



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:44 AM UTC

PDB ID : 8SER / pdb_00008ser
EMDB ID : EMD-40426
Title : Cryo-EM Structure of RyR1 + Adenosine
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.42 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:

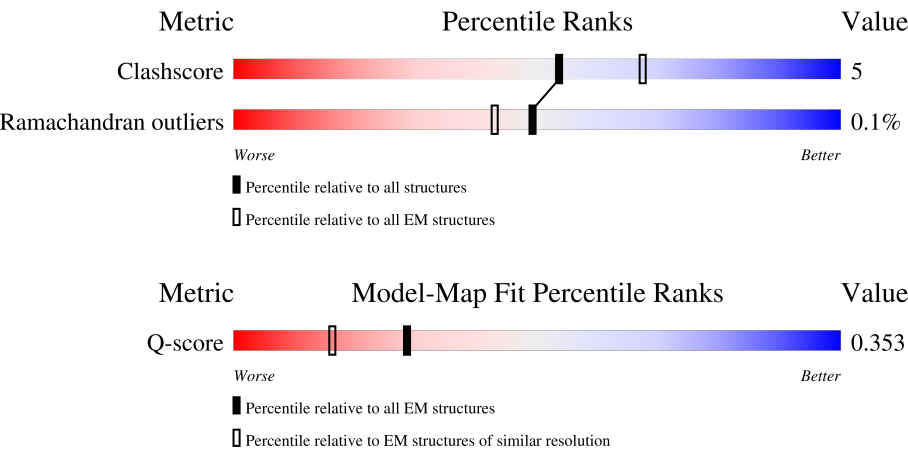
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.42 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	-
Q-score	-	25397	13959 (2.92 - 3.92)

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	5037	12% 75% 12% 13%
1	B	5037	12% 75% 12% 13%
1	C	5037	13% 74% 12% 13%
1	D	5037	12% 75% 12% 13%
2	E	350	26% 5% 69%

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Mol	Chain	Length	Quality of chain
2	F	350	 26% 5% 69%
2	G	350	 26% 5% 69%
2	H	350	 26% 5% 69%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 142952 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4376	Total 34900	C 22201	N 6022	O 6441	S 236	9	0
1	B	4376	Total 34900	C 22201	N 6022	O 6441	S 236	9	0
1	C	4376	Total 34900	C 22201	N 6022	O 6441	S 236	9	0
1	D	4376	Total 34900	C 22201	N 6022	O 6441	S 236	9	0

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	F	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	G	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	H	107	Total 818	C 516	N 144	O 154	S 4	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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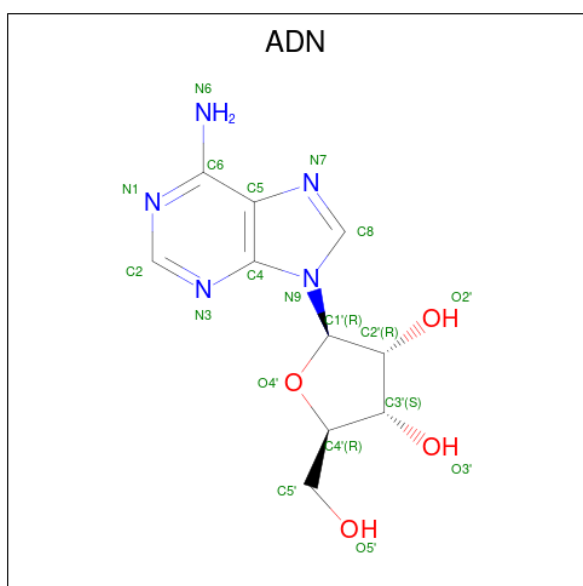
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			19	10	5	4	
3	B	1	Total	C	N	O	0
			19	10	5	4	
3	C	1	Total	C	N	O	0
			19	10	5	4	
3	D	1	Total	C	N	O	0
			19	10	5	4	

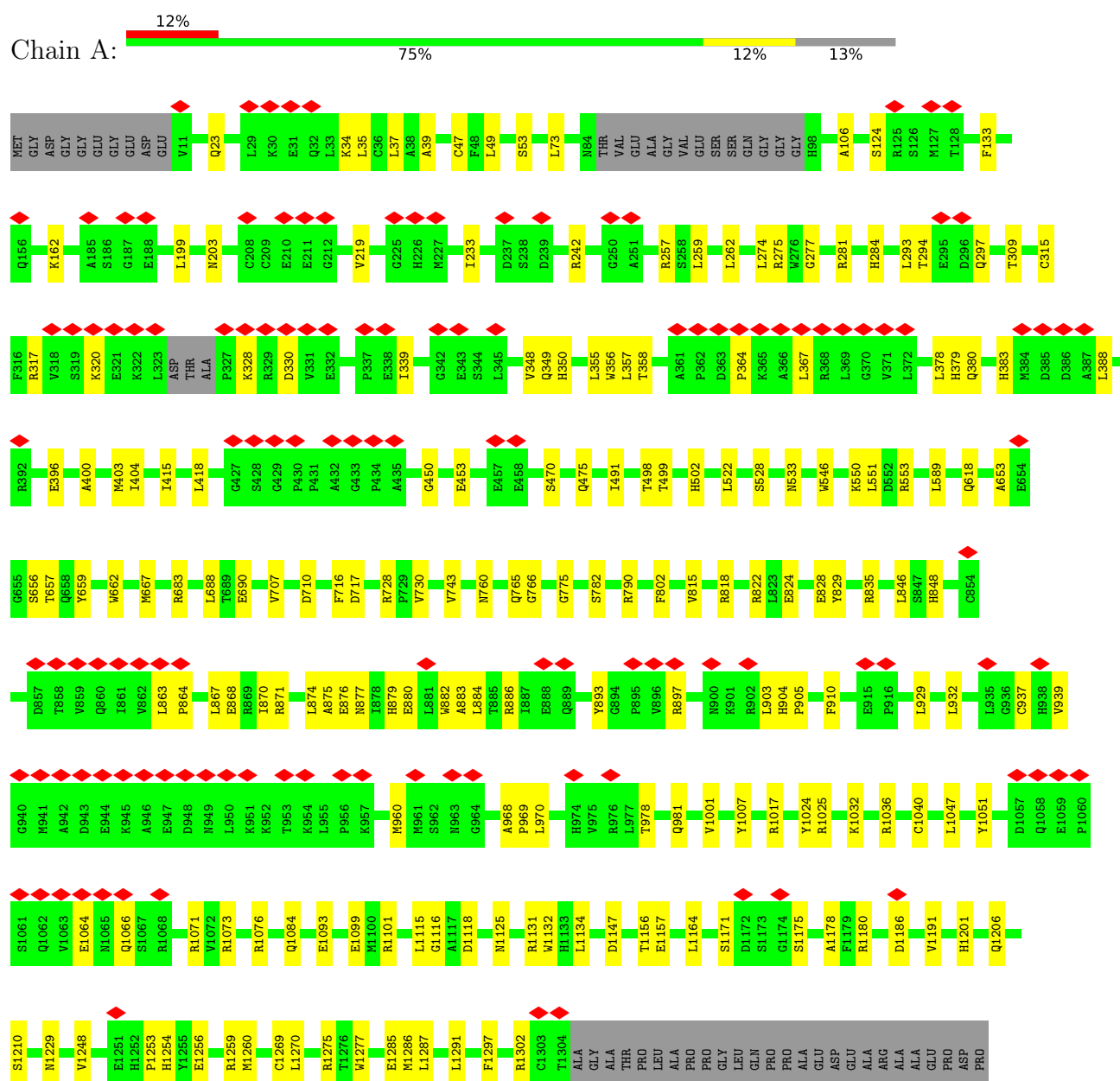
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	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.

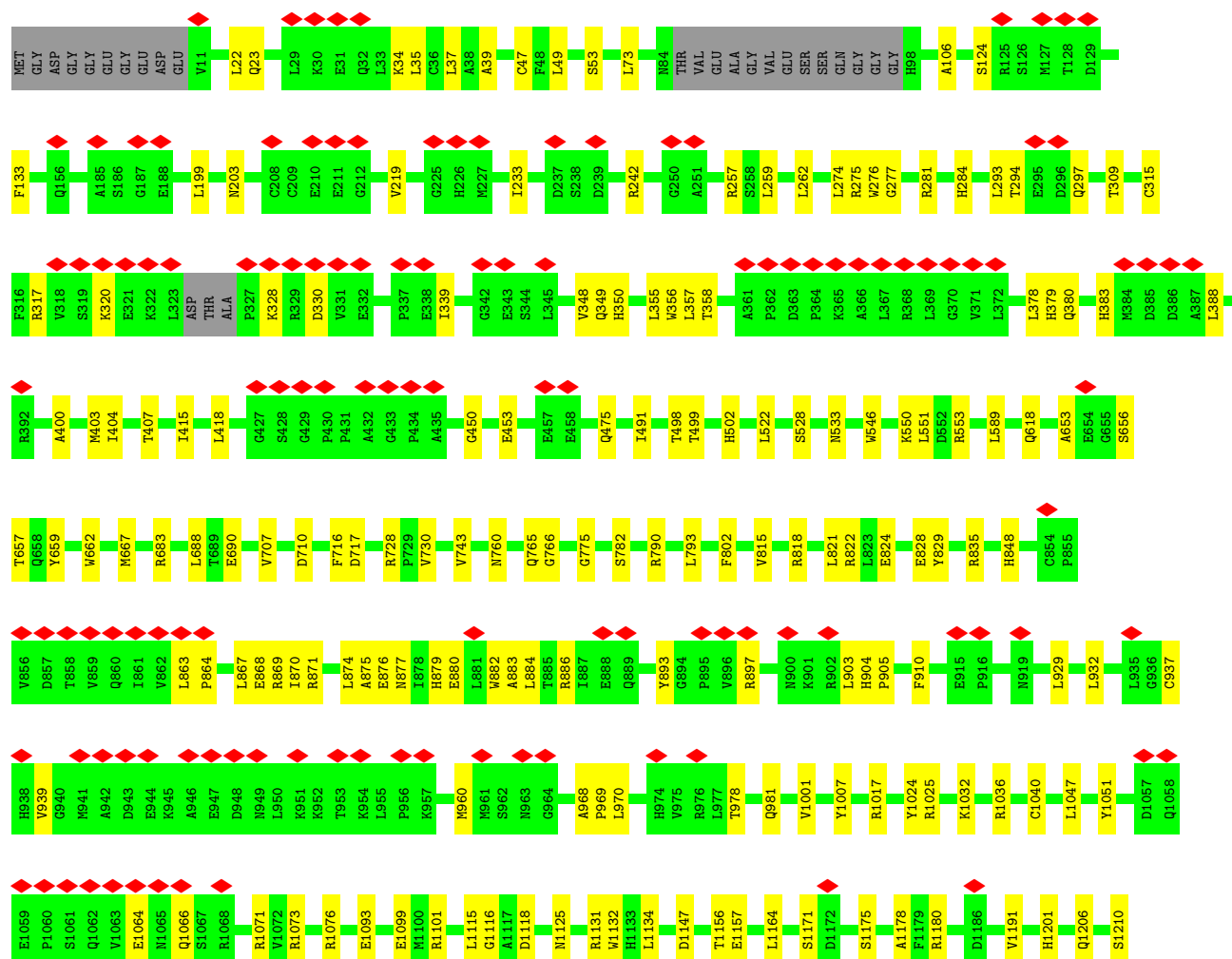
• Molecule 1: Ryanodine receptor 1

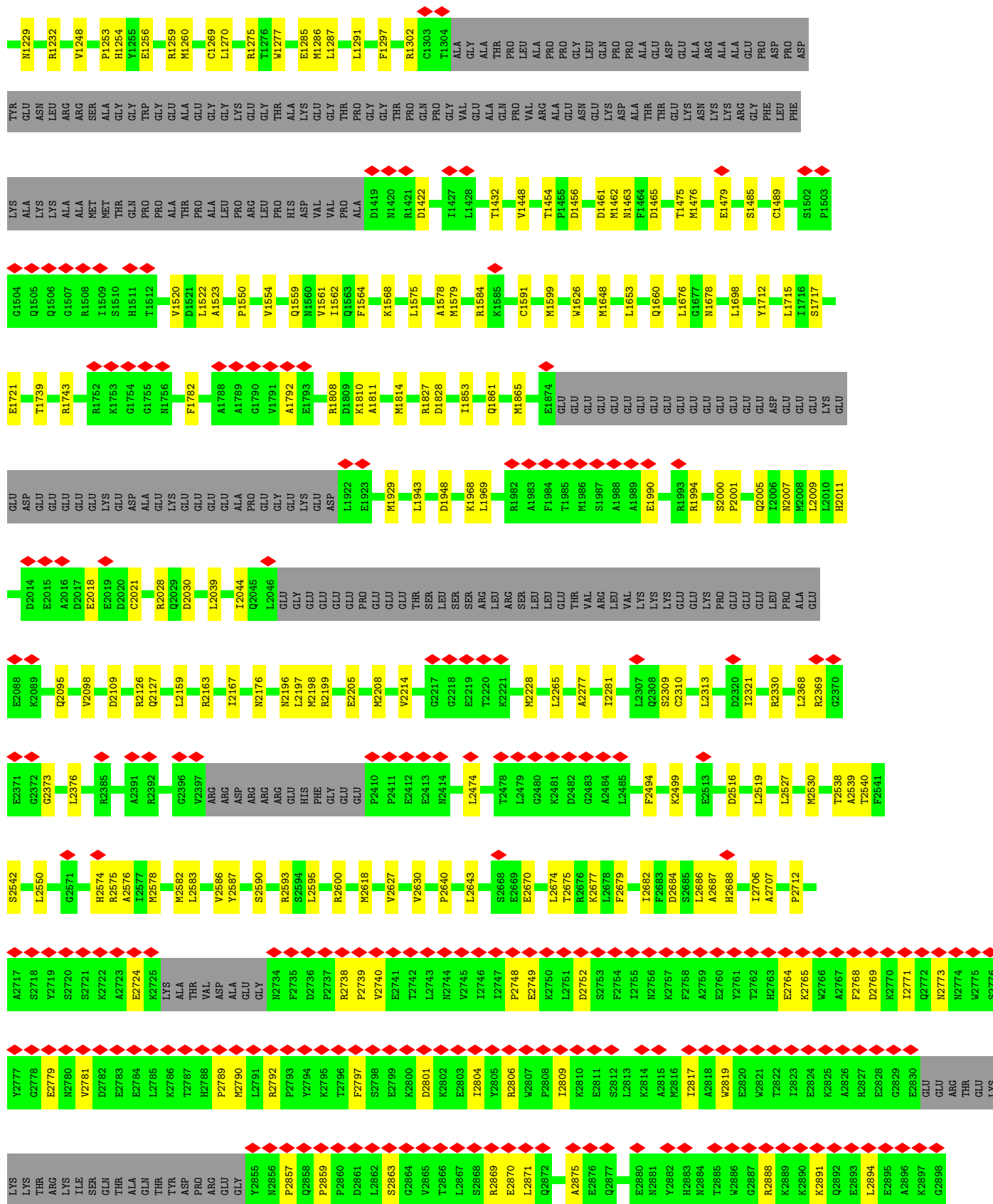




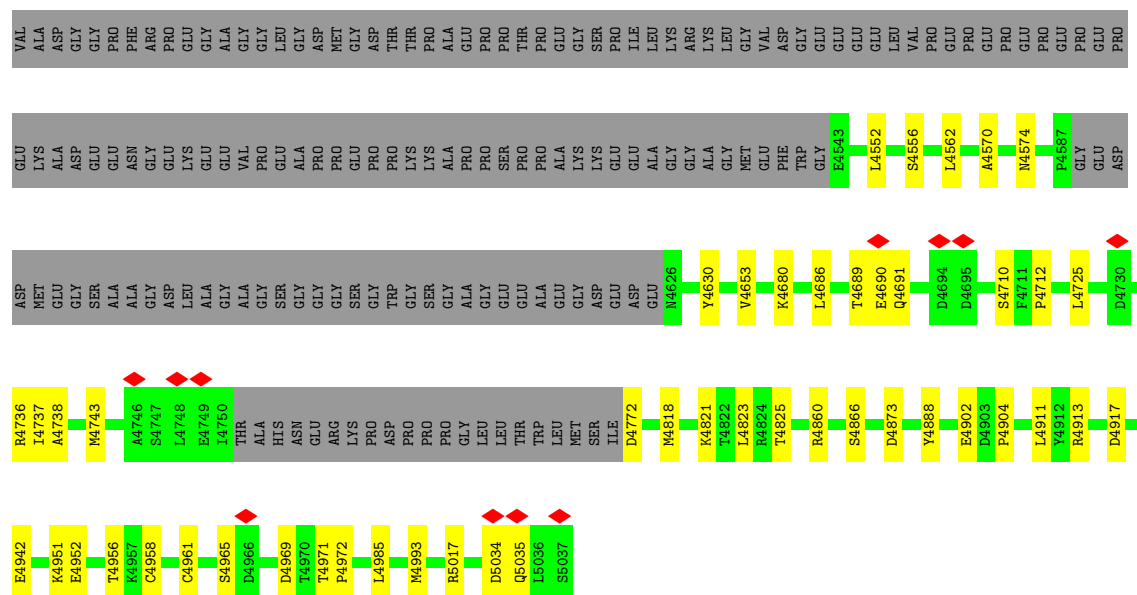


- Molecule 1: Ryanodine receptor 1

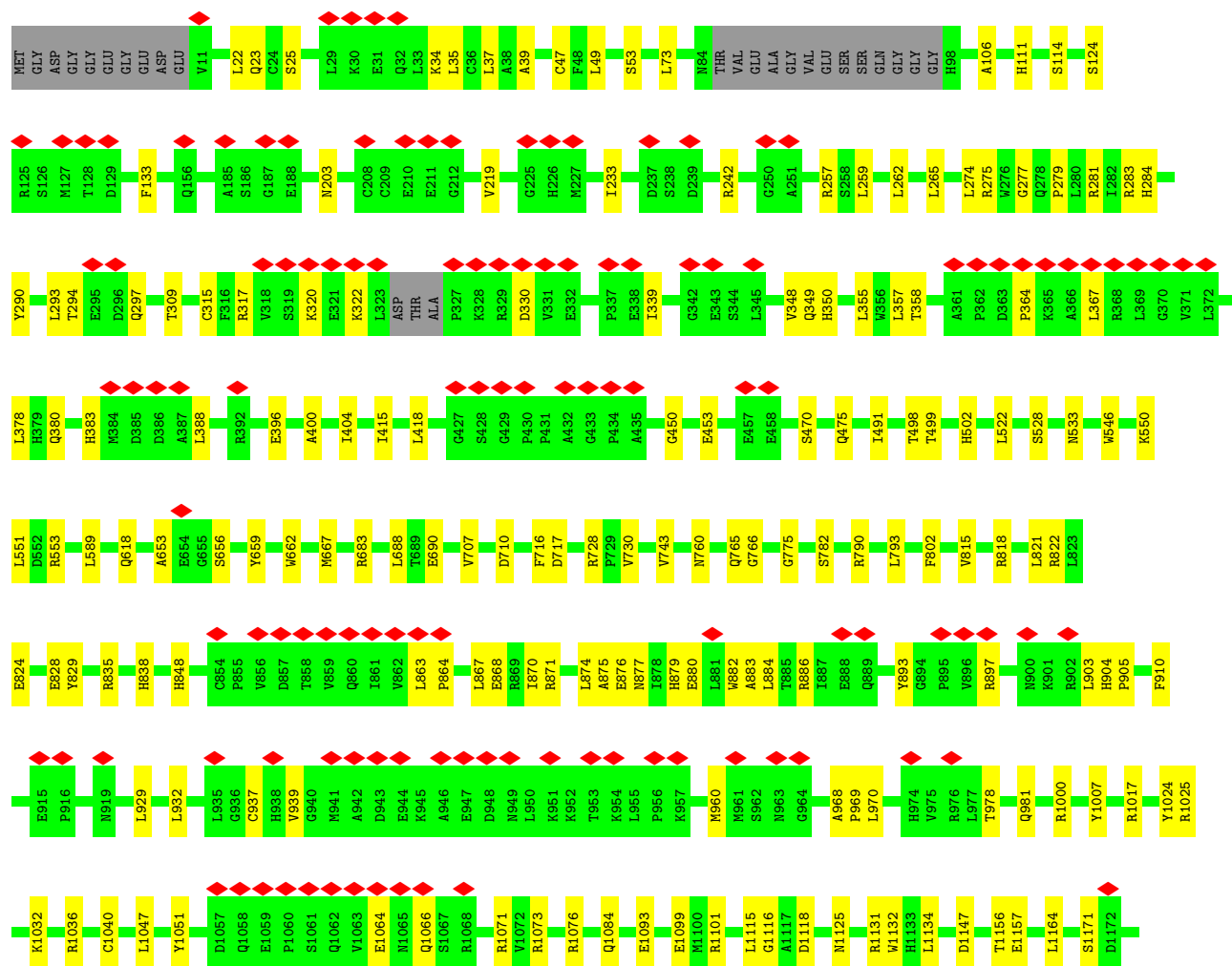
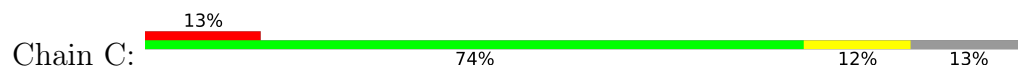






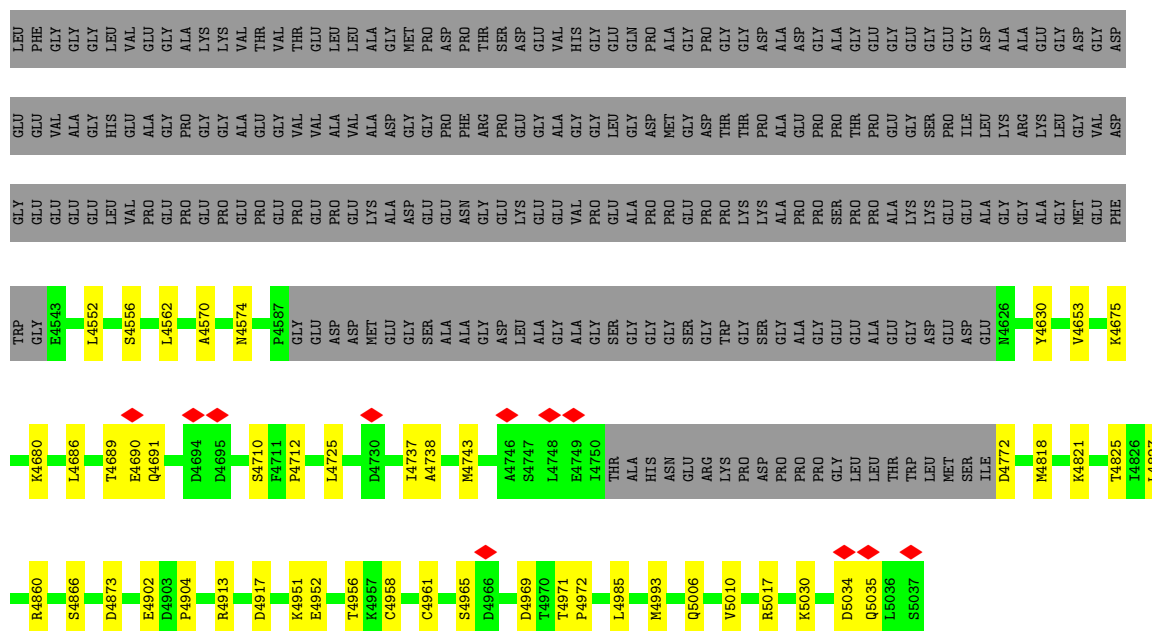


• Molecule 1: Ryanodine receptor 1

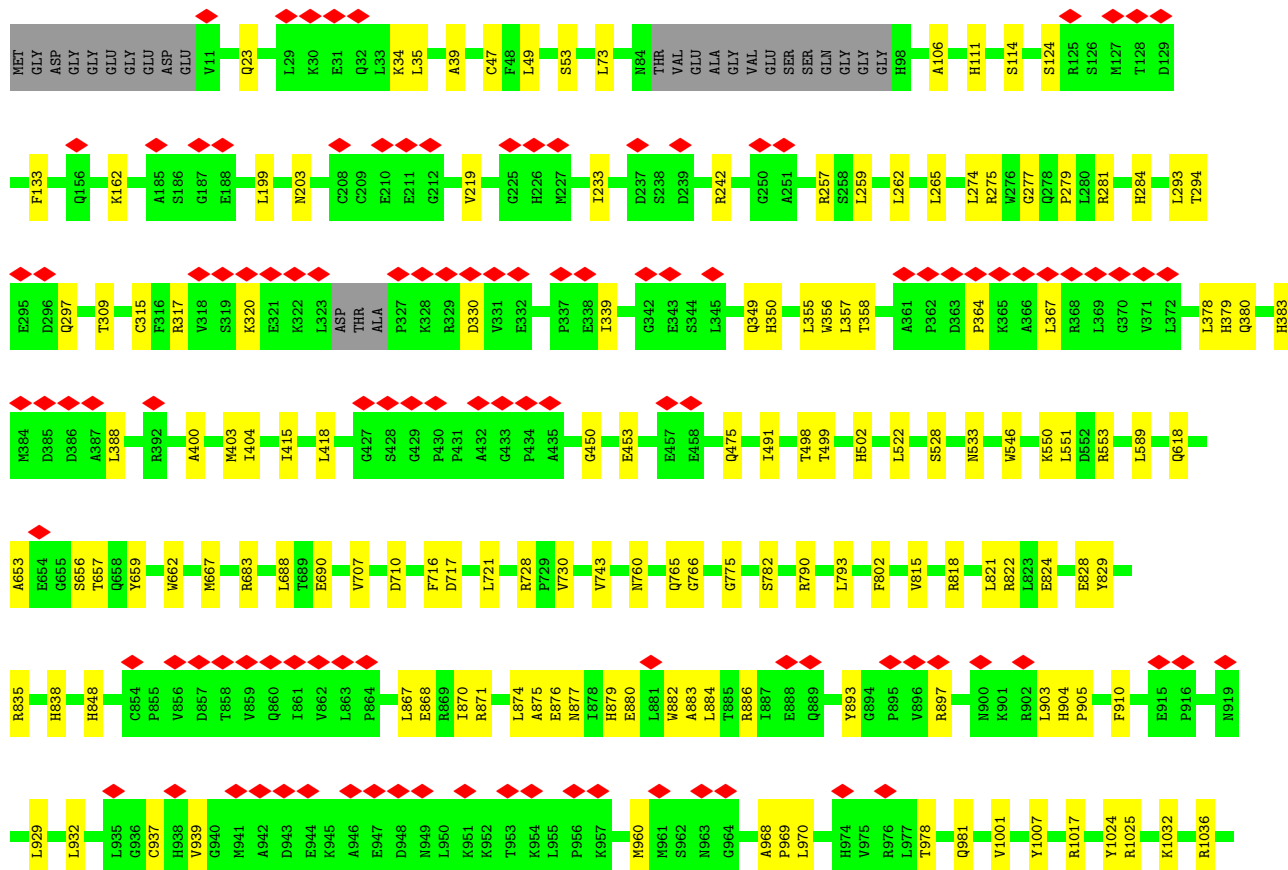
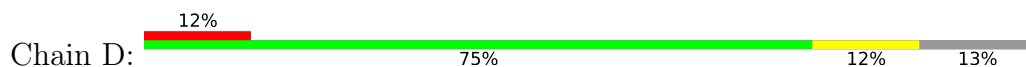




ALA	K4214	D4092	K3948	GLU	S3600	THR	E3382	E3265	H3146	K3036	GLY	A2879
ARG	E4224	F4093	K3959	GLY	A3601	LYS	A3383	K3266	H3146	K3036	LEU	E2880
LEU	G4225	Q4094	E3967	GLU	V3602	LYS	K3384	V3269	D3154	E3037	LYS	Y2881
ARG	G4226	K4095	E3968	ASN	H3605	LYS	A3385	E3271	I3157	K3045	ASP	H2882
SER	E4227	A4096	I3969	GLY	E3610	R3498	A3386	I3272	I3157	A3048	GLU	H2883
LEU	A4228	D4098	T3974	ALA	H3611	G3500	A3387	I3273	I3158	L2946		T2885
TYR		S4099	T3974	GLU	H3612	R3501	E3388	I3274	D3159	D2947		H2886
ARG		Q4100	T3974	GLU	P3612	D3501	E3389	P3275	D3160	H3052		G2887
SER	E4232	Q4101	T3974	GLU	Y3613	R3502	E3390	M3276	Q3162	R3053		R2888
LEU	I4242	K4102	Q3978		K3614	Y3503	E3391		V3163			K2889
ARG		Q4103	S3979		S3615	Q3506	E3286		S3164	G3058		R2890
ARG	E4253	F4104	L3980		K3616	Q3506	R3287		R3167	T3059		K2891
VAL	P4254	T4104	R3984		K3617	I3510	L3393		T3169	P3062		Q2892
ARG		G4105	L3985		A3618	I3514			T3169	P3062		K2891
ARG	GLU	P4106	K4002		V3619	L3514			S3171	V3065		Q2892
LEU	GLY	E4107	R3769		W3620	N3523	P3292		S3171	V3065		E2893
LEU	PRO	I4108	L3770		H3621	M3524	P3294		N3180	L3068		L2894
ARG	GLU	Q4109	H3771		K3622	I3533	A3295		N3180	L3068		E2895
THR	ALA	F4110	R3773		L3623	T3538	L3296		V3183	L3075		A2996
ALA	ASP	L4111	D4018		L3624	A3541	P3297		E3184	M3081		K2897
ALA	ASP	L4112	L4019		L3625	T3538	A3298		K3185	E2978		G2898
ARG	GLU	S4115	G3788		S3626	A3541	G3299		Q3209	A2979		G2899
GLU	ALA	E4116	T3797		K3626	L3542	A3300		L3210	V2980		G2900
ALA	MET	A4117	L3835		Q3627	K3543	P3301		L3210	V2981		T2901
THR	GLY	D4118	L3835		R3628	K3543	P3302			S2982		H2902
LEU	GLU	E4119	S3840		R3629	D3544	P3303			S2983		F2903
LEU	ALA	N4120	K3852		R3630	T3545	L3316			G2984		L2904
ALA	ALA	E4121			A3631	D3546	I3322			R2985		L2905
LEU	GLY	M4122	V4049		V3632	E3547	L3322			V2986		V2906
TRP	ALA	M4064			V3633	E3548	N3325		M3106	E2987		F2907
ALA		F4065			A3634	N3555	N3326		V3107	K2988		V2908
GLU	GLU	L4066			C3635	N3556	K3329		L3110	S2989		D2909
VAL	GLY	R4067			F3636	L3557	F3469		R3111	P2990		T2910
ALA	ALA	L4068			R3637	H3558	S3468		G3113	H2991		L2911
ARG	ALA	K4069			A3659	R3558	L3470		K3114	E2992		T2912
ALA	GLY	D4070			L3663	G3560	L3471		V3115	Q2993		
ALA	ALA	I4071			G3659	G3561	T3471		S3116	F2997		A2913
GLY	GLY	Q4133			L3663	G3562	A3472		GLN	K2914		K2914
ALA	ALA	D4138			G3681	E3564	D3473		ALA	Q3007		E2915
ALA	THR	N4142			E3682	E3564	S3474		ARG	Q3008		K2916
ALA	VAL	E4075			E3683	E3565	K3475		THR	Y3009		A2917
ALA	ALA	A4076			Q3683	G3565	S3476		GLN	F3010		R2918
GLY	ALA	D4079			E3684	L3579	K3477		VAL	N3012		D2919
ALA	GLY	Y4080			E3685	P3580	M3478		K3123	R2920		R2920
LEU	ALA	V4081			E3686	G3581	A3479		G3124	E2921		E2921
ARG	THR	F4163			E3687	R3582	LYS			F3017		K2922
ALA	ALA	T4082			E3688	E3583	ALA		M3239	T3020		K2922
LEU	ARG	D4083			E3689	E3584	GLY		V3245	P3021		A2923
TRP	LEU	P4084			E3690	D3585	ASP			G3022		Q2924
GLY	ALA	R4085			V3690	E3586	ALA			K3023		E2925
SER	ALA	E4182			E3691	A3586	GLN			L2926		L2926
	ALA	I4183			E3692	D3587	SER			V3024		L2927
	ALA	R4188			E3692	D3587	GLY			L3025		K2928
		E4196			P3695	I3592	GLY			G3026		F2929
					D3696	V3596	SER			S3027		L2930
					Q3700		ASP			G3028		Q2931
					Y3722		GLN					M2932
					E3736		GLU					N2933
							ARG					G2934
												Y2935
												A2936
												K2939

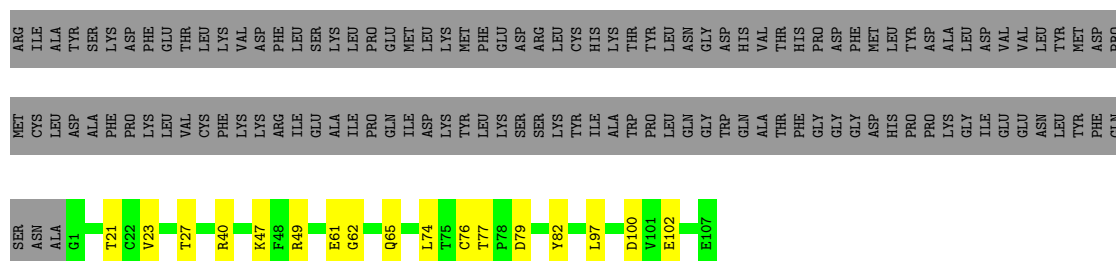


• Molecule 1: Ryanodine receptor 1

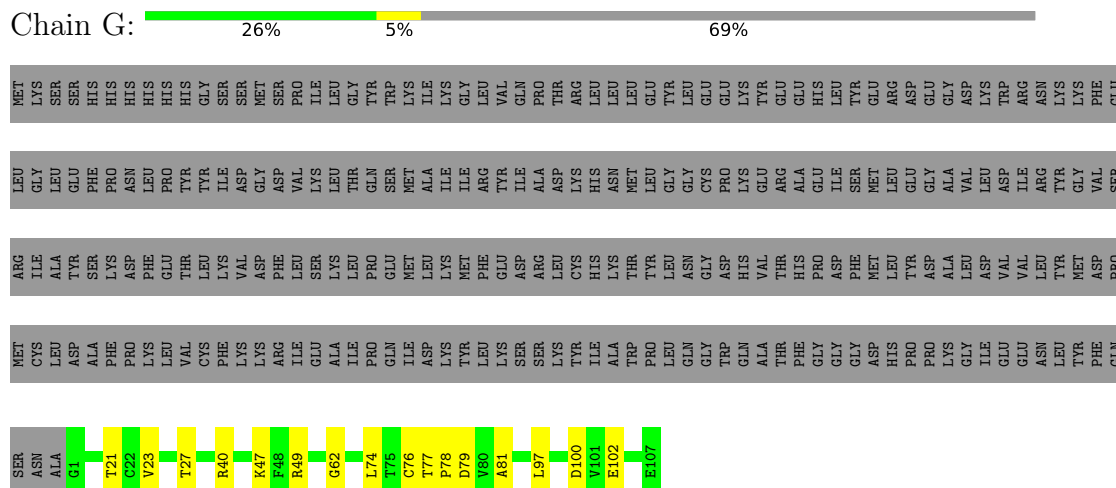




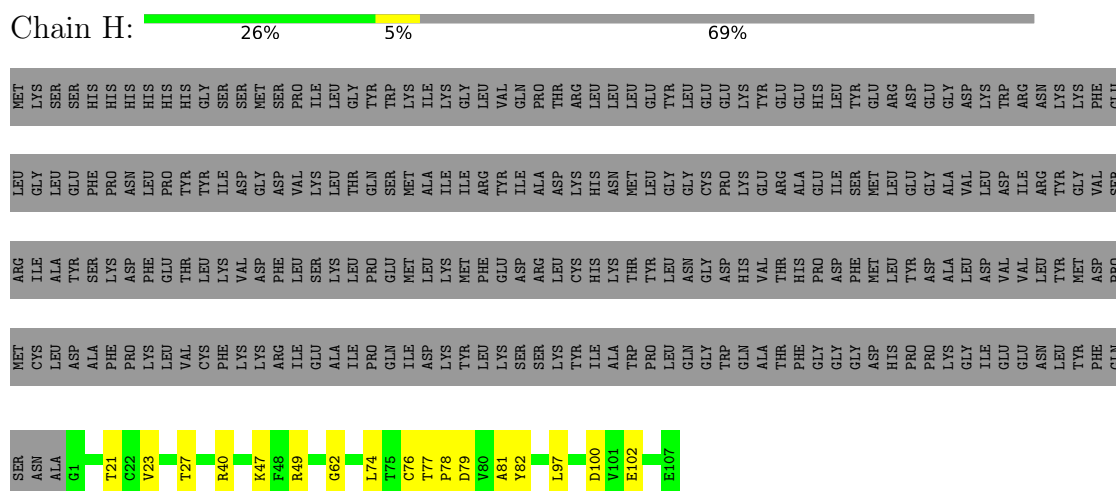




- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51504	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.346	Depositor
Minimum map value	-0.409	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.387	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, 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	0.27	0/35714	0.59	6/48365 (0.0%)
1	B	0.27	0/35714	0.59	6/48365 (0.0%)
1	C	0.27	0/35714	0.59	6/48365 (0.0%)
1	D	0.27	0/35714	0.59	6/48365 (0.0%)
2	E	0.23	0/834	0.53	0/1123
2	F	0.23	0/834	0.53	0/1123
2	G	0.23	0/834	0.53	0/1123
2	H	0.23	0/834	0.53	0/1123
All	All	0.27	0/146192	0.59	24/197952 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4178	LEU	CA-C-N	-8.77	116.13	122.18
1	A	4178	LEU	C-N-CA	-8.77	116.13	122.18
1	C	4178	LEU	CA-C-N	-8.75	116.14	122.18
1	C	4178	LEU	C-N-CA	-8.75	116.14	122.18
1	B	4178	LEU	CA-C-N	-8.73	116.16	122.18
1	B	4178	LEU	C-N-CA	-8.73	116.16	122.18
1	D	4178	LEU	CA-C-N	-8.73	116.16	122.18
1	D	4178	LEU	C-N-CA	-8.73	116.16	122.18
1	C	3615	SER	CA-C-N	5.33	131.72	121.54
1	C	3615	SER	C-N-CA	5.33	131.72	121.54
1	B	3615	SER	CA-C-N	5.32	131.70	121.54
1	B	3615	SER	C-N-CA	5.32	131.70	121.54
1	D	3615	SER	CA-C-N	5.31	131.67	121.54
1	D	3615	SER	C-N-CA	5.31	131.67	121.54
1	A	3615	SER	CA-C-N	5.30	131.67	121.54
1	A	3615	SER	C-N-CA	5.30	131.67	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4196	GLU	CB-CA-C	-5.25	102.39	110.78
1	C	4196	GLU	CB-CA-C	-5.24	102.40	110.78
1	A	4196	GLU	CB-CA-C	-5.24	102.40	110.78
1	D	4196	GLU	CB-CA-C	-5.22	102.43	110.78
1	A	905	PRO	N-CA-C	5.08	122.94	112.47
1	C	905	PRO	N-CA-C	5.07	122.92	112.47
1	D	905	PRO	N-CA-C	5.07	122.92	112.47
1	B	905	PRO	N-CA-C	5.07	122.91	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	34900	0	34530	358	0
1	B	34900	0	34530	363	0
1	C	34900	0	34530	367	0
1	D	34900	0	34530	362	0
2	E	818	0	824	8	0
2	F	818	0	824	9	0
2	G	818	0	824	8	0
2	H	818	0	824	9	0
3	A	19	0	13	0	0
3	B	19	0	13	0	0
3	C	19	0	13	0	0
3	D	19	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	142952	0	141468	1473	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 5.

All (1473) 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:B:1810:LYS:HG2	1:B:1814:MET:HE2	1.72	0.72
1:C:1810:LYS:HG2	1:C:1814:MET:HE2	1.72	0.72
1:D:1810:LYS:HG2	1:D:1814:MET:HE2	1.72	0.72
1:A:1810:LYS:HG2	1:A:1814:MET:HE2	1.72	0.72
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.64	0.70
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.64	0.69
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.65	0.68
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.65	0.68
1:C:667:MET:HE1	1:C:743:VAL:HG22	1.78	0.66
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.78	0.65
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.29	0.65
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.78	0.65
1:D:667:MET:HE1	1:D:743:VAL:HG22	1.78	0.65
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.78	0.65
1:A:1476:MET:HB2	1:A:1485:SER:HB3	1.79	0.64
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.78	0.64
1:B:667:MET:HE1	1:B:743:VAL:HG22	1.78	0.64
1:A:667:MET:HE1	1:A:743:VAL:HG22	1.78	0.64
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.79	0.64
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.80	0.64
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.29	0.64
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.29	0.64
1:D:2519:LEU:HD12	1:D:2578:MET:HE3	1.80	0.64
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.80	0.64
1:A:2519:LEU:HD12	1:A:2578:MET:HE3	1.80	0.63
1:C:1476:MET:HB2	1:C:1485:SER:HB3	1.79	0.63
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.79	0.63
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.80	0.63
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.79	0.63
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.79	0.63
1:C:3969:ILE:HD11	1:C:3980:LEU:HD13	1.80	0.63
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.79	0.63
1:D:3969:ILE:HD11	1:D:3980:LEU:HD13	1.81	0.63
1:D:1476:MET:HB2	1:D:1485:SER:HB3	1.79	0.63
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.80	0.63
1:B:1476:MET:HB2	1:B:1485:SER:HB3	1.79	0.63
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.81	0.62
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.33	0.62
1:B:2929:PHE:O	1:B:2933:ASN:ND2	2.33	0.62
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.81	0.62
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.33	0.62
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.30	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.62
1:C:2519:LEU:HD12	1:C:2578:MET:HE3	1.80	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.79	0.62
1:B:2519:LEU:HD12	1:B:2578:MET:HE3	1.80	0.62
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.32	0.62
1:C:2929:PHE:O	1:C:2933:ASN:ND2	2.33	0.62
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.80	0.62
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.81	0.61
1:A:3969:ILE:HD11	1:A:3980:LEU:HD13	1.81	0.61
1:B:3969:ILE:HD11	1:B:3980:LEU:HD13	1.81	0.61
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.32	0.61
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.33	0.61
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.80	0.61
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.33	0.61
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.33	0.61
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.81	0.61
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.61
1:A:2929:PHE:O	1:A:2933:ASN:ND2	2.33	0.61
1:D:2929:PHE:O	1:D:2933:ASN:ND2	2.33	0.61
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.34	0.61
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.83	0.61
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.83	0.61
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.29	0.61
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.83	0.61
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.83	0.61
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.82	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.61
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.83	0.60
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.32	0.60
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.34	0.60
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.83	0.60
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.82	0.60
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.83	0.60
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.84	0.60
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.83	0.60
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.34	0.60
2:G:40:ARG:NH2	2:G:102:GLU:OE1	2.34	0.60
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.84	0.60
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.35	0.60
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.30	0.60
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.35	0.60
1:A:275:ARG:HH12	1:A:330:ASP:HA	1.67	0.59
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.82	0.59
1:B:2749:GLU:HG3	1:B:2752:ASP:HB3	1.85	0.59
1:A:1575:LEU:HB3	1:A:1579:MET:HE2	1.84	0.59
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.68	0.59
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.32	0.59
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.68	0.59
1:D:2749:GLU:HG3	1:D:2752:ASP:HB3	1.85	0.59
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.82	0.59
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.32	0.59
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.32	0.59
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	1.85	0.59
1:A:2007:ASN:O	1:A:2011:HIS:HB2	2.03	0.59
1:D:275:ARG:HH12	1:D:330:ASP:HA	1.67	0.59
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.83	0.59
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.84	0.59
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.68	0.59
1:A:2749:GLU:HG3	1:A:2752:ASP:HB3	1.85	0.59
1:A:4689:THR:OG1	1:A:4690:GLU:N	2.36	0.59
1:B:275:ARG:HH12	1:B:330:ASP:HA	1.67	0.59
1:B:1285:GLU:HB2	1:B:1462:MET:HE1	1.85	0.59
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.36	0.59
1:C:1285:GLU:HB2	1:C:1462:MET:HE1	1.85	0.58
1:C:2007:ASN:O	1:C:2011:HIS:HB2	2.03	0.58
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.30	0.58
1:A:3579:LEU:HB2	1:A:3582:ARG:HG2	1.85	0.58
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.84	0.58
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.84	0.58
1:C:2749:GLU:HG3	1:C:2752:ASP:HB3	1.85	0.58
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.68	0.58
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.36	0.58
1:D:2007:ASN:O	1:D:2011:HIS:HB2	2.03	0.58
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.36	0.58
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.35	0.58
1:B:2007:ASN:O	1:B:2011:HIS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4689:THR:OG1	1:B:4690:GLU:N	2.36	0.58
1:C:4068:LEU:HD22	1:C:4111:LEU:HD11	1.86	0.58
1:C:4689:THR:OG1	1:C:4690:GLU:N	2.36	0.58
1:D:4068:LEU:HD22	1:D:4111:LEU:HD11	1.86	0.58
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.77	0.58
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	1.85	0.58
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.37	0.58
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.37	0.58
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	1.85	0.58
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.84	0.58
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.37	0.58
1:C:275:ARG:HH12	1:C:330:ASP:HA	1.67	0.58
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.36	0.58
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.35	0.58
1:B:3579:LEU:HB2	1:B:3582:ARG:HG2	1.85	0.58
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.77	0.58
1:A:882:TRP:O	1:A:886:ARG:NH1	2.37	0.58
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.77	0.58
1:A:4068:LEU:HD22	1:A:4111:LEU:HD11	1.86	0.58
1:C:1575:LEU:HB3	1:C:1579:MET:HE2	1.84	0.58
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.77	0.58
1:B:1575:LEU:HB3	1:B:1579:MET:HE2	1.84	0.58
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	1.85	0.58
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.32	0.58
1:B:4068:LEU:HD22	1:B:4111:LEU:HD11	1.86	0.58
1:C:882:TRP:O	1:C:886:ARG:NH1	2.37	0.58
1:D:4689:THR:OG1	1:D:4690:GLU:N	2.36	0.58
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.37	0.58
1:B:320:LYS:NZ	1:B:383:HIS:O	2.37	0.57
1:B:3132:THR:HG23	1:B:3136:LEU:HB3	1.86	0.57
1:D:882:TRP:O	1:D:886:ARG:NH1	2.37	0.57
1:D:1575:LEU:HB3	1:D:1579:MET:HE2	1.84	0.57
1:A:1285:GLU:HB2	1:A:1462:MET:HE1	1.85	0.57
1:D:320:LYS:NZ	1:D:383:HIS:O	2.37	0.57
1:D:3132:THR:HG23	1:D:3136:LEU:HB3	1.86	0.57
1:B:882:TRP:O	1:B:886:ARG:NH1	2.37	0.57
1:D:1285:GLU:HB2	1:D:1462:MET:HE1	1.85	0.57
1:A:2095:GLN:HA	1:A:2127:GLN:HE21	1.70	0.57
1:C:320:LYS:NZ	1:C:383:HIS:O	2.37	0.57
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.37	0.57
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.38	0.57
1:A:320:LYS:NZ	1:A:383:HIS:O	2.37	0.57
1:B:765:GLN:NE2	1:B:1479:GLU:OE1	2.38	0.57
1:D:765:GLN:NE2	1:D:1479:GLU:OE1	2.37	0.57
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.38	0.57
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.37	0.57
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.37	0.57
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.32	0.57
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.38	0.57
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.87	0.57
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.87	0.57
1:B:39:ALA:HB2	1:B:47:CYS:HA	1.86	0.57
1:C:3132:THR:HG23	1:C:3136:LEU:HB3	1.86	0.57
1:D:2095:GLN:HA	1:D:2127:GLN:HE21	1.70	0.57
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.85	0.57
1:A:3132:THR:HG23	1:A:3136:LEU:HB3	1.86	0.56
1:B:4902:GLU:O	1:B:4913:ARG:NH1	2.38	0.56
1:C:765:GLN:NE2	1:C:1479:GLU:OE1	2.38	0.56
1:C:828:GLU:O	1:C:1073:ARG:NH1	2.38	0.56
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.38	0.56
1:D:39:ALA:HB2	1:D:47:CYS:HA	1.86	0.56
1:B:828:GLU:O	1:B:1073:ARG:NH1	2.38	0.56
1:D:828:GLU:O	1:D:1073:ARG:NH1	2.38	0.56
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.38	0.56
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.87	0.56
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.38	0.56
1:C:3579:LEU:HB2	1:C:3582:ARG:HG2	1.85	0.56
1:B:2095:GLN:HA	1:B:2127:GLN:HE21	1.70	0.56
1:C:4818:MET:SD	1:C:4818:MET:N	2.78	0.56
1:A:39:ALA:HB2	1:A:47:CYS:HA	1.86	0.56
1:C:39:ALA:HB2	1:C:47:CYS:HA	1.86	0.56
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.38	0.56
1:A:4818:MET:SD	1:A:4818:MET:N	2.78	0.56
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.38	0.56
1:D:4902:GLU:O	1:D:4913:ARG:NH1	2.38	0.56
2:E:21:THR:HG22	2:E:49:ARG:HD2	1.87	0.56
2:G:21:THR:HG22	2:G:49:ARG:HD2	1.87	0.56
1:A:765:GLN:NE2	1:A:1479:GLU:OE1	2.37	0.56
1:C:688:LEU:HD23	1:C:690:GLU:H	1.71	0.56
1:D:4818:MET:SD	1:D:4818:MET:N	2.78	0.56
1:A:828:GLU:O	1:A:1073:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.38	0.56
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.87	0.56
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.87	0.56
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.32	0.56
1:C:2095:GLN:HA	1:C:2127:GLN:HE21	1.70	0.56
1:C:4902:GLU:O	1:C:4913:ARG:NH1	2.38	0.56
1:B:4818:MET:N	1:B:4818:MET:SD	2.78	0.56
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.87	0.55
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.87	0.55
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.71	0.55
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.38	0.55
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.38	0.55
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.88	0.55
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.88	0.55
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.88	0.55
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.89	0.55
1:A:688:LEU:HD23	1:A:690:GLU:H	1.71	0.55
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.38	0.55
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.89	0.55
2:H:21:THR:HG22	2:H:49:ARG:HD2	1.87	0.55
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.71	0.55
1:B:3948:LYS:HG2	1:B:4012:LEU:HD22	1.89	0.55
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.40	0.55
1:C:2538:THR:HG23	1:C:2540:THR:H	1.71	0.55
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.89	0.55
1:C:2677:LYS:NZ	1:C:2909:ASP:OD2	2.37	0.55
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.89	0.55
1:B:3219:TYR:OH	1:B:3239:MET:SD	2.65	0.55
1:C:2765:LYS:NZ	1:C:2859:PRO:O	2.39	0.55
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.87	0.55
1:D:281:ARG:NH2	1:D:309:THR:OG1	2.40	0.55
1:D:475:GLN:NE2	1:D:528:SER:O	2.40	0.55
1:D:688:LEU:HD23	1:D:690:GLU:H	1.71	0.55
1:C:475:GLN:NE2	1:C:528:SER:O	2.40	0.55
1:C:3948:LYS:HG2	1:C:4012:LEU:HD22	1.89	0.55
1:D:350:HIS:HB2	1:D:378:LEU:HD21	1.89	0.55
2:F:21:THR:HG22	2:F:49:ARG:HD2	1.87	0.55
1:A:475:GLN:NE2	1:A:528:SER:O	2.40	0.54
1:A:2538:THR:HG23	1:A:2540:THR:H	1.71	0.54
1:B:2679:PHE:HB2	1:B:2706:ILE:HG21	1.90	0.54
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:LEU:HD23	1:B:690:GLU:H	1.70	0.54
1:B:3414:ARG:NH1	1:B:3469:PHE:O	2.38	0.54
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.90	0.54
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.71	0.54
1:D:2765:LYS:NZ	1:D:2859:PRO:O	2.39	0.54
1:A:281:ARG:NH2	1:A:309:THR:OG1	2.40	0.54
1:A:1175:SER:OG	1:A:1180:ARG:NH2	2.38	0.54
1:A:2679:PHE:HB2	1:A:2706:ILE:HG21	1.89	0.54
1:B:475:GLN:NE2	1:B:528:SER:O	2.40	0.54
1:B:2538:THR:HG23	1:B:2540:THR:H	1.71	0.54
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.89	0.54
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.88	0.54
1:A:2001:PRO:HG2	1:A:3864:THR:HB	1.90	0.54
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.88	0.54
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.90	0.54
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.73	0.54
1:A:350:HIS:HB2	1:A:378:LEU:HD21	1.89	0.54
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.89	0.54
1:B:822:ARG:NH1	1:B:824:GLU:OE1	2.40	0.54
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.73	0.54
1:C:2679:PHE:HB2	1:C:2706:ILE:HG21	1.90	0.54
1:D:822:ARG:NH1	1:D:824:GLU:OE1	2.40	0.54
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.73	0.54
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.72	0.54
1:C:2001:PRO:HG2	1:C:3864:THR:HB	1.90	0.54
1:D:1792:ALA:O	1:D:2176:ASN:ND2	2.40	0.54
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	1.90	0.54
1:D:3948:LYS:HG2	1:D:4012:LEU:HD22	1.89	0.54
1:B:1792:ALA:O	1:B:2176:ASN:ND2	2.41	0.54
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.73	0.54
1:D:2679:PHE:HB2	1:D:2706:ILE:HG21	1.90	0.54
1:A:2765:LYS:NZ	1:A:2859:PRO:O	2.39	0.54
1:A:4902:GLU:O	1:A:4913:ARG:NH1	2.38	0.54
1:B:2765:LYS:NZ	1:B:2859:PRO:O	2.39	0.54
1:C:1175:SER:OG	1:C:1180:ARG:NH2	2.38	0.54
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.89	0.54
1:C:281:ARG:NH2	1:C:309:THR:OG1	2.40	0.54
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.89	0.54
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.89	0.54
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.90	0.54
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3524:MET:O	1:D:3595:ARG:NH1	2.41	0.53
1:A:3376:GLU:OE2	1:A:3450:ASN:ND2	2.40	0.53
1:A:3948:LYS:HG2	1:A:4012:LEU:HD22	1.89	0.53
1:B:350:HIS:HB2	1:B:378:LEU:HD21	1.89	0.53
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.90	0.53
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.89	0.53
1:C:822:ARG:NH1	1:C:824:GLU:OE1	2.40	0.53
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.39	0.53
1:D:3376:GLU:OE2	1:D:3450:ASN:ND2	2.40	0.53
1:B:2682:ILE:O	1:B:2686:LEU:HB2	2.09	0.53
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	1.90	0.53
1:B:4952:GLU:O	1:B:4956:THR:HB	2.09	0.53
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.41	0.53
1:D:2677:LYS:NZ	1:D:2909:ASP:OD2	2.37	0.53
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.89	0.53
1:A:3980:LEU:HD23	1:A:3985:LEU:HD22	1.90	0.53
1:B:1175:SER:OG	1:B:1180:ARG:NH2	2.38	0.53
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.73	0.53
1:C:1302:ARG:HG3	1:C:1523:ALA:HB1	1.91	0.53
1:C:2682:ILE:O	1:C:2686:LEU:HB2	2.09	0.53
1:B:2971:GLN:HE22	1:B:3045:LYS:HD3	1.74	0.53
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.42	0.53
1:B:3980:LEU:HD23	1:B:3985:LEU:HD22	1.90	0.53
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.41	0.53
1:C:3376:GLU:OE2	1:C:3450:ASN:ND2	2.40	0.53
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.90	0.53
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.73	0.53
1:D:2001:PRO:HG2	1:D:3864:THR:HB	1.90	0.53
1:D:3980:LEU:HD23	1:D:3985:LEU:HD22	1.90	0.53
1:A:499:THR:HG23	1:A:502:HIS:H	1.74	0.53
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.91	0.53
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.39	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.41	0.53
1:C:350:HIS:HB2	1:C:378:LEU:HD21	1.89	0.53
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.91	0.53
1:C:1066:GLN:OE1	1:C:1463:ASN:ND2	2.42	0.53
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.42	0.53
1:D:2971:GLN:HE22	1:D:3045:LYS:HD3	1.74	0.53
1:D:3316:LEU:HD11	1:D:3346:VAL:HA	1.91	0.53
1:A:1302:ARG:HG3	1:A:1523:ALA:HB1	1.91	0.53
1:A:1792:ALA:O	1:A:2176:ASN:ND2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1066:GLN:OE1	1:B:1463:ASN:ND2	2.41	0.53
1:B:1302:ARG:HG3	1:B:1523:ALA:HB1	1.91	0.53
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.89	0.53
1:D:2538:THR:HG23	1:D:2540:THR:H	1.71	0.53
1:D:2682:ILE:O	1:D:2686:LEU:HB2	2.09	0.53
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.42	0.53
1:D:4952:GLU:O	1:D:4956:THR:HB	2.09	0.53
1:A:822:ARG:NH1	1:A:824:GLU:OE1	2.40	0.53
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.42	0.53
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.41	0.53
1:C:2971:GLN:HE22	1:C:3045:LYS:HD3	1.74	0.53
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.42	0.53
1:A:1066:GLN:OE1	1:A:1463:ASN:ND2	2.41	0.53
1:A:2682:ILE:O	1:A:2686:LEU:HB2	2.09	0.53
1:B:499:THR:HG23	1:B:502:HIS:H	1.74	0.53
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.91	0.53
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	1.91	0.53
1:A:2971:GLN:HE22	1:A:3045:LYS:HD3	1.74	0.53
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	1.90	0.53
1:A:3940:LYS:O	1:A:4002:LYS:NZ	2.38	0.53
1:A:743:VAL:HB	1:A:760:ASN:HA	1.90	0.52
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	1.91	0.52
1:C:3414:ARG:NH1	1:C:3469:PHE:O	2.38	0.52
1:D:1066:GLN:OE1	1:D:1463:ASN:ND2	2.41	0.52
1:D:2687:ALA:O	1:D:2993:GLN:NE2	2.43	0.52
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.41	0.52
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.73	0.52
1:B:3376:GLU:OE2	1:B:3450:ASN:ND2	2.40	0.52
1:D:743:VAL:HB	1:D:760:ASN:HA	1.91	0.52
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.91	0.52
1:D:4112:LEU:O	1:D:4115:SER:OG	2.28	0.52
1:A:3157:ILE:HA	1:A:3161:VAL:HB	1.92	0.52
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.42	0.52
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.91	0.52
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.39	0.52
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.42	0.52
1:C:3980:LEU:HD23	1:C:3985:LEU:HD22	1.90	0.52
1:D:499:THR:HG23	1:D:502:HIS:H	1.74	0.52
1:D:1302:ARG:HG3	1:D:1523:ALA:HB1	1.91	0.52
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.42	0.52
1:C:2687:ALA:O	1:C:2993:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4952:GLU:O	1:C:4956:THR:HB	2.09	0.52
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.42	0.52
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.42	0.52
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.73	0.52
1:B:2001:PRO:HG2	1:B:3864:THR:HB	1.90	0.52
1:B:2677:LYS:NZ	1:B:2909:ASP:OD2	2.37	0.52
1:C:257:ARG:O	1:C:284:HIS:NE2	2.42	0.52
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.92	0.52
1:B:2687:ALA:O	1:B:2993:GLN:NE2	2.43	0.52
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.26	0.52
1:C:4020:GLN:HA	1:C:4023:MET:HB3	1.92	0.52
1:D:450:GLY:HA2	1:D:453:GLU:HG3	1.92	0.52
1:A:450:GLY:HA2	1:A:453:GLU:HG3	1.92	0.52
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.39	0.52
1:D:3219:TYR:OH	1:D:3239:MET:SD	2.65	0.52
1:A:3414:ARG:NH1	1:A:3469:PHE:O	2.39	0.52
1:B:4020:GLN:HA	1:B:4023:MET:HB3	1.92	0.52
1:C:1792:ALA:O	1:C:2176:ASN:ND2	2.40	0.52
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.92	0.52
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.75	0.52
1:A:4020:GLN:HA	1:A:4023:MET:HB3	1.92	0.52
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.42	0.52
1:C:499:THR:HG23	1:C:502:HIS:H	1.74	0.52
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.42	0.52
1:D:3940:LYS:O	1:D:4002:LYS:NZ	2.38	0.52
2:F:27:THR:HB	2:F:100:ASP:HB3	1.91	0.52
2:H:27:THR:HB	2:H:100:ASP:HB3	1.91	0.52
1:A:1811:ALA:HA	1:A:1814:MET:HE3	1.92	0.52
1:A:4917:ASP:OD2	1:D:4888:TYR:OH	2.18	0.52
1:C:743:VAL:HB	1:C:760:ASN:HA	1.91	0.52
1:C:4112:LEU:O	1:C:4115:SER:OG	2.28	0.52
1:D:1175:SER:OG	1:D:1180:ARG:NH2	2.38	0.52
1:D:3157:ILE:HA	1:D:3161:VAL:HB	1.92	0.52
1:A:4952:GLU:O	1:A:4956:THR:HB	2.09	0.51
1:B:743:VAL:HB	1:B:760:ASN:HA	1.91	0.51
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.91	0.51
1:B:3316:LEU:HD11	1:B:3346:VAL:HA	1.91	0.51
1:D:2640:PRO:HA	1:D:2643:LEU:HB3	1.92	0.51
1:D:3368:ARG:NH2	1:D:3404:ASP:OD2	2.43	0.51
1:A:2687:ALA:O	1:A:2993:GLN:NE2	2.43	0.51
1:A:3368:ARG:NH2	1:A:3404:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLY:HA2	1:C:453:GLU:HG3	1.92	0.51
1:C:1248:VAL:HG22	1:C:1599:MET:HG3	1.93	0.51
2:G:27:THR:HB	2:G:100:ASP:HB3	1.91	0.51
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.91	0.51
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.75	0.51
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.76	0.51
1:B:3368:ARG:NH2	1:B:3404:ASP:OD2	2.43	0.51
1:D:4020:GLN:HA	1:D:4023:MET:HB3	1.92	0.51
1:A:2640:PRO:HA	1:A:2643:LEU:HB3	1.93	0.51
1:B:2640:PRO:HA	1:B:2643:LEU:HB3	1.93	0.51
1:B:3157:ILE:HA	1:B:3161:VAL:HB	1.92	0.51
1:C:2640:PRO:HA	1:C:2643:LEU:HB3	1.92	0.51
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.92	0.51
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.76	0.51
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.92	0.51
1:C:3157:ILE:HA	1:C:3161:VAL:HB	1.92	0.51
1:C:3368:ARG:NH2	1:C:3404:ASP:OD2	2.43	0.51
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.75	0.51
1:D:4242:ILE:HG12	1:D:4993:MET:HB3	1.93	0.51
1:D:4866:SER:HB2	1:D:4873:ASP:H	1.75	0.51
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.26	0.51
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.75	0.51
1:A:2369[A]:ARG:HH21	1:A:2373:GLY:HA2	1.75	0.51
1:A:4680:LYS:HE3	1:A:4686:LEU:HD22	1.93	0.51
1:B:274:LEU:HB3	1:B:339:ILE:HD12	1.93	0.51
1:B:3232:LEU:HD22	1:B:3239:MET:HE1	1.93	0.51
1:B:4680:LYS:HE3	1:B:4686:LEU:HD22	1.93	0.51
1:C:1811:ALA:HA	1:C:1814:MET:HE3	1.92	0.51
1:C:3232:LEU:HD22	1:C:3239:MET:HE1	1.93	0.51
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.27	0.51
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.46	0.51
1:A:4866:SER:HB2	1:A:4873:ASP:H	1.75	0.51
1:B:450:GLY:HA2	1:B:453:GLU:HG3	1.92	0.51
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.92	0.51
1:B:1248:VAL:HG22	1:B:1599:MET:HG3	1.93	0.51
1:B:4866:SER:HB2	1:B:4873:ASP:H	1.76	0.51
1:D:2369[A]:ARG:HH21	1:D:2373:GLY:HA2	1.75	0.51
1:D:2917:ALA:HA	1:D:2920:ARG:HB3	1.92	0.51
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.46	0.51
1:B:1811:ALA:HA	1:B:1814:MET:HE3	1.93	0.51
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2369[A]:ARG:HH21	1:C:2373:GLY:HA2	1.75	0.51
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.75	0.51
1:D:3959:LYS:NZ	1:D:4022:ASP:OD2	2.43	0.51
1:A:4242:ILE:HG12	1:A:4993:MET:HB3	1.93	0.51
1:B:4112:LEU:O	1:B:4115:SER:OG	2.28	0.51
1:D:1248:VAL:HG22	1:D:1599:MET:HG3	1.93	0.51
1:A:1990:GLU:HG2	1:A:1994:ARG:HH12	1.76	0.50
1:A:2917:ALA:HA	1:A:2920:ARG:HB3	1.92	0.50
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.92	0.50
1:D:3232:LEU:HD22	1:D:3239:MET:HE1	1.93	0.50
2:E:27:THR:HB	2:E:100:ASP:HB3	1.91	0.50
1:A:274:LEU:HB3	1:A:339:ILE:HD12	1.93	0.50
1:B:1578:ALA:O	1:B:1584:ARG:NH2	2.37	0.50
1:B:2369[A]:ARG:HH21	1:B:2373:GLY:HA2	1.75	0.50
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.75	0.50
1:C:4106:PRO:O	1:C:4110:PHE:HB3	2.11	0.50
1:C:4866:SER:HB2	1:C:4873:ASP:H	1.75	0.50
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.46	0.50
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.93	0.50
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.44	0.50
1:A:3523:ASN:OD1	1:A:3582:ARG:NH2	2.44	0.50
1:A:3545:THR:HG22	1:A:3548:GLU:HG3	1.93	0.50
1:A:3695:PRO:HB2	1:A:3700:GLN:HG3	1.94	0.50
1:A:4106:PRO:O	1:A:4110:PHE:HB3	2.11	0.50
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.94	0.50
1:A:3219:TYR:OH	1:A:3239:MET:SD	2.65	0.50
1:B:403:MET:O	1:B:407:THR:OG1	2.26	0.50
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.26	0.50
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.94	0.50
1:C:4242:ILE:HG12	1:C:4993:MET:HB3	1.93	0.50
1:D:2930:LEU:HB3	1:D:2935:TYR:HB2	1.93	0.50
1:A:3959:LYS:NZ	1:A:4022:ASP:OD2	2.43	0.50
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.41	0.50
1:D:1969:LEU:HD21	1:D:2009:LEU:HD13	1.94	0.50
1:A:4562:LEU:HD22	1:A:4653:VAL:HG13	1.94	0.50
1:B:2869:ARG:NH2	1:B:2870[B]:GLU:OE2	2.45	0.50
1:B:2917:ALA:HA	1:B:2920:ARG:HB3	1.92	0.50
1:B:3545:THR:HG22	1:B:3548:GLU:HG3	1.93	0.50
1:C:1260:MET:HB2	1:C:1269:CYS:HB2	1.94	0.50
1:C:3523:ASN:OD1	1:C:3582:ARG:NH2	2.44	0.50
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1260:MET:HB2	1:B:1269:CYS:HB2	1.94	0.50
1:B:3695:PRO:HB2	1:B:3700:GLN:HG3	1.94	0.50
1:B:3959:LYS:NZ	1:B:4022:ASP:OD2	2.43	0.50
1:C:3695:PRO:HB2	1:C:3700:GLN:HG3	1.94	0.50
1:C:4562:LEU:HD22	1:C:4653:VAL:HG13	1.94	0.50
1:D:2869:ARG:NH2	1:D:2870[B]:GLU:OE2	2.45	0.50
1:D:3523:ASN:OD1	1:D:3582:ARG:NH2	2.44	0.50
1:D:3695:PRO:HB2	1:D:3700:GLN:HG3	1.94	0.50
1:D:4106:PRO:O	1:D:4110:PHE:HB3	2.11	0.50
1:A:1578:ALA:O	1:A:1584:ARG:NH2	2.37	0.50
1:A:2930:LEU:HB3	1:A:2935:TYR:HB2	1.93	0.50
1:A:3232:LEU:HD22	1:A:3239:MET:HE1	1.93	0.50
1:B:4562:LEU:HD22	1:B:4653:VAL:HG13	1.94	0.50
1:C:1969:LEU:HD21	1:C:2009:LEU:HD13	1.94	0.50
1:C:3371:LYS:NZ	1:C:3375:GLU:OE2	2.42	0.50
1:D:4680:LYS:HE3	1:D:4686:LEU:HD22	1.93	0.50
1:A:1248:VAL:HG22	1:A:1599:MET:HG3	1.93	0.50
1:A:2677:LYS:NZ	1:A:2909:ASP:OD2	2.37	0.50
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.41	0.50
1:B:257:ARG:O	1:B:284:HIS:NE2	2.42	0.50
1:B:1969:LEU:HD21	1:B:2009:LEU:HD13	1.94	0.50
1:C:2869:ARG:NH2	1:C:2870[B]:GLU:OE2	2.45	0.50
1:C:2917:ALA:HA	1:C:2920:ARG:HB3	1.92	0.50
1:D:1990:GLU:HG2	1:D:1994:ARG:HH12	1.76	0.50
1:D:3545:THR:HG22	1:D:3548:GLU:HG3	1.93	0.50
1:D:4562:LEU:HD22	1:D:4653:VAL:HG13	1.94	0.50
1:A:551:LEU:HB3	1:A:589:LEU:HD11	1.94	0.49
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.40	0.49
1:A:3236:VAL:HA	1:A:3239:MET:HG2	1.94	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:3236:VAL:HA	1:B:3239:MET:HG2	1.94	0.49
1:B:3523:ASN:OD1	1:B:3582:ARG:NH2	2.44	0.49
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.94	0.49
1:B:4106:PRO:O	1:B:4110:PHE:HB3	2.11	0.49
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.94	0.49
1:C:3545:THR:HG22	1:C:3548:GLU:HG3	1.93	0.49
1:D:1260:MET:HB2	1:D:1269:CYS:HB2	1.94	0.49
1:A:1969:LEU:HD21	1:A:2009:LEU:HD13	1.94	0.49
1:A:2309:SER:OG	1:A:2321:ILE:O	2.26	0.49
1:A:2869:ARG:NH2	1:A:2870[B]:GLU:OE2	2.45	0.49
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3106:MET:HE3	1:A:3132:THR:HB	1.95	0.49
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.94	0.49
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.44	0.49
1:B:4242:ILE:HG12	1:B:4993:MET:HB3	1.93	0.49
1:C:2724:GLU:OE1	1:C:2738:ARG:NH2	2.46	0.49
1:C:2930:LEU:HB3	1:C:2935:TYR:HB2	1.93	0.49
1:D:1811:ALA:HA	1:D:1814:MET:HE3	1.92	0.49
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.94	0.49
1:D:3106:MET:HE3	1:D:3132:THR:HB	1.95	0.49
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.26	0.49
1:A:2527:LEU:HD13	1:A:2582:MET:HG2	1.95	0.49
1:A:3371:LYS:NZ	1:A:3375:GLU:OE2	2.42	0.49
1:A:4630:TYR:OH	1:B:4860:ARG:NH2	2.42	0.49
1:B:475:GLN:OE1	1:B:533:ASN:ND2	2.46	0.49
1:B:2930:LEU:HB3	1:B:2935:TYR:HB2	1.93	0.49
1:C:274:LEU:HB3	1:C:339:ILE:HD12	1.93	0.49
1:C:3959:LYS:NZ	1:C:4022:ASP:OD2	2.43	0.49
1:D:274:LEU:HB3	1:D:339:ILE:HD12	1.93	0.49
1:D:3236:VAL:HA	1:D:3239:MET:HG2	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1260:MET:HB2	1:A:1269:CYS:HB2	1.94	0.49
1:B:2527:LEU:HD13	1:B:2582:MET:HG2	1.95	0.49
1:B:3106:MET:HE3	1:B:3132:THR:HB	1.95	0.49
1:D:2724:GLU:OE1	1:D:2738:ARG:NH2	2.46	0.49
1:B:1990:GLU:HG2	1:B:1994:ARG:HH12	1.76	0.49
1:B:2724:GLU:OE1	1:B:2738:ARG:NH2	2.46	0.49
1:B:2769:ASP:O	1:B:2773:ASN:HB2	2.13	0.49
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.46	0.49
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.95	0.49
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.95	0.49
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.95	0.49
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.94	0.49
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.95	0.49
1:B:551:LEU:HB3	1:B:589:LEU:HD11	1.94	0.49
1:C:3940:LYS:O	1:C:4002:LYS:NZ	2.38	0.49
1:C:4725:LEU:HA	1:C:4737:ILE:HG21	1.95	0.49
1:D:551:LEU:HB3	1:D:589:LEU:HD11	1.95	0.49
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.95	0.49
1:C:4680:LYS:HE3	1:C:4686:LEU:HD22	1.93	0.49
1:D:2891:LYS:HA	1:D:2894:LEU:HB3	1.95	0.49
1:D:3371:LYS:NZ	1:D:3375:GLU:OE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:OE1	1:A:533:ASN:ND2	2.46	0.49
1:B:3103:ILE:HG21	1:B:3168:THR:HG23	1.95	0.49
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.26	0.49
1:C:3106:MET:HE3	1:C:3132:THR:HB	1.95	0.49
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.95	0.49
1:A:1171:SER:OG	1:A:1175:SER:O	2.24	0.48
1:B:3164:SER:HA	1:B:3167:ARG:HE	1.78	0.48
1:C:1990:GLU:HG2	1:C:1994:ARG:HH12	1.77	0.48
1:C:3103:ILE:HG21	1:C:3168:THR:HG23	1.95	0.48
1:C:3236:VAL:HA	1:C:3239:MET:HG2	1.94	0.48
1:D:358:THR:HG21	1:D:383:HIS:H	1.78	0.48
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.95	0.48
1:D:3414:ARG:NH1	1:D:3469:PHE:O	2.38	0.48
1:A:358:THR:HG21	1:A:383:HIS:H	1.78	0.48
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.47	0.48
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.13	0.48
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.95	0.48
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.94	0.48
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.48
1:C:2527:LEU:HD13	1:C:2582:MET:HG2	1.95	0.48
1:C:2967:MET:HE3	1:C:2971:GLN:HE21	1.78	0.48
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.96	0.48
1:D:2527:LEU:HD13	1:D:2582:MET:HG2	1.95	0.48
1:D:2707:ALA:HB1	1:D:3009:TYR:HD1	1.78	0.48
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.12	0.48
2:E:77:THR:HG22	2:E:79:ASP:H	1.79	0.48
1:A:2891:LYS:HA	1:A:2894:LEU:HB3	1.95	0.48
1:A:3037:GLU:HB3	1:A:3088:VAL:HG21	1.95	0.48
1:A:4112:LEU:O	1:A:4115:SER:OG	2.28	0.48
1:B:358:THR:HG21	1:B:383:HIS:H	1.78	0.48
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.47	0.48
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.96	0.48
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.95	0.48
1:C:358:THR:HG21	1:C:383:HIS:H	1.78	0.48
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.22	0.48
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.46	0.48
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.94	0.48
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.96	0.48
1:A:2769:ASP:O	1:A:2773:ASN:HB2	2.13	0.48
1:B:1422:ASP:OD2	1:B:1568:LYS:NZ	2.38	0.48
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.95	0.48
1:C:1743[A]:ARG:HE	1:C:1743[A]:ARG:HB2	1.49	0.48
1:C:2891:LYS:HA	1:C:2894:LEU:HB3	1.95	0.48
1:C:3164:SER:HA	1:C:3167:ARG:HE	1.79	0.48
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.13	0.48
1:D:257:ARG:O	1:D:284:HIS:NE2	2.42	0.48
1:D:2967:MET:HE3	1:D:2971:GLN:HE21	1.78	0.48
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.43	0.48
1:A:2724:GLU:OE1	1:A:2738:ARG:NH2	2.46	0.48
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.47	0.48
1:B:2967:MET:HE3	1:B:2971:GLN:HE21	1.78	0.48
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.26	0.48
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.95	0.48
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.44	0.48
2:F:77:THR:HG22	2:F:79:ASP:H	1.78	0.48
2:H:77:THR:HG22	2:H:79:ASP:H	1.79	0.48
1:A:2516:ASP:OD1	1:A:2516:ASP:N	2.46	0.48
1:A:3164:SER:HA	1:A:3167:ARG:HE	1.79	0.48
1:B:1171:SER:OG	1:B:1175:SER:O	2.24	0.48
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.13	0.48
1:B:4018:ASP:HA	1:B:4021:LYS:HB3	1.96	0.48
1:C:551:LEU:HB3	1:C:589:LEU:HD11	1.95	0.48
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.94	0.48
1:C:2707:ALA:HB1	1:C:3009:TYR:HD1	1.78	0.48
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.47	0.48
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.95	0.48
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.95	0.48
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.95	0.48
1:B:4097:MET:HE2	1:B:4111:LEU:HD23	1.96	0.48
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.96	0.48
1:C:3596:VAL:O	1:C:3600:SER:OG	2.21	0.48
1:D:2769:ASP:O	1:D:2773:ASN:HB2	2.13	0.48
1:D:4725:LEU:HA	1:D:4737:ILE:HG21	1.95	0.48
2:F:62:GLY:HA3	2:F:74:LEU:HD21	1.96	0.48
1:A:2739:PRO:HG3	1:A:2888:ARG:HG2	1.96	0.48
1:B:3371:LYS:NZ	1:B:3375:GLU:OE2	2.42	0.48
1:C:2769:ASP:O	1:C:2773:ASN:HB2	2.13	0.48
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.95	0.48
1:D:2516:ASP:OD1	1:D:2516:ASP:N	2.46	0.48
2:G:62:GLY:HA3	2:G:74:LEU:HD21	1.96	0.48
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4097:MET:HE2	1:A:4111:LEU:HD23	1.96	0.48
1:B:2739:PRO:HG3	1:B:2888:ARG:HG2	1.96	0.48
1:C:2739:PRO:HG3	1:C:2888:ARG:HG2	1.96	0.48
1:C:4018:ASP:HA	1:C:4021:LYS:HB3	1.96	0.48
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.96	0.48
1:D:1171:SER:OG	1:D:1175:SER:O	2.24	0.48
1:D:3037:GLU:HB3	1:D:3088:VAL:HG21	1.95	0.48
1:D:3164:SER:HA	1:D:3167:ARG:HE	1.79	0.48
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.47	0.48
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.47	0.48
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.95	0.48
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.47	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.48
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.96	0.48
1:D:3103:ILE:HG21	1:D:3168:THR:HG23	1.95	0.48
1:A:2576:ALA:HB1	1:A:2618:MET:HG2	1.96	0.47
1:A:2707:ALA:HB1	1:A:3009:TYR:HD1	1.78	0.47
1:A:3110:LEU:O	1:A:3180:ASN:ND2	2.47	0.47
1:A:4725:LEU:HA	1:A:4737:ILE:HG21	1.95	0.47
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.40	0.47
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.95	0.47
1:D:2576:ALA:HB1	1:D:2618:MET:HG2	1.96	0.47
2:G:77:THR:HG22	2:G:79:ASP:H	1.78	0.47
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.47	0.47
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.95	0.47
1:A:3354:LEU:HA	1:A:3358:PHE:HB2	1.96	0.47
1:B:4725:LEU:HA	1:B:4737:ILE:HG21	1.95	0.47
1:C:3622:LYS:HB2	1:C:3626:LYS:HG2	1.96	0.47
1:C:4097:MET:HE2	1:C:4111:LEU:HD23	1.96	0.47
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.47
1:D:3354:LEU:HA	1:D:3358:PHE:HB2	1.96	0.47
2:E:62:GLY:HA3	2:E:74:LEU:HD21	1.96	0.47
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.96	0.47
1:A:257:ARG:O	1:A:284:HIS:NE2	2.42	0.47
1:A:3103:ILE:HG21	1:A:3168:THR:HG23	1.95	0.47
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.22	0.47
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.47
1:D:4725:LEU:HB2	1:D:4743:MET:HE1	1.97	0.47
1:A:2967:MET:HE3	1:A:2971:GLN:HE21	1.78	0.47
1:A:4018:ASP:HA	1:A:4021:LYS:HB3	1.96	0.47
1:A:4725:LEU:HB2	1:A:4743:MET:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:ALA:O	1:B:879:HIS:ND1	2.47	0.47
1:B:2891:LYS:HA	1:B:2894:LEU:HB3	1.95	0.47
1:B:3110:LEU:O	1:B:3180:ASN:ND2	2.47	0.47
1:C:2677:LYS:HE2	1:C:2677:LYS:HB3	1.67	0.47
1:C:3110:LEU:O	1:C:3180:ASN:ND2	2.47	0.47
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.43	0.47
1:A:3622:LYS:HB2	1:A:3626:LYS:HG2	1.96	0.47
1:A:4738:ALA:HA	1:A:4743:MET:HE3	1.96	0.47
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.97	0.47
1:B:4738:ALA:HA	1:B:4743:MET:HE3	1.96	0.47
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.97	0.47
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.97	0.47
1:B:2576:ALA:HB1	1:B:2618:MET:HG2	1.96	0.47
1:B:2707:ALA:HB1	1:B:3009:TYR:HD1	1.78	0.47
1:B:3037:GLU:HB3	1:B:3088:VAL:HG21	1.95	0.47
1:B:3271:GLU:OE2	1:B:3337:ARG:NH2	2.44	0.47
1:B:3354:LEU:HA	1:B:3358:PHE:HB2	1.96	0.47
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.95	0.47
1:C:3354:LEU:HA	1:C:3358:PHE:HB2	1.96	0.47
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	1.96	0.47
1:D:1698:LEU:HA	1:D:1712:TYR:HE1	1.80	0.47
1:D:4018:ASP:HA	1:D:4021:LYS:HB3	1.96	0.47
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.97	0.47
1:A:710:ASP:OD1	1:A:710:ASP:N	2.48	0.47
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.88	0.47
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.48	0.47
1:A:4044:MET:HE2	1:A:4146:LEU:HD11	1.97	0.47
1:B:1256:GLU:HB3	1:B:1275:ARG:HD2	1.97	0.47
1:B:4965:SER:O	1:B:4969:ASP:HB2	2.15	0.47
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.48	0.47
1:C:2474:LEU:HD13	1:C:2550:LEU:HD21	1.96	0.47
1:C:3592:ILE:HG22	1:C:3595:ARG:HH21	1.80	0.47
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.48	0.47
1:D:2214:VAL:HG21	1:D:2228:MET:HE1	1.96	0.47
1:D:2739:PRO:HG3	1:D:2888:ARG:HG2	1.96	0.47
1:D:3622:LYS:HB2	1:D:3626:LYS:HG2	1.96	0.47
1:D:4044:MET:HE2	1:D:4146:LEU:HD11	1.97	0.47
1:D:4097:MET:HE2	1:D:4111:LEU:HD23	1.96	0.47
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.96	0.47
1:A:2159:LEU:HG	1:A:2163:ARG:HE	1.80	0.47
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.96	0.47
1:B:2474:LEU:HD13	1:B:2550:LEU:HD21	1.96	0.47
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.88	0.47
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.88	0.47
1:D:2474:LEU:HD13	1:D:2550:LEU:HD21	1.96	0.47
1:D:2677:LYS:HE2	1:D:2677:LYS:HB3	1.67	0.47
1:A:875:ALA:O	1:A:879:HIS:ND1	2.47	0.47
1:B:233:ILE:O	1:B:257:ARG:NH2	2.48	0.47
1:B:2214:VAL:HG21	1:B:2228:MET:HE1	1.96	0.47
1:B:2764:GLU:HG3	1:B:2857:PRO:HB3	1.97	0.47
1:B:3622:LYS:HB2	1:B:3626:LYS:HG2	1.96	0.47
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.97	0.47
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.48	0.47
1:C:2214:VAL:HG21	1:C:2228:MET:HE1	1.96	0.47
1:C:3037:GLU:HB3	1:C:3088:VAL:HG21	1.95	0.47
1:C:3159:ASP:OD1	1:C:3159:ASP:N	2.44	0.47
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.97	0.47
2:H:62:GLY:HA3	2:H:74:LEU:HD21	1.96	0.47
1:A:1698:LEU:HA	1:A:1712:TYR:HE1	1.80	0.47
1:A:1743[A]:ARG:HE	1:A:1743[A]:ARG:HB2	1.49	0.47
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.48	0.47
1:B:1698:LEU:HA	1:B:1712:TYR:HE1	1.80	0.47
1:B:3592:ILE:HG22	1:B:3595:ARG:HH21	1.80	0.47
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.43	0.47
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.48	0.47
1:D:2768:PHE:HA	1:D:2771:ILE:HG22	1.97	0.47
1:A:1084:GLN:NE2	1:A:1186:ASP:O	2.42	0.46
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.43	0.46
1:B:3329:ILE:O	1:B:3403:ARG:NH2	2.48	0.46
1:C:2764:GLU:HG3	1:C:2857:PRO:HB3	1.97	0.46
1:D:710:ASP:OD1	1:D:710:ASP:N	2.48	0.46
1:D:1297:PHE:HD1	1:D:1522:LEU:HA	1.80	0.46
1:D:2159:LEU:HG	1:D:2163:ARG:HE	1.80	0.46
1:A:1256:GLU:HB3	1:A:1275:ARG:HD2	1.97	0.46
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.96	0.46
1:B:2309:SER:OG	1:B:2321:ILE:O	2.26	0.46
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.33	0.46
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.38	0.46
1:B:4044:MET:HE2	1:B:4146:LEU:HD11	1.97	0.46
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.96	0.46
1:C:1698:LEU:HA	1:C:1712:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2159:LEU:HG	1:C:2163:ARG:HE	1.80	0.46
1:C:2576:ALA:HB1	1:C:2618:MET:HG2	1.96	0.46
1:D:3110:LEU:O	1:D:3180:ASN:ND2	2.47	0.46
1:A:4965:SER:O	1:A:4969:ASP:HB2	2.15	0.46
1:A:4971:THR:HG22	1:A:4972:PRO:HD2	1.98	0.46
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.97	0.46
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.83	0.46
1:C:1968:LYS:NZ	1:C:2030:ASP:OD2	2.49	0.46
1:C:4065:PHE:O	1:C:4133:GLN:NE2	2.49	0.46
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.76	0.46
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.97	0.46
1:A:1968:LYS:NZ	1:A:2030:ASP:OD2	2.49	0.46
1:A:2214:VAL:HG21	1:A:2228:MET:HE1	1.96	0.46
1:A:2768:PHE:HA	1:A:2771:ILE:HG22	1.97	0.46
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.48	0.46
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.40	0.46
1:C:1297:PHE:HD1	1:C:1522:LEU:HA	1.80	0.46
1:C:2684:ASP:O	1:C:2688:HIS:ND1	2.46	0.46
1:C:4044:MET:HE2	1:C:4146:LEU:HD11	1.97	0.46
1:C:4738:ALA:HA	1:C:4743:MET:HE3	1.96	0.46
1:D:659:TYR:O	1:D:662:TRP:NE1	2.49	0.46
1:D:4065:PHE:O	1:D:4133:GLN:NE2	2.49	0.46
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.98	0.46
1:A:2863:SER:HA	1:A:2928:LYS:HG3	1.98	0.46
1:A:4736:ARG:HE	1:A:4736:ARG:HB3	1.58	0.46
1:B:2863:SER:HA	1:B:2928:LYS:HG3	1.98	0.46
1:C:659:TYR:O	1:C:662:TRP:NE1	2.49	0.46
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.97	0.46
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.97	0.46
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.97	0.46
1:D:815:VAL:O	1:D:1007:TYR:OH	2.29	0.46
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.98	0.46
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.88	0.46
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.48	0.46
1:B:4065:PHE:O	1:B:4133:GLN:NE2	2.49	0.46
1:B:4971:THR:HG22	1:B:4972:PRO:HD2	1.98	0.46
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.96	0.46
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.81	0.46
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.97	0.46
1:A:2684:ASP:O	1:A:2688:HIS:ND1	2.46	0.46
1:A:3592:ILE:HG22	1:A:3595:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2684:ASP:O	1:B:2688:HIS:ND1	2.46	0.46
1:B:4725:LEU:HB2	1:B:4743:MET:HE1	1.97	0.46
1:C:357:LEU:HD11	1:C:388:LEU:HD11	1.98	0.46
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.33	0.46
1:C:4725:LEU:HB2	1:C:4743:MET:HE1	1.97	0.46
1:D:1968:LYS:NZ	1:D:2030:ASP:OD2	2.49	0.46
1:D:2764:GLU:HG3	1:D:2857:PRO:HB3	1.97	0.46
1:D:3592:ILE:HG22	1:D:3595:ARG:HH21	1.80	0.46
1:D:4738:ALA:HA	1:D:4743:MET:HE3	1.96	0.46
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.97	0.46
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.37	0.46
1:D:2863:SER:HA	1:D:2928:LYS:HG3	1.98	0.46
1:A:4049:VAL:HA	1:A:4163:PHE:HZ	1.81	0.46
1:B:2159:LEU:HG	1:B:2163:ARG:HE	1.80	0.46
1:B:3107:VAL:O	1:B:3111:ARG:HB2	2.16	0.46
1:B:4049:VAL:HA	1:B:4163:PHE:HZ	1.81	0.46
1:B:4552:LEU:O	1:B:4556:SER:OG	2.34	0.46
1:C:2205:GLU:O	1:C:2208:MET:N	2.49	0.46
1:C:2863:SER:HA	1:C:2928:LYS:HG3	1.98	0.46
1:C:4049:VAL:HA	1:C:4163:PHE:HZ	1.81	0.46
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.97	0.46
1:D:3107:VAL:O	1:D:3111:ARG:HB2	2.16	0.46
1:D:4965:SER:O	1:D:4969:ASP:HB2	2.15	0.46
1:A:491:ILE:HD11	1:A:522:LEU:HB3	1.98	0.46
1:A:2764:GLU:HG3	1:A:2857:PRO:HB3	1.97	0.46
1:A:3081:MET:HE3	1:A:3092:LEU:HD23	1.98	0.46
1:B:1968:LYS:NZ	1:B:2030:ASP:OD2	2.49	0.46
1:B:3081:MET:HE3	1:B:3092:LEU:HD23	1.98	0.46
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.97	0.46
1:C:491:ILE:HD11	1:C:522:LEU:HB3	1.98	0.46
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.81	0.46
1:C:3107:VAL:O	1:C:3111:ARG:HB2	2.16	0.46
1:D:3266:MET:HB3	1:D:3269:VAL:HB	1.99	0.46
1:D:4971:THR:HG22	1:D:4972:PRO:HD2	1.98	0.46
1:A:3107:VAL:O	1:A:3111:ARG:HB2	2.16	0.45
1:C:2516:ASP:N	1:C:2516:ASP:OD1	2.46	0.45
1:C:2768:PHE:HA	1:C:2771:ILE:HG22	1.97	0.45
1:C:4965:SER:O	1:C:4969:ASP:HB2	2.15	0.45
1:D:3081:MET:HE3	1:D:3092:LEU:HD23	1.98	0.45
1:D:3329:ILE:O	1:D:3403:ARG:NH2	2.48	0.45
1:A:1297:PHE:HD1	1:A:1522:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2205:GLU:O	1:A:2208:MET:N	2.49	0.45
1:A:2474:LEU:HD13	1:A:2550:LEU:HD21	1.96	0.45
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.81	0.45
1:A:3788:GLY:HA2	1:A:3835:LEU:HG	1.98	0.45
1:B:815:VAL:O	1:B:1007:TYR:OH	2.29	0.45
1:B:1297:PHE:HD1	1:B:1522:LEU:HA	1.80	0.45
1:C:3081:MET:HE3	1:C:3092:LEU:HD23	1.98	0.45
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.48	0.45
1:D:3409:TYR:HE2	1:D:3510:ILE:HG12	1.82	0.45
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.48	0.45
1:B:357:LEU:HD11	1:B:388:LEU:HD11	1.98	0.45
1:B:2768:PHE:HA	1:B:2771:ILE:HG22	1.97	0.45
1:C:3980:LEU:HD22	1:C:4030:LEU:HD21	1.98	0.45
1:A:1432:THR:HA	1:A:1520:VAL:O	2.17	0.45
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.83	0.45
1:B:3788:GLY:HA2	1:B:3835:LEU:HG	1.98	0.45
1:B:3875:MET:HE3	1:B:3875:MET:HB3	1.85	0.45
1:C:3409:TYR:HE2	1:C:3510:ILE:HG12	1.82	0.45
1:D:1948:ASP:OD1	1:D:2126:ARG:NH2	2.42	0.45
2:E:23:VAL:HG13	2:E:47:LYS:HG2	1.98	0.45
1:A:1465:ASP:OD1	1:A:1465:ASP:N	2.50	0.45
1:B:491:ILE:HD11	1:B:522:LEU:HB3	1.99	0.45
1:C:233:ILE:O	1:C:257:ARG:NH2	2.48	0.45
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.98	0.45
1:C:1578:ALA:O	1:C:1584:ARG:NH2	2.37	0.45
1:C:2670:GLU:HG2	1:C:2912:THR:HB	1.98	0.45
1:C:2765:LYS:HA	1:C:2765:LYS:HD3	1.76	0.45
1:D:1864:LYS:NZ	1:D:1871:PHE:O	2.47	0.45
1:D:2205:GLU:O	1:D:2208:MET:N	2.49	0.45
2:F:23:VAL:HG13	2:F:47:LYS:HG2	1.98	0.45
2:G:23:VAL:HG13	2:G:47:LYS:HG2	1.98	0.45
1:A:4214:LYS:HE2	1:A:4985:LEU:HD11	1.99	0.45
1:B:4214:LYS:HE2	1:B:4985:LEU:HD11	1.99	0.45
1:C:1432:THR:HA	1:C:1520:VAL:O	2.17	0.45
1:D:357:LEU:HD11	1:D:388:LEU:HD11	1.98	0.45
1:D:1256:GLU:HB3	1:D:1275:ARG:HD2	1.97	0.45
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.49	0.45
1:A:3980:LEU:HD22	1:A:4030:LEU:HD21	1.98	0.45
1:B:710:ASP:N	1:B:710:ASP:OD1	2.48	0.45
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.17	0.45
1:B:2265:LEU:O	1:B:2330:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2670:GLU:HG2	1:B:2912:THR:HB	1.98	0.45
1:C:710:ASP:OD1	1:C:710:ASP:N	2.48	0.45
1:C:2368:LEU:HD11	1:C:2376:LEU:HD12	1.99	0.45
1:C:3219:TYR:OH	1:C:3239:MET:SD	2.65	0.45
1:C:3266:MET:HB3	1:C:3269:VAL:HB	1.99	0.45
1:D:233:ILE:O	1:D:257:ARG:NH2	2.48	0.45
1:D:1698:LEU:HA	1:D:1712:TYR:CE1	2.52	0.45
1:A:653:ALA:HB3	1:A:656:SER:HB2	1.99	0.45
1:A:4065:PHE:O	1:A:4133:GLN:NE2	2.49	0.45
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.45
1:B:2368:LEU:HD11	1:B:2376:LEU:HD12	1.99	0.45
1:C:775:GLY:H	1:C:848:HIS:CE1	2.35	0.45
1:C:2265:LEU:O	1:C:2330:ARG:NH1	2.50	0.45
1:D:2670:GLU:HG2	1:D:2912:THR:HB	1.98	0.45
1:A:294:THR:HG23	1:A:297:GLN:H	1.82	0.45
1:A:2368:LEU:HD11	1:A:2376:LEU:HD12	1.99	0.45
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.99	0.45
1:C:743:VAL:HG21	1:C:802:PHE:HE2	1.82	0.45
1:C:790:ARG:HA	1:C:1626:TRP:O	2.17	0.45
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.17	0.45
1:C:4552:LEU:O	1:C:4556:SER:OG	2.34	0.45
1:D:491:ILE:HD11	1:D:522:LEU:HB3	1.98	0.45
1:D:653:ALA:HB3	1:D:656:SER:HB2	1.99	0.45
1:D:743:VAL:HG21	1:D:802:PHE:HE2	1.82	0.45
1:D:1432:THR:HA	1:D:1520:VAL:O	2.17	0.45
1:D:1648:MET:HE2	1:D:1648:MET:HB3	1.92	0.45
1:D:3980:LEU:HD22	1:D:4030:LEU:HD21	1.98	0.45
2:H:23:VAL:HG13	2:H:47:LYS:HG2	1.98	0.45
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.48	0.45
1:A:2265:LEU:O	1:A:2330:ARG:NH1	2.50	0.45
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.52	0.45
1:A:4888:TYR:OH	1:B:4917:ASP:OD2	2.27	0.45
1:B:659:TYR:O	1:B:662:TRP:NE1	2.49	0.45
1:B:743:VAL:HG21	1:B:802:PHE:HE2	1.82	0.45
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.98	0.45
1:B:1465:ASP:N	1:B:1465:ASP:OD1	2.50	0.45
1:B:1782:PHE:O	2:F:82:TYR:OH	2.32	0.45
1:C:1256:GLU:HB3	1:C:1275:ARG:HD2	1.97	0.45
1:C:1698:LEU:HA	1:C:1712:TYR:CE1	2.52	0.45
1:C:2686:LEU:HB3	1:C:2997:PHE:HE1	1.82	0.45
1:C:3924:LEU:HD22	1:C:3984:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4971:THR:HG22	1:C:4972:PRO:HD2	1.98	0.45
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.40	0.45
1:D:2265:LEU:O	1:D:2330:ARG:NH1	2.50	0.45
1:A:1698:LEU:HA	1:A:1712:TYR:CE1	2.52	0.44
1:A:2670:GLU:HG2	1:A:2912:THR:HB	1.98	0.44
1:B:2686:LEU:HB3	1:B:2997:PHE:HE1	1.82	0.44
1:C:3271:GLU:OE2	1:C:3337:ARG:NH2	2.44	0.44
1:D:294:THR:HG23	1:D:297:GLN:H	1.82	0.44
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.17	0.44
1:D:2368:LEU:HD11	1:D:2376:LEU:HD12	1.99	0.44
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	1.98	0.44
1:A:262:LEU:HD13	1:A:274:LEU:HD11	2.00	0.44
1:A:659:TYR:O	1:A:662:TRP:NE1	2.49	0.44
1:B:790:ARG:HA	1:B:1626:TRP:O	2.17	0.44
1:B:3924:LEU:HD22	1:B:3984:ARG:HG2	1.99	0.44
1:B:3980:LEU:HD22	1:B:4030:LEU:HD21	1.98	0.44
1:C:3270:ILE:HA	1:C:3274:LEU:HD12	2.00	0.44
1:D:34:LYS:H	1:D:53:SER:HB3	1.82	0.44
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.98	0.44
1:D:3924:LEU:HD22	1:D:3984:ARG:HG2	1.99	0.44
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.99	0.44
1:A:3051:ARG:NH2	1:A:3102:ASP:OD1	2.50	0.44
1:A:3409:TYR:HE2	1:A:3510:ILE:HG12	1.82	0.44
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.49	0.44
1:B:3266:MET:HB3	1:B:3269:VAL:HB	1.99	0.44
1:C:34:LYS:H	1:C:53:SER:HB3	1.82	0.44
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.51	0.44
1:C:2309:SER:OG	1:C:2321:ILE:O	2.26	0.44
1:D:2686:LEU:HB3	1:D:2997:PHE:HE1	1.82	0.44
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.17	0.44
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.82	0.44
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.50	0.44
1:A:3924:LEU:HD22	1:A:3984:ARG:HG2	1.99	0.44
1:A:4552:LEU:O	1:A:4556:SER:OG	2.34	0.44
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.99	0.44
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	2.00	0.44
1:C:815:VAL:O	1:C:1007:TYR:OH	2.29	0.44
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.49	0.44
1:D:2018:GLU:HB3	1:D:2028:ARG:HH12	1.82	0.44
1:A:743:VAL:HG21	1:A:802:PHE:HE2	1.82	0.44
1:A:835:ARG:NH2	1:A:1210:SER:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3301:PRO:HA	1:A:3302:PRO:HD3	1.91	0.44
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.51	0.44
1:B:1698:LEU:HA	1:B:1712:TYR:CE1	2.52	0.44
1:B:2205:GLU:O	1:B:2208:MET:N	2.49	0.44
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.52	0.44
1:C:3788:GLY:HA2	1:C:3835:LEU:HG	1.98	0.44
1:D:262:LEU:HD13	1:D:274:LEU:HD11	2.00	0.44
1:D:790:ARG:HA	1:D:1626:TRP:O	2.17	0.44
1:A:34:LYS:H	1:A:53:SER:HB3	1.82	0.44
1:B:1432:THR:HA	1:B:1520:VAL:O	2.17	0.44
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.81	0.44
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.52	0.44
1:C:73:LEU:O	1:C:106:ALA:N	2.40	0.44
1:D:835:ARG:NH2	1:D:1210:SER:O	2.51	0.44
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.52	0.44
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.82	0.44
1:A:233:ILE:O	1:A:257:ARG:NH2	2.48	0.44
1:B:775:GLY:H	1:B:848:HIS:CE1	2.35	0.44
1:B:2039:LEU:HD22	1:B:2044:ILE:HG13	2.00	0.44
1:B:2869:ARG:NH2	1:B:2947:ASP:OD1	2.51	0.44
1:B:4736:ARG:HE	1:B:4736:ARG:HB3	1.58	0.44
1:C:835:ARG:NH2	1:C:1210:SER:O	2.51	0.44
1:C:1286:MET:HE3	1:C:1287:LEU:H	1.83	0.44
1:C:4958:CYS:HB3	1:C:4961:CYS:SG	2.58	0.44
1:D:775:GLY:H	1:D:848:HIS:CE1	2.35	0.44
1:D:1465:ASP:OD1	1:D:1465:ASP:N	2.50	0.44
1:D:4049:VAL:HA	1:D:4163:PHE:HZ	1.81	0.44
1:D:4214:LYS:HE2	1:D:4985:LEU:HD11	1.99	0.44
1:A:790:ARG:HA	1:A:1626:TRP:O	2.17	0.44
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.26	0.44
1:B:3270:ILE:HA	1:B:3274:LEU:HD12	2.00	0.44
1:C:294:THR:HG23	1:C:297:GLN:H	1.82	0.44
1:C:653:ALA:HB3	1:C:656:SER:HB2	1.99	0.44
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.51	0.44
1:A:357:LEU:HD11	1:A:388:LEU:HD11	1.98	0.44
1:A:2494:PHE:HE2	1:A:2499:LYS:HE3	1.83	0.44
1:B:653:ALA:HB3	1:B:656:SER:HB2	1.99	0.44
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.83	0.44
1:B:2494:PHE:HE2	1:B:2499:LYS:HE3	1.83	0.44
1:C:396:GLU:OE2	1:C:470:SER:OG	2.29	0.44
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1948:ASP:OD1	1:C:2126:ARG:NH2	2.42	0.44
1:C:2159:LEU:HD21	1:C:2163:ARG:HH21	1.83	0.44
1:C:2869:ARG:NH2	1:C:2947:ASP:OD1	2.51	0.44
1:C:4214:LYS:HE2	1:C:4985:LEU:HD11	1.99	0.44
1:D:2869:ARG:NH2	1:D:2947:ASP:OD1	2.51	0.44
1:D:3270:ILE:HA	1:D:3274:LEU:HD12	1.99	0.44
1:D:5034:ASP:OD2	1:D:5035:GLN:NE2	2.51	0.44
1:A:403:MET:HE2	1:A:403:MET:HB3	1.88	0.43
1:A:775:GLY:H	1:A:848:HIS:CE1	2.35	0.43
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.33	0.43
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.37	0.43
1:B:1476:MET:HE2	1:B:1476:MET:HB3	1.92	0.43
1:B:1743[A]:ARG:HE	1:B:1743[A]:ARG:HB2	1.49	0.43
1:B:2516:ASP:OD1	1:B:2516:ASP:N	2.46	0.43
1:B:3409:TYR:HE2	1:B:3510:ILE:HG12	1.82	0.43
1:C:2627:VAL:HG21	1:C:2674:LEU:HG	2.00	0.43
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.99	0.43
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.49	0.43
1:D:2970:SER:HA	1:D:2973:PHE:CE2	2.53	0.43
1:A:877:ASN:HA	1:A:970:LEU:H	1.84	0.43
1:A:893:TYR:HB3	1:A:960:MET:HE2	2.00	0.43
1:B:294:THR:HG23	1:B:297:GLN:H	1.82	0.43
1:B:1286:MET:HE3	1:B:1287:LEU:H	1.83	0.43
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.83	0.43
1:D:1782:PHE:O	2:H:82:TYR:OH	2.32	0.43
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.33	0.43
1:B:884:LEU:HD13	1:B:968:ALA:H	1.83	0.43
1:C:2018:GLU:HB3	1:C:2028:ARG:HH12	1.82	0.43
1:C:5034:ASP:OD2	1:C:5035:GLN:NE2	2.51	0.43
1:D:2039:LEU:HD22	1:D:2044:ILE:HG13	2.00	0.43
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.99	0.43
1:A:2039:LEU:HD22	1:A:2044:ILE:HG13	2.00	0.43
1:A:4958:CYS:HB3	1:A:4961:CYS:SG	2.58	0.43
1:C:2675:THR:HG22	1:C:2706:ILE:HG23	2.00	0.43
1:C:4951:LYS:HE3	1:C:4951:LYS:HB3	1.82	0.43
1:D:73:LEU:O	1:D:106:ALA:N	2.40	0.43
1:D:3271:GLU:OE2	1:D:3337:ARG:NH2	2.44	0.43
1:A:2018:GLU:HB3	1:A:2028:ARG:HH12	1.82	0.43
1:A:2869:ARG:NH2	1:A:2947:ASP:OD1	2.51	0.43
1:A:3266:MET:HB3	1:A:3269:VAL:HB	1.99	0.43
1:A:5034:ASP:OD2	1:A:5035:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:ARG:NH2	1:B:1210:SER:O	2.51	0.43
1:C:111:HIS:ND1	1:C:114:SER:OG	2.39	0.43
1:C:877:ASN:HA	1:C:970:LEU:H	1.84	0.43
1:C:4630:TYR:OH	1:D:4860:ARG:NH2	2.47	0.43
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.52	0.43
1:A:1286:MET:HE3	1:A:1287:LEU:H	1.83	0.43
1:A:2686:LEU:HB3	1:A:2997:PHE:HE1	1.82	0.43
1:A:3245:VAL:HG23	1:A:3248:ARG:H	1.84	0.43
1:B:34:LYS:H	1:B:53:SER:HB3	1.82	0.43
1:B:2018:GLU:HB3	1:B:2028:ARG:HH12	1.82	0.43
1:B:2277:ALA:O	1:B:2281:ILE:HG13	2.18	0.43
1:B:2712:PRO:HG3	1:B:3013:HIS:CD2	2.54	0.43
1:C:2277:ALA:O	1:C:2281:ILE:HG13	2.18	0.43
1:C:2970:SER:HA	1:C:2973:PHE:CE2	2.53	0.43
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.51	0.43
1:A:1864:LYS:NZ	1:A:1871:PHE:O	2.47	0.43
1:A:2159:LEU:HD21	1:A:2163:ARG:HH21	1.83	0.43
1:A:2277:ALA:O	1:A:2281:ILE:HG13	2.18	0.43
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.67	0.43
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.48	0.43
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.43
1:C:1465:ASP:OD1	1:C:1465:ASP:N	2.50	0.43
1:C:2494:PHE:HE2	1:C:2499:LYS:HE3	1.83	0.43
1:D:2494:PHE:HE2	1:D:2499:LYS:HE3	1.83	0.43
1:D:2712:PRO:HG3	1:D:3013:HIS:CD2	2.54	0.43
1:A:884:LEU:HD13	1:A:968:ALA:H	1.83	0.43
1:A:3270:ILE:HA	1:A:3274:LEU:HD12	2.00	0.43
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.52	0.43
1:B:262:LEU:HD13	1:B:274:LEU:HD11	1.99	0.43
1:B:2675:THR:HG22	1:B:2706:ILE:HG23	2.00	0.43
1:C:262:LEU:HD13	1:C:274:LEU:HD11	2.00	0.43
1:C:884:LEU:HD13	1:C:968:ALA:H	1.83	0.43
1:C:2712:PRO:HG3	1:C:3013:HIS:CD2	2.54	0.43
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.84	0.43
1:D:877:ASN:HA	1:D:970:LEU:H	1.84	0.43
1:D:2159:LEU:HD21	1:D:2163:ARG:HH21	1.83	0.43
1:D:2574:HIS:CD2	1:D:2575:ARG:HG2	2.54	0.43
1:D:2779:GLU:HG3	1:D:2792:ARG:HG2	2.01	0.43
1:D:4627:MET:HE3	1:D:4627:MET:HB3	1.93	0.43
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.90	0.43
1:C:1291:LEU:HD12	1:C:1550:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1812:LEU:HD23	1:C:1812:LEU:HA	1.90	0.43
1:C:2779:GLU:HG3	1:C:2792:ARG:HG2	2.01	0.43
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.99	0.43
1:C:3888:LEU:HD23	1:C:3888:LEU:HA	1.91	0.43
1:D:2277:ALA:O	1:D:2281:ILE:HG13	2.18	0.43
1:D:2627:VAL:HG21	1:D:2674:LEU:HG	2.00	0.43
1:D:4958:CYS:HB3	1:D:4961:CYS:SG	2.58	0.43
1:A:2779:GLU:HG3	1:A:2792:ARG:HG2	2.01	0.43
1:A:3051:ARG:HA	1:A:3131:TYR:CE1	2.54	0.43
1:A:4652:LEU:HD12	1:A:4652:LEU:HA	1.92	0.43
1:B:893:TYR:HB3	1:B:960:MET:HE2	2.01	0.43
1:B:1116:GLY:O	1:B:1134:LEU:N	2.52	0.43
1:B:2627:VAL:HG21	1:B:2674:LEU:HG	2.00	0.43
1:B:4958:CYS:HB3	1:B:4961:CYS:SG	2.58	0.43
1:C:716:PHE:HE1	1:C:730:VAL:HG21	1.84	0.43
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.48	0.43
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	2.01	0.43
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.83	0.43
1:C:2583:LEU:HA	1:C:2586:VAL:HG12	2.01	0.43
1:C:3245:VAL:HG23	1:C:3248:ARG:H	1.84	0.43
1:D:1286:MET:HE3	1:D:1287:LEU:H	1.83	0.43
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.50	0.43
1:D:2583:LEU:HA	1:D:2586:VAL:HG12	2.01	0.43
1:A:815:VAL:O	1:A:1007:TYR:OH	2.29	0.42
1:A:1116:GLY:O	1:A:1134:LEU:N	2.52	0.42
1:B:877:ASN:HA	1:B:970:LEU:H	1.83	0.42
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	2.01	0.42
1:B:1291:LEU:HD12	1:B:1550:PRO:HG2	2.01	0.42
1:B:2159:LEU:HD21	1:B:2163:ARG:HH21	1.83	0.42
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.53	0.42
1:B:5034:ASP:OD2	1:B:5035:GLN:NE2	2.51	0.42
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.83	0.42
1:C:1256:GLU:HB3	1:C:1275:ARG:HH11	1.84	0.42
1:C:3051:ARG:HA	1:C:3131:TYR:CE1	2.54	0.42
1:D:3051:ARG:HA	1:D:3131:TYR:CE1	2.54	0.42
1:A:162:LYS:H	1:A:162:LYS:HG2	1.67	0.42
1:A:2574:HIS:CD2	1:A:2575:ARG:HG2	2.54	0.42
1:A:2712:PRO:HG3	1:A:3013:HIS:CD2	2.54	0.42
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.53	0.42
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	2.00	0.42
1:A:4675:LYS:HE3	1:A:4675:LYS:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.50	0.42
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.52	0.42
1:D:716:PHE:HE1	1:D:730:VAL:HG21	1.84	0.42
1:A:2583:LEU:HA	1:A:2586:VAL:HG12	2.01	0.42
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.20	0.42
1:B:2583:LEU:HA	1:B:2586:VAL:HG12	2.01	0.42
1:B:2779:GLU:HG3	1:B:2792:ARG:HG2	2.01	0.42
1:C:1171:SER:OG	1:C:1175:SER:O	2.24	0.42
1:C:2039:LEU:HD22	1:C:2044:ILE:HG13	2.00	0.42
1:D:893:TYR:HB3	1:D:960:MET:HE2	2.01	0.42
1:D:2675:THR:HG22	1:D:2706:ILE:HG23	2.00	0.42
1:D:4181:ILE:HD12	1:D:4183:ILE:HG23	2.01	0.42
1:A:124:SER:HB2	1:A:133:PHE:HA	2.01	0.42
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.84	0.42
1:B:4128:PHE:HA	1:B:4131:ARG:HH21	1.85	0.42
1:B:4710:SER:OG	1:B:4772:ASP:OD2	2.38	0.42
1:C:1116:GLY:O	1:C:1134:LEU:N	2.52	0.42
1:C:2574:HIS:CD2	1:C:2575:ARG:HG2	2.54	0.42
1:C:4181:ILE:HD12	1:C:4183:ILE:HG23	2.01	0.42
1:D:124:SER:HB2	1:D:133:PHE:HA	2.01	0.42
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.20	0.42
1:D:2170:MET:HE3	1:D:2170:MET:HB3	1.94	0.42
1:D:3007:ASN:O	1:D:3011:THR:OG1	2.22	0.42
1:D:3245:VAL:HG23	1:D:3248:ARG:H	1.84	0.42
1:D:4552:LEU:O	1:D:4556:SER:OG	2.34	0.42
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.91	0.42
1:A:2675:THR:HG22	1:A:2706:ILE:HG23	2.00	0.42
1:A:4677:LEU:HD12	1:A:4677:LEU:HA	1.85	0.42
1:B:716:PHE:HE1	1:B:730:VAL:HG21	1.84	0.42
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.29	0.42
1:B:2574:HIS:CD2	1:B:2575:ARG:HG2	2.54	0.42
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.67	0.42
1:B:4630:TYR:OH	1:C:4860:ARG:NH2	2.47	0.42
1:B:4911:LEU:HD13	1:B:4911:LEU:HA	1.90	0.42
1:C:2825:LYS:HE2	1:C:2825:LYS:HB2	1.91	0.42
1:C:3329:ILE:O	1:C:3403:ARG:NH2	2.49	0.42
1:C:3514:LEU:HD11	1:C:3602:VAL:HG13	2.02	0.42
1:D:111:HIS:ND1	1:D:114:SER:OG	2.39	0.42
1:D:400:ALA:O	1:D:404:ILE:HD12	2.19	0.42
1:D:498:THR:HA	1:D:553:ARG:HH12	1.85	0.42
1:D:884:LEU:HD13	1:D:968:ALA:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1256:GLU:HB3	1:D:1275:ARG:HH11	1.84	0.42
1:D:1422:ASP:OD2	1:D:1568:LYS:NZ	2.38	0.42
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.52	0.42
1:A:73:LEU:O	1:A:106:ALA:N	2.40	0.42
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.50	0.42
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.02	0.42
1:B:3245:VAL:HG23	1:B:3248:ARG:H	1.84	0.42
1:B:3514:LEU:HD11	1:B:3602:VAL:HG13	2.02	0.42
1:C:400:ALA:O	1:C:404:ILE:HD12	2.19	0.42
1:C:893:TYR:HB3	1:C:960:MET:HE2	2.00	0.42
1:C:3582:ARG:HA	1:C:3582:ARG:HD3	1.87	0.42
1:D:199:LEU:HD12	1:D:199:LEU:HA	1.87	0.42
1:D:1578:ALA:O	1:D:1584:ARG:NH2	2.37	0.42
1:A:1256:GLU:HB3	1:A:1275:ARG:HH11	1.84	0.42
1:A:2627:VAL:HG21	1:A:2674:LEU:HG	2.00	0.42
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.02	0.42
1:B:400:ALA:O	1:B:404:ILE:HD12	2.19	0.42
1:B:2587:TYR:O	1:B:2590:SER:OG	2.26	0.42
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.52	0.42
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.29	0.42
1:C:5030:LYS:HB2	1:C:5030:LYS:HE2	1.90	0.42
1:D:162:LYS:H	1:D:162:LYS:HG2	1.67	0.42
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.55	0.42
2:H:76:CYS:HB2	2:H:97:LEU:HB2	2.02	0.42
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.55	0.42
1:A:2538:THR:OG1	1:A:2539:ALA:N	2.53	0.42
1:A:4181:ILE:HD12	1:A:4183:ILE:HG23	2.01	0.42
1:A:4944:ARG:NE	1:B:4942:GLU:OE1	2.53	0.42
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.55	0.42
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.82	0.42
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.55	0.42
1:D:1084:GLN:NE2	1:D:1186:ASP:O	2.42	0.42
1:D:4823:LEU:HD23	1:D:4823:LEU:HA	1.83	0.42
2:E:76:CYS:HB2	2:E:97:LEU:HB2	2.02	0.42
1:A:328:LYS:HE2	1:A:328:LYS:HB2	1.92	0.42
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.87	0.42
1:B:1861:GLN:O	1:B:1865:MET:HG3	2.20	0.42
1:C:4675:LYS:HB3	1:C:4675:LYS:HE3	1.83	0.42
1:D:3068:LEU:HG	1:D:3139:VAL:HG11	2.02	0.42
1:A:657:THR:HG22	1:A:1001:VAL:HG21	2.02	0.42
1:A:2781:VAL:HG22	1:A:2790:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:THR:HA	1:B:553:ARG:HH12	1.85	0.42
1:B:3051:ARG:HA	1:B:3131:TYR:CE1	2.54	0.42
1:B:4057:MET:HE3	1:B:4057:MET:HB2	1.88	0.42
1:C:1422:ASP:OD2	1:C:1568:LYS:NZ	2.38	0.42
1:C:1861:GLN:O	1:C:1865:MET:HG3	2.20	0.42
1:C:2610:LEU:HD23	1:C:2610:LEU:HA	1.94	0.42
1:C:4128:PHE:HA	1:C:4131:ARG:HH21	1.85	0.42
1:D:403:MET:HE2	1:D:403:MET:HB3	1.88	0.42
1:D:1291:LEU:HD12	1:D:1550:PRO:HG2	2.01	0.42
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	2.02	0.42
1:D:1861:GLN:O	1:D:1865:MET:HG3	2.20	0.42
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.02	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.20	0.41
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.90	0.41
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.02	0.41
1:B:1256:GLU:HB3	1:B:1275:ARG:HH11	1.84	0.41
1:B:1648:MET:HE2	1:B:1648:MET:HB3	1.92	0.41
1:B:2806:ARG:HA	1:B:2809:ILE:HD13	2.02	0.41
1:B:4181:ILE:HD12	1:B:4183:ILE:HG23	2.01	0.41
1:C:1717:SER:HA	1:C:1721:GLU:HG2	2.02	0.41
1:C:2748:PRO:HG2	1:C:2817:ILE:HD13	2.02	0.41
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.02	0.41
1:D:1739:THR:O	1:D:1743[B]:ARG:HG3	2.20	0.41
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	2.01	0.41
1:D:4584:ASP:OD1	1:D:4584:ASP:N	2.51	0.41
1:A:2527:LEU:HA	1:A:2530:MET:HG3	2.02	0.41
1:A:3514:LEU:HD11	1:A:3602:VAL:HG13	2.01	0.41
1:B:2781:VAL:HG22	1:B:2790:MET:HB2	2.02	0.41
1:B:3068:LEU:HD23	1:B:3139:VAL:HG21	2.02	0.41
1:B:3068:LEU:HG	1:B:3139:VAL:HG11	2.02	0.41
1:B:3201:MET:HE3	1:B:3201:MET:HB2	1.93	0.41
1:C:25:SER:O	1:C:25:SER:OG	2.38	0.41
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	2.02	0.41
1:D:1229:ASN:HB2	1:D:1827:ARG:HG3	2.01	0.41
1:D:1717:SER:HA	1:D:1721:GLU:HG2	2.02	0.41
1:A:219:VAL:HG12	1:A:259:LEU:HD12	2.03	0.41
1:A:348:VAL:HB	1:A:357:LEU:HD22	2.03	0.41
1:A:400:ALA:O	1:A:404:ILE:HD12	2.19	0.41
1:A:1717:SER:HA	1:A:1721:GLU:HG2	2.02	0.41
1:A:1861:GLN:O	1:A:1865:MET:HG3	2.20	0.41
1:A:3261:ALA:HB1	1:A:3265:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:SER:HB2	1:B:133:PHE:HA	2.01	0.41
1:B:1717:SER:HA	1:B:1721:GLU:HG2	2.02	0.41
1:B:3110:LEU:HD23	1:B:3183:VAL:HG22	2.02	0.41
1:B:3582:ARG:HD3	1:B:3582:ARG:HA	1.87	0.41
1:C:219:VAL:HG12	1:C:259:LEU:HD12	2.03	0.41
1:C:322:LYS:HD3	1:C:322:LYS:HA	1.95	0.41
1:C:1269:CYS:HA	1:C:1564:PHE:O	2.20	0.41
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	2.01	0.41
1:C:2781:VAL:HG22	1:C:2790:MET:HB2	2.02	0.41
1:D:2748:PRO:HG2	1:D:2817:ILE:HD13	2.02	0.41
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.87	0.41
1:A:1291:LEU:HD12	1:A:1550:PRO:HG2	2.01	0.41
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.22	0.41
1:A:3110:LEU:HD23	1:A:3183:VAL:HG22	2.02	0.41
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.52	0.41
1:C:1476:MET:HE2	1:C:1476:MET:HB3	1.92	0.41
1:C:2197:LEU:HB3	1:C:2198:MET:HE2	2.02	0.41
1:C:2538:THR:OG1	1:C:2539:ALA:N	2.53	0.41
1:C:2806:ARG:HA	1:C:2809:ILE:HD13	2.02	0.41
1:C:2878:LEU:HD12	1:C:2878:LEU:HA	1.90	0.41
1:C:3051:ARG:NH2	1:C:3102:ASP:OD1	2.50	0.41
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.56	0.41
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.21	0.41
1:A:2748:PRO:HG2	1:A:2817:ILE:HD13	2.02	0.41
1:A:4064:MET:HE1	1:A:4111:LEU:HB2	2.02	0.41
1:A:4710:SER:OG	1:A:4772:ASP:OD2	2.38	0.41
1:A:4821:LYS:O	1:A:4825:THR:HG23	2.21	0.41
1:B:348:VAL:HB	1:B:357:LEU:HD22	2.03	0.41
1:B:2748:PRO:HG2	1:B:2817:ILE:HD13	2.02	0.41
1:B:3078:ARG:NE	1:B:3155:ASP:OD2	2.40	0.41
1:B:3260:GLY:HA2	1:B:3325:ASN:ND2	2.36	0.41
1:B:4888:TYR:OH	1:C:4917:ASP:OD2	2.31	0.41
1:C:498:THR:HA	1:C:553:ARG:HH12	1.85	0.41
1:C:3068:LEU:HG	1:C:3139:VAL:HG11	2.02	0.41
1:D:3694:LYS:HA	1:D:3695:PRO:HD3	1.90	0.41
1:A:498:THR:HA	1:A:553:ARG:HH12	1.85	0.41
1:A:1229:ASN:HB2	1:A:1827:ARG:HG3	2.01	0.41
1:A:1739:THR:O	1:A:1743[B]:ARG:HG3	2.20	0.41
1:A:3068:LEU:HG	1:A:3139:VAL:HG11	2.02	0.41
1:B:219:VAL:HG12	1:B:259:LEU:HD12	2.03	0.41
1:B:657:THR:HG22	1:B:1001:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2197:LEU:HB3	1:B:2198:MET:HE2	2.02	0.41
1:B:4064:MET:HE1	1:B:4111:LEU:HB2	2.02	0.41
1:C:1739:THR:O	1:C:1743[B]:ARG:HG3	2.21	0.41
1:C:2927:LEU:HD12	1:C:2927:LEU:HA	1.92	0.41
1:C:3260:GLY:HA2	1:C:3325:ASN:ND2	2.36	0.41
1:C:4710:SER:OG	1:C:4772:ASP:OD2	2.37	0.41
1:C:4827:LEU:HD23	1:C:4827:LEU:HA	1.94	0.41
1:D:265:LEU:HD22	1:D:279:PRO:HB2	2.03	0.41
1:D:1249:PRO:HA	1:D:1250:PRO:HD3	1.97	0.41
1:D:2684:ASP:O	1:D:2688:HIS:ND1	2.46	0.41
1:D:3110:LEU:HD23	1:D:3183:VAL:HG22	2.02	0.41
1:D:4098:ASP:OD1	1:D:4098:ASP:N	2.54	0.41
2:F:76:CYS:HB2	2:F:97:LEU:HB2	2.02	0.41
2:G:76:CYS:HB2	2:G:97:LEU:HB2	2.02	0.41
1:A:2806:ARG:HA	1:A:2809:ILE:HD13	2.03	0.41
1:A:4584:ASP:OD1	1:A:4584:ASP:N	2.51	0.41
1:A:4942:GLU:OE1	1:D:4944:ARG:NE	2.53	0.41
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	2.02	0.41
1:B:2527:LEU:HA	1:B:2530:MET:HG3	2.03	0.41
1:C:124:SER:HB2	1:C:133:PHE:HA	2.01	0.41
1:C:415:ILE:HA	1:C:418:LEU:HD12	2.03	0.41
1:C:3068:LEU:HD23	1:C:3139:VAL:HG21	2.02	0.41
1:C:3696:ASP:OD1	1:C:3696:ASP:N	2.53	0.41
1:D:219:VAL:HG12	1:D:259:LEU:HD12	2.03	0.41
1:D:2276:ALA:O	1:D:2279:SER:OG	2.39	0.41
1:D:2757:LYS:HG2	1:D:2929:PHE:HZ	1.86	0.41
1:D:3106:MET:HE1	1:D:3133:THR:H	1.86	0.41
1:A:716:PHE:HE1	1:A:730:VAL:HG21	1.84	0.41
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.02	0.41
1:A:2197:LEU:HB3	1:A:2198:MET:HE2	2.02	0.41
1:A:2790:MET:HE3	1:A:2790:MET:HB3	1.92	0.41
1:A:3068:LEU:HD23	1:A:3139:VAL:HG21	2.02	0.41
1:A:4128:PHE:HA	1:A:4131:ARG:HH21	1.85	0.41
1:B:415:ILE:HA	1:B:418:LEU:HD12	2.03	0.41
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.56	0.41
1:B:1948:ASP:OD1	1:B:2126:ARG:NH2	2.42	0.41
1:B:3261:ALA:HB1	1:B:3265:GLU:HG3	2.03	0.41
1:C:2906:VAL:HG23	1:C:2911:LEU:HD23	2.03	0.41
1:C:3852:LYS:HE3	1:C:3852:LYS:HB3	1.94	0.41
1:D:2781:VAL:HA	1:D:2789:PRO:HB2	2.03	0.41
1:D:2806:ARG:HA	1:D:2809:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3969:ILE:HD13	1:D:3969:ILE:HA	1.88	0.41
1:D:4064:MET:HE1	1:D:4111:LEU:HB2	2.02	0.41
1:D:4710:SER:OG	1:D:4772:ASP:OD2	2.38	0.41
1:A:356:TRP:O	1:A:379:HIS:N	2.54	0.41
1:A:415:ILE:HA	1:A:418:LEU:HD12	2.03	0.41
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.85	0.41
1:A:2542:SER:OG	1:A:2593:ARG:O	2.39	0.41
1:A:3271:GLU:OE2	1:A:3337:ARG:NH2	2.44	0.41
1:A:4090:LYS:HE2	1:A:4090:LYS:HB3	1.91	0.41
1:B:1739:THR:O	1:B:1743[B]:ARG:HG3	2.20	0.41
1:B:3272:ILE:O	1:B:3276:MET:HG2	2.21	0.41
1:B:3301:PRO:HA	1:B:3302:PRO:HD3	1.91	0.41
1:B:3696:ASP:N	1:B:3696:ASP:OD1	2.53	0.41
1:B:4821:LYS:O	1:B:4825:THR:HG23	2.21	0.41
1:B:4951:LYS:HE3	1:B:4951:LYS:HB3	1.82	0.41
1:C:265:LEU:HD22	1:C:279:PRO:HB2	2.03	0.41
1:C:348:VAL:HB	1:C:357:LEU:HD22	2.03	0.41
1:C:2781:VAL:HA	1:C:2789:PRO:HB2	2.03	0.41
1:D:415:ILE:HA	1:D:418:LEU:HD12	2.03	0.41
1:D:766:GLY:HA2	1:D:1475:THR:O	2.21	0.41
1:D:1762:LEU:HD12	1:D:1863:LEU:HD13	2.03	0.41
1:D:2250:MET:HE2	1:D:2250:MET:HB2	1.91	0.41
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.54	0.41
1:D:2906:VAL:HG23	1:D:2911:LEU:HD23	2.03	0.41
1:D:3260:GLY:HA2	1:D:3325:ASN:ND2	2.36	0.41
1:D:3261:ALA:HB1	1:D:3265:GLU:HG3	2.03	0.41
1:D:3514:LEU:HD11	1:D:3602:VAL:HG13	2.02	0.41
2:G:78:PRO:HA	2:G:81:ALA:HB3	2.03	0.41
1:A:766:GLY:HA2	1:A:1475:THR:O	2.21	0.41
1:A:2757:LYS:HG2	1:A:2929:PHE:HZ	1.86	0.41
1:A:3260:GLY:HA2	1:A:3325:ASN:ND2	2.36	0.41
1:A:3291:ALA:HA	1:A:3292:PRO:HD3	1.88	0.41
1:B:276:TRP:O	1:B:328:LYS:NZ	2.44	0.41
1:B:2538:THR:OG1	1:B:2539:ALA:N	2.53	0.41
1:B:3209:GLN:HG2	1:B:3210:LEU:HG	2.03	0.41
1:B:3713:LYS:HB2	1:B:3713:LYS:HE2	1.93	0.41
1:C:880:GLU:HB3	1:C:883:ALA:HB3	2.02	0.41
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.56	0.41
1:C:3722:TYR:OH	1:C:3797:THR:OG1	2.29	0.41
1:C:3974:THR:O	1:C:3978:GLN:HG2	2.21	0.41
1:C:4821:LYS:O	1:C:4825:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:THR:HG22	1:D:1001:VAL:HG21	2.02	0.41
1:D:793:LEU:HD12	1:D:821:LEU:HD21	2.03	0.41
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.56	0.41
1:D:880:GLU:HB3	1:D:883:ALA:HB3	2.02	0.41
1:D:3068:LEU:HD23	1:D:3139:VAL:HG21	2.02	0.41
1:A:396:GLU:OE2	1:A:470:SER:OG	2.29	0.40
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	2.02	0.40
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	2.01	0.40
1:A:3694:LYS:HA	1:A:3695:PRO:HD3	1.91	0.40
1:A:5006:GLN:O	1:A:5010:VAL:HG12	2.21	0.40
1:B:73:LEU:O	1:B:106:ALA:N	2.40	0.40
1:B:766:GLY:HA2	1:B:1475:THR:O	2.21	0.40
1:B:793:LEU:HD12	1:B:821:LEU:HD21	2.03	0.40
1:B:2781:VAL:HA	1:B:2789:PRO:HB2	2.03	0.40
1:C:283:ARG:NH1	1:C:290:TYR:OH	2.53	0.40
1:C:766:GLY:HA2	1:C:1475:THR:O	2.21	0.40
1:C:3110:LEU:HD23	1:C:3183:VAL:HG22	2.02	0.40
1:D:2197:LEU:HB3	1:D:2198:MET:HE2	2.02	0.40
1:D:4801:LEU:HD23	1:D:4801:LEU:HA	1.93	0.40
2:H:78:PRO:HA	2:H:81:ALA:HB3	2.03	0.40
1:A:1948:ASP:OD1	1:A:2126:ARG:NH2	2.42	0.40
1:A:2906:VAL:HG23	1:A:2911:LEU:HD23	2.03	0.40
1:A:3974:THR:O	1:A:3978:GLN:HG2	2.22	0.40
1:A:4066:LEU:HD22	1:A:4133:GLN:HE22	1.86	0.40
1:B:1929:MET:HE2	1:B:1929:MET:HB3	1.97	0.40
1:C:1084:GLN:NE2	1:C:1186:ASP:O	2.42	0.40
1:C:2463:LEU:HA	1:C:2466:LEU:HD12	2.03	0.40
1:C:2527:LEU:HA	1:C:2530:MET:HG3	2.03	0.40
1:C:2542:SER:OG	1:C:2593:ARG:O	2.39	0.40
1:C:3272:ILE:O	1:C:3276:MET:HG2	2.21	0.40
1:D:356:TRP:O	1:D:379:HIS:N	2.54	0.40
1:D:1116:GLY:O	1:D:1134:LEU:N	2.52	0.40
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.29	0.40
1:D:2781:VAL:HG22	1:D:2790:MET:HB2	2.02	0.40
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.87	0.40
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.93	0.40
1:D:4677:LEU:HD12	1:D:4677:LEU:HA	1.85	0.40
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.29	0.40
1:A:4951:LYS:HE3	1:A:4951:LYS:HB3	1.83	0.40
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.51	0.40
1:B:3051:ARG:NH2	1:B:3102:ASP:OD1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.56	0.40
1:C:2258:LEU:HD23	1:C:2258:LEU:HA	1.96	0.40
1:C:2905:LEU:HD23	1:C:2905:LEU:HA	1.95	0.40
1:C:3209:GLN:HG2	1:C:3210:LEU:HG	2.03	0.40
1:C:5006:GLN:O	1:C:5010:VAL:HG12	2.21	0.40
1:D:1466:LEU:HD23	1:D:1466:LEU:HA	1.95	0.40
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.56	0.40
1:A:3272:ILE:O	1:A:3276:MET:HG2	2.21	0.40
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	2.02	0.40
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.54	0.40
1:B:3106:MET:HE1	1:B:3133:THR:H	1.86	0.40
1:B:3974:THR:O	1:B:3978:GLN:HG2	2.21	0.40
1:C:22:LEU:HD12	1:C:37:LEU:HD12	2.03	0.40
1:C:364:PRO:HD2	1:C:367:LEU:HD12	2.04	0.40
1:C:793:LEU:HD12	1:C:821:LEU:HD21	2.03	0.40
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.54	0.40
1:C:4064:MET:HE1	1:C:4111:LEU:HB2	2.02	0.40
1:D:4675:LYS:HE3	1:D:4675:LYS:HB3	1.83	0.40
2:E:78:PRO:HA	2:E:81:ALA:HB3	2.03	0.40
1:A:364:PRO:HD2	1:A:367:LEU:HD12	2.04	0.40
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	2.04	0.40
1:B:22:LEU:HD12	1:B:37:LEU:HD12	2.03	0.40
1:B:356:TRP:O	1:B:379:HIS:N	2.54	0.40
1:B:2542:SER:OG	1:B:2593:ARG:O	2.39	0.40
1:B:2906:VAL:HG23	1:B:2911:LEU:HD23	2.03	0.40
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.93	0.40
1:C:2711:PRO:HA	1:C:2712:PRO:HD3	2.00	0.40
1:C:4066:LEU:HD22	1:C:4133:GLN:HE22	1.86	0.40
1:D:364:PRO:HD2	1:D:367:LEU:HD12	2.04	0.40
1:D:721:LEU:HD23	1:D:721:LEU:HA	1.90	0.40
1:D:2690:LYS:HA	1:D:2690:LYS:HD2	1.92	0.40
1:D:3974:THR:O	1:D:3978:GLN:HG2	2.21	0.40
1:D:4128:PHE:HA	1:D:4131:ARG:HH21	1.85	0.40
2:F:61:GLU:O	2:F:65:GLN:HG3	2.22	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	4353/5037 (86%)	4168 (96%)	182 (4%)	3 (0%)	48	78
1	B	4353/5037 (86%)	4168 (96%)	182 (4%)	3 (0%)	48	78
1	C	4353/5037 (86%)	4167 (96%)	183 (4%)	3 (0%)	48	78
1	D	4353/5037 (86%)	4167 (96%)	183 (4%)	3 (0%)	48	78
2	E	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	F	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	G	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	H	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
All	All	17832/21548 (83%)	17062 (96%)	758 (4%)	12 (0%)	49	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3616	LYS
1	A	4712	PRO
1	B	3616	LYS
1	B	4712	PRO
1	C	3616	LYS
1	C	4712	PRO
1	D	3616	LYS
1	D	4712	PRO
1	A	4691	GLN
1	B	4691	GLN
1	C	4691	GLN
1	D	4691	GLN

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADN	A	5101	-	21,21,21	0.19	0	31,31,31	0.32	0
3	ADN	D	5101	-	21,21,21	0.19	0	31,31,31	0.32	0
3	ADN	B	5101	-	21,21,21	0.19	0	31,31,31	0.32	0
3	ADN	C	5101	-	21,21,21	0.19	0	31,31,31	0.32	0

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
3	ADN	A	5101	-	-	3/6/22/22	0/3/3/3
3	ADN	D	5101	-	-	3/6/22/22	0/3/3/3
3	ADN	B	5101	-	-	3/6/22/22	0/3/3/3
3	ADN	C	5101	-	-	3/6/22/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

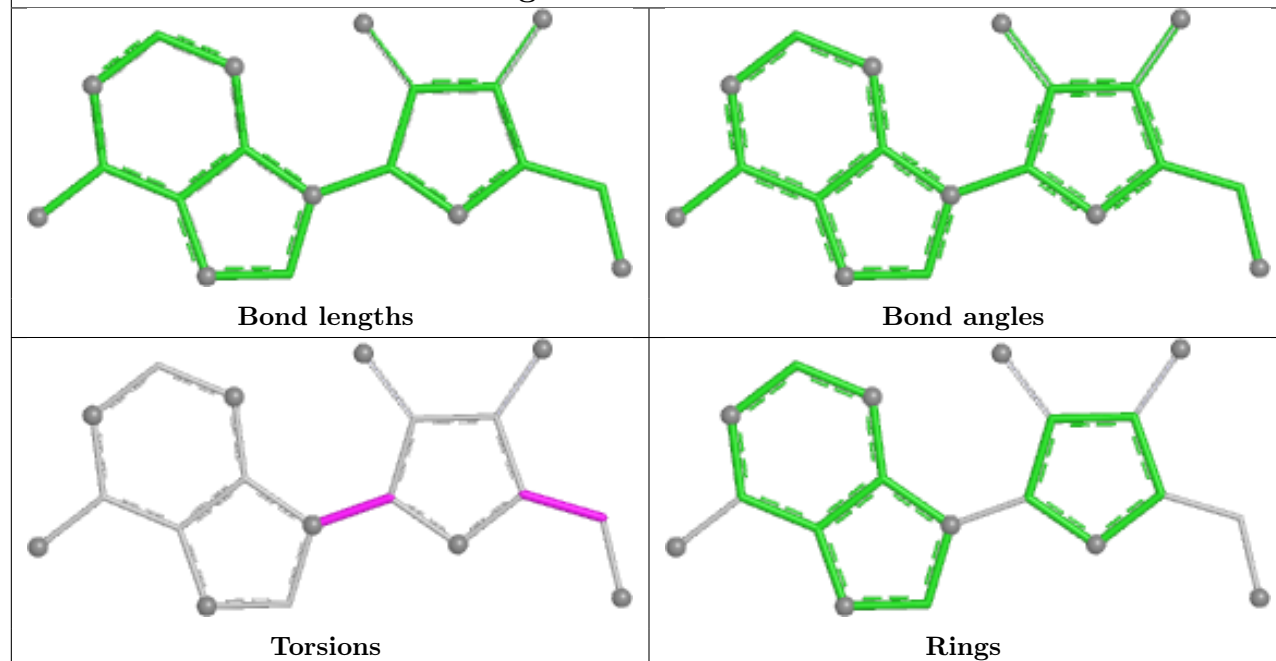
Mol	Chain	Res	Type	Atoms
3	A	5101	ADN	C3'-C4'-C5'-O5'
3	B	5101	ADN	C3'-C4'-C5'-O5'
3	C	5101	ADN	C3'-C4'-C5'-O5'
3	D	5101	ADN	C3'-C4'-C5'-O5'
3	A	5101	ADN	O4'-C4'-C5'-O5'
3	B	5101	ADN	O4'-C4'-C5'-O5'
3	C	5101	ADN	O4'-C4'-C5'-O5'
3	D	5101	ADN	O4'-C4'-C5'-O5'
3	A	5101	ADN	O4'-C1'-N9-C8
3	B	5101	ADN	O4'-C1'-N9-C8
3	C	5101	ADN	O4'-C1'-N9-C8
3	D	5101	ADN	O4'-C1'-N9-C8

There are no ring outliers.

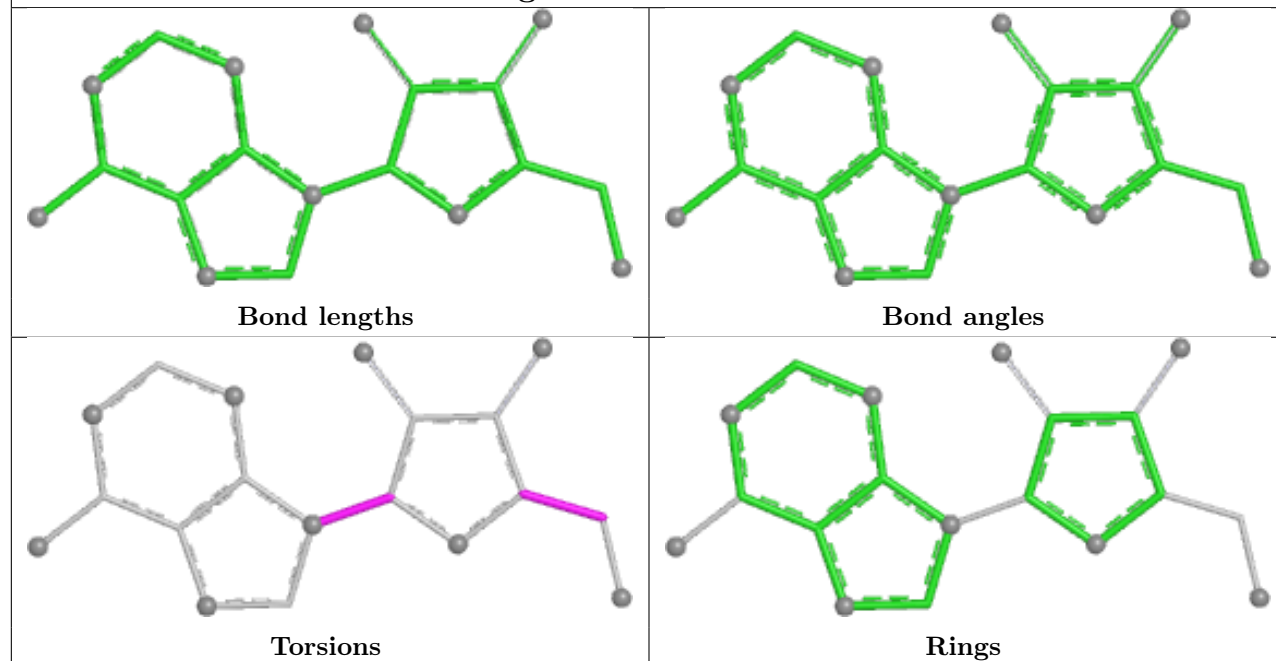
No monomer is involved in short contacts.

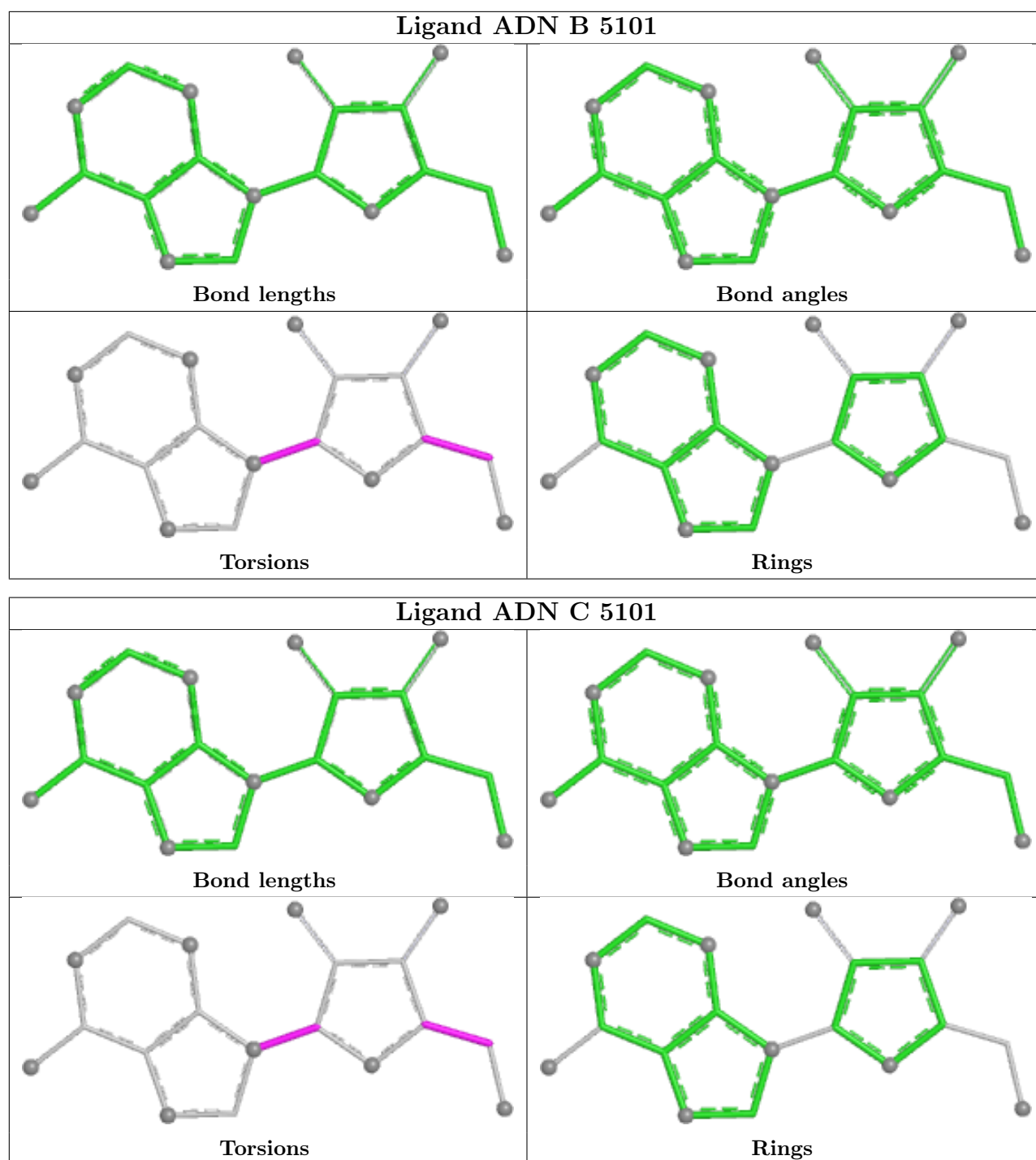
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand ADN A 5101



Ligand ADN D 5101





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.

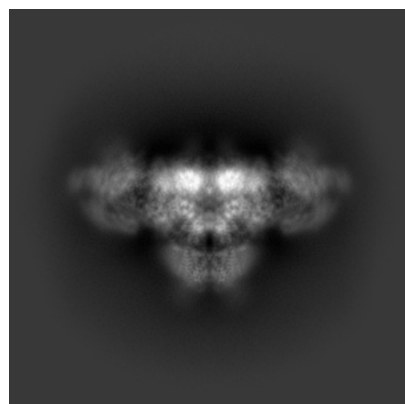
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40426. These allow visual inspection of the internal detail of the map and identification of artifacts.

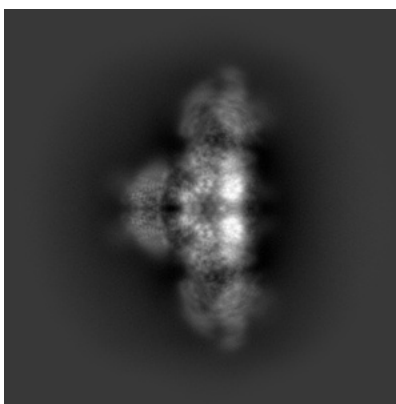
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

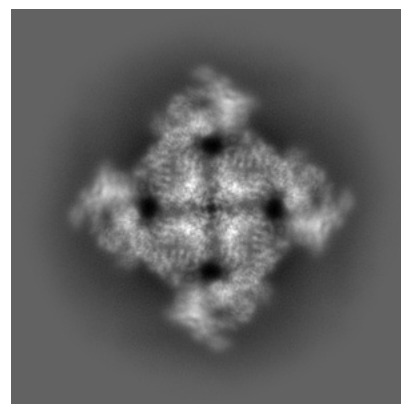
6.1.1 Primary map



X

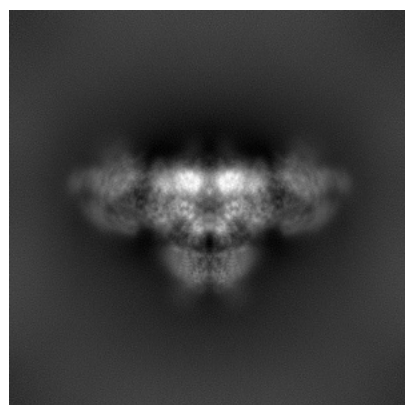


Y

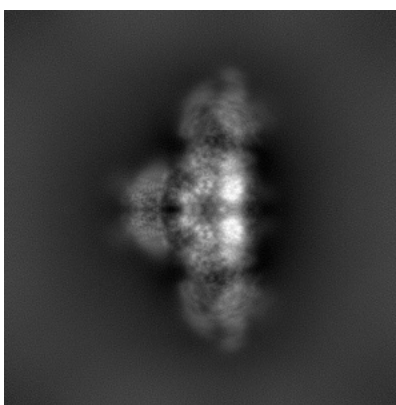


Z

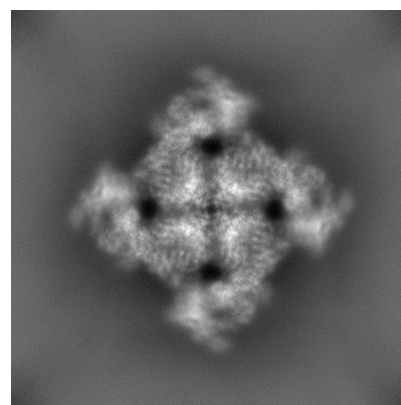
6.1.2 Raw map



X



Y

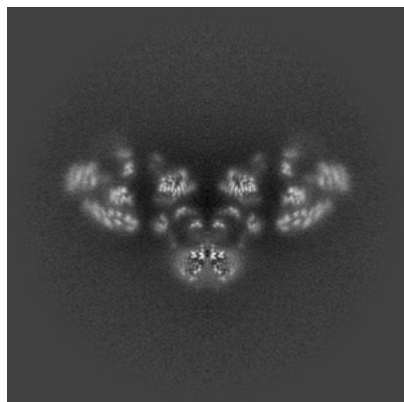


Z

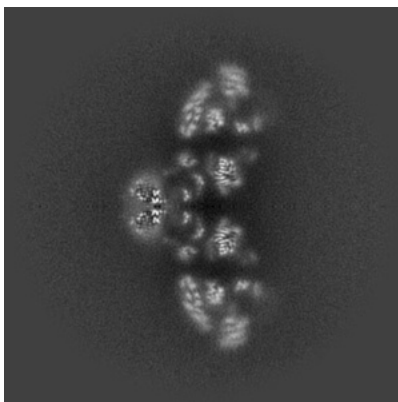
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

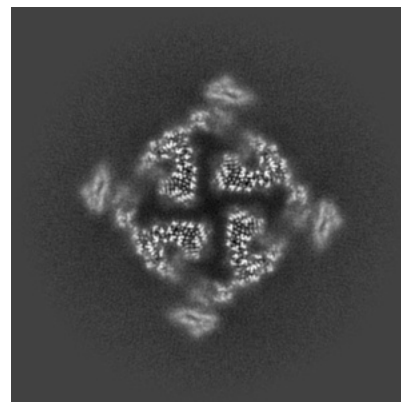
6.2.1 Primary map



X Index: 200

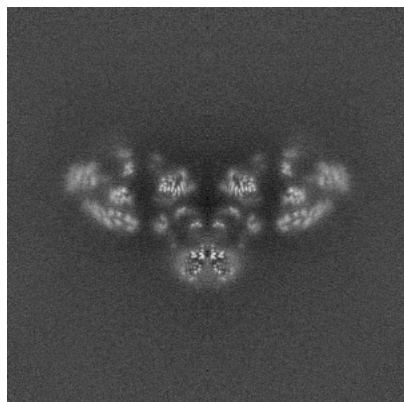


Y Index: 200

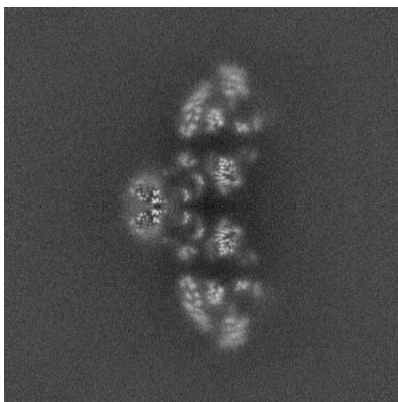


Z Index: 200

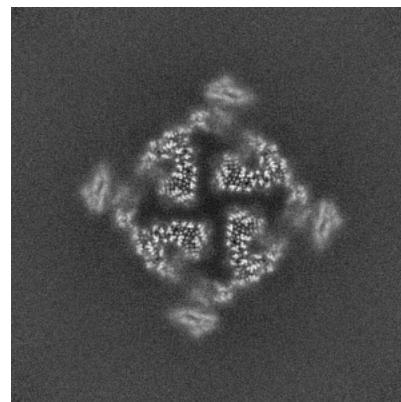
6.2.2 Raw map



X Index: 200



Y Index: 200

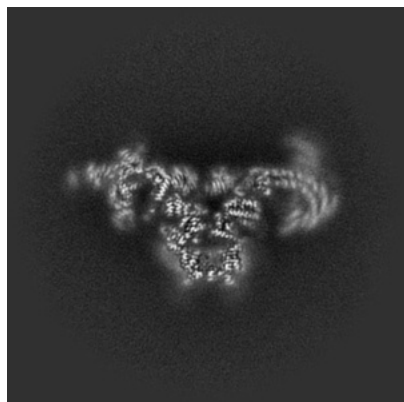


Z Index: 200

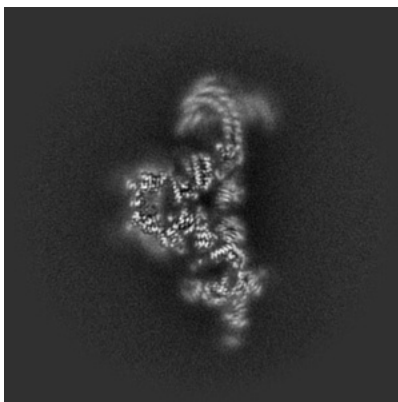
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

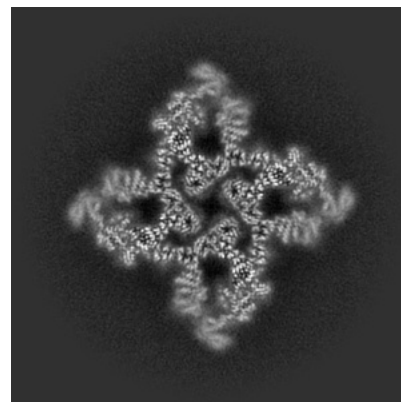
6.3.1 Primary map



X Index: 218

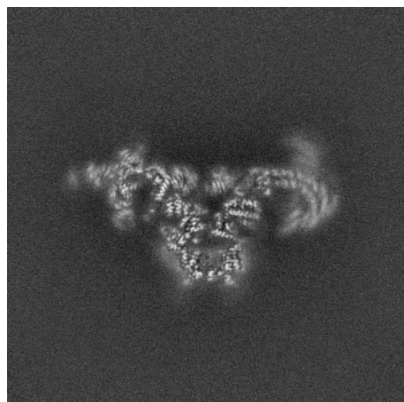


Y Index: 182

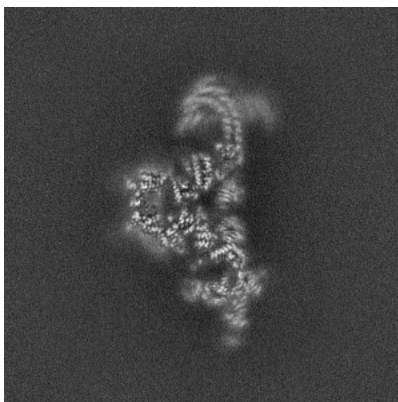


Z Index: 225

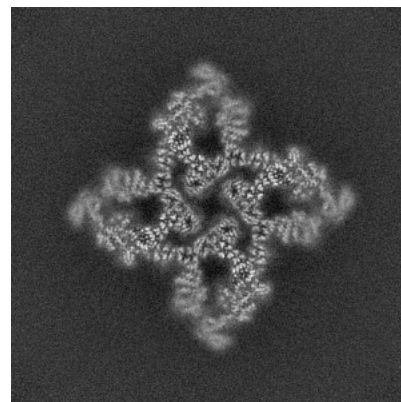
6.3.2 Raw map



X Index: 218



Y Index: 182

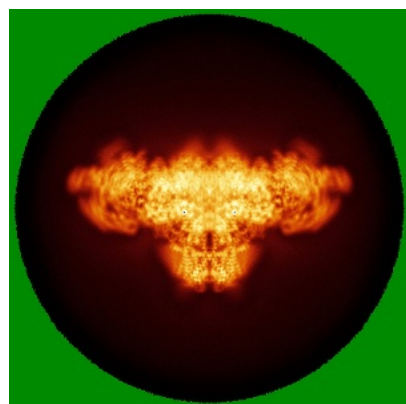


Z Index: 225

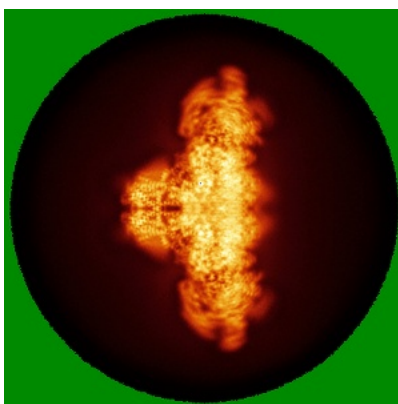
The images above show the largest variance slices of the map in three orthogonal directions.

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

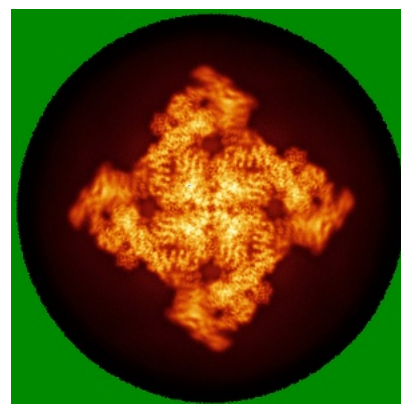
6.4.1 Primary map



X

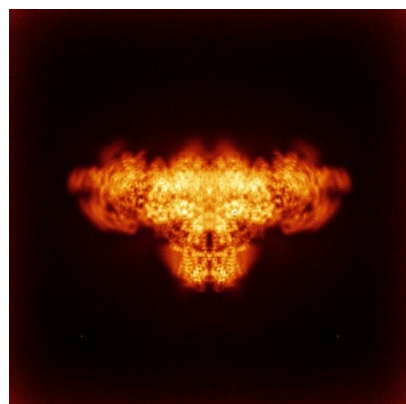


Y

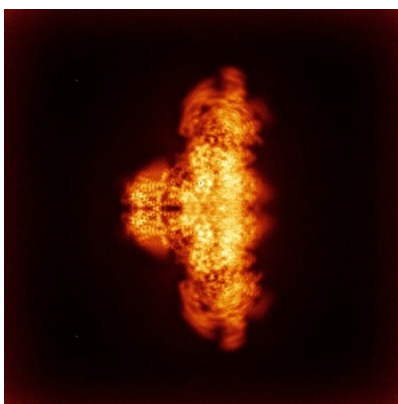


Z

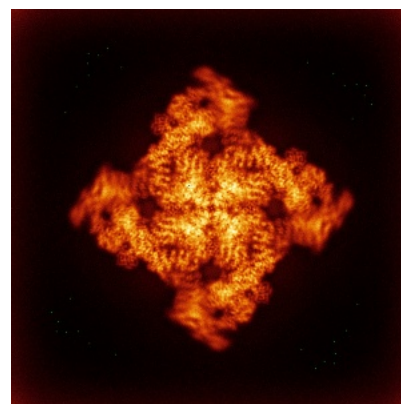
6.4.2 Raw map



X



Y

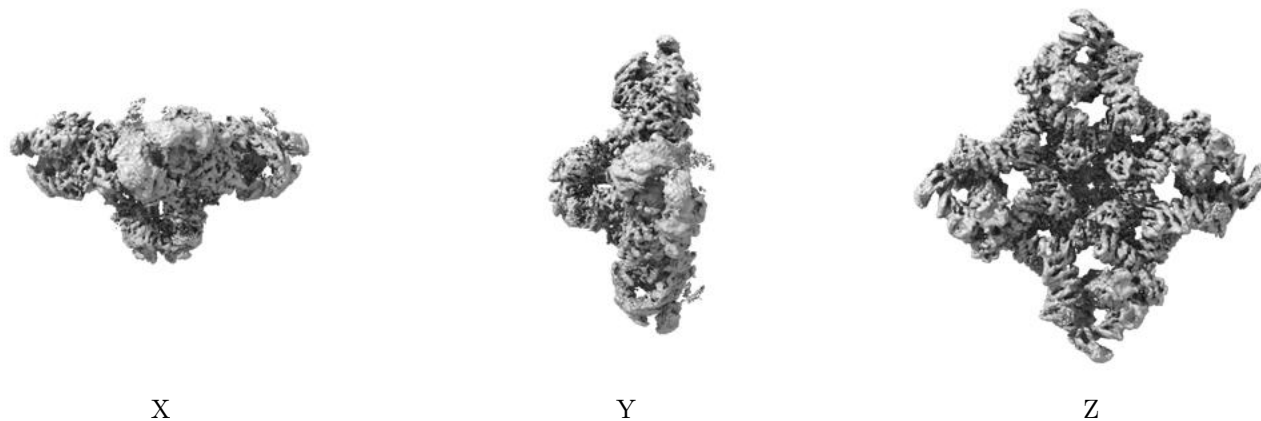


Z

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.

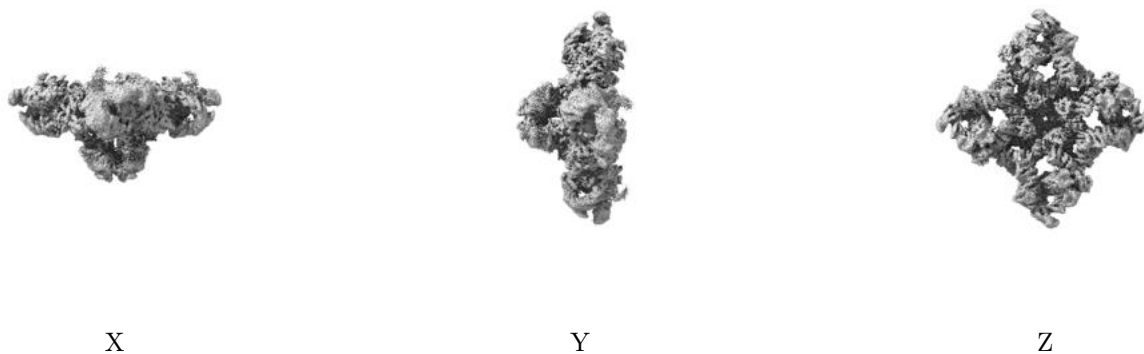
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.387. 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.

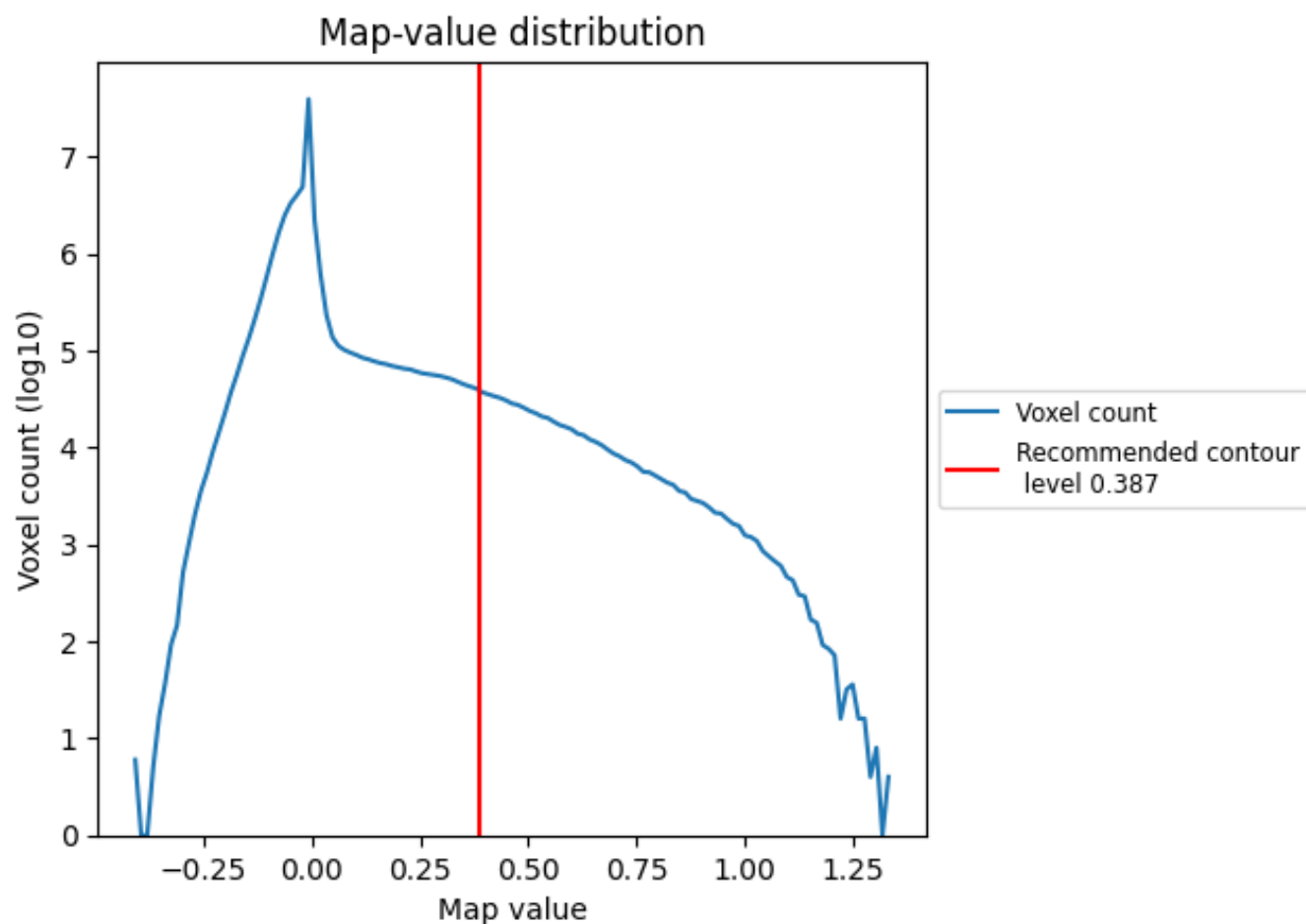
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

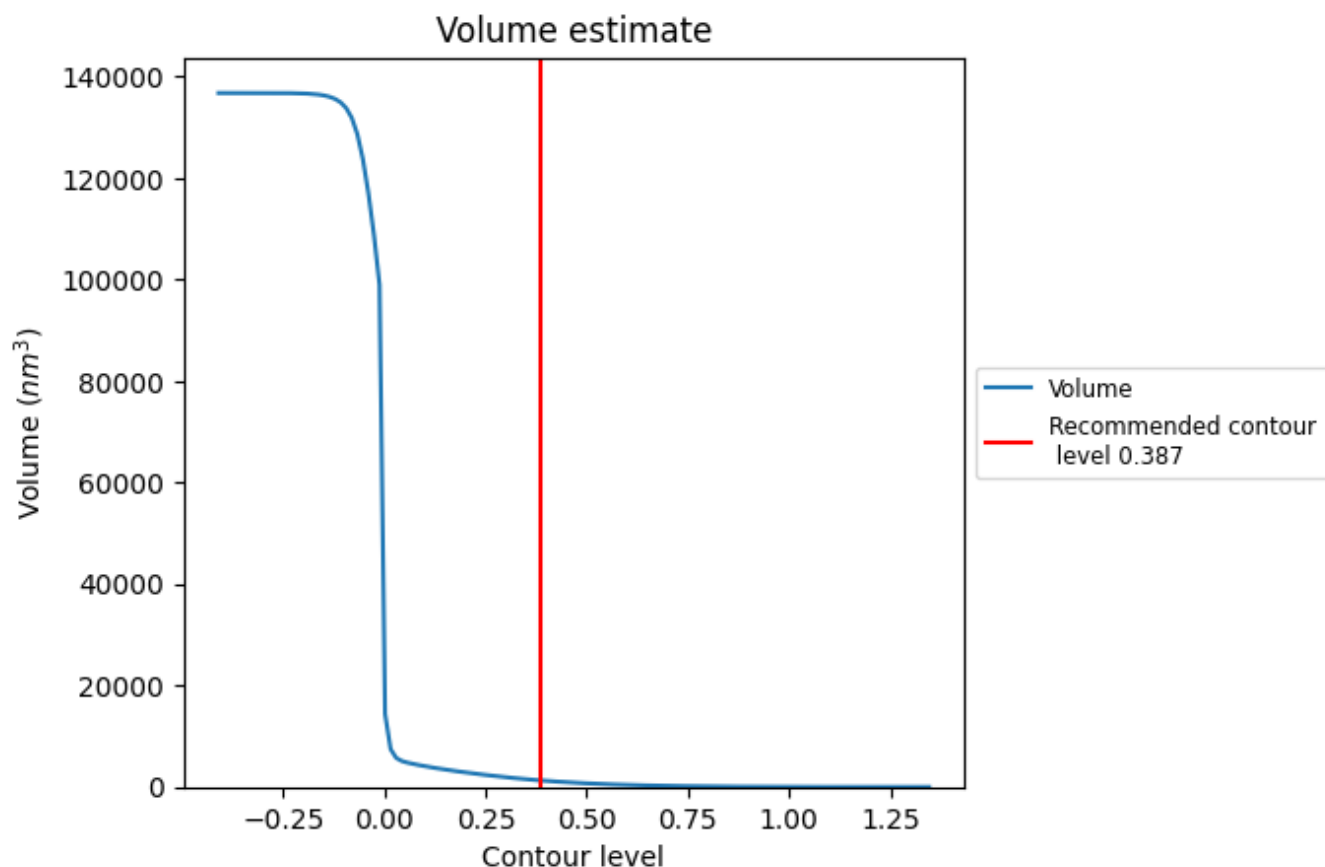
This section contains the results of statistical analysis of the map.

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.

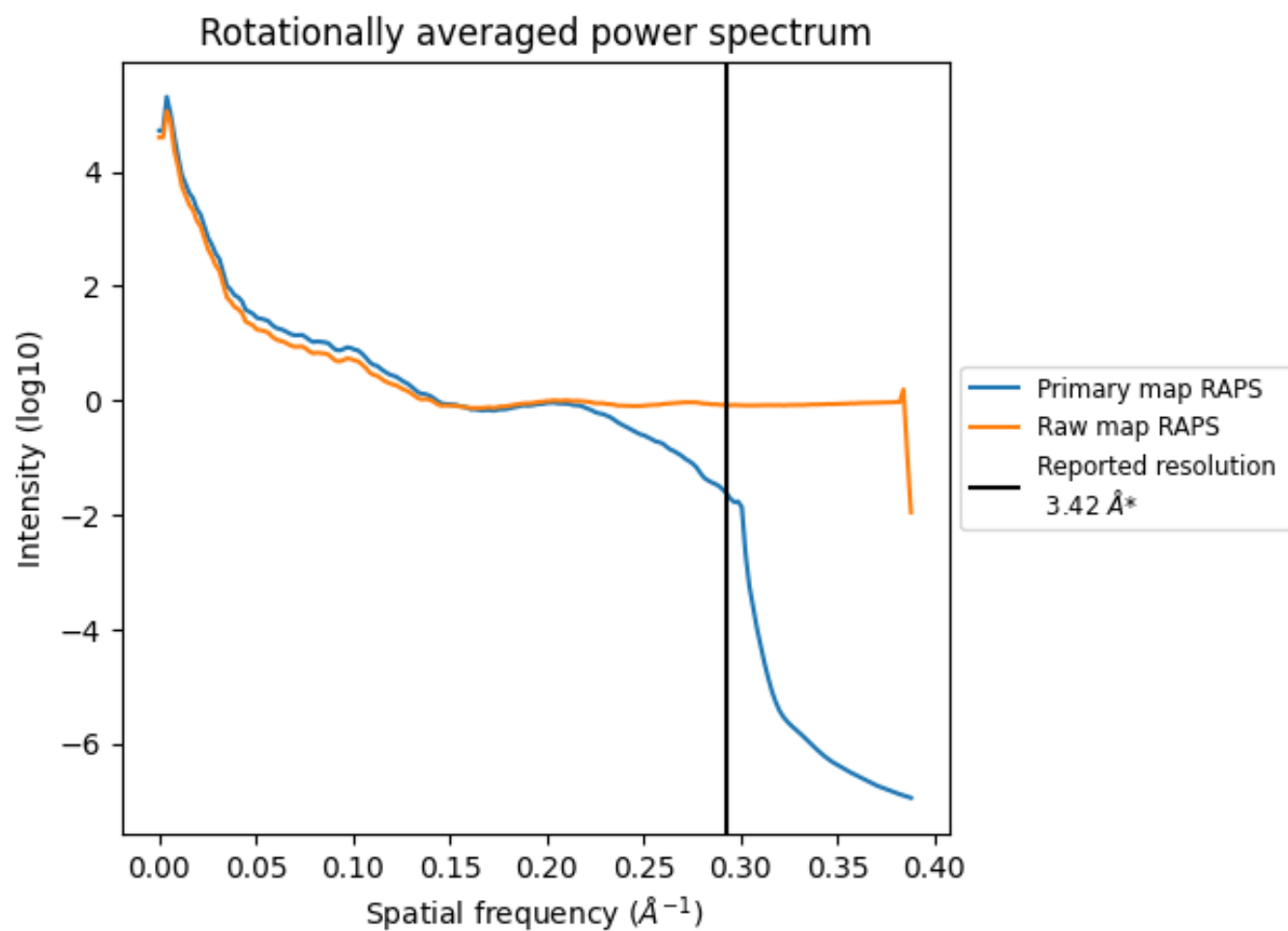
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1280 nm³; this corresponds to an approximate mass of 1156 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 ⓘ

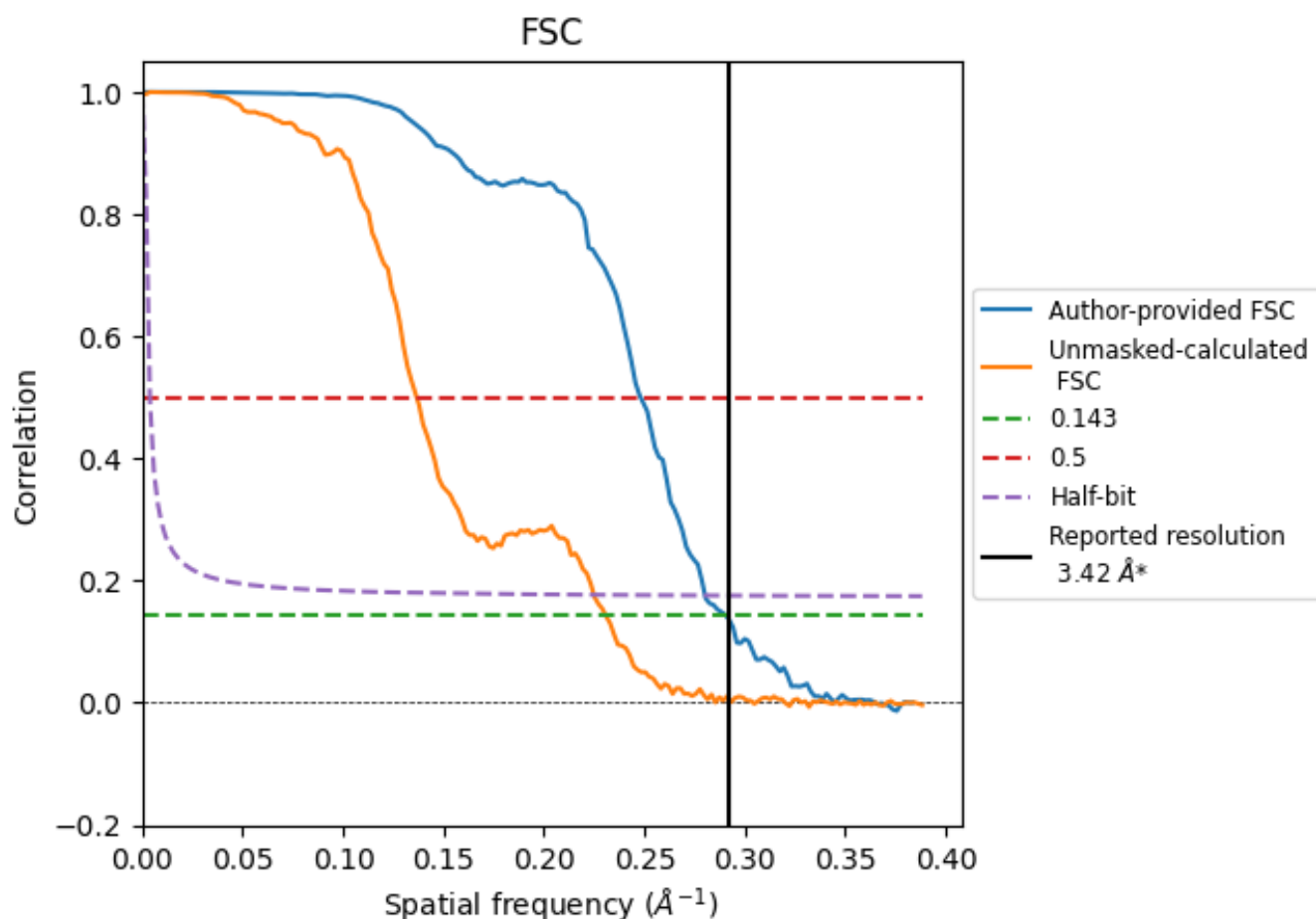


*Reported resolution corresponds to spatial frequency of 0.292 $\text{\AA}^{-1}$

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 0.292 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.44	4.03	3.57
Unmasked-calculated*	4.33	7.32	4.45

*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 4.33 differs from the reported value 3.42 by more than 10 %

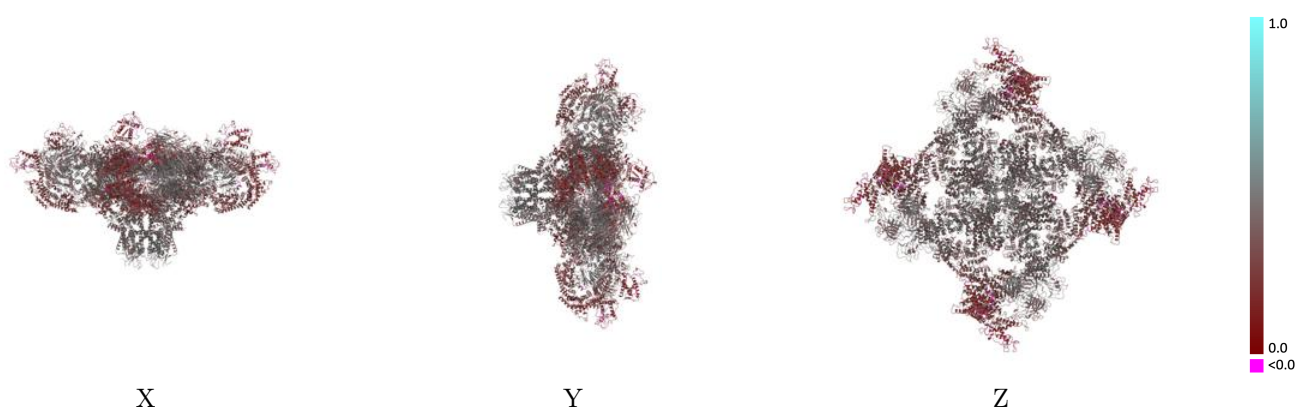
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-40426 and PDB model 8SER. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

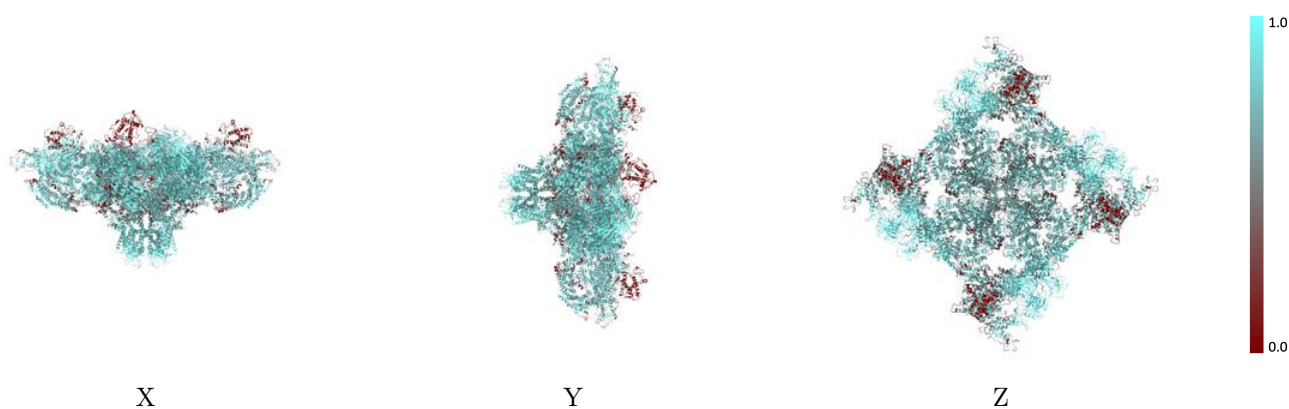
This section was not generated.

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



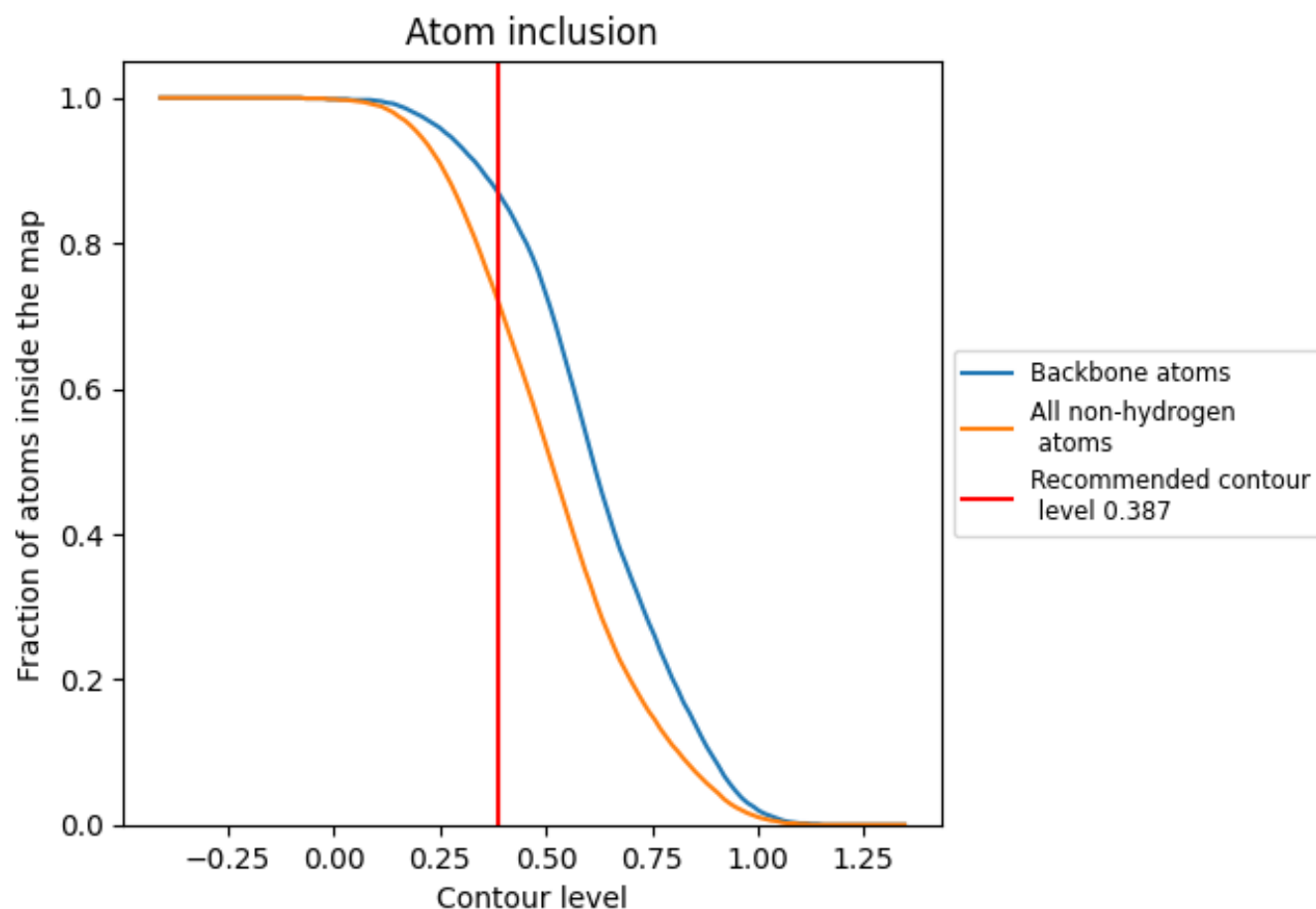
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.387).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.387) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.3530
A	0.7170	0.3510
B	0.7170	0.3510
C	0.7170	0.3510
D	0.7170	0.3520
E	0.8730	0.4230
F	0.8730	0.4230
G	0.8730	0.4240
H	0.8730	0.4250

1.0

0.0

<0.0