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:VAL:CG1	1:B:1064:LEU:HD13	2.46	0.45
1:D:830:GLU:OE1	1:D:830:GLU:N	2.49	0.45
1:D:2468:VAL:HG11	1:D:2521:THR:HG22	1.99	0.45
1:B:2461:PRO:HG3	1:B:2514:ALA:HB1	1.99	0.45
1:B:3678:LYS:NZ	1:B:3682:GLU:OE1	2.48	0.45
1:A:2468:VAL:HG11	1:A:2521:THR:HG22	1.99	0.44
1:A:2790:ARG:NH1	1:A:2791:THR:O	2.50	0.44
1:B:145:PHE:O	1:B:205:ALA:N	2.44	0.44
1:B:179:ASP:N	1:B:179:ASP:OD1	2.50	0.44
1:B:2468:VAL:HG11	1:B:2521:THR:HG22	1.99	0.44
1:D:612:ASP:O	1:D:616:SER:CB	2.65	0.44
1:D:721:ASP:O	1:D:724:SER:OG	2.12	0.44
1:B:411:GLU:OE1	1:B:411:GLU:N	2.50	0.44
1:C:409:GLN:NE2	1:C:3864:ASN:OD1	2.50	0.44
1:D:1504:ASN:OD1	1:D:1526:LYS:NZ	2.50	0.44
1:A:1681:VAL:HG12	1:A:1686:LEU:HD21	2.00	0.44
1:B:548:CYS:SG	1:B:578:VAL:HG22	2.57	0.44
1:B:1172:THR:O	1:B:1172:THR:OG1	2.33	0.44
1:C:18:ASP:OD1	1:C:18:ASP:N	2.47	0.44
1:C:179:ASP:OD1	1:C:179:ASP:N	2.50	0.44
1:C:2175:VAL:HG11	1:C:2219:TYR:OH	2.17	0.44
1:A:3923:ILE:HD13	1:A:3984:MET:SD	2.57	0.44
1:B:579:LEU:HD11	1:B:616:SER:O	2.17	0.44
1:C:579:LEU:HD11	1:C:616:SER:O	2.18	0.44
1:C:2154:PHE:CB	1:C:2161:MET:HE3	2.47	0.44
1:D:179:ASP:OD1	1:D:179:ASP:N	2.50	0.44
1:D:509:SER:OG	1:D:510:SER:N	2.51	0.44
1:A:4821:ARG:NH1	1:D:4828:ASP:OD1	2.50	0.44
1:B:164:PRO:O	1:B:182:ILE:HD12	2.18	0.44
1:C:3923:ILE:HD13	1:C:3984:MET:SD	2.57	0.44
1:B:1550:SER:HA	1:B:1553:VAL:HG12	1.99	0.44
1:C:164:PRO:O	1:C:182:ILE:HD12	2.17	0.44
1:B:2790:ARG:NH1	1:B:2791:THR:O	2.51	0.44
1:C:1614:GLU:N	1:C:1619:LEU:O	2.50	0.44
1:C:2468:VAL:HG11	1:C:2521:THR:HG22	1.99	0.44
1:C:4828:ASP:OD1	1:D:4821:ARG:NH1	2.50	0.44
1:A:2461:PRO:HG3	1:A:2514:ALA:HB1	1.99	0.44
1:A:4828:ASP:OD1	1:B:4821:ARG:NH1	2.51	0.44
1:B:237:LEU:N	1:B:404:ASN:O	2.51	0.44
1:B:4828:ASP:OD1	1:C:4821:ARG:NH1	2.51	0.44
1:D:45:ARG:NH2	1:D:458:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:PRO:O	1:D:182:ILE:HD12	2.18	0.44
1:D:1506:LEU:N	1:D:1524:ASN:OD1	2.47	0.44
1:D:1614:GLU:N	1:D:1619:LEU:O	2.50	0.44
1:A:1613:SER:O	1:A:1613:SER:OG	2.32	0.44
1:A:509:SER:OG	1:A:510:SER:N	2.51	0.43
1:B:40:GLU:OE2	1:B:125:TYR:OH	2.36	0.43
1:B:1927:PHE:CG	1:B:2031:LEU:HD22	2.53	0.43
1:B:4802:ASP:OD1	1:B:4802:ASP:N	2.48	0.43
1:B:4962:GLU:O	1:B:4964:GLN:N	2.51	0.43
1:D:2154:PHE:CB	1:D:2161:MET:HE3	2.47	0.43
1:D:4962:GLU:O	1:D:4964:GLN:N	2.51	0.43
1:B:1681:VAL:HG12	1:B:1686:LEU:HD21	2.00	0.43
1:C:1613:SER:O	1:C:1613:SER:OG	2.32	0.43
1:C:2461:PRO:HG3	1:C:2514:ALA:HB1	2.01	0.43
1:A:3678:LYS:NZ	1:A:3682:GLU:OE1	2.48	0.43
1:C:237:LEU:N	1:C:404:ASN:O	2.51	0.43
1:C:1927:PHE:CG	1:C:2031:LEU:HD22	2.53	0.43
1:C:2094:ILE:O	1:C:2098:VAL:HG13	2.18	0.43
1:C:4962:GLU:O	1:C:4964:GLN:N	2.51	0.43
1:D:758:CYS:SG	1:D:767:SER:OG	2.76	0.43
1:D:1681:VAL:HG12	1:D:1686:LEU:HD21	2.00	0.43
1:D:2094:ILE:O	1:D:2098:VAL:HG13	2.18	0.43
1:D:2404:GLU:CB	1:D:2407:LEU:HD13	2.48	0.43
1:D:2461:PRO:HG3	1:D:2514:ALA:HB1	2.00	0.43
1:D:4615:TYR:O	1:D:4619:GLN:NE2	2.52	0.43
1:A:164:PRO:O	1:A:182:ILE:HD12	2.18	0.43
1:C:2790:ARG:NH1	1:C:2791:THR:O	2.51	0.43
1:C:4073:GLU:OE1	1:C:4073:GLU:N	2.51	0.43
1:D:3496:SER:O	1:D:3500:THR:OG1	2.30	0.43
1:A:579:LEU:HD11	1:A:616:SER:O	2.17	0.43
1:A:4073:GLU:N	1:A:4073:GLU:OE1	2.51	0.43
1:B:600:LEU:HD12	1:B:600:LEU:O	2.18	0.43
1:B:2636:GLU:OE1	1:B:2636:GLU:N	2.48	0.43
1:B:3011:GLY:O	1:B:3015:ARG:NE	2.52	0.43
1:B:4073:GLU:OE1	1:B:4073:GLU:N	2.51	0.43
1:B:4615:TYR:O	1:B:4619:GLN:NE2	2.52	0.43
1:C:45:ARG:NH2	1:C:458:ASP:OD2	2.50	0.43
1:C:600:LEU:O	1:C:600:LEU:HD12	2.18	0.43
1:D:411:GLU:OE1	1:D:411:GLU:N	2.50	0.43
1:D:1613:SER:O	1:D:1613:SER:OG	2.32	0.43
1:D:1927:PHE:CG	1:D:2031:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2636:GLU:OE1	1:D:2636:GLU:N	2.49	0.43
1:A:758:CYS:SG	1:A:767:SER:OG	2.77	0.43
1:A:2175:VAL:HG11	1:A:2219:TYR:OH	2.18	0.43
1:B:2404:GLU:CB	1:B:2407:LEU:HD13	2.48	0.43
1:C:509:SER:OG	1:C:510:SER:N	2.51	0.43
1:C:1550:SER:HA	1:C:1553:VAL:HG12	2.00	0.43
1:C:2404:GLU:CB	1:C:2407:LEU:HD13	2.48	0.43
1:C:4615:TYR:O	1:C:4619:GLN:NE2	2.51	0.43
1:A:179:ASP:OD1	1:A:179:ASP:N	2.50	0.43
1:B:1504:ASN:OD1	1:B:1524:ASN:ND2	2.51	0.43
1:C:758:CYS:SG	1:C:767:SER:OG	2.76	0.43
1:C:1734:THR:HG22	1:C:1756:THR:OG1	2.19	0.43
1:C:3011:GLY:O	1:C:3015:ARG:NE	2.52	0.43
1:D:3738:MET:O	1:D:3742:THR:HG23	2.19	0.43
1:A:2094:ILE:O	1:A:2098:VAL:HG13	2.18	0.43
1:A:2404:GLU:CB	1:A:2407:LEU:HD13	2.48	0.43
1:A:3738:MET:O	1:A:3742:THR:HG23	2.19	0.43
1:B:375:GLN:N	1:B:390:LYS:O	2.52	0.43
1:B:509:SER:OG	1:B:510:SER:N	2.51	0.43
1:D:1734:THR:HG22	1:D:1756:THR:OG1	2.19	0.43
1:A:3995:GLY:C	1:A:4108:MET:HE1	2.44	0.43
1:A:4962:GLU:O	1:A:4964:GLN:N	2.51	0.43
1:B:2094:ILE:O	1:B:2098:VAL:HG13	2.18	0.43
1:D:237:LEU:N	1:D:404:ASN:O	2.51	0.43
1:D:600:LEU:HD12	1:D:600:LEU:O	2.18	0.43
1:D:1255:LEU:HD13	1:D:1451:HIS:CE1	2.54	0.43
1:B:436:LEU:HD11	1:B:445:ILE:HG23	2.01	0.42
1:C:587:ASN:N	1:C:587:ASN:OD1	2.52	0.42
1:D:579:LEU:HD21	1:D:586:LEU:CD1	2.49	0.42
1:D:587:ASN:OD1	1:D:587:ASN:N	2.52	0.42
1:D:1550:SER:HA	1:D:1553:VAL:HG12	1.99	0.42
1:C:636:LEU:O	1:C:642:LEU:HD21	2.19	0.42
1:C:3738:MET:O	1:C:3742:THR:HG23	2.18	0.42
1:A:40:GLU:OE2	1:A:125:TYR:OH	2.36	0.42
1:A:579:LEU:HD21	1:A:586:LEU:CD1	2.49	0.42
1:A:1255:LEU:HD13	1:A:1451:HIS:CE1	2.55	0.42
1:C:3995:GLY:C	1:C:4108:MET:HE1	2.44	0.42
1:D:579:LEU:HD11	1:D:616:SER:O	2.18	0.42
1:D:2175:VAL:HG11	1:D:2219:TYR:OH	2.18	0.42
1:A:855:VAL:HG12	1:A:1084:ARG:HD3	2.01	0.42
1:A:1927:PHE:CG	1:A:2031:LEU:HD22	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:LEU:HD11	1:D:445:ILE:HG23	2.01	0.42
1:D:3011:GLY:O	1:D:3015:ARG:NE	2.51	0.42
1:D:3995:GLY:C	1:D:4108:MET:HE1	2.44	0.42
1:A:600:LEU:HD12	1:A:600:LEU:O	2.18	0.42
1:B:636:LEU:O	1:B:642:LEU:HD21	2.20	0.42
1:B:1255:LEU:HD13	1:B:1451:HIS:CE1	2.54	0.42
1:B:1734:THR:HG22	1:B:1756:THR:OG1	2.19	0.42
1:B:3738:MET:O	1:B:3742:THR:HG23	2.19	0.42
1:B:3995:GLY:C	1:B:4108:MET:HE1	2.44	0.42
1:C:1255:LEU:HD13	1:C:1451:HIS:CE1	2.54	0.42
1:C:2313:GLU:O	1:C:2317:ASN:ND2	2.52	0.42
1:A:237:LEU:N	1:A:404:ASN:O	2.51	0.42
1:A:823:TYR:O	1:A:826:VAL:HG23	2.20	0.42
1:B:823:TYR:O	1:B:826:VAL:HG23	2.20	0.42
1:C:436:LEU:HD11	1:C:445:ILE:HG23	2.01	0.42
1:C:2095:GLY:O	1:C:2099:ARG:NH1	2.53	0.42
1:D:4765:GLN:OE1	1:D:4765:GLN:N	2.52	0.42
1:A:3011:GLY:O	1:A:3015:ARG:NE	2.52	0.42
1:B:61:ASP:OD2	1:B:298:ARG:NH1	2.53	0.42
1:B:579:LEU:HD21	1:B:586:LEU:CD1	2.50	0.42
1:D:375:GLN:N	1:D:390:LYS:O	2.52	0.42
1:A:45:ARG:NH2	1:A:458:ASP:OD2	2.50	0.42
1:A:968:LYS:CD	1:A:981:MET:HE2	2.50	0.42
1:B:537:LEU:O	1:B:537:LEU:HD22	2.20	0.42
1:C:1681:VAL:HG12	1:C:1686:LEU:HD21	2.01	0.42
1:C:1812:GLY:O	1:C:1814:THR:N	2.53	0.42
1:D:2313:GLU:O	1:D:2317:ASN:ND2	2.53	0.42
1:A:2095:GLY:O	1:A:2099:ARG:NH1	2.53	0.42
1:A:3356:ASP:O	1:A:3360:THR:OG1	2.16	0.42
1:B:45:ARG:NH2	1:B:458:ASP:OD2	2.50	0.42
1:B:968:LYS:CD	1:B:981:MET:HE2	2.50	0.42
1:C:579:LEU:HD21	1:C:586:LEU:CD1	2.49	0.42
1:A:61:ASP:OD2	1:A:298:ARG:NH1	2.53	0.42
1:A:1614:GLU:N	1:A:1619:LEU:O	2.50	0.42
1:B:504:ARG:O	1:B:507:VAL:HG13	2.20	0.42
1:C:40:GLU:OE2	1:C:125:TYR:OH	2.37	0.42
1:C:537:LEU:HD22	1:C:537:LEU:O	2.20	0.42
1:C:711:GLU:OE1	1:C:1639:SER:OG	2.38	0.42
1:D:1731:THR:O	1:D:1734:THR:OG1	2.38	0.42
1:D:4942:MET:O	1:D:4946:ARG:N	2.50	0.42
1:A:504:ARG:O	1:A:507:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ASN:OD1	1:B:587:ASN:N	2.52	0.41
1:C:2275:SER:OG	1:C:2383:MET:HE3	2.20	0.41
1:D:823:TYR:O	1:D:826:VAL:HG23	2.20	0.41
1:A:2107:ILE:HG22	1:A:2157:HIS:CE1	2.55	0.41
1:B:1731:THR:O	1:B:1734:THR:OG1	2.37	0.41
1:B:2495:LEU:HD13	1:B:2872:PRO:HD2	2.02	0.41
1:C:566:GLU:HG2	1:C:1587:LEU:HD21	2.02	0.41
1:C:2495:LEU:HD13	1:C:2872:PRO:HD2	2.02	0.41
1:D:2260:ASP:OD1	1:D:2260:ASP:N	2.53	0.41
1:A:1083:GLU:O	1:A:1209:VAL:HG23	2.20	0.41
1:A:1734:THR:HG22	1:A:1756:THR:OG1	2.19	0.41
1:A:2260:ASP:OD1	1:A:2260:ASP:N	2.53	0.41
1:B:2107:ILE:HG22	1:B:2157:HIS:CE1	2.55	0.41
1:D:504:ARG:O	1:D:507:VAL:HG13	2.20	0.41
1:A:1016:TRP:O	1:A:1017:THR:OG1	2.37	0.41
1:A:2275:SER:OG	1:A:2383:MET:HE3	2.20	0.41
1:B:1083:GLU:O	1:B:1209:VAL:HG23	2.20	0.41
1:B:1633:ILE:N	1:B:1637:ASN:OD1	2.53	0.41
1:C:414:ARG:O	1:C:418:VAL:HG13	2.21	0.41
1:C:823:TYR:O	1:C:826:VAL:HG23	2.20	0.41
1:C:1168:MET:HE2	1:C:1197:VAL:HG13	2.02	0.41
1:D:2495:LEU:HD13	1:D:2872:PRO:HD2	2.02	0.41
1:D:4073:GLU:N	1:D:4073:GLU:OE1	2.51	0.41
1:A:566:GLU:HG2	1:A:1587:LEU:HD21	2.03	0.41
1:A:1118:SER:OG	1:A:1119:ARG:N	2.53	0.41
1:B:414:ARG:O	1:B:418:VAL:HG13	2.21	0.41
1:B:1118:SER:OG	1:B:1119:ARG:N	2.53	0.41
1:B:1614:GLU:N	1:B:1619:LEU:O	2.50	0.41
1:B:2313:GLU:O	1:B:2317:ASN:ND2	2.52	0.41
1:D:414:ARG:O	1:D:418:VAL:HG13	2.21	0.41
1:D:2095:GLY:O	1:D:2099:ARG:NH1	2.53	0.41
1:A:537:LEU:HD22	1:A:537:LEU:O	2.20	0.41
1:A:2313:GLU:O	1:A:2317:ASN:ND2	2.53	0.41
1:B:1613:SER:O	1:B:1613:SER:OG	2.32	0.41
1:B:1641:ASP:OD1	1:B:1642:ILE:N	2.54	0.41
1:C:1118:SER:OG	1:C:1119:ARG:N	2.53	0.41
1:C:1641:ASP:OD1	1:C:1642:ILE:N	2.54	0.41
1:C:2260:ASP:N	1:C:2260:ASP:OD1	2.53	0.41
1:C:4903:GLY:O	1:C:4906:THR:OG1	2.35	0.41
1:D:1641:ASP:OD1	1:D:1642:ILE:N	2.54	0.41
1:A:1038:LEU:HD13	1:A:1042:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2081:ARG:O	1:A:2085:VAL:HG23	2.21	0.41
1:B:566:GLU:HG2	1:B:1587:LEU:HD21	2.03	0.41
1:C:209:GLN:OE1	1:C:210:THR:N	2.54	0.41
1:C:1083:GLU:O	1:C:1209:VAL:HG23	2.20	0.41
1:D:537:LEU:HD22	1:D:537:LEU:O	2.20	0.41
1:D:579:LEU:HD21	1:D:586:LEU:HD12	2.03	0.41
1:D:4666:SER:O	1:D:4670:GLY:N	2.54	0.41
1:B:2095:GLY:O	1:B:2099:ARG:NH1	2.53	0.41
1:C:504:ARG:O	1:C:507:VAL:HG13	2.20	0.41
1:C:968:LYS:CD	1:C:981:MET:HE2	2.50	0.41
1:C:1946:VAL:HG12	1:C:1947:MET:H	1.86	0.41
1:D:4500:MET:HE1	1:D:4584:PHE:HB3	2.03	0.41
1:A:436:LEU:HD11	1:A:445:ILE:HG23	2.01	0.41
1:A:4500:MET:HE1	1:A:4584:PHE:HB3	2.03	0.41
1:A:4666:SER:O	1:A:4670:GLY:N	2.54	0.41
1:B:536:LEU:HD12	1:B:537:LEU:N	2.36	0.41
1:B:758:CYS:SG	1:B:767:SER:OG	2.79	0.41
1:B:2260:ASP:OD1	1:B:2260:ASP:N	2.53	0.41
1:B:2576:CYS:N	1:B:2578:GLN:OE1	2.54	0.41
1:B:4765:GLN:OE1	1:B:4765:GLN:N	2.52	0.41
1:C:2039:LYS:NZ	1:C:2040:LYS:O	2.42	0.41
1:C:4765:GLN:OE1	1:C:4765:GLN:N	2.52	0.41
1:C:4826:ILE:HG13	1:C:4830:ILE:HD12	2.03	0.41
1:D:40:GLU:OE2	1:D:125:TYR:OH	2.36	0.41
1:D:536:LEU:HD12	1:D:537:LEU:N	2.36	0.41
1:D:1038:LEU:HD13	1:D:1042:THR:HG21	2.02	0.41
1:D:1168:MET:HE2	1:D:1197:VAL:HG13	2.02	0.41
1:D:2107:ILE:HG22	1:D:2157:HIS:CE1	2.55	0.41
1:D:3356:ASP:O	1:D:3360:THR:OG1	2.16	0.41
1:A:4615:TYR:O	1:A:4619:GLN:NE2	2.54	0.41
1:B:715:GLY:O	1:B:717:GLY:N	2.54	0.41
1:C:2081:ARG:O	1:C:2085:VAL:HG23	2.21	0.41
1:C:3864:ASN:OD1	1:C:3865:THR:OG1	2.15	0.41
1:D:1118:SER:OG	1:D:1119:ARG:N	2.54	0.41
1:D:1946:VAL:HG12	1:D:1947:MET:H	1.86	0.41
1:D:2039:LYS:NZ	1:D:2040:LYS:O	2.43	0.41
1:D:2636:GLU:OE1	1:D:2679:TYR:OH	2.30	0.41
1:B:534:TYR:CD1	1:B:537:LEU:HD12	2.56	0.40
1:B:939:THR:O	1:B:943:LEU:HD22	2.22	0.40
1:B:1168:MET:HE2	1:B:1197:VAL:HG13	2.03	0.40
1:B:2081:ARG:O	1:B:2085:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2107:ILE:HG22	1:C:2157:HIS:CE1	2.55	0.40
1:D:534:TYR:CD1	1:D:537:LEU:HD12	2.56	0.40
1:D:711:GLU:OE1	1:D:1639:SER:OG	2.38	0.40
1:D:2576:CYS:N	1:D:2578:GLN:OE1	2.54	0.40
1:A:375:GLN:N	1:A:390:LYS:O	2.52	0.40
1:A:587:ASN:OD1	1:A:587:ASN:N	2.53	0.40
1:A:715:GLY:O	1:A:717:GLY:N	2.54	0.40
1:A:939:THR:O	1:A:943:LEU:HD22	2.22	0.40
1:A:1633:ILE:N	1:A:1637:ASN:OD1	2.54	0.40
1:A:1641:ASP:OD1	1:A:1642:ILE:N	2.54	0.40
1:C:375:GLN:N	1:C:390:LYS:O	2.52	0.40
1:C:411:GLU:OE1	1:C:411:GLU:N	2.50	0.40
1:C:579:LEU:HD21	1:C:586:LEU:HD12	2.03	0.40
1:C:1176:THR:O	1:C:1176:THR:OG1	2.39	0.40
1:D:61:ASP:OD2	1:D:298:ARG:NH1	2.53	0.40
1:D:968:LYS:CD	1:D:981:MET:HE2	2.50	0.40
1:D:2275:SER:OG	1:D:2383:MET:HE3	2.20	0.40
1:A:152:ASP:O	1:A:154:THR:HG23	2.22	0.40
1:A:4765:GLN:OE1	1:A:4765:GLN:N	2.52	0.40
1:B:1177:LEU:HD12	1:B:1182:LEU:HD11	2.03	0.40
1:B:2275:SER:OG	1:B:2383:MET:HE3	2.20	0.40
1:D:715:GLY:O	1:D:717:GLY:N	2.54	0.40
1:D:2008:ILE:HG23	1:D:2012:GLU:CB	2.51	0.40
1:A:364:GLN:NE2	1:A:369:GLY:O	2.54	0.40
1:A:534:TYR:CD1	1:A:537:LEU:HD12	2.56	0.40
1:A:3864:ASN:OD1	1:A:3865:THR:OG1	2.15	0.40
1:B:4500:MET:HE1	1:B:4584:PHE:HB3	2.03	0.40
1:C:536:LEU:HD12	1:C:537:LEU:N	2.36	0.40
1:C:3269:SER:O	1:C:3347:MET:HE3	2.21	0.40
1:C:4500:MET:HE1	1:C:4584:PHE:HB3	2.03	0.40
1:D:134:SER:O	1:D:134:SER:OG	2.35	0.40
1:D:1083:GLU:O	1:D:1209:VAL:HG23	2.20	0.40
1:A:1946:VAL:HG12	1:A:1947:MET:H	1.86	0.40
1:B:1031:ARG:HG2	1:B:1038:LEU:HD11	2.04	0.40
1:B:1812:GLY:O	1:B:1814:THR:N	2.53	0.40
1:C:715:GLY:O	1:C:717:GLY:N	2.54	0.40
1:C:1177:LEU:HD12	1:C:1182:LEU:HD11	2.04	0.40
1:D:193:HIS:CG	1:D:206:ALA:HB3	2.57	0.40
1:D:566:GLU:HG2	1:D:1587:LEU:HD21	2.03	0.40
1:D:896:ASN:OD1	1:D:896:ASN:N	2.55	0.40
1:D:946:LEU:HD21	1:D:995:MET:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2468:VAL:HG11	1:D:2521:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3849/4966 (78%)	3318 (86%)	523 (14%)	8 (0%)	43	71
1	B	3849/4966 (78%)	3325 (86%)	517 (13%)	7 (0%)	43	71
1	C	3849/4966 (78%)	3323 (86%)	516 (13%)	10 (0%)	36	66
1	D	3849/4966 (78%)	3329 (86%)	512 (13%)	8 (0%)	43	71
2	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
All	All	15816/20292 (78%)	13687 (86%)	2096 (13%)	33 (0%)	44	71

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	B	607	ASN
1	B	1501	ASN
1	C	607	ASN
1	C	1497	GLY
1	C	2133	MET
1	D	607	ASN
1	D	1501	ASN
1	A	1501	ASN

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Mol	Chain	Res	Type
1	A	2230	SER
1	B	2230	SER
1	C	1500	ARG
1	C	1501	ASN
1	C	2230	SER
1	D	2230	SER
1	A	1262	PRO
1	A	1500	ARG
1	B	1262	PRO
1	C	1262	PRO
1	D	1262	PRO
1	D	2658	GLN
1	A	1781	PRO
1	B	1781	PRO
1	C	1781	PRO
1	D	1781	PRO
1	A	2231	PRO
1	B	2231	PRO
1	B	2285	PRO
1	C	2231	PRO
1	D	2231	PRO
1	A	2285	PRO
1	C	2285	PRO
1	D	2285	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	3181/4355 (73%)	3124 (98%)	57 (2%)	51	70
1	B	3181/4355 (73%)	3127 (98%)	54 (2%)	53	71
1	C	3181/4355 (73%)	3137 (99%)	44 (1%)	59	74
1	D	3181/4355 (73%)	3125 (98%)	56 (2%)	51	70
2	E	88/88 (100%)	87 (99%)	1 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	88/88 (100%)	87 (99%)	1 (1%)	65	76
2	G	88/88 (100%)	87 (99%)	1 (1%)	65	76
2	H	88/88 (100%)	87 (99%)	1 (1%)	65	76
All	All	13076/17772 (74%)	12861 (98%)	215 (2%)	54	72

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	CYS
1	A	132	CYS
1	A	246	THR
1	A	419	ILE
1	A	470	LEU
1	A	501	CYS
1	A	531	ASN
1	A	536	LEU
1	A	537	LEU
1	A	540	LEU
1	A	541	ILE
1	A	544	ASN
1	A	555	LEU
1	A	578	VAL
1	A	644	LEU
1	A	648	LEU
1	A	704	SER
1	A	759	LEU
1	A	1032	LEU
1	A	1432	ILE
1	A	1502	ASN
1	A	1503	SER
1	A	1506	LEU
1	A	1540	LEU
1	A	1557	GLU
1	A	1609	VAL
1	A	1621	GLN
1	A	1639	SER
1	A	1946	VAL
1	A	1951	ASN
1	A	2111	SER
1	A	2435	ILE
1	A	2519	LEU

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Mol	Chain	Res	Type
1	A	2610	THR
1	A	2659	GLU
1	A	2678	ASP
1	A	2679	TYR
1	A	2839	MET
1	A	2897	ILE
1	A	3613	HIS
1	A	3798	SER
1	A	3843	GLN
1	A	3853	PHE
1	A	3878	LEU
1	A	3924	GLN
1	A	3937	SER
1	A	3953	MET
1	A	4124	VAL
1	A	4518	TYR
1	A	4556	VAL
1	A	4621	SER
1	A	4698	ASN
1	A	4800	THR
1	A	4818	VAL
1	A	4830	ILE
1	A	4879	VAL
1	A	4890	CYS
1	B	47	CYS
1	B	132	CYS
1	B	138	SER
1	B	246	THR
1	B	419	ILE
1	B	470	LEU
1	B	501	CYS
1	B	531	ASN
1	B	536	LEU
1	B	537	LEU
1	B	540	LEU
1	B	541	ILE
1	B	544	ASN
1	B	552	SER
1	B	555	LEU
1	B	578	VAL
1	B	644	LEU
1	B	648	LEU

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Mol	Chain	Res	Type
1	B	704	SER
1	B	759	LEU
1	B	1032	LEU
1	B	1049	SER
1	B	1503	SER
1	B	1506	LEU
1	B	1540	LEU
1	B	1609	VAL
1	B	1621	GLN
1	B	1627	GLN
1	B	1946	VAL
1	B	2039	LYS
1	B	2111	SER
1	B	2129	LEU
1	B	2435	ILE
1	B	2519	LEU
1	B	2610	THR
1	B	2678	ASP
1	B	2839	MET
1	B	2897	ILE
1	B	3613	HIS
1	B	3798	SER
1	B	3843	GLN
1	B	3853	PHE
1	B	3878	LEU
1	B	3924	GLN
1	B	3937	SER
1	B	3953	MET
1	B	4518	TYR
1	B	4556	VAL
1	B	4698	ASN
1	B	4800	THR
1	B	4818	VAL
1	B	4830	ILE
1	B	4879	VAL
1	B	4890	CYS
1	C	47	CYS
1	C	132	CYS
1	C	419	ILE
1	C	470	LEU
1	C	501	CYS
1	C	531	ASN

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Mol	Chain	Res	Type
1	C	536	LEU
1	C	537	LEU
1	C	540	LEU
1	C	541	ILE
1	C	544	ASN
1	C	578	VAL
1	C	644	LEU
1	C	646	THR
1	C	704	SER
1	C	759	LEU
1	C	1032	LEU
1	C	1166	VAL
1	C	1300	MET
1	C	1506	LEU
1	C	1540	LEU
1	C	1609	VAL
1	C	1621	GLN
1	C	1946	VAL
1	C	2111	SER
1	C	2435	ILE
1	C	2610	THR
1	C	2839	MET
1	C	2897	ILE
1	C	3613	HIS
1	C	3798	SER
1	C	3853	PHE
1	C	3878	LEU
1	C	3924	GLN
1	C	3937	SER
1	C	3953	MET
1	C	4182	LYS
1	C	4556	VAL
1	C	4800	THR
1	C	4807	ASP
1	C	4818	VAL
1	C	4830	ILE
1	C	4879	VAL
1	C	4890	CYS
1	D	47	CYS
1	D	132	CYS
1	D	419	ILE
1	D	470	LEU

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Mol	Chain	Res	Type
1	D	501	CYS
1	D	531	ASN
1	D	536	LEU
1	D	537	LEU
1	D	540	LEU
1	D	541	ILE
1	D	544	ASN
1	D	552	SER
1	D	578	VAL
1	D	614	LEU
1	D	644	LEU
1	D	704	SER
1	D	759	LEU
1	D	1032	LEU
1	D	1166	VAL
1	D	1300	MET
1	D	1429	SER
1	D	1506	LEU
1	D	1540	LEU
1	D	1557	GLU
1	D	1609	VAL
1	D	1621	GLN
1	D	1627	GLN
1	D	1946	VAL
1	D	1951	ASN
1	D	2111	SER
1	D	2435	ILE
1	D	2519	LEU
1	D	2610	THR
1	D	2651	LEU
1	D	2655	LYS
1	D	2682	SER
1	D	2839	MET
1	D	2897	ILE
1	D	3613	HIS
1	D	3798	SER
1	D	3843	GLN
1	D	3853	PHE
1	D	3878	LEU
1	D	3924	GLN
1	D	3937	SER
1	D	3953	MET

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Mol	Chain	Res	Type
1	D	4182	LYS
1	D	4518	TYR
1	D	4556	VAL
1	D	4698	ASN
1	D	4800	THR
1	D	4807	ASP
1	D	4818	VAL
1	D	4830	ILE
1	D	4879	VAL
1	D	4890	CYS
2	E	38	SER
2	F	38	SER
2	G	38	SER
2	H	38	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	150	GLN
1	A	409	GLN
1	A	490	GLN
1	A	650	ASN
1	A	746	GLN
1	A	781	ASN
1	A	930	ASN
1	A	1547	GLN
1	A	2058	GLN
1	A	2308	ASN
1	A	2440	GLN
1	A	2691	GLN
1	A	2829	ASN
1	A	2896	GLN
1	A	3721	GLN
1	A	3900	GLN
1	A	3931	GLN
1	A	3948	HIS
1	A	4056	HIS
1	A	4074	ASN
1	B	150	GLN
1	B	208	GLN
1	B	409	GLN

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Mol	Chain	Res	Type
1	B	490	GLN
1	B	746	GLN
1	B	781	ASN
1	B	1547	GLN
1	B	2308	ASN
1	B	2440	GLN
1	B	2691	GLN
1	B	2829	ASN
1	B	2896	GLN
1	B	3081	HIS
1	B	3721	GLN
1	B	3900	GLN
1	B	3931	GLN
1	B	3948	HIS
1	B	4056	HIS
1	B	4761	HIS
1	C	150	GLN
1	C	394	HIS
1	C	409	GLN
1	C	490	GLN
1	C	496	ASN
1	C	650	ASN
1	C	746	GLN
1	C	781	ASN
1	C	930	ASN
1	C	1451	HIS
1	C	1547	GLN
1	C	2090	GLN
1	C	2308	ASN
1	C	2440	GLN
1	C	2691	GLN
1	C	2829	ASN
1	C	2896	GLN
1	C	3081	HIS
1	C	3721	GLN
1	C	3900	GLN
1	C	3931	GLN
1	C	3948	HIS
1	C	4056	HIS
1	C	4074	ASN
1	C	4761	HIS
1	D	409	GLN

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Mol	Chain	Res	Type
1	D	490	GLN
1	D	650	ASN
1	D	746	GLN
1	D	781	ASN
1	D	1547	GLN
1	D	2090	GLN
1	D	2308	ASN
1	D	2440	GLN
1	D	2691	GLN
1	D	2829	ASN
1	D	3721	GLN
1	D	3900	GLN
1	D	3931	GLN
1	D	3948	HIS
1	D	4056	HIS
1	D	4074	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

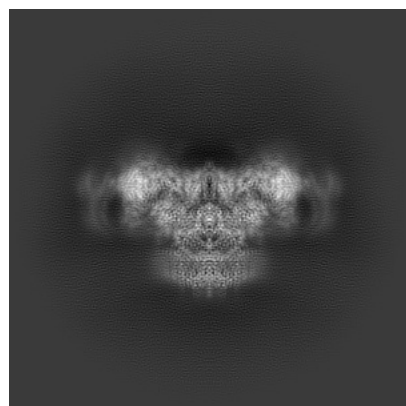
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21861. These allow visual inspection of the internal detail of the map and identification of artifacts.

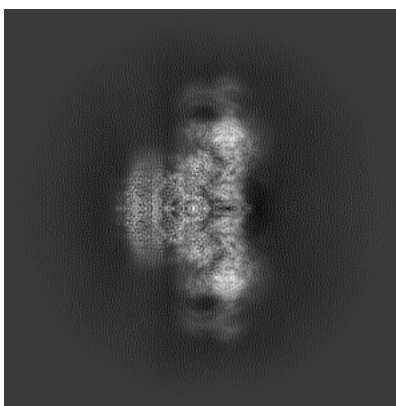
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

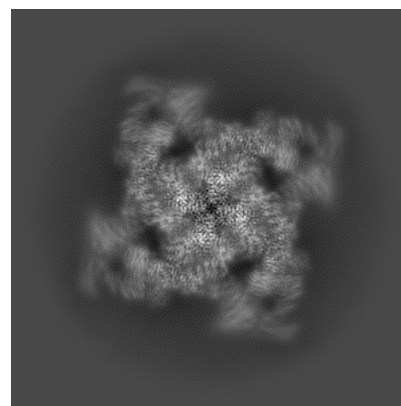
6.1.1 Primary map



X

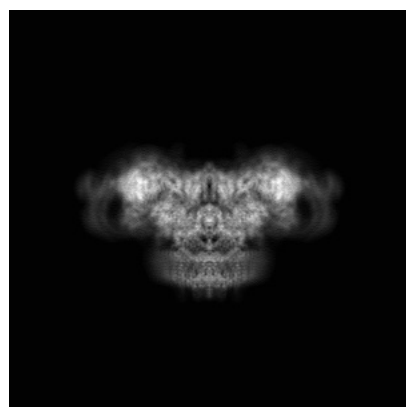


Y

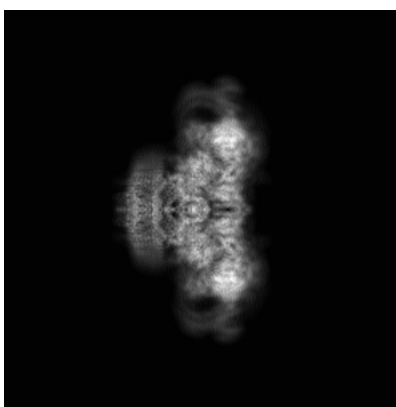


Z

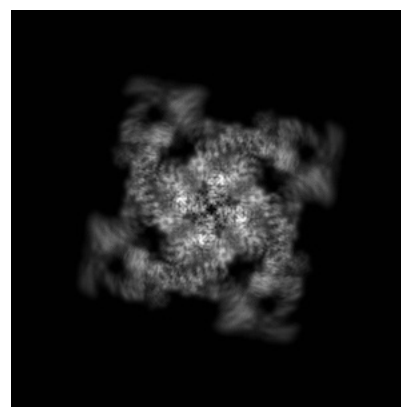
6.1.2 Raw map



X



Y



Z

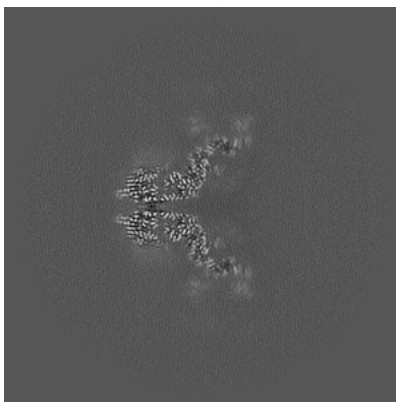
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

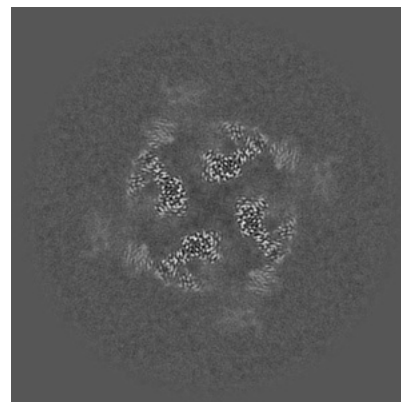
6.2.1 Primary map



X Index: 232

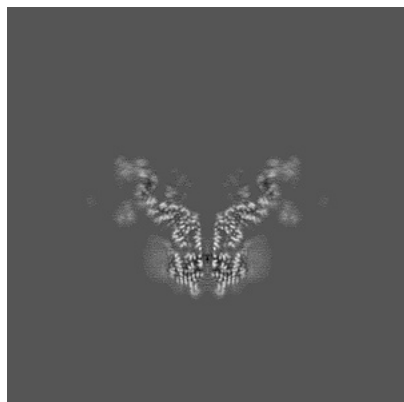


Y Index: 232

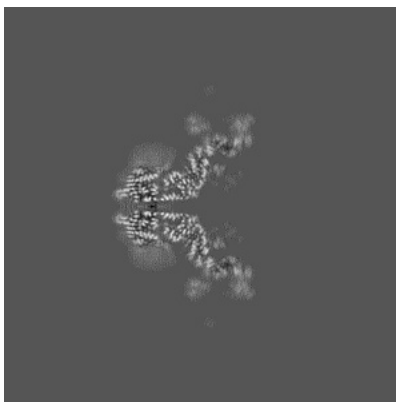


Z Index: 232

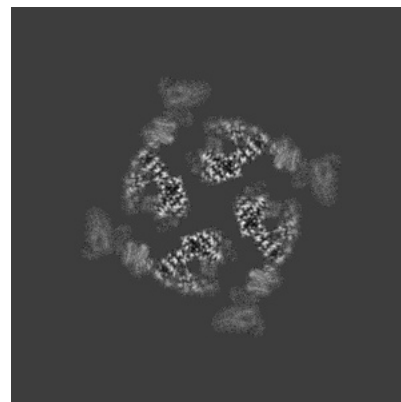
6.2.2 Raw map



X Index: 232



Y Index: 232



Z Index: 232

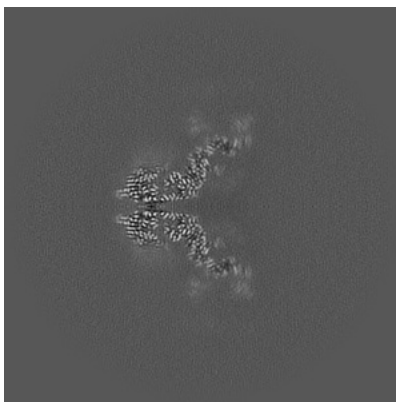
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

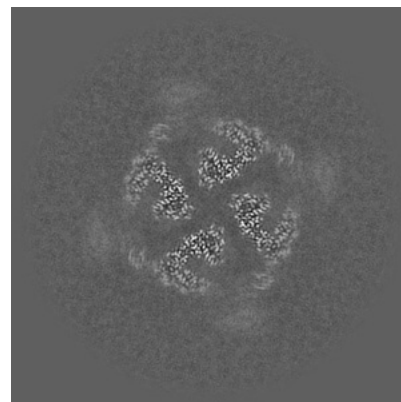
6.3.1 Primary map



X Index: 232

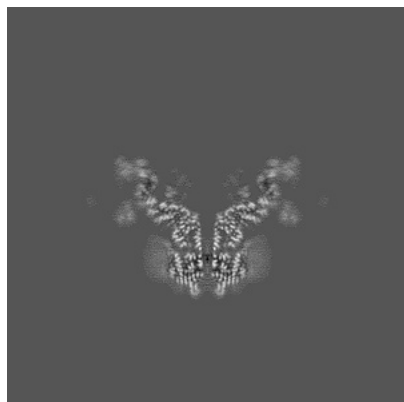


Y Index: 232

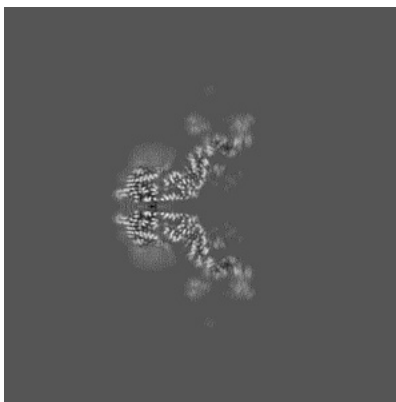


Z Index: 227

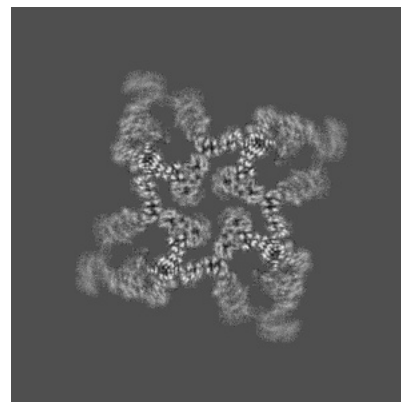
6.3.2 Raw map



X Index: 232



Y Index: 232

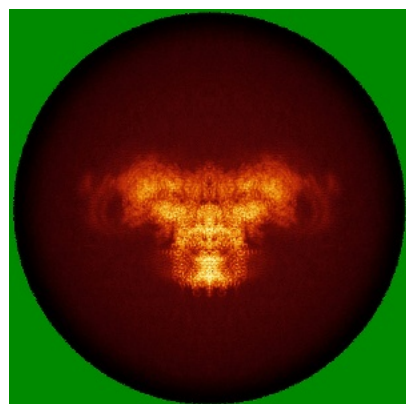


Z Index: 259

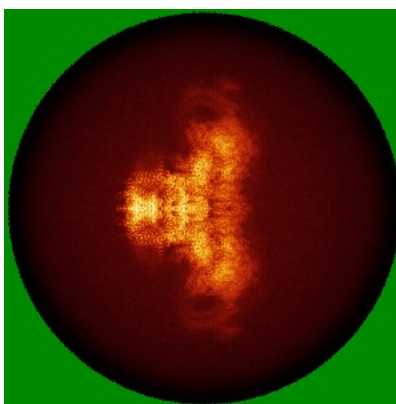
The images above show the largest variance slices of the map in three orthogonal directions.

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

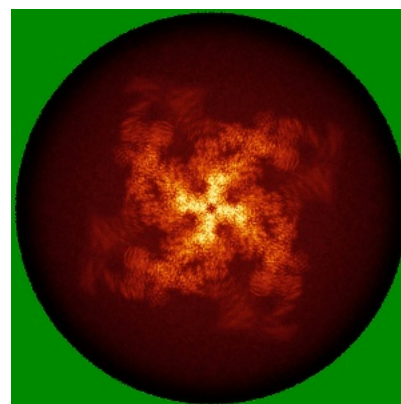
6.4.1 Primary map



X

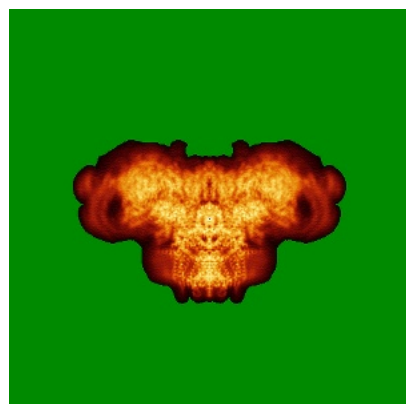


Y

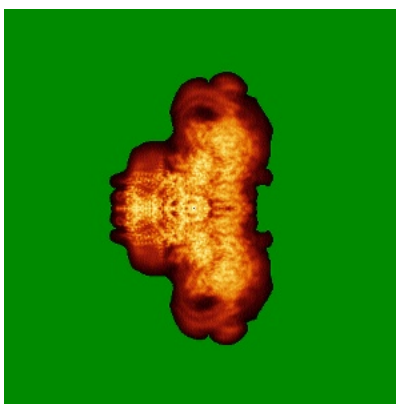


Z

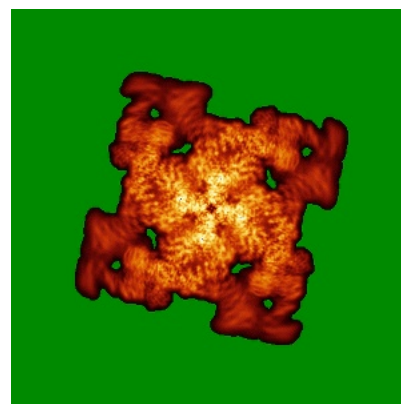
6.4.2 Raw map



X



Y

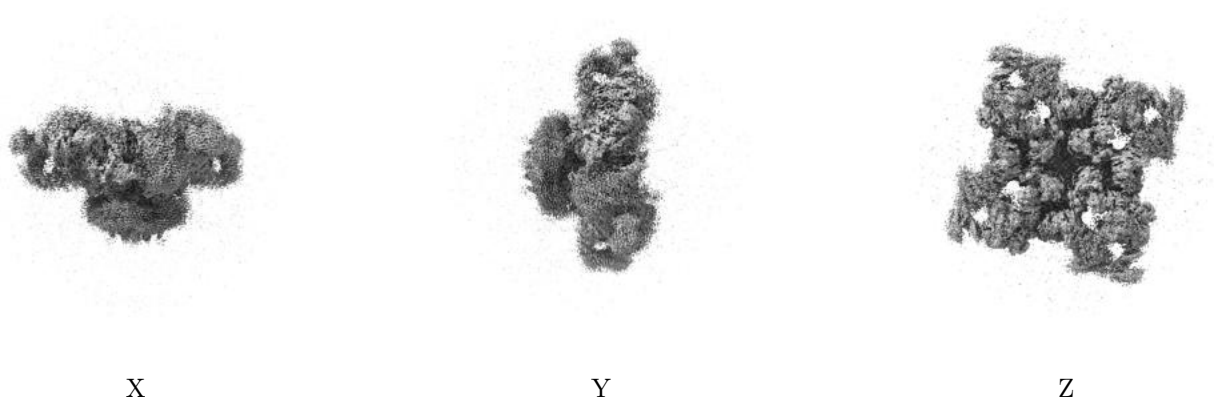


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

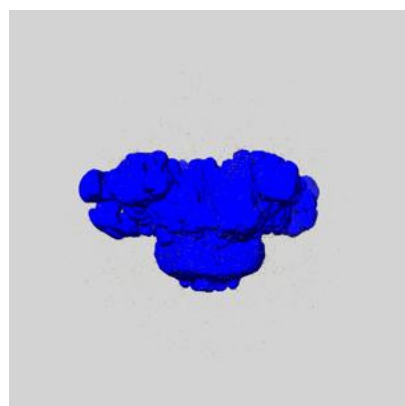
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

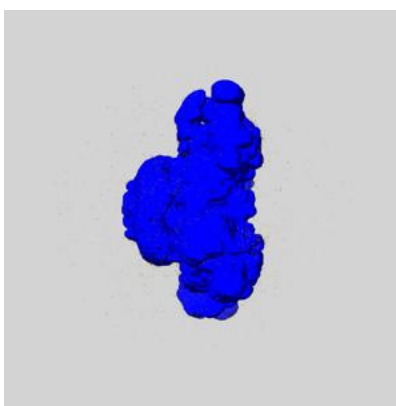
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

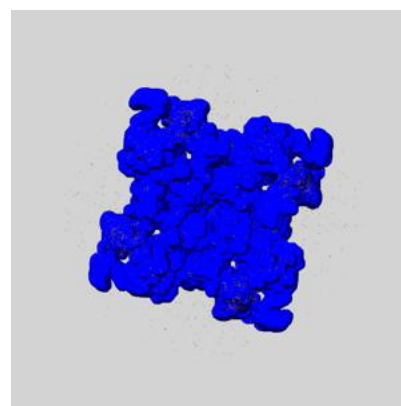
6.6.1 emd_21861_msk_1.map [i](#)



X



Y

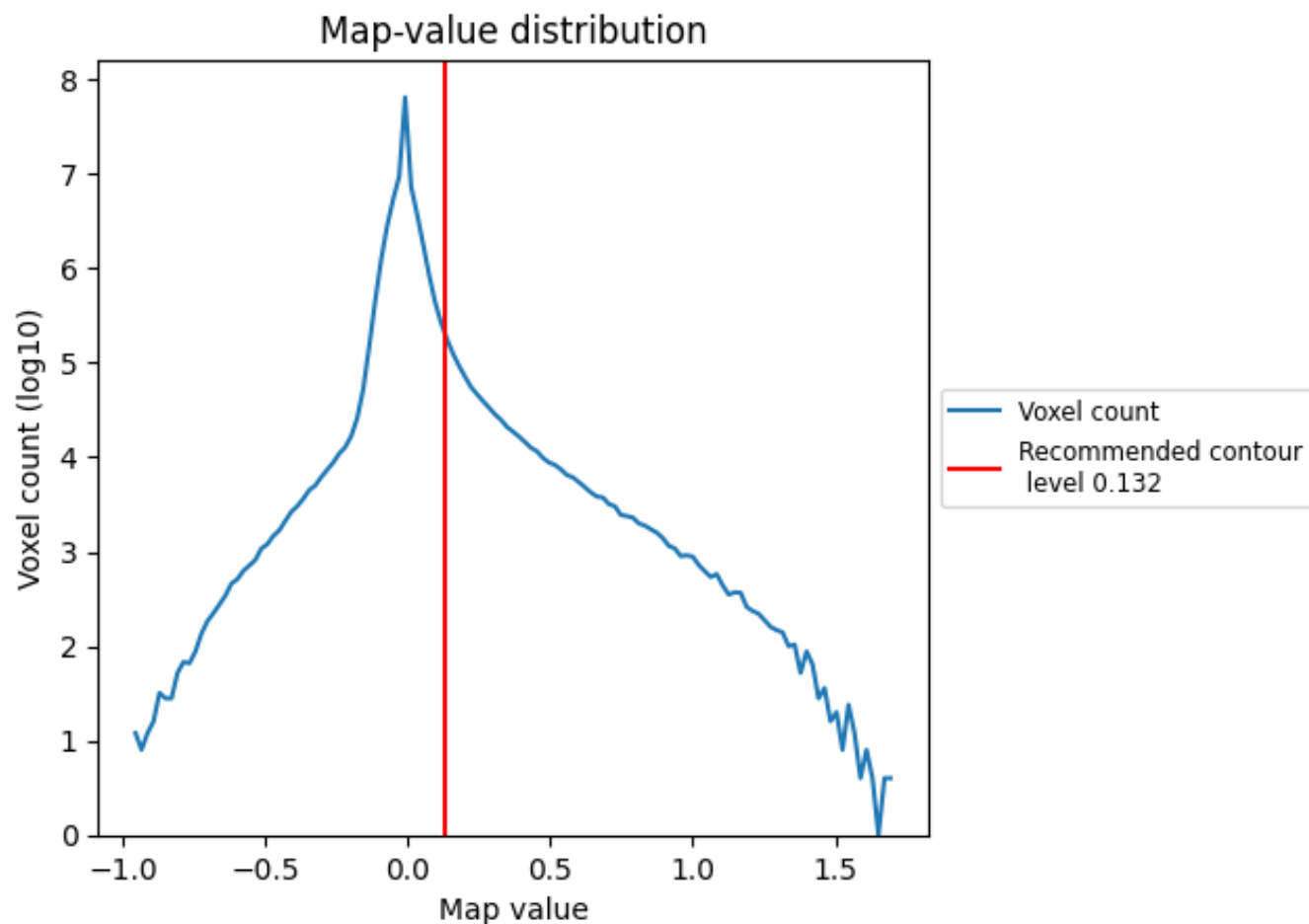


Z

7 Map analysis [i](#)

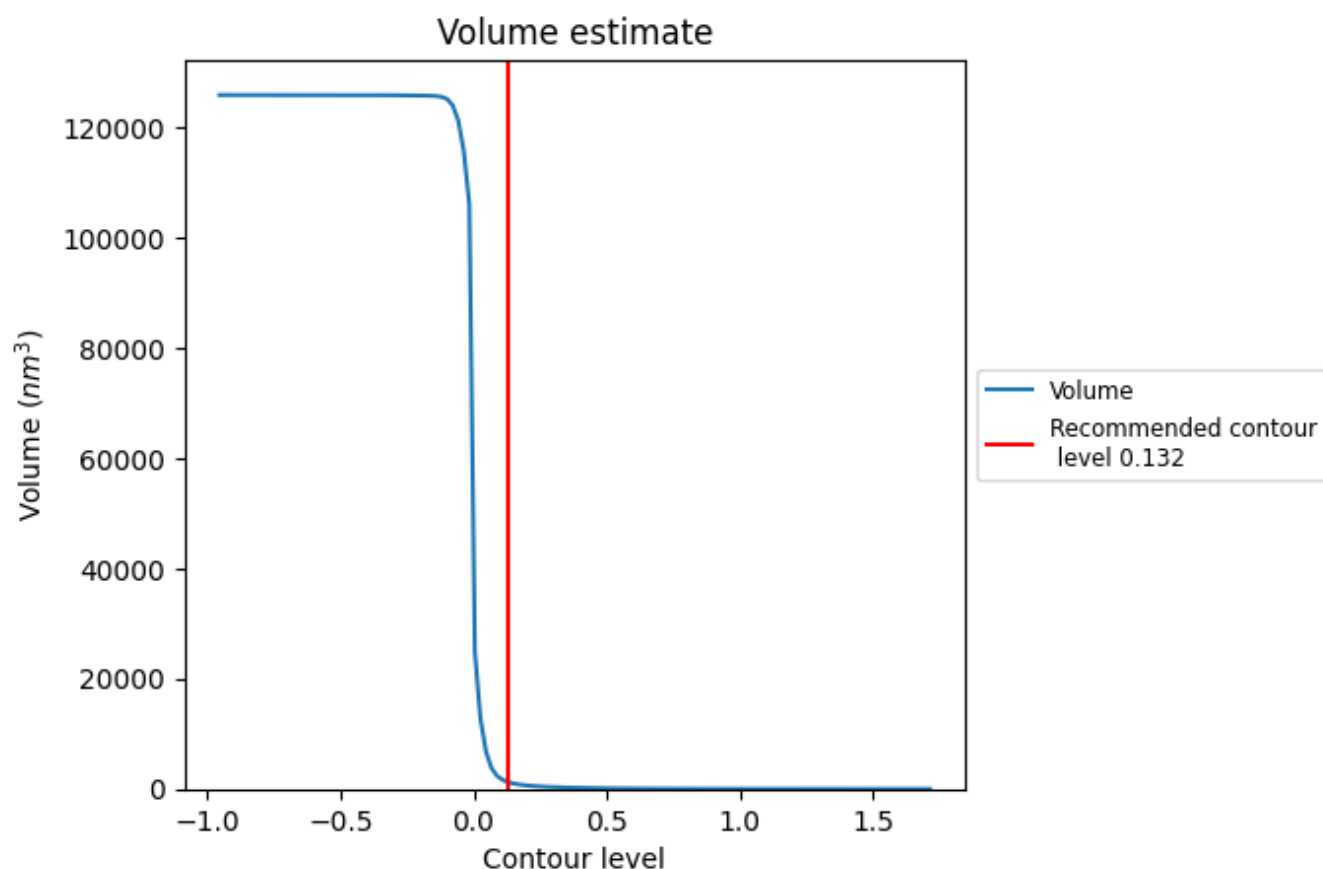
This section contains the results of statistical analysis of the map.

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.

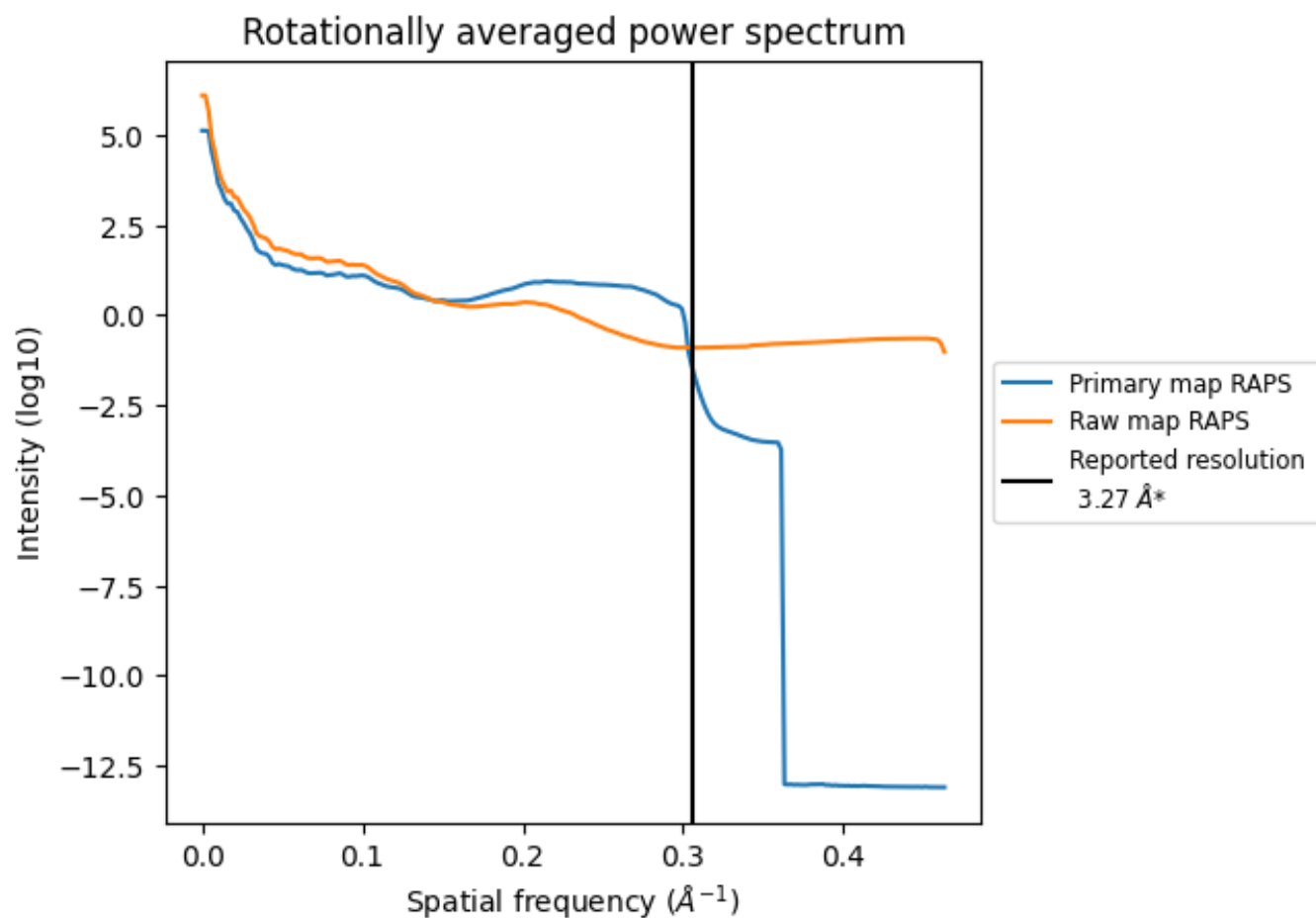
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1213 nm^3 ; this corresponds to an approximate mass of 1096 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 ⓘ

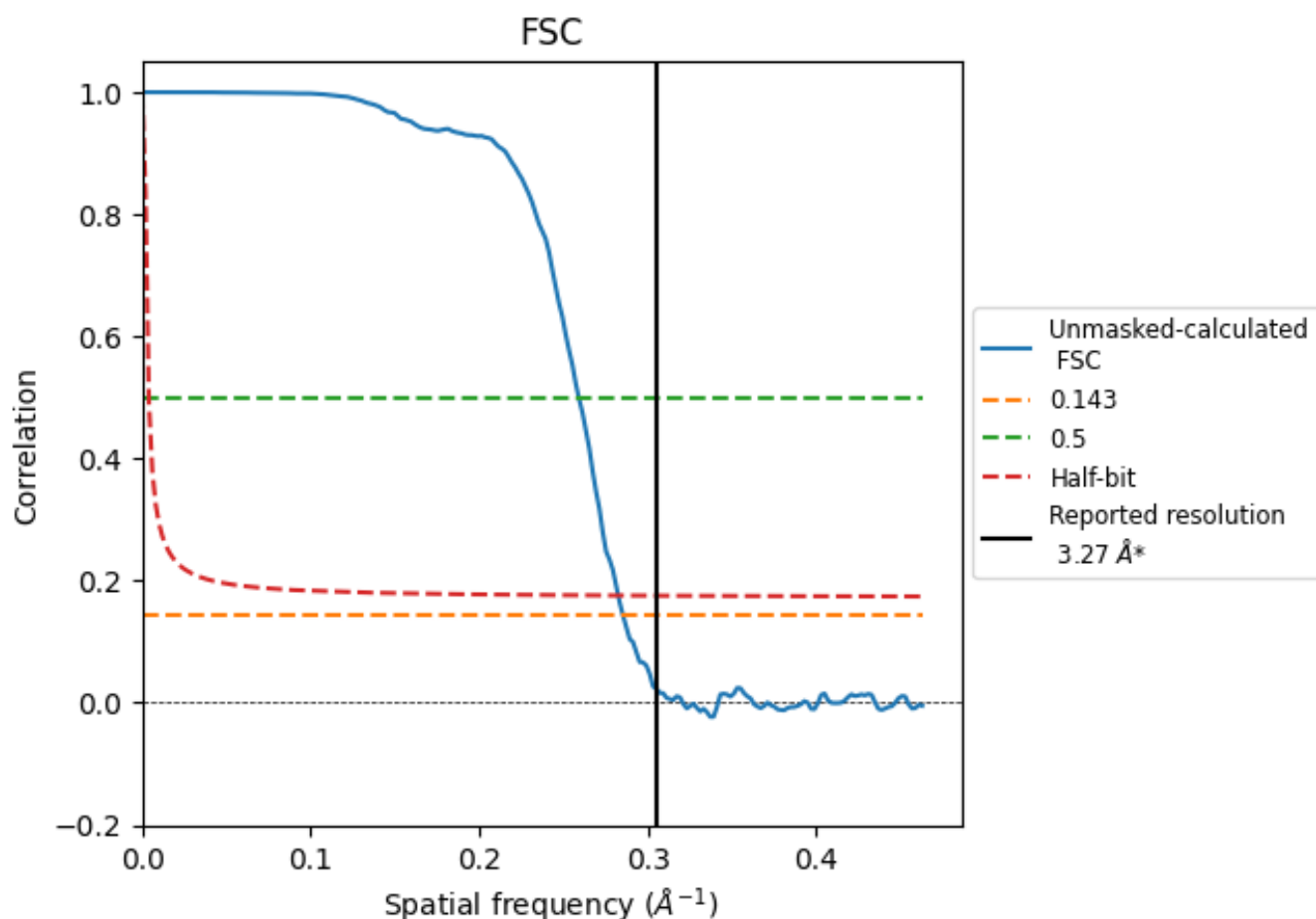


*Reported resolution corresponds to spatial frequency of $0.306 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.306 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	3.86	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

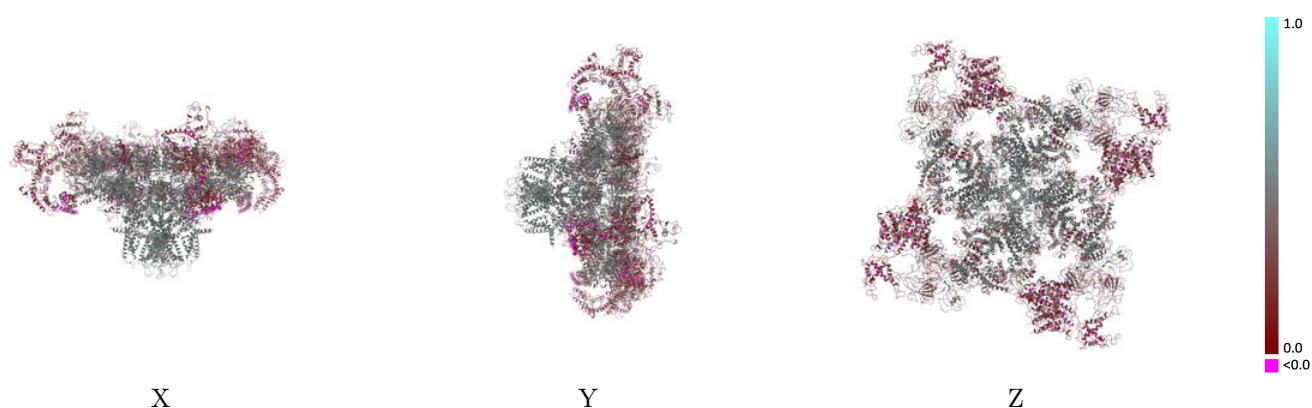
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21861 and PDB model 6WOU. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

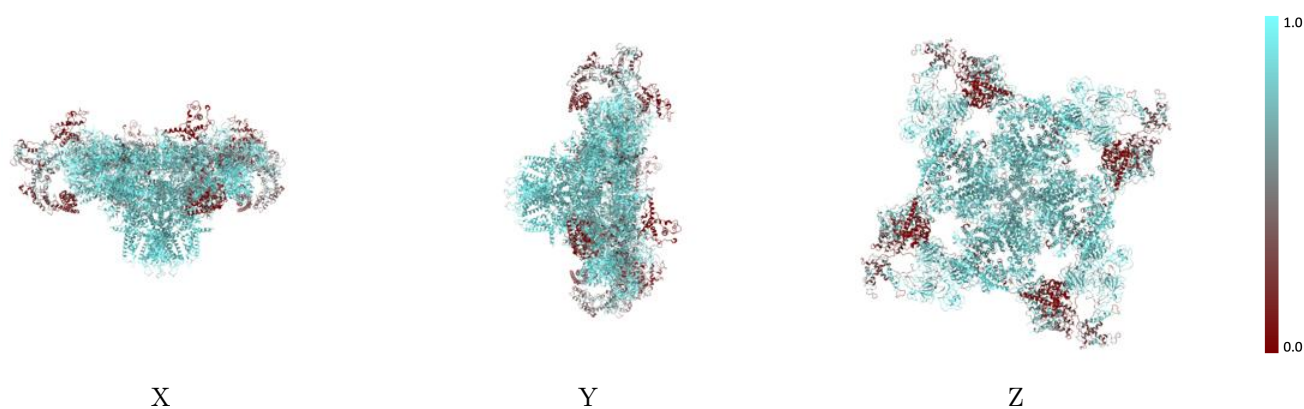
This section was not generated.

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



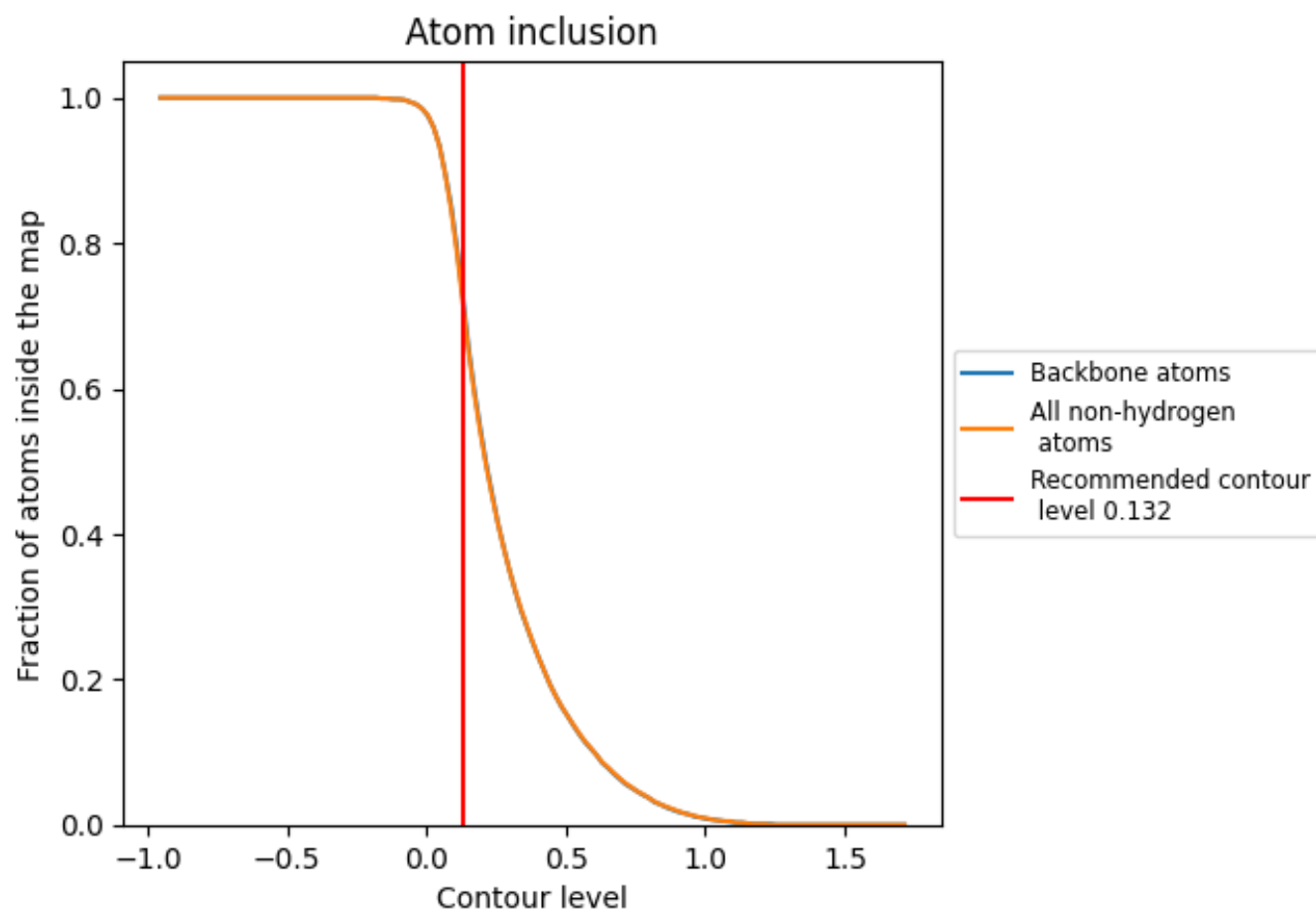
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.132).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7120	0.3760
A	0.7110	0.3740
B	0.7110	0.3730
C	0.7110	0.3740
D	0.7110	0.3740
E	0.8710	0.4550
F	0.8720	0.4560
G	0.8670	0.4560
H	0.8690	0.4580

1.0

0.0

<0.0