



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 05:05 PM EST

PDB ID : 7JMG
EMDB ID : EMD-22393
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 22 - State 2 (S2)
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2020-07-31
Resolution : 4.50 Å(reported)
Based on initial model : 5TB4

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

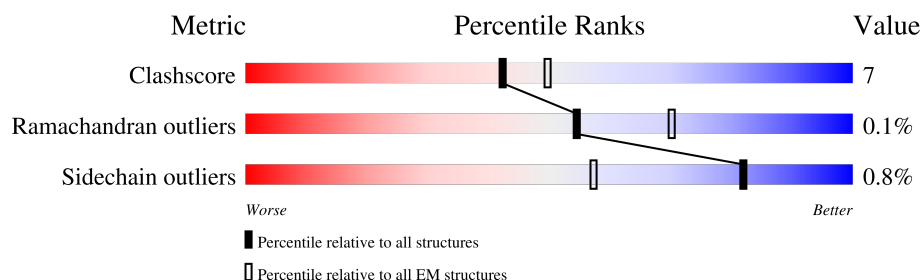
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	4687	<div> <div>21%</div> <div>74%</div> <div>14%</div> <div>11%</div> </div>
1	E	4687	<div> <div>25%</div> <div>74%</div> <div>14%</div> <div>11%</div> </div>
1	G	4687	<div> <div>26%</div> <div>74%</div> <div>14%</div> <div>11%</div> </div>
1	I	4687	<div> <div>24%</div> <div>74%</div> <div>14%</div> <div>11%</div> </div>
2	A	107	<div> <div>17%</div> <div>75%</div> <div>25%</div> </div>
2	F	107	<div> <div>24%</div> <div>78%</div> <div>22%</div> </div>
2	H	107	<div> <div>31%</div> <div>77%</div> <div>23%</div> </div>
2	J	107	<div> <div>25%</div> <div>74%</div> <div>26%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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 type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0

3 Residue-property plots

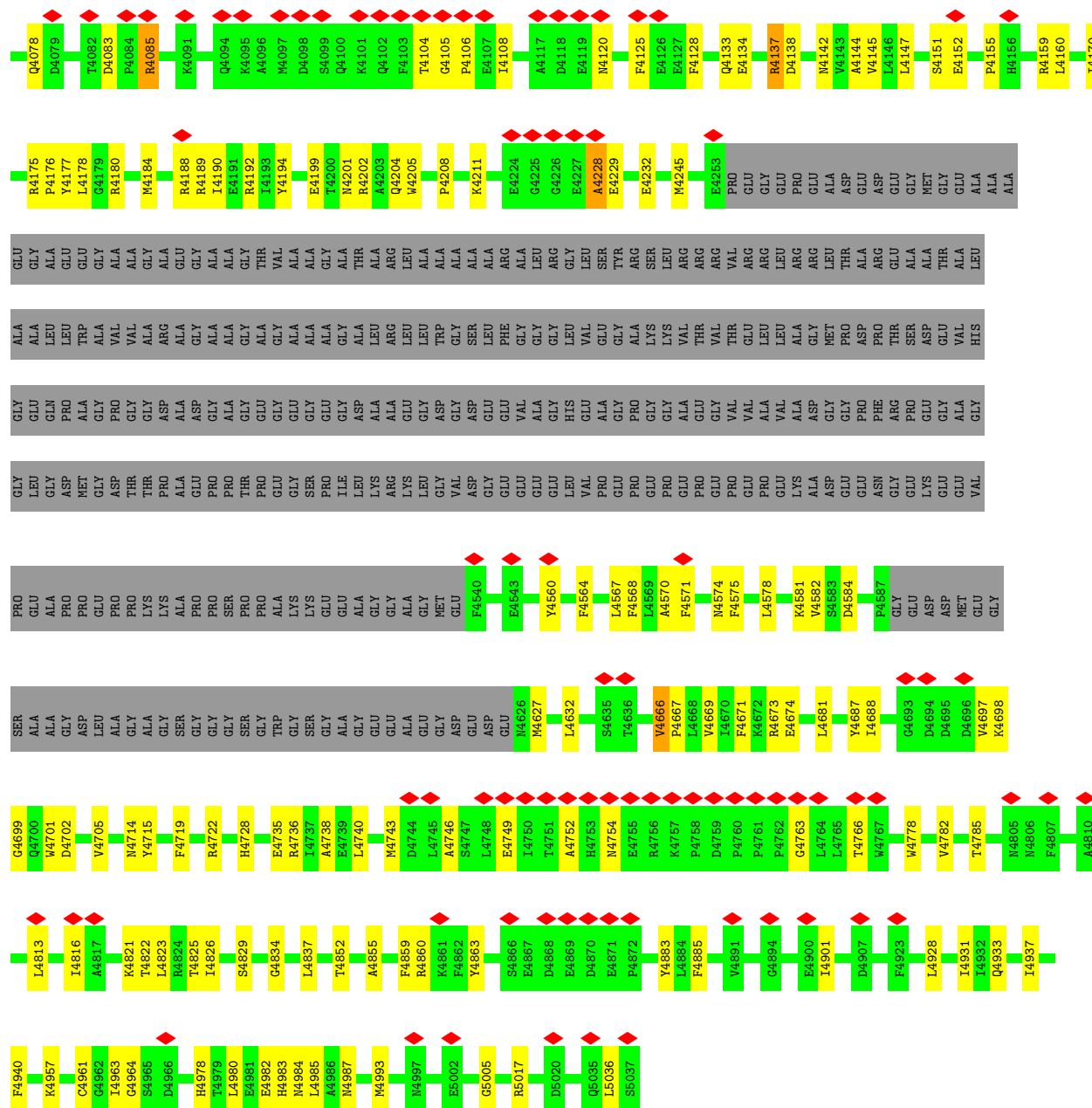
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 type 1

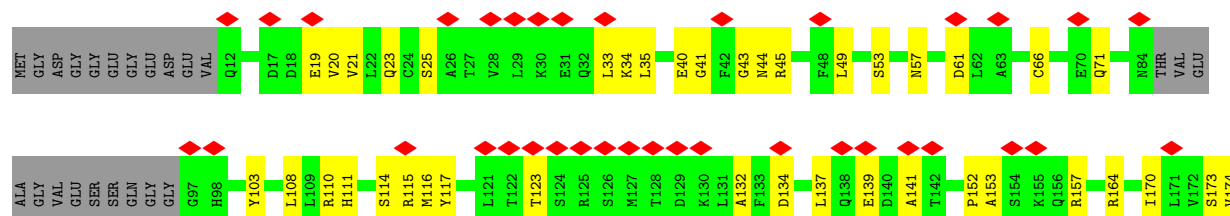
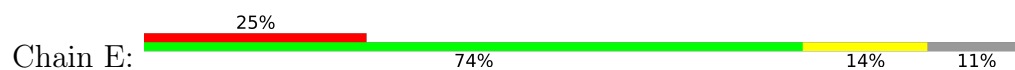


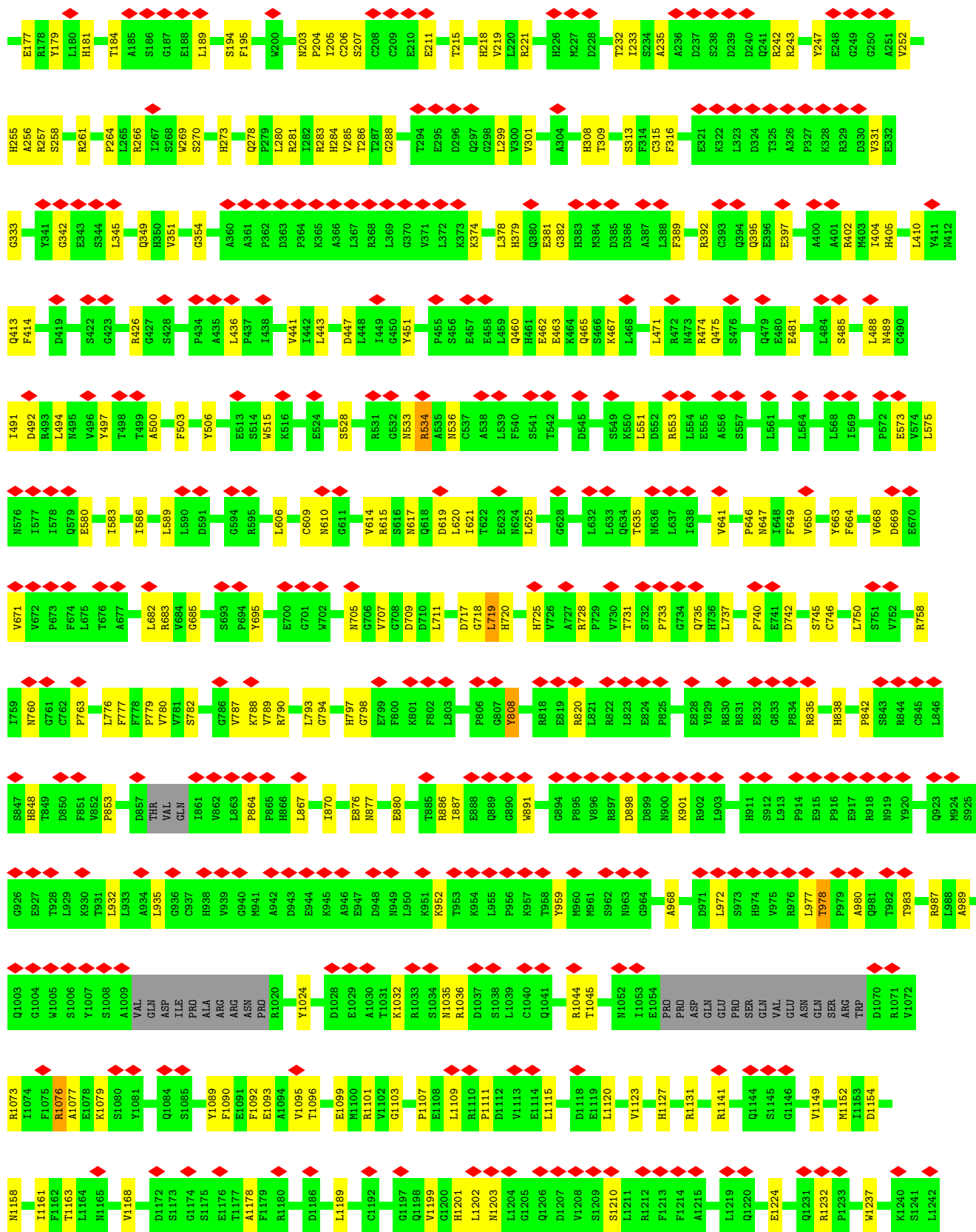


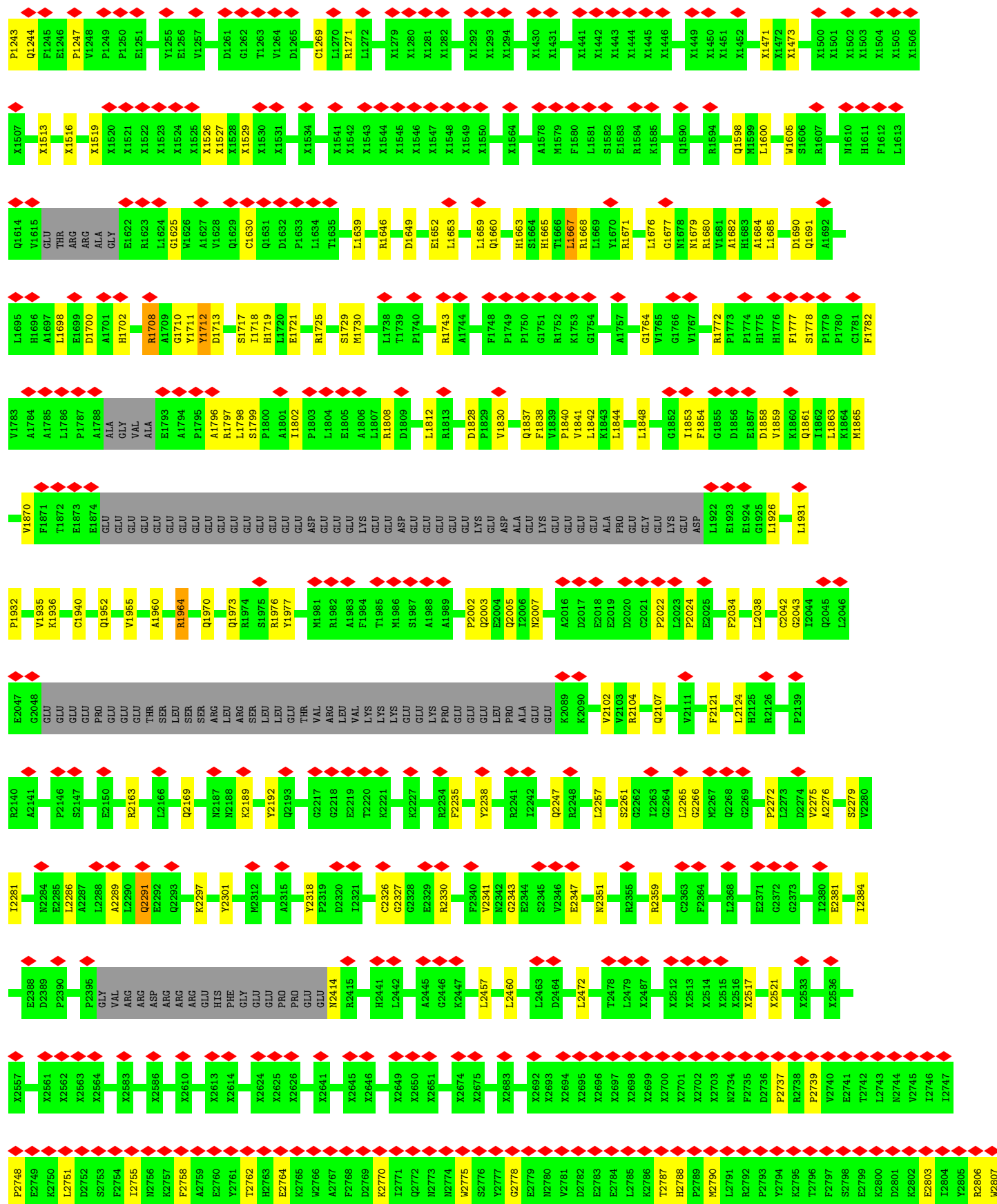




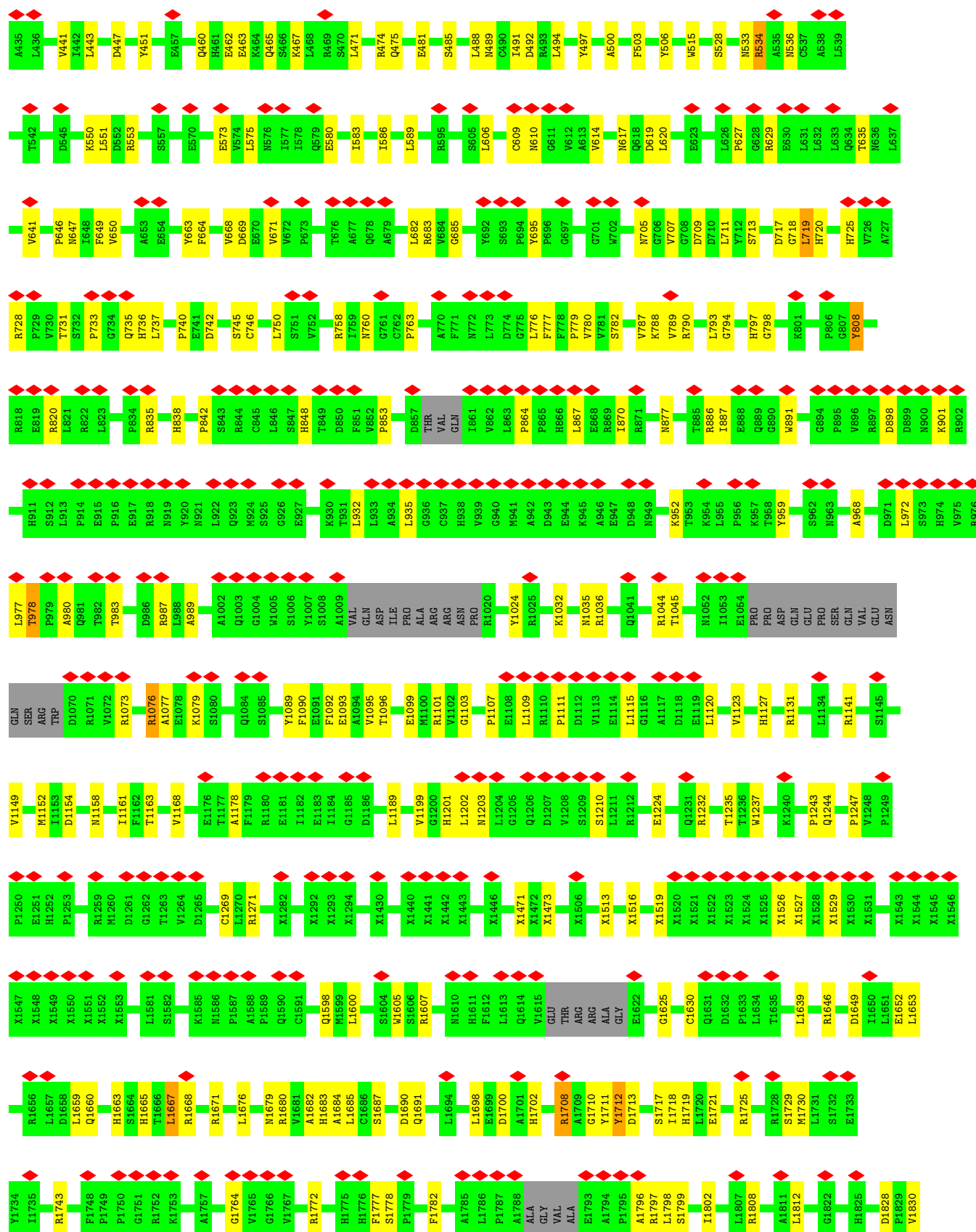
● Molecule 1: ryanodine receptor type 1





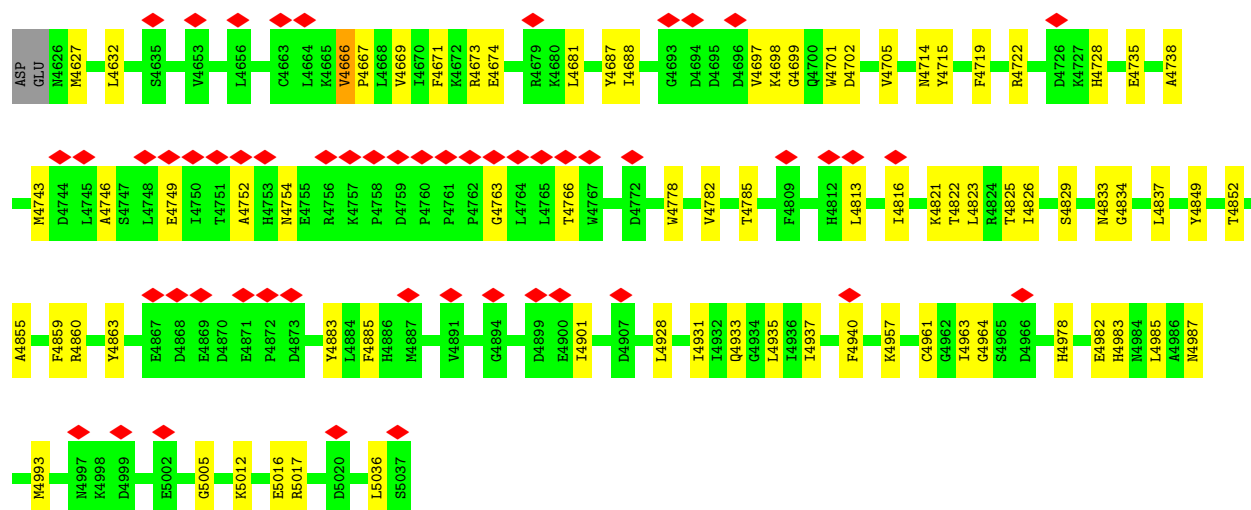


MET	R4159	K4069	E3945	V3859	L3764	E3684	X3559	X3336	X3192	K2928	S2868	GLY	P2808
GLY	L4160	D4070	Q3946	N3860	Q3767	E3685	X3560	X3345	X3193	P2929	R2869	GLU	T2809
ALA			N3950	E3861	L3770	E3686	X3561	X3346	X3194	L2930	E2870	ALA	K2810
ALA	I4170	G4073	F3951	D3862		E3687	X3562	X3347	X3195	Q2931	L2871	GLY	E2811
GLY	R4175	S4074	Q3960	T3864	R3773	E3688	X3564	X3348	X3196	M2932	Q2872	GLY	S2812
ALA	P4176	E4075	F3951	T3865	G3774	E3689	X3564	X3349	X3197	N2933	L2873	GLY	L2813
GLY	Y4177		N3963	T3866	A3775	V3690	X3565	X3350	X3216	G2934	M2874	GLY	K2814
GLY	L4178	Q4078	T3966	I3867		E3691	X3566	X3351	X3217	Y2935	A2875	GLY	A2815
GLY	R4180	D4079		N3868	V3779	E3692	X3567	X3352	X3218	E2876	Q2877	GLY	M2816
ALA	I4183	T4082	G3971	Q3869	Q3781	H3704	X3568	X3353	X3219	T2938	L2878	GLY	A2818
ALA	M4184	P4083	C3973	N3870	S3784		X3569	X3354	X3220	R2939	A2879	GLY	W2819
GLY	R4189	D4084	N3976	G3871	A3785	T3708	X3576	X3355	X3235	E2890	E2880	GLY	W2819
GLY	I4190	R4085	C3971	E3872	C3786	A3709		X3356	X3236	X2942	E2880	GLY	E2820
ALA	E4191		N3976	V3873	K3787	L3710		X3357	X3241	X2943	N2881	GLY	W2821
ALA	I4192	K4091	R3984	K3874	G3788	T3711		X3358	X3242	X2944	Y2882	GLY	T2822
GLY	I4193			M3875	E3789	K3712		X3359	X3243	X2945	H2883	GLY	T2823
THR	Y4194			A3876	T3790	S3714		X3360	X3243	X2946	N2884	GLY	E2824
VAL	E4199	Q4094	V3990	D3877	G3791	K3715		X3363	X3244	X2947	T2885	GLY	K2825
ALA	L4200	A4096	G3991	D3878	A3792	L3716		X3366	X3245	X2948	W2886	GLY	A2826
ALA	M4201	M4097	L3993	E3879		D3717		X3370	X3246	X2949	G2887	GLY	R2827
GLY	R4202	D4098	H3994	R3886	S3796	E3718		X3373	X3247		K2888	GLY	E2828
ALA	F3996	S4099	V3997	R3887	K3799	D3719		X3370	X3248	X2971	K2889	GLY	G2829
ALA	A4203	Q4100	A3997	L3886	L3805	Y3720		X3373	X3249	X2975	K2890	GLY	E2830
ALA	Q4204	K4101	H3998	L3887	N3806	L3721		X3381	X3250	X2976	K2891	GLY	GLU
ARG	W4205	F4102	K4002	D3888	G3807	Y3722		X3388	X3251	X2976	Q2892	GLY	ARG
LEU	E4206	T4103	L4003	N3889	G3808	M3723		X3389	X3252	X2995	E2893	GLY	THR
ALA	M4207	S4106	S4008	F3890	A3724	A3725		X3391	X3253	X3013	L2894	GLY	GLU
ALA	P4208	P4107	L4013	N3899	D3818	K3731		X3392	X3254	X3014	E2895	GLY	LYS
ALA	K4211	I4108	V4024	N3901	Y3819	H3734		X3393	X3255	X3015	A2896	GLY	LYS
ALA	E4224	E4116	L4027	T3905	F3829	L3735		X3394	X3256	X3016	K2897	GLY	THR
LEU	G4225	A4117	M4034	Q3906	Q3830	E3736		X3395	X3266	X3017	G2898	GLY	ARG
ARG	G4226	D4118	M4044	T3907	F3831	E3737		X3398	X3270	X3021	G2899	GLY	LYS
LEU	E4227	E4119	M4044	T3910	Q3832	G3738		X3432	X3273	X3022	T2901	GLY	ILE
SER	A4228	E4121	M4044	Q3907	L3833	E3739		X3433	X3274	X3023	H2902	GLY	THR
ARG	E4229	F4125	M4044	T3912	A3834	N3741		X3434	X3277	X3045	P2903	GLY	ALA
ARG	E4232		M4044	T3915	L3835	E3740		X3435	X3277	X3046	L2904	GLY	GLN
ARG	M4245		M4044	T3915	L3835	N3741		X3436	X3277	X3047	P2906	GLY	THR
VAL	E4253		M4044	T3915	L3835	E3741		X3436	X3277	X3048	V2906	GLY	ASP
ARG	PRO		M4044	T3915	L3835	E3741		X3436	X3277	X3049	P2907	GLY	ARG
GLY	GLY		M4044	T3915	L3835	E3741		X3436	X3277	X3050	Y2908	GLY	GLY
LEU	GLY		M4044	T3915	L3835	E3741		X3436	X3277	X3053	D2909	GLY	V2855
ARG	GLY		M4044	T3915	L3835	E3741		X3436	X3277	X3053	T2910	GLY	P2856
THR	ASP		M4044	T3915	L3835	E3741		X3436	X3277	X3053	L2911	GLY	P2857
THR	ASP		M4044	T3915	L3835	E3741		X3436	X3277	X3053	T2912	GLY	Q2858
ARG	GLY		M4044	T3915	L3835	E3741		X3436	X3277	X3053	A2913	GLY	P2859
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	K2914	GLY	P2860
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	E2915	GLY	L2862
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	K2916	GLY	S2863
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	A2917	GLY	G2864
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	R2918	GLY	V2865
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	D2919	GLY	T2866
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	E2921	GLY	L2867
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	K2922	GLY	
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	A2923	GLY	
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	Q2924	GLY	
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	E2925	GLY	
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	L2926	GLY	
			M4044	T3915	L3835	E3741		X3436	X3277	X3053	L2927	GLY	

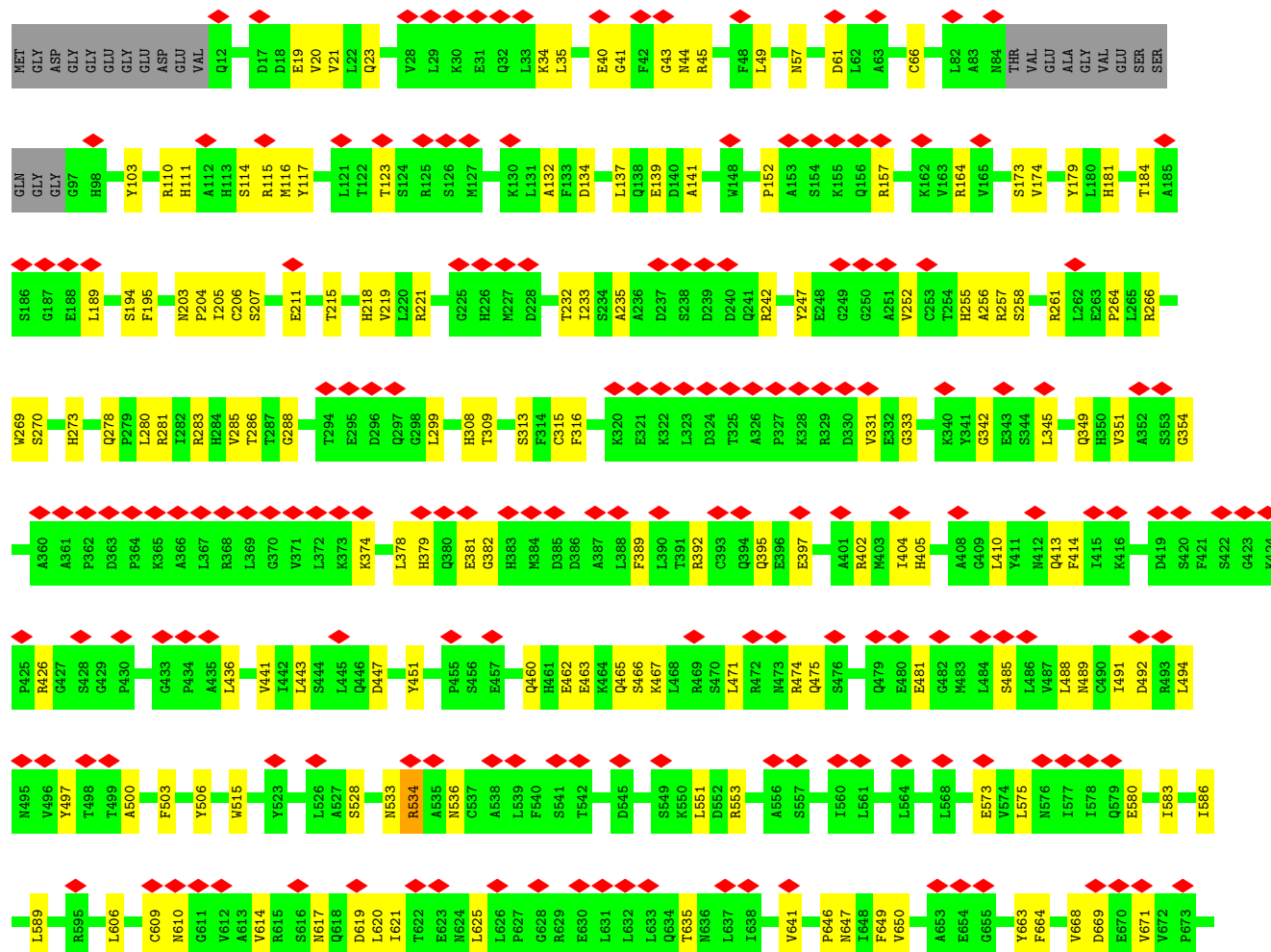
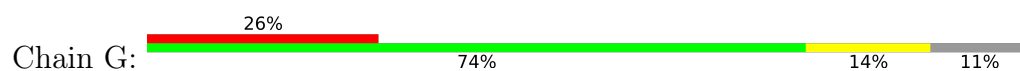




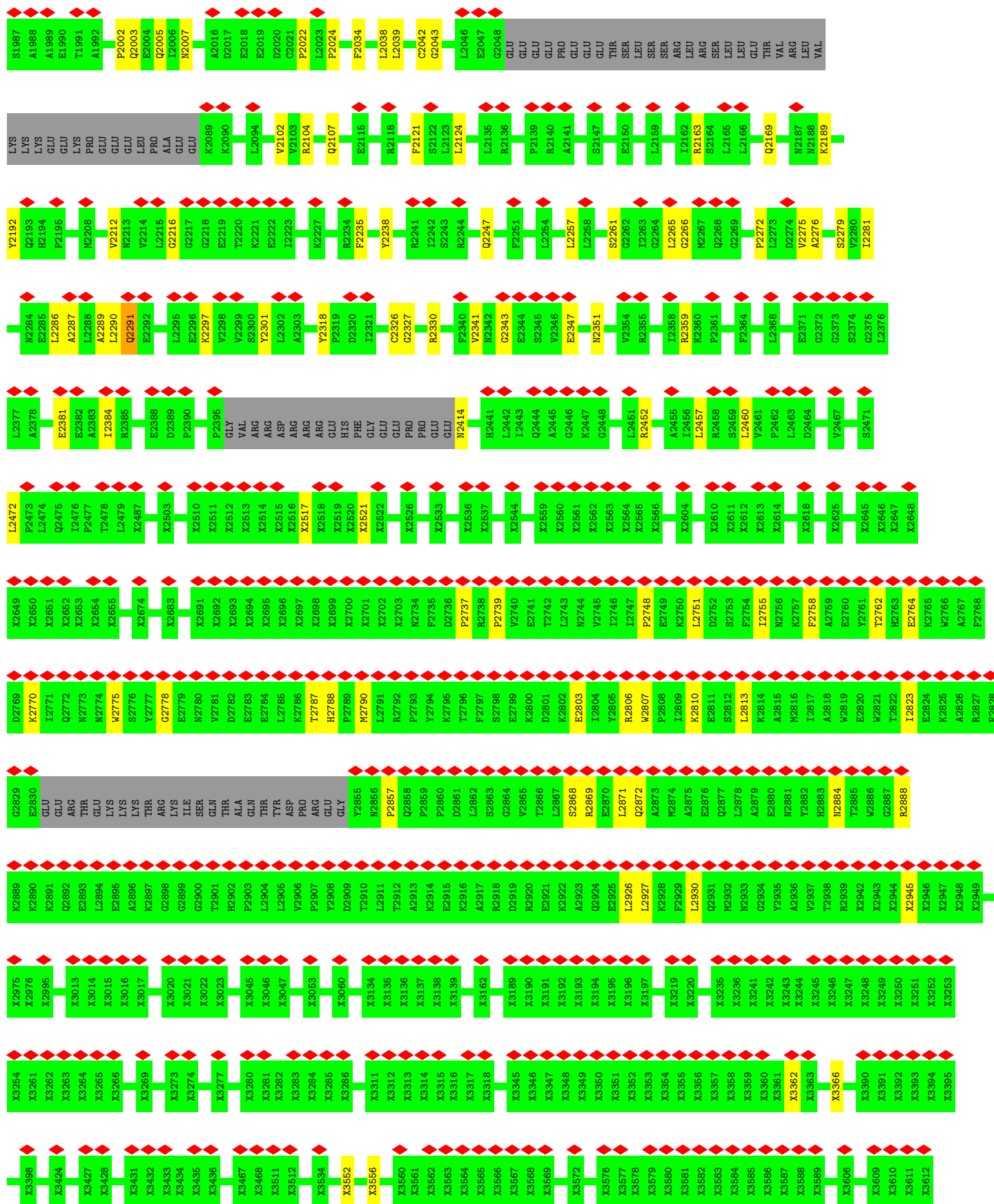




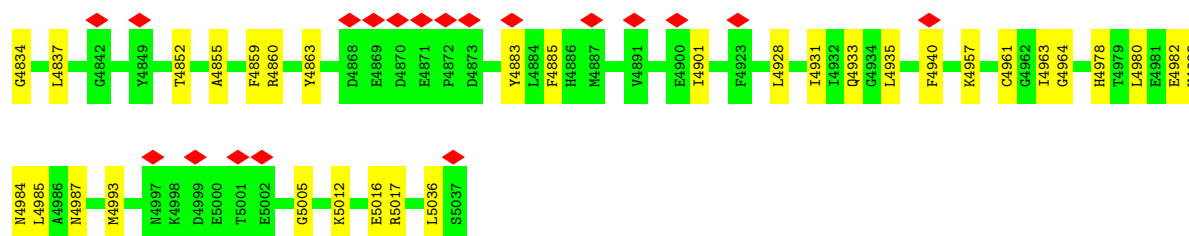
• Molecule 1: ryanodine receptor type 1



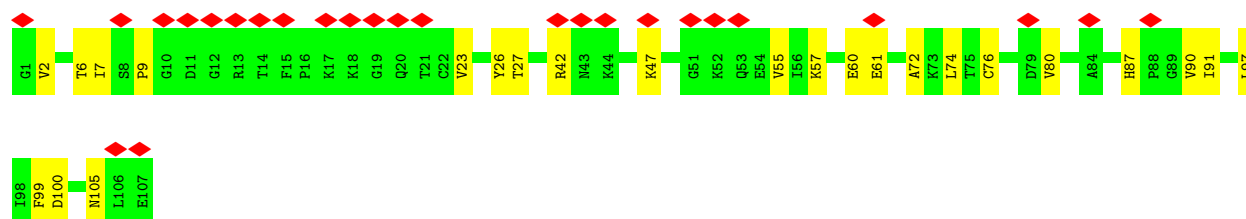
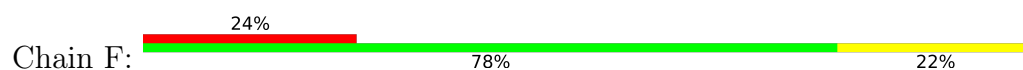




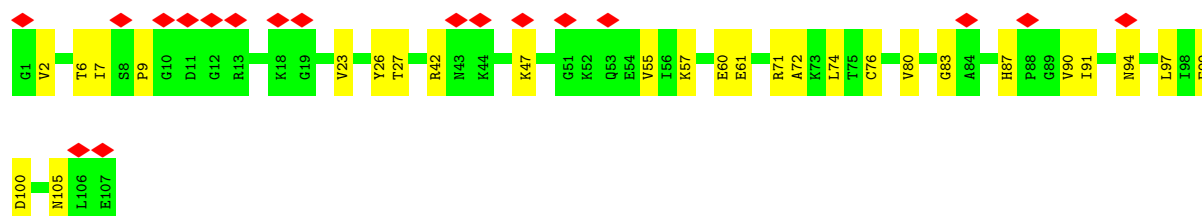
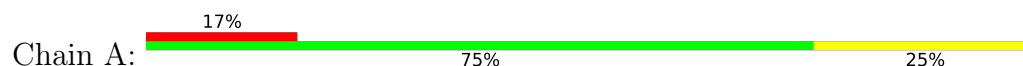




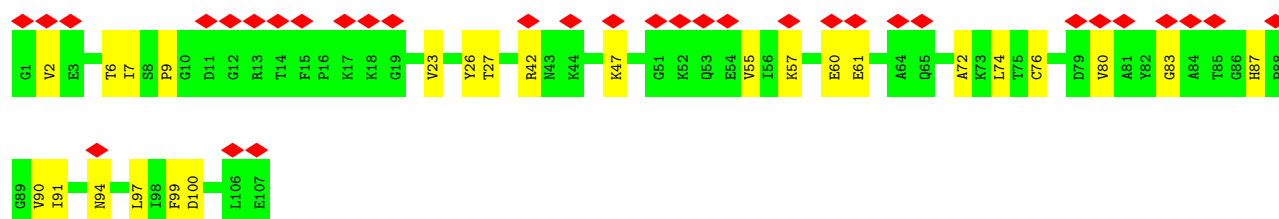
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



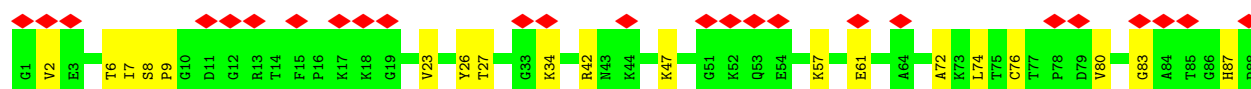
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

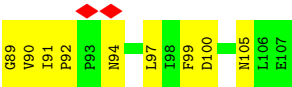


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.555	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.33	0/25428	0.56	5/34534 (0.0%)
1	E	0.33	0/25428	0.56	6/34534 (0.0%)
1	G	0.33	0/25428	0.56	5/34534 (0.0%)
1	I	0.33	0/25428	0.56	5/34534 (0.0%)
2	A	0.33	0/834	0.56	0/1123
2	F	0.33	0/834	0.56	0/1123
2	H	0.33	0/834	0.56	0/1123
2	J	0.33	0/834	0.56	0/1123
All	All	0.33	0/105048	0.56	21/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	12
1	E	0	12
1	G	0	12
1	I	0	12
All	All	0	48

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	719	LEU	CA-CB-CG	6.77	130.87	115.30
1	E	719	LEU	CA-CB-CG	6.76	130.85	115.30
1	G	719	LEU	CA-CB-CG	6.75	130.81	115.30
1	B	719	LEU	CA-CB-CG	6.74	130.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3764	LEU	CA-CB-CG	6.40	130.03	115.30
1	G	3764	LEU	CA-CB-CG	6.40	130.03	115.30
1	B	3764	LEU	CA-CB-CG	6.37	129.96	115.30
1	I	3764	LEU	CA-CB-CG	6.37	129.95	115.30
1	E	1667	LEU	CA-CB-CG	5.76	128.56	115.30
1	G	1667	LEU	CA-CB-CG	5.75	128.51	115.30
1	B	1667	LEU	CA-CB-CG	5.73	128.49	115.30
1	I	1667	LEU	CA-CB-CG	5.72	128.47	115.30
1	I	977	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	977	LEU	CA-CB-CG	5.55	128.06	115.30
1	E	977	LEU	CA-CB-CG	5.54	128.05	115.30
1	G	977	LEU	CA-CB-CG	5.54	128.03	115.30
1	G	2291	GLN	C-N-CA	5.08	134.41	121.70
1	I	2291	GLN	C-N-CA	5.06	134.34	121.70
1	E	2291	GLN	C-N-CA	5.05	134.32	121.70
1	B	2291	GLN	C-N-CA	5.05	134.32	121.70
1	E	4985	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1676	LEU	Peptide
1	B	1690	ASP	Peptide
1	B	1712	TYR	Peptide
1	B	1828	ASP	Peptide
1	B	2291	GLN	Peptide
1	B	2343	GLY	Peptide
1	B	2472	LEU	Peptide
1	B	2807	TRP	Peptide
1	B	3971	GLY	Peptide
1	B	4228	ALA	Peptide
1	B	4666	VAL	Peptide
1	B	808	TYR	Peptide
1	E	1676	LEU	Peptide
1	E	1690	ASP	Peptide
1	E	1712	TYR	Peptide
1	E	1828	ASP	Peptide
1	E	2291	GLN	Peptide
1	E	2343	GLY	Peptide
1	E	2472	LEU	Peptide
1	E	2807	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	E	3971	GLY	Peptide
1	E	4228	ALA	Peptide
1	E	4666	VAL	Peptide
1	E	808	TYR	Peptide
1	G	1676	LEU	Peptide
1	G	1690	ASP	Peptide
1	G	1712	TYR	Peptide
1	G	1828	ASP	Peptide
1	G	2291	GLN	Peptide
1	G	2343	GLY	Peptide
1	G	2472	LEU	Peptide
1	G	2807	TRP	Peptide
1	G	3971	GLY	Peptide
1	G	4228	ALA	Peptide
1	G	4666	VAL	Peptide
1	G	808	TYR	Peptide
1	I	1676	LEU	Peptide
1	I	1690	ASP	Peptide
1	I	1712	TYR	Peptide
1	I	1828	ASP	Peptide
1	I	2291	GLN	Peptide
1	I	2343	GLY	Peptide
1	I	2472	LEU	Peptide
1	I	2807	TRP	Peptide
1	I	3971	GLY	Peptide
1	I	4228	ALA	Peptide
1	I	4666	VAL	Peptide
1	I	808	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	29369	0	24714	390	0
1	E	29369	0	24715	385	0
1	G	29369	0	24713	387	0
1	I	29369	0	24715	388	0
2	A	818	0	824	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	818	0	824	14	0
2	H	818	0	824	14	0
2	J	818	0	824	20	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102153	1593	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 7.

All (1593) 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:E:4674:GLU:HG3	1:E:4714:ASN:HB3	1.69	0.75
1:G:4674:GLU:HG3	1:G:4714:ASN:HB3	1.69	0.74
1:B:4674:GLU:HG3	1:B:4714:ASN:HB3	1.69	0.73
1:I:4674:GLU:HG3	1:I:4714:ASN:HB3	1.69	0.73
1:G:788:LYS:HG2	1:G:1630:CYS:H	1.56	0.71
1:I:4855:ALA:HA	1:I:4859:PHE:HB2	1.73	0.70
1:B:788:LYS:HG2	1:B:1630:CYS:H	1.56	0.70
1:E:788:LYS:HG2	1:E:1630:CYS:H	1.56	0.70
1:E:4855:ALA:HA	1:E:4859:PHE:HB2	1.73	0.70
1:I:788:LYS:HG2	1:I:1630:CYS:H	1.56	0.70
1:B:4855:ALA:HA	1:B:4859:PHE:HB2	1.73	0.69
1:G:4855:ALA:HA	1:G:4859:PHE:HB2	1.73	0.69
1:B:103:TYR:HB3	1:B:152:PRO:HD3	1.76	0.67
1:G:1671:ARG:NH2	1:G:1710:GLY:O	2.27	0.67
1:B:1671:ARG:NH2	1:B:1710:GLY:O	2.27	0.67
1:E:1671:ARG:NH2	1:E:1710:GLY:O	2.27	0.67
1:I:1671:ARG:NH2	1:I:1710:GLY:O	2.27	0.67
1:G:4957:LYS:HG2	1:G:4964:GLY:HA2	1.76	0.67
1:E:103:TYR:HB3	1:E:152:PRO:HD3	1.76	0.67
1:G:103:TYR:HB3	1:G:152:PRO:HD3	1.76	0.67
1:E:4961:CYS:SG	1:E:4978:HIS:NE2	2.68	0.67
1:E:4957:LYS:HG2	1:E:4964:GLY:HA2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.29	0.66
1:I:4957:LYS:HG2	1:I:4964:GLY:HA2	1.77	0.66
1:I:745:SER:HB2	1:I:758:ARG:HB3	1.78	0.66
1:G:745:SER:HB2	1:G:758:ARG:HB3	1.77	0.66
1:B:745:SER:HB2	1:B:758:ARG:HB3	1.78	0.66
1:B:2359:ARG:NH1	1:I:179:TYR:OH	2.29	0.66
1:E:745:SER:HB2	1:E:758:ARG:HB3	1.78	0.66
1:G:219:VAL:HG13	1:G:285:VAL:HG21	1.78	0.66
1:G:281:ARG:NH2	1:G:309:THR:OG1	2.29	0.66
1:B:4961:CYS:SG	1:B:4978:HIS:NE2	2.69	0.66
1:I:103:TYR:HB3	1:I:152:PRO:HD3	1.76	0.66
1:G:4961:CYS:SG	1:G:4978:HIS:NE2	2.69	0.66
1:I:4961:CYS:SG	1:I:4978:HIS:NE2	2.69	0.66
1:B:219:VAL:HG13	1:B:285:VAL:HG21	1.78	0.65
1:B:4957:LYS:HG2	1:B:4964:GLY:HA2	1.77	0.65
1:E:281:ARG:NH2	1:E:309:THR:OG1	2.29	0.65
1:B:256:ALA:HB1	1:B:286:THR:HG21	1.79	0.65
1:E:219:VAL:HG13	1:E:285:VAL:HG21	1.78	0.65
1:I:219:VAL:HG13	1:I:285:VAL:HG21	1.78	0.65
1:I:256:ALA:HB1	1:I:286:THR:HG21	1.79	0.65
1:G:1247:PRO:HA	1:G:1598:GLN:HA	1.79	0.65
1:I:650:VAL:HB	1:I:777:PHE:HB2	1.79	0.65
1:E:426:ARG:HB2	1:E:506:TYR:HA	1.79	0.65
1:E:650:VAL:HB	1:E:777:PHE:HB2	1.79	0.65
1:I:1247:PRO:HA	1:I:1598:GLN:HA	1.79	0.65
1:G:989:ALA:O	1:G:1035:ASN:ND2	2.30	0.64
1:E:379:HIS:HD2	1:E:382:GLY:H	1.44	0.64
1:E:989:ALA:O	1:E:1035:ASN:ND2	2.30	0.64
1:G:1092:PHE:HB3	1:G:1149:VAL:HB	1.79	0.64
1:B:379:HIS:HD2	1:B:382:GLY:H	1.44	0.64
1:B:989:ALA:O	1:B:1035:ASN:ND2	2.30	0.64
1:E:1092:PHE:HB3	1:E:1149:VAL:HB	1.79	0.64
1:I:111:HIS:HD2	1:I:114:SER:H	1.46	0.64
1:G:256:ALA:HB1	1:G:286:THR:HG21	1.79	0.64
1:E:1247:PRO:HA	1:E:1598:GLN:HA	1.79	0.64
1:E:256:ALA:HB1	1:E:286:THR:HG21	1.79	0.64
1:G:426:ARG:HB2	1:G:506:TYR:HA	1.79	0.64
1:B:650:VAL:HB	1:B:777:PHE:HB2	1.79	0.64
1:I:281:ARG:NH2	1:I:309:THR:OG1	2.29	0.64
1:B:426:ARG:HB2	1:B:506:TYR:HA	1.79	0.64
1:G:379:HIS:HD2	1:G:382:GLY:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:650:VAL:HB	1:G:777:PHE:HB2	1.79	0.64
1:E:606:LEU:O	1:E:617:ASN:ND2	2.31	0.64
1:B:111:HIS:HD2	1:B:114:SER:H	1.46	0.63
1:B:1247:PRO:HA	1:B:1598:GLN:HA	1.79	0.63
1:I:989:ALA:O	1:I:1035:ASN:ND2	2.30	0.63
1:I:606:LEU:O	1:I:617:ASN:ND2	2.31	0.63
1:G:111:HIS:HD2	1:G:114:SER:H	1.46	0.63
1:G:606:LEU:O	1:G:617:ASN:ND2	2.31	0.63
1:E:497:TYR:HB3	1:E:500:ALA:HB2	1.81	0.63
1:I:426:ARG:HB2	1:I:506:TYR:HA	1.79	0.63
1:I:379:HIS:HD2	1:I:382:GLY:H	1.45	0.63
1:I:4192:ARG:HH12	1:I:4982:GLU:HG2	1.64	0.63
1:G:4192:ARG:HH12	1:G:4982:GLU:HG2	1.64	0.63
1:I:2755:ILE:HD13	1:I:2810:LYS:HG2	1.81	0.63
1:G:742:ASP:HA	1:G:760:ASN:HD21	1.64	0.63
1:I:1092:PHE:HB3	1:I:1149:VAL:HB	1.79	0.62
1:G:315:CYS:SG	1:G:316:PHE:N	2.72	0.62
1:B:315:CYS:SG	1:B:316:PHE:N	2.72	0.62
1:B:1092:PHE:HB3	1:B:1149:VAL:HB	1.79	0.62
1:B:2755:ILE:HD13	1:B:2810:LYS:HG2	1.81	0.62
1:E:4860:ARG:HD2	1:G:4582:VAL:HG11	1.81	0.62
1:G:497:TYR:HB3	1:G:500:ALA:HB2	1.81	0.62
1:B:606:LEU:O	1:B:617:ASN:ND2	2.31	0.62
1:B:609:CYS:SG	1:B:610:ASN:N	2.73	0.62
1:I:315:CYS:SG	1:I:316:PHE:N	2.72	0.62
1:B:4582:VAL:HG11	1:I:4860:ARG:HD2	1.82	0.62
1:E:742:ASP:HA	1:E:760:ASN:HD21	1.64	0.62
1:I:497:TYR:HB3	1:I:500:ALA:HB2	1.81	0.62
1:E:111:HIS:HD2	1:E:114:SER:H	1.46	0.62
1:E:315:CYS:SG	1:E:316:PHE:N	2.72	0.62
1:B:742:ASP:HA	1:B:760:ASN:HD21	1.64	0.62
1:E:2755:ILE:HD13	1:E:2810:LYS:HG2	1.81	0.62
1:E:3937:TYR:O	1:E:4002:LYS:NZ	2.32	0.62
1:I:3937:TYR:O	1:I:4002:LYS:NZ	2.32	0.62
1:I:742:ASP:HA	1:I:760:ASN:HD21	1.64	0.61
1:E:2003:GLN:O	1:E:2007:ASN:ND2	2.34	0.61
1:G:2003:GLN:O	1:G:2007:ASN:ND2	2.34	0.61
1:B:4192:ARG:HH12	1:B:4982:GLU:HG2	1.63	0.61
1:I:2003:GLN:O	1:I:2007:ASN:ND2	2.34	0.61
1:G:2755:ILE:HD13	1:G:2810:LYS:HG2	1.81	0.61
1:B:497:TYR:HB3	1:B:500:ALA:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:853:PRO:HB3	1:I:1024:TYR:H	1.66	0.61
2:F:6:THR:HA	2:F:72:ALA:HA	1.82	0.61
1:G:609:CYS:SG	1:G:610:ASN:N	2.73	0.61
1:B:1519:UNK:HA	1:B:1526:UNK:HA	1.83	0.61
1:E:4192:ARG:HH12	1:E:4982:GLU:HG2	1.64	0.61
1:I:609:CYS:SG	1:I:610:ASN:N	2.73	0.61
1:G:1743:ARG:O	1:G:1964:ARG:NH2	2.33	0.61
1:E:1519:UNK:HA	1:E:1526:UNK:HA	1.82	0.61
1:E:4201:ASN:O	1:E:4205:TRP:N	2.34	0.61
1:I:635:THR:O	2:J:34:LYS:NZ	2.34	0.61
1:B:4201:ASN:O	1:B:4205:TRP:N	2.34	0.61
2:H:6:THR:HA	2:H:72:ALA:HA	1.82	0.61
1:B:853:PRO:HB3	1:B:1024:TYR:H	1.66	0.61
1:E:609:CYS:SG	1:E:610:ASN:N	2.73	0.61
1:E:1743:ARG:O	1:E:1964:ARG:NH2	2.33	0.61
1:B:1743:ARG:O	1:B:1964:ARG:NH2	2.33	0.61
1:G:3937:TYR:O	1:G:4002:LYS:NZ	2.32	0.61
1:B:1700:ASP:OD2	1:B:1708:ARG:NH2	2.35	0.60
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.32	0.60
2:J:6:THR:HA	2:J:72:ALA:HA	1.83	0.60
1:B:1232:ARG:HD2	1:B:1702:HIS:HB3	1.83	0.60
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.34	0.60
1:B:2452:ARG:HH12	1:I:177:GLU:HG3	1.66	0.60
1:E:1700:ASP:OD2	1:E:1708:ARG:NH2	2.35	0.60
1:I:4201:ASN:O	1:I:4205:TRP:N	2.34	0.60
1:G:1232:ARG:HD2	1:G:1702:HIS:HB3	1.83	0.60
1:B:4201:ASN:ND2	1:B:4993:MET:SD	2.75	0.60
1:E:179:TYR:OH	1:G:2359:ARG:NH1	2.34	0.60
1:G:853:PRO:HB3	1:G:1024:TYR:H	1.66	0.60
2:A:6:THR:HA	2:A:72:ALA:HA	1.82	0.60
1:I:1721:GLU:OE2	1:I:1725:ARG:NH2	2.32	0.60
1:E:646:PRO:HD2	1:E:779:PRO:HB2	1.83	0.60
1:I:4201:ASN:ND2	1:I:4993:MET:SD	2.75	0.60
1:E:4201:ASN:ND2	1:E:4993:MET:SD	2.75	0.60
1:I:1700:ASP:OD2	1:I:1708:ARG:NH2	2.35	0.60
1:I:842:PRO:HD3	1:I:1073:ARG:HG3	1.84	0.60
1:I:1743:ARG:O	1:I:1964:ARG:NH2	2.33	0.60
1:G:4201:ASN:ND2	1:G:4993:MET:SD	2.75	0.60
1:E:842:PRO:HD3	1:E:1073:ARG:HG3	1.84	0.59
1:E:1232:ARG:HD2	1:E:1702:HIS:HB3	1.83	0.59
1:I:1152:MET:HB2	1:I:1161:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3990:VAL:HG13	1:G:4051:SER:HB2	1.84	0.59
1:G:4201:ASN:O	1:G:4205:TRP:N	2.34	0.59
1:E:853:PRO:HB3	1:E:1024:TYR:H	1.66	0.59
1:E:4134:GLU:O	1:E:4137:ARG:NH2	2.35	0.59
1:B:4134:GLU:O	1:B:4137:ARG:NH2	2.35	0.59
1:I:1232:ARG:HD2	1:I:1702:HIS:HB3	1.83	0.59
1:G:646:PRO:HD2	1:G:779:PRO:HB2	1.83	0.59
1:B:842:PRO:HD3	1:B:1073:ARG:HG3	1.84	0.59
1:G:1101:ARG:HE	1:G:1115:LEU:HB3	1.67	0.59
1:G:1700:ASP:OD2	1:G:1708:ARG:NH2	2.35	0.59
1:E:1101:ARG:HE	1:E:1115:LEU:HB3	1.67	0.59
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.84	0.59
1:G:1152:MET:HB2	1:G:1161:ILE:HB	1.84	0.59
1:G:4134:GLU:O	1:G:4137:ARG:NH2	2.35	0.59
1:G:842:PRO:HD3	1:G:1073:ARG:HG3	1.84	0.59
1:E:1721:GLU:OE2	1:E:1725:ARG:NH2	2.32	0.59
1:B:3990:VAL:HG13	1:B:4051:SER:HB2	1.84	0.58
1:I:719:LEU:HD22	1:I:735:GLN:HG2	1.85	0.58
1:I:4134:GLU:O	1:I:4137:ARG:NH2	2.35	0.58
1:G:575:LEU:HD22	1:G:609:CYS:HB3	1.85	0.58
1:B:4056:GLU:HA	1:B:4059:LEU:HB2	1.85	0.58
2:A:26:TYR:OH	2:A:42:ARG:NH2	2.36	0.58
1:E:575:LEU:HD22	1:E:609:CYS:HB3	1.86	0.58
1:G:1519:UNK:HA	1:G:1526:UNK:HA	1.83	0.58
1:B:132:ALA:HA	1:B:194:SER:HB2	1.85	0.58
1:I:646:PRO:HD2	1:I:779:PRO:HB2	1.83	0.58
2:H:26:TYR:OH	2:H:42:ARG:NH2	2.36	0.58
1:E:3897:ASN:O	1:E:3901:ASN:ND2	2.37	0.58
1:E:3990:VAL:HG13	1:E:4051:SER:HB2	1.84	0.58
1:I:1101:ARG:HE	1:I:1115:LEU:HB3	1.67	0.58
1:I:3990:VAL:HG13	1:I:4051:SER:HB2	1.84	0.58
1:B:646:PRO:HD2	1:B:779:PRO:HB2	1.83	0.58
1:E:719:LEU:HD22	1:E:735:GLN:HG2	1.85	0.58
1:I:132:ALA:HA	1:I:194:SER:HB2	1.85	0.58
1:I:575:LEU:HD22	1:I:609:CYS:HB3	1.86	0.58
1:I:3897:ASN:O	1:I:3901:ASN:ND2	2.37	0.58
1:E:132:ALA:HA	1:E:194:SER:HB2	1.85	0.58
1:E:1152:MET:HB2	1:E:1161:ILE:HB	1.84	0.58
1:G:3897:ASN:O	1:G:3901:ASN:ND2	2.37	0.58
1:B:221:ARG:NH2	1:B:255:HIS:O	2.37	0.58
1:B:1101:ARG:HE	1:B:1115:LEU:HB3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2189:LYS:HA	1:B:2192:TYR:HD2	1.69	0.58
1:B:575:LEU:HD22	1:B:609:CYS:HB3	1.86	0.57
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.37	0.57
1:E:4056:GLU:HA	1:E:4059:LEU:HB2	1.85	0.57
2:J:26:TYR:OH	2:J:42:ARG:NH2	2.36	0.57
1:E:2189:LYS:HA	1:E:2192:TYR:HD2	1.69	0.57
1:I:671:VAL:HG22	1:I:740:PRO:HG3	1.87	0.57
1:G:2022:PRO:HB2	1:G:2024:PRO:HD2	1.87	0.57
2:F:26:TYR:OH	2:F:42:ARG:NH2	2.36	0.57
1:B:3897:ASN:O	1:B:3901:ASN:ND2	2.37	0.57
1:I:1667:LEU:HD23	1:I:1671:ARG:HH12	1.70	0.57
1:G:132:ALA:HA	1:G:194:SER:HB2	1.85	0.57
1:G:2189:LYS:HA	1:G:2192:TYR:HD2	1.69	0.57
1:G:4673:ARG:HH22	1:G:4698:LYS:HB2	1.69	0.57
1:B:671:VAL:HG22	1:B:740:PRO:HG3	1.87	0.57
1:I:4056:GLU:HA	1:I:4059:LEU:HB2	1.85	0.57
1:I:4813:LEU:HD12	1:I:4816:ILE:HD11	1.87	0.57
1:B:2737:PRO:O	1:B:2888:ARG:NH2	2.37	0.57
1:E:671:VAL:HG22	1:E:740:PRO:HG3	1.87	0.57
1:E:2737:PRO:O	1:E:2888:ARG:NH2	2.37	0.57
1:I:2189:LYS:HA	1:I:2192:TYR:HD2	1.69	0.57
1:G:719:LEU:HD22	1:G:735:GLN:HG2	1.85	0.57
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.87	0.57
2:A:23:VAL:HG22	2:A:47:LYS:HG2	1.87	0.57
2:J:23:VAL:HG22	2:J:47:LYS:HG2	1.87	0.57
1:B:1667:LEU:HD23	1:B:1671:ARG:HH12	1.69	0.57
1:B:4673:ARG:HH22	1:B:4698:LYS:HB2	1.69	0.57
1:B:4813:LEU:HD12	1:B:4816:ILE:HD11	1.87	0.57
1:E:4813:LEU:HD12	1:E:4816:ILE:HD11	1.87	0.57
1:I:221:ARG:NH2	1:I:255:HIS:O	2.37	0.57
1:I:2359:ARG:NH1	1:G:179:TYR:OH	2.37	0.57
1:I:2737:PRO:O	1:I:2888:ARG:NH2	2.37	0.57
1:G:1721:GLU:OE2	1:G:1725:ARG:NH2	2.32	0.57
1:G:2737:PRO:O	1:G:2888:ARG:NH2	2.38	0.57
1:G:4813:LEU:HD12	1:G:4816:ILE:HD11	1.87	0.57
1:B:1679:ASN:ND2	1:B:1798:LEU:O	2.38	0.57
1:I:1519:UNK:HA	1:I:1526:UNK:HA	1.85	0.57
1:G:57:ASN:HD22	1:G:308:HIS:HB2	1.69	0.57
1:G:717:ASP:OD1	1:G:720:HIS:ND1	2.38	0.57
1:E:1109:LEU:HA	1:E:1120:LEU:HD21	1.87	0.57
1:G:671:VAL:HG22	1:G:740:PRO:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:LEU:HD22	1:B:735:GLN:HG2	1.85	0.57
1:B:1960:ALA:O	1:B:1964:ARG:NE	2.38	0.57
1:E:1679:ASN:ND2	1:E:1798:LEU:O	2.38	0.57
1:I:1109:LEU:HA	1:I:1120:LEU:HD21	1.87	0.57
1:G:1079:LYS:NZ	1:G:1107:PRO:O	2.36	0.57
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.78	0.56
1:E:1960:ALA:O	1:E:1964:ARG:NE	2.39	0.56
1:I:4673:ARG:HH22	1:I:4698:LYS:HB2	1.69	0.56
1:B:695:TYR:OH	1:B:1073:ARG:NH1	2.38	0.56
1:B:717:ASP:OD1	1:B:720:HIS:ND1	2.38	0.56
1:E:4151:SER:HA	1:E:4160:LEU:HD21	1.87	0.56
1:I:1679:ASN:ND2	1:I:1798:LEU:O	2.38	0.56
1:I:2022:PRO:HB2	1:I:2024:PRO:HD2	1.87	0.56
1:G:1808:ARG:NH1	1:G:1853:ILE:O	2.37	0.56
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.87	0.56
1:B:57:ASN:HD22	1:B:308:HIS:HB2	1.69	0.56
1:E:2022:PRO:HB2	1:E:2024:PRO:HD2	1.87	0.56
1:E:4673:ARG:HH22	1:E:4698:LYS:HB2	1.69	0.56
1:I:57:ASN:HD22	1:I:308:HIS:HB2	1.69	0.56
1:I:695:TYR:OH	1:I:1073:ARG:NH1	2.38	0.56
1:I:717:ASP:OD1	1:I:720:HIS:ND1	2.38	0.56
1:G:972:LEU:O	1:G:1044:ARG:NH2	2.39	0.56
1:G:1667:LEU:HD23	1:G:1671:ARG:HH12	1.70	0.56
1:G:4056:GLU:HA	1:G:4059:LEU:HB2	1.85	0.56
1:G:4151:SER:HA	1:G:4160:LEU:HD21	1.87	0.56
1:B:4151:SER:HA	1:B:4160:LEU:HD21	1.86	0.56
1:B:4933:GLN:HE22	1:E:4937:ILE:HD11	1.71	0.56
1:E:2318:TYR:HH	1:E:2414:ASN:N	2.04	0.56
1:G:3764:LEU:HG	1:G:3767:GLN:HB3	1.88	0.56
1:E:57:ASN:HD22	1:E:308:HIS:HB2	1.69	0.56
1:I:1808:ARG:NH1	1:I:1853:ILE:O	2.37	0.56
1:G:221:ARG:NH2	1:G:255:HIS:O	2.37	0.56
1:G:4184:MET:HB3	1:G:4190:ILE:HD13	1.87	0.56
1:E:1808:ARG:NH1	1:E:1853:ILE:O	2.38	0.56
1:I:4151:SER:HA	1:I:4160:LEU:HD21	1.87	0.56
2:J:27:THR:HB	2:J:100:ASP:HB3	1.87	0.56
1:B:1079:LYS:NZ	1:B:1107:PRO:O	2.36	0.56
1:G:695:TYR:OH	1:G:1073:ARG:NH1	2.38	0.56
1:G:1679:ASN:ND2	1:G:1798:LEU:O	2.38	0.56
2:A:27:THR:HB	2:A:100:ASP:HB3	1.87	0.56
1:B:4184:MET:HB3	1:B:4190:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ARG:HH21	1:E:115:ARG:HB3	1.71	0.56
1:E:717:ASP:OD1	1:E:720:HIS:ND1	2.38	0.56
1:E:1093:GLU:OE1	1:E:1201:HIS:NE2	2.38	0.56
1:I:1777:PHE:HA	1:I:1799:SER:HB2	1.88	0.56
1:G:110:ARG:HH21	1:G:115:ARG:HB3	1.71	0.56
1:G:1973:GLN:O	1:G:1977:TYR:N	2.36	0.56
1:B:2318:TYR:HH	1:B:2414:ASN:N	2.04	0.56
1:E:534:ARG:NH2	1:E:573:GLU:OE2	2.39	0.56
1:E:1079:LYS:NZ	1:E:1107:PRO:O	2.36	0.56
1:E:3889:GLN:OE1	1:E:3960:GLN:NE2	2.39	0.56
1:E:4232:GLU:OE2	1:E:5017:ARG:NH1	2.39	0.56
1:I:206:CYS:SG	1:I:207:SER:N	2.78	0.56
1:I:451:TYR:O	1:I:474:ARG:NH1	2.39	0.56
1:G:1777:PHE:HA	1:G:1799:SER:HB2	1.87	0.56
1:B:2022:PRO:HB2	1:B:2024:PRO:HD2	1.87	0.55
1:E:1667:LEU:HD23	1:E:1671:ARG:HH12	1.69	0.55
1:G:1109:LEU:HA	1:G:1120:LEU:HD21	1.87	0.55
1:G:1960:ALA:O	1:G:1964:ARG:NE	2.38	0.55
1:G:4687:TYR:OH	1:G:4699:GLY:O	2.25	0.55
1:B:1109:LEU:HA	1:B:1120:LEU:HD21	1.87	0.55
1:E:221:ARG:NH2	1:E:255:HIS:O	2.37	0.55
1:I:23:GLN:OE1	1:I:203:ASN:ND2	2.40	0.55
1:I:647:ASN:ND2	1:I:820:ARG:O	2.36	0.55
1:G:2318:TYR:HH	1:G:2414:ASN:N	2.04	0.55
1:E:451:TYR:O	1:E:474:ARG:NH1	2.39	0.55
1:I:2318:TYR:HH	1:I:2414:ASN:N	2.04	0.55
1:G:20:VAL:HG12	1:G:204:PRO:HA	1.89	0.55
1:B:647:ASN:ND2	1:B:820:ARG:O	2.36	0.55
1:B:3889:GLN:OE1	1:B:3960:GLN:NE2	2.39	0.55
1:E:683:ARG:HB2	1:E:782:SER:HB3	1.89	0.55
1:E:695:TYR:OH	1:E:1073:ARG:NH1	2.38	0.55
1:E:972:LEU:O	1:E:1044:ARG:NH2	2.39	0.55
1:E:1973:GLN:O	1:E:1977:TYR:N	2.36	0.55
1:G:3889:GLN:OE1	1:G:3960:GLN:NE2	2.39	0.55
2:F:27:THR:HB	2:F:100:ASP:HB3	1.87	0.55
1:B:110:ARG:HH21	1:B:115:ARG:HB3	1.70	0.55
1:B:488:LEU:O	1:B:492:ASP:N	2.39	0.55
1:B:4232:GLU:OE2	1:B:5017:ARG:NH1	2.39	0.55
1:E:23:GLN:OE1	1:E:203:ASN:ND2	2.40	0.55
1:E:1777:PHE:HA	1:E:1799:SER:HB2	1.87	0.55
1:I:887:ILE:HG21	1:I:959:TYR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1960:ALA:O	1:I:1964:ARG:NE	2.38	0.55
1:G:206:CYS:SG	1:G:207:SER:N	2.78	0.55
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.40	0.55
1:E:4184:MET:HB3	1:E:4190:ILE:HD13	1.87	0.55
1:E:4687:TYR:OH	1:E:4699:GLY:O	2.25	0.55
1:B:887:ILE:HG21	1:B:959:TYR:HA	1.88	0.55
1:E:20:VAL:HG12	1:E:204:PRO:HA	1.89	0.55
1:E:887:ILE:HG21	1:E:959:TYR:HA	1.88	0.55
1:E:1931:LEU:HB3	1:E:1935:VAL:HB	1.89	0.55
1:E:2042:CYS:SG	1:E:2043:GLY:N	2.78	0.55
1:I:3932:ASP:HA	1:I:3935:TRP:HD1	1.72	0.55
1:G:887:ILE:HG21	1:G:959:TYR:HA	1.88	0.55
1:G:3932:ASP:HA	1:G:3935:TRP:HD1	1.72	0.55
1:B:972:LEU:O	1:B:1044:ARG:NH2	2.39	0.55
1:B:1093:GLU:OE1	1:B:1201:HIS:NE2	2.39	0.55
1:B:1777:PHE:HA	1:B:1799:SER:HB2	1.87	0.55
1:I:110:ARG:HH21	1:I:115:ARG:HB3	1.70	0.55
1:I:4184:MET:HB3	1:I:4190:ILE:HD13	1.87	0.55
1:B:641:VAL:HG21	1:B:705:ASN:HA	1.89	0.55
1:B:3764:LEU:HG	1:B:3767:GLN:HB3	1.88	0.55
1:E:3932:ASP:HA	1:E:3935:TRP:HD1	1.72	0.55
1:I:641:VAL:HG21	1:I:705:ASN:HA	1.89	0.55
1:I:3889:GLN:OE1	1:I:3960:GLN:NE2	2.39	0.55
1:I:4687:TYR:OH	1:I:4699:GLY:O	2.25	0.55
1:G:2042:CYS:SG	1:G:2043:GLY:N	2.78	0.55
1:B:2281:ILE:HG23	1:B:2341:VAL:HG11	1.89	0.55
1:E:647:ASN:ND2	1:E:820:ARG:O	2.36	0.55
1:I:283:ARG:HH21	1:I:402:ARG:HH12	1.55	0.55
1:I:534:ARG:NH2	1:I:573:GLU:OE2	2.39	0.55
1:I:1667:LEU:O	1:I:1671:ARG:NH1	2.40	0.55
1:I:1973:GLN:O	1:I:1977:TYR:N	2.36	0.55
1:B:683:ARG:HB2	1:B:782:SER:HB3	1.89	0.54
1:I:1079:LYS:NZ	1:I:1107:PRO:O	2.36	0.54
1:I:1093:GLU:OE1	1:I:1201:HIS:NE2	2.39	0.54
1:I:4232:GLU:OE2	1:I:5017:ARG:NH1	2.39	0.54
1:G:683:ARG:HB2	1:G:782:SER:HB3	1.89	0.54
1:G:2748:PRO:HD2	1:G:2751:LEU:HD12	1.89	0.54
1:B:1667:LEU:O	1:B:1671:ARG:NH1	2.40	0.54
1:I:2748:PRO:HD2	1:I:2751:LEU:HD12	1.89	0.54
1:G:23:GLN:OE1	1:G:203:ASN:ND2	2.39	0.54
1:G:1931:LEU:HB3	1:G:1935:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:HIS:N	2:F:91:ILE:O	2.41	0.54
1:I:20:VAL:HG12	1:I:204:PRO:HA	1.89	0.54
2:H:27:THR:HB	2:H:100:ASP:HB3	1.87	0.54
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.25	0.54
1:G:1667:LEU:O	1:G:1671:ARG:NH1	2.40	0.54
1:B:1931:LEU:HB3	1:B:1935:VAL:HB	1.89	0.54
1:E:3764:LEU:HG	1:E:3767:GLN:HB3	1.88	0.54
2:J:87:HIS:N	2:J:91:ILE:O	2.41	0.54
1:B:551:LEU:HD11	1:B:589:LEU:HD13	1.89	0.54
1:B:3932:ASP:HA	1:B:3935:TRP:HD1	1.72	0.54
1:E:206:CYS:SG	1:E:207:SER:N	2.78	0.54
1:I:313:SER:HB3	1:I:351:VAL:HB	1.90	0.54
1:I:619:ASP:OD1	1:I:1680:ARG:NH1	2.41	0.54
1:I:2042:CYS:SG	1:I:2043:GLY:N	2.78	0.54
2:H:87:HIS:N	2:H:91:ILE:O	2.41	0.54
1:B:19:GLU:HB2	1:B:206:CYS:HB3	1.90	0.54
1:G:2281:ILE:HG23	1:G:2341:VAL:HG11	1.89	0.54
1:G:4834:GLY:HA2	1:G:4837:LEU:HD12	1.90	0.54
1:B:731:THR:OG1	1:B:1519:UNK:O	2.26	0.54
1:E:488:LEU:O	1:E:492:ASP:N	2.39	0.54
1:E:1667:LEU:O	1:E:1671:ARG:NH1	2.40	0.54
1:E:2748:PRO:HD2	1:E:2751:LEU:HD12	1.89	0.54
1:I:2281:ILE:HG23	1:I:2341:VAL:HG11	1.89	0.54
1:I:3764:LEU:HG	1:I:3767:GLN:HB3	1.88	0.54
1:I:4567:LEU:HD12	1:I:4816:ILE:HD12	1.90	0.54
1:G:313:SER:HB3	1:G:351:VAL:HB	1.90	0.54
1:G:4232:GLU:OE2	1:G:5017:ARG:NH1	2.39	0.54
1:E:313:SER:HB3	1:E:351:VAL:HB	1.90	0.54
2:A:87:HIS:N	2:A:91:ILE:O	2.40	0.54
1:B:20:VAL:HG12	1:B:204:PRO:HA	1.89	0.54
1:B:206:CYS:SG	1:B:207:SER:N	2.78	0.54
1:B:451:TYR:O	1:B:474:ARG:NH1	2.39	0.54
1:B:4567:LEU:HD12	1:B:4816:ILE:HD12	1.90	0.54
1:E:4567:LEU:HD12	1:E:4816:ILE:HD12	1.90	0.54
1:G:488:LEU:O	1:G:492:ASP:N	2.39	0.54
1:I:972:LEU:O	1:I:1044:ARG:NH2	2.39	0.53
1:G:19:GLU:HB2	1:G:206:CYS:HB3	1.90	0.53
1:G:619:ASP:OD1	1:G:1680:ARG:NH1	2.41	0.53
1:G:4178:LEU:HD11	1:G:4194:TYR:HB3	1.90	0.53
1:G:4567:LEU:HD12	1:G:4816:ILE:HD12	1.90	0.53
1:B:313:SER:HB3	1:B:351:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1111:PRO:HD3	1:B:1605:TRP:HE1	1.74	0.53
1:E:177:GLU:HG3	1:G:2452:ARG:HH12	1.72	0.53
1:E:641:VAL:HG21	1:E:705:ASN:HA	1.89	0.53
1:I:19:GLU:HB2	1:I:206:CYS:HB3	1.89	0.53
1:I:551:LEU:HD11	1:I:589:LEU:HD13	1.89	0.53
1:G:641:VAL:HG21	1:G:705:ASN:HA	1.89	0.53
1:G:647:ASN:ND2	1:G:820:ARG:O	2.36	0.53
1:E:283:ARG:HH21	1:E:402:ARG:HH12	1.55	0.53
1:E:683:ARG:NH1	1:E:707:VAL:O	2.40	0.53
1:E:4178:LEU:HD11	1:E:4194:TYR:HB3	1.90	0.53
1:E:4834:GLY:HA2	1:E:4837:LEU:HD12	1.90	0.53
1:I:683:ARG:HB2	1:I:782:SER:HB3	1.89	0.53
1:G:551:LEU:HD11	1:G:589:LEU:HD13	1.89	0.53
1:I:1111:PRO:HD3	1:I:1605:TRP:HE1	1.74	0.53
1:I:1649:ASP:HB3	1:I:1652:GLU:HG2	1.91	0.53
1:B:41:GLY:O	1:B:45:ARG:NH1	2.42	0.53
1:I:488:LEU:O	1:I:492:ASP:N	2.39	0.53
1:I:1931:LEU:HB3	1:I:1935:VAL:HB	1.89	0.53
1:G:534:ARG:NH2	1:G:573:GLU:OE2	2.39	0.53
1:G:838:HIS:HA	1:G:1201:HIS:HB3	1.90	0.53
1:B:534:ARG:NH2	1:B:573:GLU:OE2	2.39	0.53
1:E:19:GLU:HB2	1:E:206:CYS:HB3	1.90	0.53
1:B:283:ARG:HH21	1:B:402:ARG:HH12	1.55	0.53
1:B:619:ASP:OD1	1:B:1680:ARG:NH1	2.41	0.53
1:B:4834:GLY:HA2	1:B:4837:LEU:HD12	1.90	0.53
1:E:41:GLY:O	1:E:45:ARG:NH1	2.42	0.53
1:I:4834:GLY:HA2	1:I:4837:LEU:HD12	1.90	0.53
1:B:1032:LYS:O	1:B:1036:ARG:N	2.40	0.53
1:B:4178:LEU:HD11	1:B:4194:TYR:HB3	1.90	0.53
1:E:551:LEU:HD11	1:E:589:LEU:HD13	1.89	0.53
1:E:2281:ILE:HG23	1:E:2341:VAL:HG11	1.89	0.53
1:I:683:ARG:NH1	1:I:707:VAL:O	2.40	0.53
1:I:4178:LEU:HD11	1:I:4194:TYR:HB3	1.90	0.53
1:G:451:TYR:O	1:G:474:ARG:NH1	2.39	0.53
1:G:1111:PRO:HD3	1:G:1605:TRP:HE1	1.74	0.53
1:I:4584:ASP:HA	1:I:4627:MET:HA	1.91	0.53
1:G:728:ARG:NH2	1:G:1527:UNK:O	2.42	0.53
1:G:1649:ASP:HB3	1:G:1652:GLU:HG2	1.91	0.53
1:G:3946:GLN:OE1	1:G:3950:ASN:ND2	2.42	0.53
1:B:2748:PRO:HD2	1:B:2751:LEU:HD12	1.89	0.53
1:G:463:GLU:OE2	1:G:467:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1093:GLU:OE1	1:G:1201:HIS:NE2	2.39	0.53
1:B:463:GLU:OE2	1:B:467:LYS:NZ	2.42	0.52
1:B:1649:ASP:HB3	1:B:1652:GLU:HG2	1.91	0.52
1:E:4584:ASP:HA	1:E:4627:MET:HA	1.91	0.52
1:I:278:GLN:N	1:I:315:CYS:SG	2.82	0.52
1:B:3973:CYS:SG	1:B:3976:ASN:ND2	2.82	0.52
1:E:123:THR:OG1	1:E:134:ASP:OD1	2.28	0.52
1:E:463:GLU:OE2	1:E:467:LYS:NZ	2.42	0.52
1:E:3973:CYS:SG	1:E:3976:ASN:ND2	2.82	0.52
1:I:838:HIS:HA	1:I:1201:HIS:HB3	1.90	0.52
1:E:731:THR:OG1	1:E:1519:UNK:O	2.27	0.52
1:E:838:HIS:HA	1:E:1201:HIS:HB3	1.90	0.52
1:E:1131:ARG:NH1	1:E:1178:ALA:O	2.42	0.52
1:E:3946:GLN:OE1	1:E:3950:ASN:ND2	2.42	0.52
1:I:41:GLY:O	1:I:45:ARG:NH1	2.42	0.52
1:B:1077:ALA:HB3	1:B:1189:LEU:HD11	1.92	0.52
1:B:2420:HIS:ND1	1:B:2493:UNK:O	2.32	0.52
1:E:728:ARG:NH2	1:E:1527:UNK:O	2.42	0.52
1:I:1032:LYS:O	1:I:1036:ARG:N	2.40	0.52
1:G:41:GLY:O	1:G:45:ARG:NH1	2.42	0.52
1:B:1694:LEU:O	1:B:1712:TYR:OH	2.24	0.52
1:B:2347:GLU:O	1:B:2351:ASN:N	2.43	0.52
1:E:1111:PRO:HD3	1:E:1605:TRP:HE1	1.74	0.52
1:I:221:ARG:NE	1:I:258:SER:OG	2.43	0.52
1:G:1653:LEU:HB3	1:G:1660:GLN:HB2	1.91	0.52
1:B:395:GLN:NE2	1:B:397:GLU:OE1	2.43	0.52
1:B:3946:GLN:OE1	1:B:3950:ASN:ND2	2.42	0.52
1:E:40:GLU:HB3	1:E:44:ASN:HB3	1.92	0.52
1:I:123:THR:OG1	1:I:134:ASP:OD1	2.28	0.52
1:I:3946:GLN:OE1	1:I:3950:ASN:ND2	2.42	0.52
1:I:4560:TYR:O	1:I:4564:PHE:N	2.41	0.52
1:G:40:GLU:HB3	1:G:44:ASN:HB3	1.92	0.52
1:G:1077:ALA:HB3	1:G:1189:LEU:HD11	1.92	0.52
1:G:1665:HIS:HA	1:G:1668:ARG:HG2	1.92	0.52
1:B:40:GLU:HB3	1:B:44:ASN:HB3	1.92	0.52
1:B:838:HIS:HA	1:B:1201:HIS:HB3	1.90	0.52
1:B:4155:PRO:HD2	1:B:5036:LEU:HD23	1.92	0.52
1:E:1649:ASP:HB3	1:E:1652:GLU:HG2	1.91	0.52
1:E:2457:LEU:HD23	1:E:2460:LEU:HD12	1.92	0.52
1:E:4155:PRO:HD2	1:E:5036:LEU:HD23	1.92	0.52
1:I:463:GLU:OE2	1:I:467:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3973:CYS:SG	1:I:3976:ASN:ND2	2.83	0.52
1:G:283:ARG:HH21	1:G:402:ARG:HH12	1.55	0.52
1:G:2347:GLU:O	1:G:2351:ASN:N	2.43	0.52
1:B:1653:LEU:HB3	1:B:1660:GLN:HB2	1.91	0.52
1:E:1077:ALA:HB3	1:E:1189:LEU:HD11	1.92	0.52
1:I:1653:LEU:HB3	1:I:1660:GLN:HB2	1.91	0.52
1:G:1032:LYS:O	1:G:1036:ARG:N	2.40	0.52
1:B:1764:GLY:HA3	1:B:1859:VAL:HG11	1.92	0.52
1:E:395:GLN:NE2	1:E:397:GLU:OE1	2.43	0.52
1:E:619:ASP:OD1	1:E:1680:ARG:NH1	2.41	0.52
1:E:978:THR:HB	1:E:980:ALA:H	1.75	0.52
1:E:1665:HIS:HA	1:E:1668:ARG:HG2	1.92	0.52
1:I:40:GLU:HB3	1:I:44:ASN:HB3	1.92	0.52
1:I:1131:ARG:NH1	1:I:1178:ALA:O	2.42	0.52
1:I:1764:GLY:HA3	1:I:1859:VAL:HG11	1.92	0.52
1:I:4075:GLU:HA	1:I:4078:GLN:HB2	1.92	0.52
1:G:3973:CYS:SG	1:G:3976:ASN:ND2	2.82	0.52
1:B:123:THR:OG1	1:B:134:ASP:OD1	2.28	0.51
1:B:1237:TRP:HH2	1:B:1652:GLU:HA	1.75	0.51
1:B:1721:GLU:OE2	1:B:1725:ARG:NH2	2.32	0.51
1:B:4584:ASP:HA	1:B:4627:MET:HA	1.91	0.51
1:I:1271:ARG:HA	1:I:1471:UNK:HA	1.91	0.51
1:G:978:THR:HB	1:G:980:ALA:H	1.75	0.51
1:E:1271:ARG:HA	1:E:1471:UNK:HA	1.91	0.51
1:I:1077:ALA:HB3	1:I:1189:LEU:HD11	1.92	0.51
1:E:278:GLN:N	1:E:315:CYS:SG	2.82	0.51
1:E:309:THR:O	1:E:313:SER:OG	2.27	0.51
1:E:1764:GLY:HA3	1:E:1859:VAL:HG11	1.92	0.51
1:I:952:LYS:HB3	1:I:968:ALA:HB1	1.92	0.51
1:I:2347:GLU:O	1:I:2351:ASN:N	2.43	0.51
1:G:4155:PRO:HD2	1:G:5036:LEU:HD23	1.92	0.51
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.92	0.51
1:E:2347:GLU:O	1:E:2351:ASN:N	2.43	0.51
1:G:4075:GLU:HA	1:G:4078:GLN:HB2	1.92	0.51
1:B:111:HIS:CD2	1:B:114:SER:H	2.28	0.51
1:B:2457:LEU:HD23	1:B:2460:LEU:HD12	1.92	0.51
1:G:278:GLN:N	1:G:315:CYS:SG	2.82	0.51
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.42	0.51
1:E:61:ASP:OD1	1:E:402:ARG:NH2	2.44	0.51
1:E:1653:LEU:HB3	1:E:1660:GLN:HB2	1.91	0.51
1:E:4849:TYR:HE1	1:G:4578:LEU:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:728:ARG:NH2	1:I:1527:UNK:O	2.43	0.51
1:I:1237:TRP:HH2	1:I:1652:GLU:HA	1.76	0.51
1:I:4155:PRO:HD2	1:I:5036:LEU:HD23	1.92	0.51
1:G:242:ARG:NH1	1:G:481:GLU:OE1	2.39	0.51
2:J:74:LEU:HB2	2:J:99:PHE:HB2	1.92	0.51
1:E:4697:VAL:O	1:E:4701:TRP:N	2.44	0.51
1:G:1764:GLY:HA3	1:G:1859:VAL:HG11	1.92	0.51
1:G:2457:LEU:HD23	1:G:2460:LEU:HD12	1.92	0.51
1:B:952:LYS:HB3	1:B:968:ALA:HB1	1.92	0.51
1:B:978:THR:HB	1:B:980:ALA:H	1.75	0.51
1:B:1665:HIS:HA	1:B:1668:ARG:HG2	1.92	0.51
1:E:952:LYS:HB3	1:E:968:ALA:HB1	1.92	0.51
1:E:1237:TRP:HH2	1:E:1652:GLU:HA	1.75	0.51
1:E:1729:SER:O	1:E:2163:ARG:NH1	2.44	0.51
1:E:1865:MET:HB3	1:E:1926:LEU:HB2	1.93	0.51
1:G:952:LYS:HB3	1:G:968:ALA:HB1	1.92	0.51
1:B:61:ASP:OD1	1:B:402:ARG:NH2	2.44	0.51
1:G:4584:ASP:HA	1:G:4627:MET:HA	1.91	0.51
2:H:74:LEU:HB2	2:H:99:PHE:HB2	1.92	0.51
1:E:2927:LEU:HD23	1:E:2930:LEU:HD12	1.93	0.50
1:G:123:THR:OG1	1:G:134:ASP:OD1	2.28	0.50
1:B:683:ARG:NH1	1:B:707:VAL:O	2.40	0.50
1:B:1698:LEU:N	1:B:1712:TYR:OH	2.45	0.50
1:B:1973:GLN:O	1:B:1977:TYR:N	2.36	0.50
1:B:3762:ARG:H	1:B:4754:ASN:HA	1.76	0.50
1:G:4885:PHE:HE2	1:G:4901:ILE:HD11	1.77	0.50
1:B:1865:MET:HB3	1:B:1926:LEU:HB2	1.93	0.50
1:E:221:ARG:NE	1:E:258:SER:OG	2.43	0.50
1:E:1698:LEU:N	1:E:1712:TYR:OH	2.45	0.50
1:E:2803:GLU:OE2	1:E:2806:ARG:NH1	2.44	0.50
1:E:4885:PHE:HE2	1:E:4901:ILE:HD11	1.77	0.50
1:I:731:THR:OG1	1:I:1519:UNK:O	2.30	0.50
1:I:1698:LEU:N	1:I:1712:TYR:OH	2.45	0.50
1:I:2803:GLU:OE2	1:I:2806:ARG:NH1	2.44	0.50
1:I:4582:VAL:HG11	1:G:4860:ARG:HD2	1.94	0.50
2:H:2:VAL:HG21	2:H:61:GLU:HB2	1.94	0.50
1:B:1729:SER:O	1:B:2163:ARG:NH1	2.45	0.50
1:B:3781:GLN:HA	1:B:3784:SER:HB3	1.94	0.50
1:E:4075:GLU:HA	1:E:4078:GLN:HB2	1.91	0.50
1:I:1848:LEU:HB3	1:I:1853:ILE:HB	1.94	0.50
1:I:4885:PHE:HE2	1:I:4901:ILE:HD11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4697:VAL:O	1:G:4701:TRP:N	2.44	0.50
1:B:886:ARG:HB3	1:B:891:TRP:HB2	1.94	0.50
1:I:1729:SER:O	1:I:2163:ARG:NH1	2.44	0.50
1:I:4697:VAL:O	1:I:4701:TRP:N	2.44	0.50
1:G:1237:TRP:HH2	1:G:1652:GLU:HA	1.75	0.50
2:F:2:VAL:HG21	2:F:61:GLU:HB2	1.94	0.50
1:B:2803:GLU:OE2	1:B:2806:ARG:NH1	2.44	0.50
1:E:1713:ASP:O	1:E:1717:SER:N	2.44	0.50
1:I:1865:MET:HB3	1:I:1926:LEU:HB2	1.93	0.50
1:I:2457:LEU:HD23	1:I:2460:LEU:HD12	1.92	0.50
1:G:3817:LEU:HD13	1:G:3899:PHE:HD1	1.77	0.50
1:B:309:THR:O	1:B:313:SER:OG	2.27	0.50
1:B:728:ARG:NH2	1:B:1527:UNK:O	2.45	0.50
1:B:4075:GLU:HA	1:B:4078:GLN:HB2	1.92	0.50
1:E:3780:LEU:HD11	1:E:3816:MET:HG3	1.94	0.50
1:I:61:ASP:OD1	1:I:402:ARG:NH2	2.44	0.50
1:G:61:ASP:OD1	1:G:402:ARG:NH2	2.44	0.50
1:G:2803:GLU:OE2	1:G:2806:ARG:NH1	2.44	0.50
1:G:3780:LEU:HD11	1:G:3816:MET:HG3	1.94	0.50
2:A:74:LEU:HB2	2:A:99:PHE:HB2	1.92	0.50
1:B:221:ARG:NE	1:B:258:SER:OG	2.43	0.50
1:B:278:GLN:N	1:B:315:CYS:SG	2.82	0.50
1:E:3762:ARG:H	1:E:4754:ASN:HA	1.76	0.50
1:I:1665:HIS:HA	1:I:1668:ARG:HG2	1.92	0.50
1:I:2927:LEU:HD23	1:I:2930:LEU:HD12	1.93	0.50
1:I:3840:SER:OG	1:I:3875:MET:O	2.24	0.50
1:G:1865:MET:HB3	1:G:1926:LEU:HB2	1.94	0.50
1:B:3780:LEU:HD11	1:B:3816:MET:HG3	1.94	0.50
1:I:395:GLN:NE2	1:I:397:GLU:OE1	2.43	0.50
1:I:2770:LYS:HB3	1:I:2775:TRP:HB2	1.94	0.50
1:G:886:ARG:HB3	1:G:891:TRP:HB2	1.94	0.50
1:G:1131:ARG:NH1	1:G:1178:ALA:O	2.42	0.50
1:G:1698:LEU:N	1:G:1712:TYR:OH	2.44	0.50
1:G:2758:PHE:O	1:G:2762:THR:N	2.45	0.50
2:A:2:VAL:HG21	2:A:61:GLU:HB2	1.94	0.50
1:G:261:ARG:HB3	1:G:283:ARG:HB3	1.94	0.49
1:B:2002:PRO:HA	1:B:2005:GLN:HB3	1.94	0.49
1:E:886:ARG:HB3	1:E:891:TRP:HB2	1.94	0.49
1:E:3843:ASP:H	1:E:3874:VAL:HG13	1.78	0.49
1:E:4749:GLU:HA	1:E:4752:ALA:HB3	1.94	0.49
1:G:3781:GLN:HA	1:G:3784:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4138:ASP:O	1:E:4142:ASN:ND2	2.46	0.49
1:I:682:LEU:HD13	1:I:787:VAL:HG11	1.94	0.49
1:I:978:THR:HB	1:I:980:ALA:H	1.75	0.49
1:G:4138:ASP:O	1:G:4142:ASN:ND2	2.46	0.49
1:B:4885:PHE:HE2	1:B:4901:ILE:HD11	1.77	0.49
1:I:3780:LEU:HD11	1:I:3816:MET:HG3	1.94	0.49
1:G:731:THR:OG1	1:G:1519:UNK:O	2.29	0.49
1:B:2927:LEU:HD23	1:B:2930:LEU:HD12	1.93	0.49
1:I:485:SER:O	1:I:489:ASN:N	2.44	0.49
1:I:2002:PRO:HA	1:I:2005:GLN:HB3	1.94	0.49
1:G:395:GLN:NE2	1:G:397:GLU:OE1	2.43	0.49
1:G:683:ARG:NH1	1:G:707:VAL:O	2.40	0.49
1:G:1729:SER:O	1:G:2163:ARG:NH1	2.44	0.49
1:G:1848:LEU:HB3	1:G:1853:ILE:HB	1.94	0.49
1:B:280:LEU:HD21	1:B:316:PHE:HE2	1.78	0.49
1:E:280:LEU:HD21	1:E:316:PHE:HE2	1.78	0.49
1:E:1848:LEU:HB3	1:E:1853:ILE:HB	1.94	0.49
1:E:2770:LYS:HB3	1:E:2775:TRP:HB2	1.94	0.49
1:I:886:ARG:HB3	1:I:891:TRP:HB2	1.94	0.49
1:I:3817:LEU:HD13	1:I:3899:PHE:HD1	1.77	0.49
1:G:2770:LYS:HB3	1:G:2775:TRP:HB2	1.94	0.49
1:G:3762:ARG:H	1:G:4754:ASN:HA	1.76	0.49
2:J:2:VAL:HG21	2:J:61:GLU:HB2	1.94	0.49
1:B:3843:ASP:H	1:B:3874:VAL:HG13	1.77	0.49
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.46	0.49
1:B:4749:GLU:HA	1:B:4752:ALA:HB3	1.94	0.49
1:E:3781:GLN:HA	1:E:3784:SER:HB3	1.93	0.49
1:I:111:HIS:CD2	1:I:114:SER:H	2.28	0.49
1:I:1970:GLN:HB2	1:I:3642:TYR:HA	1.95	0.49
1:I:2758:PHE:O	1:I:2762:THR:N	2.45	0.49
1:I:4138:ASP:O	1:I:4142:ASN:ND2	2.46	0.49
1:G:111:HIS:CD2	1:G:114:SER:H	2.28	0.49
1:G:280:LEU:HD21	1:G:316:PHE:HE2	1.78	0.49
1:G:485:SER:O	1:G:489:ASN:N	2.44	0.49
1:E:3755:GLU:OE1	1:E:3762:ARG:NH1	2.46	0.49
1:I:3762:ARG:H	1:I:4754:ASN:HA	1.76	0.49
1:I:3781:GLN:HA	1:I:3784:SER:HB3	1.94	0.49
1:G:1271:ARG:HA	1:G:1471:UNK:HA	1.93	0.49
1:B:1848:LEU:HB3	1:B:1853:ILE:HB	1.94	0.49
1:I:261:ARG:HB3	1:I:283:ARG:HB3	1.94	0.49
1:I:3755:GLU:OE1	1:I:3762:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2927:LEU:HD23	1:G:2930:LEU:HD12	1.93	0.49
2:J:7:ILE:HG22	2:J:9:PRO:HD2	1.95	0.49
1:B:261:ARG:HB3	1:B:283:ARG:HB3	1.94	0.49
1:B:475:GLN:NE2	1:B:528:SER:O	2.46	0.49
1:B:580:GLU:HG3	1:B:620:LEU:HD22	1.94	0.49
1:B:3755:GLU:OE1	1:B:3762:ARG:NH1	2.46	0.49
1:E:580:GLU:HG3	1:E:620:LEU:HD22	1.94	0.49
1:E:3817:LEU:HD13	1:E:3899:PHE:HD1	1.77	0.49
1:I:460:GLN:HG2	1:I:462:GLU:H	1.78	0.49
1:I:4928:LEU:HA	1:I:4931:ILE:HD12	1.95	0.49
1:G:1830:VAL:HB	1:G:1837:GLN:HA	1.95	0.49
1:G:3840:SER:OG	1:G:3875:MET:O	2.24	0.49
1:B:3817:LEU:HD13	1:B:3899:PHE:HD1	1.77	0.48
1:I:280:LEU:HD21	1:I:316:PHE:HE2	1.78	0.48
1:G:580:GLU:HG3	1:G:620:LEU:HD22	1.94	0.48
1:G:3755:GLU:OE1	1:G:3762:ARG:NH1	2.46	0.48
1:B:1970:GLN:HB2	1:B:3642:TYR:HA	1.95	0.48
1:B:2758:PHE:O	1:B:2762:THR:N	2.45	0.48
1:E:2381:GLU:HA	1:E:2384:ILE:HD12	1.95	0.48
1:G:221:ARG:NE	1:G:258:SER:OG	2.43	0.48
1:G:309:THR:O	1:G:313:SER:OG	2.27	0.48
1:G:4749:GLU:HA	1:G:4752:ALA:HB3	1.94	0.48
1:I:45:ARG:NH2	1:I:447:ASP:OD1	2.45	0.48
1:I:1243:PRO:HB2	1:I:1600:LEU:HD13	1.95	0.48
1:B:709:ASP:O	1:B:725:HIS:ND1	2.46	0.48
1:B:4228:ALA:O	1:B:4232:GLU:N	2.46	0.48
1:B:4560:TYR:O	1:B:4564:PHE:N	2.41	0.48
1:E:4560:TYR:O	1:E:4564:PHE:N	2.41	0.48
1:I:4749:GLU:HA	1:I:4752:ALA:HB3	1.94	0.48
1:G:682:LEU:HD13	1:G:787:VAL:HG11	1.95	0.48
1:G:3843:ASP:H	1:G:3874:VAL:HG13	1.77	0.48
1:G:3910:THR:HG23	1:G:3911:THR:HG23	1.96	0.48
1:B:1269:CYS:HA	1:B:1473:UNK:HA	1.94	0.48
1:B:2770:LYS:HB3	1:B:2775:TRP:HB2	1.94	0.48
1:E:1032:LYS:O	1:E:1036:ARG:N	2.40	0.48
1:E:3910:THR:HG23	1:E:3911:THR:HG23	1.96	0.48
1:I:242:ARG:NH1	1:I:481:GLU:OE1	2.39	0.48
1:B:43:GLY:N	1:B:447:ASP:OD2	2.46	0.48
1:B:460:GLN:HG2	1:B:462:GLU:H	1.78	0.48
1:B:682:LEU:HD13	1:B:787:VAL:HG11	1.95	0.48
1:B:3910:THR:HG23	1:B:3911:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:GLN:NE2	1:E:528:SER:O	2.46	0.48
1:E:2002:PRO:HA	1:E:2005:GLN:HB3	1.94	0.48
1:E:4852:THR:HG21	1:E:4883:TYR:HB2	1.96	0.48
1:I:736:HIS:HB3	2:J:8:SER:H	1.79	0.48
1:I:1830:VAL:HB	1:I:1837:GLN:HA	1.95	0.48
1:I:3910:THR:HG23	1:I:3911:THR:HG23	1.96	0.48
1:G:1095:VAL:HB	1:G:1199:VAL:HG23	1.96	0.48
1:B:1830:VAL:HB	1:B:1837:GLN:HA	1.95	0.48
1:E:682:LEU:HD13	1:E:787:VAL:HG11	1.95	0.48
1:E:1812:LEU:HD21	1:E:1861:GLN:HG2	1.96	0.48
1:E:4928:LEU:HA	1:E:4931:ILE:HD12	1.95	0.48
1:I:475:GLN:NE2	1:I:528:SER:O	2.46	0.48
1:I:3843:ASP:H	1:I:3874:VAL:HG13	1.77	0.48
1:G:709:ASP:O	1:G:725:HIS:ND1	2.46	0.48
1:G:1691:GLN:HE22	1:G:1802:ILE:HG12	1.79	0.48
1:B:1659:LEU:O	1:B:1663:HIS:N	2.43	0.48
1:B:4697:VAL:O	1:B:4701:TRP:N	2.44	0.48
1:E:43:GLY:N	1:E:447:ASP:OD2	2.46	0.48
1:E:288:GLY:HA3	1:E:405:HIS:CE1	2.49	0.48
1:E:709:ASP:HB3	1:E:725:HIS:CE1	2.49	0.48
1:E:1830:VAL:HB	1:E:1837:GLN:HA	1.95	0.48
1:E:4228:ALA:O	1:E:4232:GLU:N	2.46	0.48
1:G:475:GLN:NE2	1:G:528:SER:O	2.46	0.48
2:F:7:ILE:HG22	2:F:9:PRO:HD2	1.95	0.48
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.95	0.48
1:B:242:ARG:NH1	1:B:481:GLU:OE1	2.39	0.48
1:B:1812:LEU:HD21	1:B:1861:GLN:HG2	1.96	0.48
1:B:2257:LEU:HD11	1:B:2276:ALA:HB2	1.96	0.48
1:B:2868:SER:O	1:B:2872:GLN:N	2.47	0.48
1:B:4666:VAL:HG23	1:B:4669:VAL:HB	1.96	0.48
1:E:261:ARG:HB3	1:E:283:ARG:HB3	1.94	0.48
1:E:460:GLN:HG2	1:E:462:GLU:H	1.78	0.48
1:E:485:SER:O	1:E:489:ASN:N	2.44	0.48
1:E:2868:SER:O	1:E:2872:GLN:N	2.47	0.48
1:I:43:GLY:N	1:I:447:ASP:OD2	2.47	0.48
1:I:1713:ASP:O	1:I:1717:SER:N	2.44	0.48
1:B:2381:GLU:HA	1:B:2384:ILE:HD12	1.95	0.48
1:B:4852:THR:HG21	1:B:4883:TYR:HB2	1.96	0.48
1:B:4928:LEU:HA	1:B:4931:ILE:HD12	1.95	0.48
1:E:1243:PRO:HB2	1:E:1600:LEU:HD13	1.95	0.48
1:I:111:HIS:HB2	1:I:137:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2257:LEU:HD11	1:I:2276:ALA:HB2	1.96	0.48
1:I:2868:SER:O	1:I:2872:GLN:N	2.47	0.48
1:I:4681:LEU:HD21	1:I:4687:TYR:HD2	1.78	0.48
1:G:288:GLY:HA3	1:G:405:HIS:CE1	2.49	0.48
1:G:4928:LEU:HA	1:G:4931:ILE:HD12	1.95	0.48
1:B:709:ASP:HB3	1:B:725:HIS:CE1	2.49	0.47
1:E:709:ASP:O	1:E:725:HIS:ND1	2.46	0.47
1:E:2758:PHE:O	1:E:2762:THR:N	2.45	0.47
1:B:111:HIS:HB2	1:B:137:LEU:HD11	1.96	0.47
1:B:404:ILE:HG21	1:B:481:GLU:HG3	1.97	0.47
1:B:1516:UNK:N	1:B:1529:UNK:O	2.47	0.47
1:E:1095:VAL:HB	1:E:1199:VAL:HG23	1.96	0.47
1:E:1691:GLN:HE22	1:E:1802:ILE:HG12	1.79	0.47
1:E:1970:GLN:HB2	1:E:3642:TYR:HA	1.95	0.47
1:I:288:GLY:HA3	1:I:405:HIS:CE1	2.49	0.47
1:I:1659:LEU:O	1:I:1663:HIS:N	2.43	0.47
1:G:1243:PRO:HB2	1:G:1600:LEU:HD13	1.95	0.47
1:G:4228:ALA:O	1:G:4232:GLU:N	2.46	0.47
2:H:7:ILE:HG22	2:H:9:PRO:HD2	1.95	0.47
1:B:4681:LEU:HD21	1:B:4687:TYR:HD2	1.78	0.47
1:E:35:LEU:HD13	1:E:49:LEU:HD13	1.95	0.47
1:I:580:GLU:HG3	1:I:620:LEU:HD22	1.95	0.47
1:I:709:ASP:HB3	1:I:725:HIS:CE1	2.49	0.47
1:I:1095:VAL:HB	1:I:1199:VAL:HG23	1.96	0.47
1:G:1970:GLN:HB2	1:G:3642:TYR:HA	1.95	0.47
1:G:2002:PRO:HA	1:G:2005:GLN:HB3	1.94	0.47
1:G:4666:VAL:HG23	1:G:4669:VAL:HB	1.96	0.47
1:G:4681:LEU:HD21	1:G:4687:TYR:HD2	1.78	0.47
1:G:4763:GLY:O	1:G:4766:THR:OG1	2.31	0.47
1:G:1269:CYS:HA	1:G:1473:UNK:HA	1.96	0.47
1:B:3830:GLN:HA	1:B:3833:GLN:HG2	1.96	0.47
1:E:877:ASN:HD22	1:E:1045:THR:HG23	1.79	0.47
1:E:4681:LEU:HD21	1:E:4687:TYR:HD2	1.79	0.47
1:I:35:LEU:HD13	1:I:49:LEU:HD13	1.95	0.47
1:I:669:ASP:OD2	1:I:790:ARG:NH2	2.47	0.47
1:G:460:GLN:HG2	1:G:462:GLU:H	1.78	0.47
1:G:709:ASP:HB3	1:G:725:HIS:CE1	2.49	0.47
1:G:4571:PHE:O	1:G:4575:PHE:N	2.47	0.47
2:A:7:ILE:HG22	2:A:9:PRO:HD2	1.95	0.47
1:E:242:ARG:NH1	1:E:481:GLU:OE1	2.39	0.47
1:I:404:ILE:HG21	1:I:481:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:709:ASP:O	1:I:725:HIS:ND1	2.46	0.47
1:I:776:LEU:HG	1:I:848:HIS:HA	1.97	0.47
1:I:2381:GLU:HA	1:I:2384:ILE:HD12	1.95	0.47
1:I:3830:GLN:HA	1:I:3833:GLN:HG2	1.96	0.47
1:I:4826:ILE:O	1:I:4829:SER:OG	2.29	0.47
1:G:776:LEU:HG	1:G:848:HIS:HA	1.97	0.47
1:G:877:ASN:HD22	1:G:1045:THR:HG23	1.79	0.47
1:B:669:ASP:OD2	1:B:790:ARG:NH2	2.47	0.47
1:B:1095:VAL:HB	1:B:1199:VAL:HG23	1.96	0.47
1:E:776:LEU:HG	1:E:848:HIS:HA	1.97	0.47
1:E:3890:LEU:HA	1:E:3893:GLU:HB2	1.97	0.47
1:I:4180:ARG:O	1:I:4987:ASN:ND2	2.47	0.47
1:I:4782:VAL:O	1:I:4785:THR:OG1	2.28	0.47
1:G:404:ILE:HG21	1:G:481:GLU:HG3	1.97	0.47
1:G:669:ASP:OD2	1:G:790:ARG:NH2	2.47	0.47
1:G:1713:ASP:O	1:G:1717:SER:N	2.44	0.47
1:G:1812:LEU:HD21	1:G:1861:GLN:HG2	1.96	0.47
1:G:2381:GLU:HA	1:G:2384:ILE:HD12	1.96	0.47
1:G:3676:ASP:OD1	1:G:3676:ASP:N	2.48	0.47
1:G:4180:ARG:O	1:G:4987:ASN:ND2	2.48	0.47
1:G:4852:THR:HG21	1:G:4883:TYR:HB2	1.96	0.47
2:J:76:CYS:HB2	2:J:97:LEU:HB2	1.97	0.47
1:B:179:TYR:OH	1:E:2359:ARG:NH1	2.47	0.47
1:B:288:GLY:HA3	1:B:405:HIS:CE1	2.49	0.47
1:B:776:LEU:HG	1:B:848:HIS:HA	1.97	0.47
1:B:1679:ASN:HA	1:B:1682:ALA:HB3	1.97	0.47
1:B:4578:LEU:HD21	1:I:4849:TYR:HE1	1.80	0.47
1:E:111:HIS:CD2	1:E:114:SER:H	2.28	0.47
1:E:111:HIS:HB2	1:E:137:LEU:HD11	1.96	0.47
1:E:3963:ASN:O	1:E:3966:THR:OG1	2.29	0.47
1:I:264:PRO:HG2	1:I:270:SER:HB2	1.97	0.47
1:I:410:LEU:HD12	1:I:413:GLN:HE21	1.80	0.47
1:B:264:PRO:HG2	1:B:270:SER:HB2	1.97	0.47
1:B:664:PHE:HB2	1:B:746:CYS:HB2	1.97	0.47
1:B:2034:PHE:O	1:B:2038:LEU:N	2.48	0.47
1:B:4980:LEU:O	1:B:4984:ASN:ND2	2.43	0.47
1:E:649:PHE:HB3	1:E:776:LEU:HD13	1.97	0.47
1:E:1973:GLN:HA	1:E:1976:ARG:HB3	1.97	0.47
1:I:1691:GLN:HE22	1:I:1802:ILE:HG12	1.79	0.47
1:I:4852:THR:HG21	1:I:4883:TYR:HB2	1.96	0.47
1:B:614:VAL:HA	1:B:2169:GLN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1243:PRO:HB2	1:B:1600:LEU:HD13	1.96	0.47
1:E:410:LEU:HD12	1:E:413:GLN:HE21	1.80	0.47
1:E:4180:ARG:O	1:E:4987:ASN:ND2	2.48	0.47
1:E:4204:GLN:NE2	1:E:4245:MET:SD	2.88	0.47
1:E:4570:ALA:O	1:E:4574:ASN:ND2	2.48	0.47
1:E:4763:GLY:O	1:E:4766:THR:OG1	2.31	0.47
1:I:685:GLY:N	1:I:780:VAL:O	2.39	0.47
1:I:1163:THR:HA	1:I:1168:VAL:HA	1.97	0.47
1:I:2034:PHE:O	1:I:2038:LEU:N	2.48	0.47
1:G:664:PHE:HB2	1:G:746:CYS:HB2	1.97	0.47
1:G:2034:PHE:O	1:G:2038:LEU:N	2.48	0.47
1:B:2739:PRO:HB3	1:B:2884:ASN:HB3	1.98	0.46
1:E:669:ASP:OD2	1:E:790:ARG:NH2	2.47	0.46
1:E:4666:VAL:HG23	1:E:4669:VAL:HB	1.96	0.46
1:I:614:VAL:HA	1:I:2169:GLN:HB3	1.97	0.46
1:I:4571:PHE:O	1:I:4575:PHE:N	2.47	0.46
1:I:4581:LYS:HB2	1:I:4632:LEU:HB2	1.97	0.46
1:G:35:LEU:HD13	1:G:49:LEU:HD13	1.95	0.46
1:G:43:GLY:N	1:G:447:ASP:OD2	2.46	0.46
1:E:404:ILE:HG21	1:E:481:GLU:HG3	1.97	0.46
1:E:664:PHE:HB2	1:E:746:CYS:HB2	1.97	0.46
1:E:1163:THR:HA	1:E:1168:VAL:HA	1.97	0.46
1:E:2257:LEU:HD11	1:E:2276:ALA:HB2	1.96	0.46
1:E:3830:GLN:HA	1:E:3833:GLN:HG2	1.96	0.46
1:E:4826:ILE:HG23	1:E:4940:PHE:HZ	1.81	0.46
1:I:877:ASN:HD22	1:I:1045:THR:HG23	1.79	0.46
1:I:1679:ASN:HA	1:I:1682:ALA:HB3	1.97	0.46
1:I:1812:LEU:HD21	1:I:1861:GLN:HG2	1.96	0.46
1:I:4228:ALA:O	1:I:4232:GLU:N	2.46	0.46
1:G:1679:ASN:HA	1:G:1682:ALA:HB3	1.97	0.46
1:G:2257:LEU:HD11	1:G:2276:ALA:HB2	1.96	0.46
1:B:1639:LEU:HD12	1:B:1653:LEU:HD21	1.98	0.46
1:B:3890:LEU:HA	1:B:3893:GLU:HB2	1.97	0.46
1:E:111:HIS:N	1:E:116:MET:O	2.44	0.46
1:G:410:LEU:HD12	1:G:413:GLN:HE21	1.80	0.46
1:G:583:ILE:HA	1:G:586:ILE:HD12	1.98	0.46
1:G:1973:GLN:HA	1:G:1976:ARG:HB3	1.98	0.46
1:B:139:GLU:O	1:B:141:ALA:N	2.49	0.46
1:B:835:ARG:HD3	1:B:1210:SER:HA	1.98	0.46
1:B:877:ASN:HD22	1:B:1045:THR:HG23	1.79	0.46
1:B:1691:GLN:HE22	1:B:1802:ILE:HG12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3840:SER:OG	1:B:3875:MET:O	2.24	0.46
1:B:4180:ARG:O	1:B:4987:ASN:ND2	2.48	0.46
1:E:2739:PRO:HB3	1:E:2884:ASN:HB3	1.98	0.46
1:I:664:PHE:HB2	1:I:746:CYS:HB2	1.97	0.46
1:I:4177:TYR:HA	1:I:4202:ARG:HH22	1.80	0.46
1:G:111:HIS:HB2	1:G:137:LEU:HD11	1.96	0.46
1:G:139:GLU:O	1:G:141:ALA:N	2.49	0.46
1:G:3830:GLN:HA	1:G:3833:GLN:HG2	1.96	0.46
1:B:3832:ILE:O	1:B:3836:MET:N	2.47	0.46
1:B:4674:GLU:HB3	1:B:4715:TYR:HB2	1.98	0.46
1:E:685:GLY:N	1:E:780:VAL:O	2.39	0.46
1:E:835:ARG:HD3	1:E:1210:SER:HA	1.98	0.46
1:E:4177:TYR:HE1	1:E:4199:GLU:HB2	1.81	0.46
1:I:3890:LEU:HA	1:I:3893:GLU:HB2	1.97	0.46
1:I:3971:GLY:H	1:I:5005:GLY:HA3	1.80	0.46
1:I:4666:VAL:HG23	1:I:4669:VAL:HB	1.96	0.46
1:I:4763:GLY:O	1:I:4766:THR:OG1	2.31	0.46
1:G:264:PRO:HG2	1:G:270:SER:HB2	1.97	0.46
1:G:838:HIS:CE1	1:G:1201:HIS:HD2	2.34	0.46
1:G:4826:ILE:O	1:G:4829:SER:OG	2.28	0.46
2:H:76:CYS:HB2	2:H:97:LEU:HB2	1.97	0.46
1:B:485:SER:O	1:B:489:ASN:N	2.44	0.46
1:B:583:ILE:HA	1:B:586:ILE:HD12	1.98	0.46
1:B:649:PHE:HB3	1:B:776:LEU:HD13	1.98	0.46
1:B:718:GLY:HA3	1:B:737:LEU:HA	1.97	0.46
1:B:1163:THR:HA	1:B:1168:VAL:HA	1.97	0.46
1:B:3905:THR:HA	1:B:3912:THR:HG23	1.98	0.46
1:B:4937:ILE:HD11	1:I:4933:GLN:HE22	1.80	0.46
1:E:184:THR:HB	1:E:189:LEU:HG	1.98	0.46
1:E:264:PRO:HG2	1:E:270:SER:HB2	1.97	0.46
1:E:3971:GLY:H	1:E:5005:GLY:HA3	1.80	0.46
1:I:139:GLU:O	1:I:141:ALA:N	2.49	0.46
1:I:4570:ALA:O	1:I:4574:ASN:ND2	2.49	0.46
1:B:3971:GLY:H	1:B:5005:GLY:HA3	1.80	0.46
1:E:1639:LEU:HD12	1:E:1653:LEU:HD21	1.98	0.46
1:E:2034:PHE:O	1:E:2038:LEU:N	2.48	0.46
1:I:309:THR:O	1:I:313:SER:OG	2.27	0.46
1:I:583:ILE:HA	1:I:586:ILE:HD12	1.98	0.46
1:I:4826:ILE:HG23	1:I:4940:PHE:HZ	1.80	0.46
1:G:184:THR:HB	1:G:189:LEU:HG	1.98	0.46
1:G:2257:LEU:O	1:G:2261:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4177:TYR:HA	1:G:4202:ARG:HH22	1.81	0.46
1:B:410:LEU:HD12	1:B:413:GLN:HE21	1.80	0.46
1:B:4581:LYS:HB2	1:B:4632:LEU:HB2	1.97	0.46
1:E:45:ARG:NH2	1:E:447:ASP:OD1	2.45	0.46
1:E:718:GLY:HA3	1:E:737:LEU:HA	1.97	0.46
1:E:983:THR:O	1:E:987:ARG:N	2.47	0.46
1:I:718:GLY:HA3	1:I:737:LEU:HA	1.97	0.46
1:I:1684:ALA:HA	1:I:1782:PHE:HZ	1.81	0.46
1:I:3963:ASN:O	1:I:3966:THR:OG1	2.29	0.46
1:I:4822:THR:O	1:I:4825:THR:OG1	2.30	0.46
1:G:395:GLN:HG3	1:G:397:GLU:H	1.81	0.46
1:G:649:PHE:HB3	1:G:776:LEU:HD13	1.98	0.46
1:G:718:GLY:HA3	1:G:737:LEU:HA	1.97	0.46
1:G:1163:THR:HA	1:G:1168:VAL:HA	1.97	0.46
1:B:2257:LEU:O	1:B:2261:SER:N	2.49	0.46
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.49	0.46
1:E:215:THR:HG22	1:E:273:HIS:HA	1.98	0.46
1:E:614:VAL:HA	1:E:2169:GLN:HB3	1.97	0.46
1:E:4177:TYR:HA	1:E:4202:ARG:HH22	1.80	0.46
1:E:4980:LEU:O	1:E:4984:ASN:ND2	2.43	0.46
1:I:184:THR:HB	1:I:189:LEU:HG	1.98	0.46
1:I:2739:PRO:HB3	1:I:2884:ASN:HB3	1.98	0.46
1:I:3658:LYS:HA	1:I:3661:TRP:CD2	2.51	0.46
1:G:4581:LYS:HB2	1:G:4632:LEU:HB2	1.97	0.46
1:B:1713:ASP:O	1:B:1717:SER:N	2.44	0.46
1:B:4826:ILE:HG23	1:B:4940:PHE:HZ	1.81	0.46
1:E:1269:CYS:HA	1:E:1473:UNK:HA	1.97	0.46
1:E:3905:THR:HA	1:E:3912:THR:HG23	1.98	0.46
1:I:2813:LEU:HD21	1:I:2926:LEU:HD11	1.98	0.46
1:G:614:VAL:HA	1:G:2169:GLN:HB3	1.97	0.46
1:G:3658:LYS:HA	1:G:3661:TRP:CD2	2.51	0.46
1:G:4083:ASP:HA	1:G:4085:ARG:HH11	1.81	0.46
1:G:4570:ALA:O	1:G:4574:ASN:ND2	2.49	0.46
1:B:184:THR:HB	1:B:189:LEU:HG	1.98	0.45
1:B:2869:ARG:HA	1:B:2872:GLN:HB3	1.99	0.45
1:B:3658:LYS:HA	1:B:3661:TRP:CD2	2.51	0.45
1:E:139:GLU:O	1:E:141:ALA:N	2.49	0.45
1:E:583:ILE:HA	1:E:586:ILE:HD12	1.98	0.45
1:E:1679:ASN:HA	1:E:1682:ALA:HB3	1.97	0.45
1:E:3658:LYS:HA	1:E:3661:TRP:CD2	2.51	0.45
1:I:101:LEU:HB3	1:I:150:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:649:PHE:HB3	1:I:776:LEU:HD13	1.98	0.45
1:I:835:ARG:HD3	1:I:1210:SER:HA	1.98	0.45
1:I:2257:LEU:O	1:I:2261:SER:N	2.49	0.45
1:I:3805:LEU:HA	1:I:3809:ASN:HB2	1.98	0.45
1:G:215:THR:HG22	1:G:273:HIS:HA	1.98	0.45
1:G:235:ALA:HA	1:G:257:ARG:HD3	1.98	0.45
1:G:1639:LEU:HD12	1:G:1653:LEU:HD21	1.98	0.45
1:E:2257:LEU:O	1:E:2261:SER:N	2.49	0.45
1:E:2813:LEU:HD21	1:E:2926:LEU:HD11	1.98	0.45
1:E:4003:LEU:HB2	1:E:4013:LEU:HD13	1.99	0.45
1:I:3905:THR:HA	1:I:3912:THR:HG23	1.98	0.45
1:G:1203:ASN:ND2	1:G:1210:SER:O	2.49	0.45
1:G:2869:ARG:HA	1:G:2872:GLN:HB3	1.98	0.45
1:G:3971:GLY:H	1:G:5005:GLY:HA3	1.80	0.45
1:B:266:ARG:NH2	1:B:269:TRP:O	2.50	0.45
1:B:1271:ARG:HA	1:B:1471:UNK:HA	1.98	0.45
1:B:2764:GLU:HG3	1:B:2857:PRO:HB2	1.99	0.45
1:B:3963:ASN:O	1:B:3966:THR:OG1	2.29	0.45
1:E:331:VAL:HG12	1:E:333:GLY:H	1.82	0.45
1:E:733:PRO:HD2	1:E:763:PRO:HD2	1.97	0.45
1:E:1708:ARG:HG2	1:E:1711:TYR:CE2	2.52	0.45
1:E:4581:LYS:HB2	1:E:4632:LEU:HB2	1.97	0.45
1:I:733:PRO:HD2	1:I:763:PRO:HD2	1.98	0.45
1:I:2266:GLY:O	1:I:2330:ARG:NH2	2.50	0.45
1:I:2764:GLU:HG3	1:I:2857:PRO:HB2	1.99	0.45
1:I:4083:ASP:HA	1:I:4085:ARG:HH11	1.81	0.45
1:I:4177:TYR:HE1	1:I:4199:GLU:HB2	1.81	0.45
1:G:2266:GLY:O	1:G:2330:ARG:NH2	2.50	0.45
1:G:2739:PRO:HB3	1:G:2884:ASN:HB3	1.98	0.45
1:G:4204:GLN:NE2	1:G:4245:MET:SD	2.88	0.45
1:B:395:GLN:HG3	1:B:397:GLU:H	1.81	0.45
1:B:838:HIS:CE1	1:B:1201:HIS:HD2	2.34	0.45
1:B:1684:ALA:HA	1:B:1782:PHE:HZ	1.81	0.45
1:B:3805:LEU:HA	1:B:3809:ASN:HB2	1.98	0.45
1:E:838:HIS:CE1	1:E:1201:HIS:HD2	2.34	0.45
1:E:2764:GLU:HG3	1:E:2857:PRO:HB2	1.99	0.45
1:E:4674:GLU:HB3	1:E:4715:TYR:HB2	1.98	0.45
1:I:215:THR:HG22	1:I:273:HIS:HA	1.98	0.45
1:I:235:ALA:HA	1:I:257:ARG:HD3	1.98	0.45
1:I:1203:ASN:ND2	1:I:1210:SER:O	2.49	0.45
1:I:2869:ARG:HA	1:I:2872:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3646:THR:O	1:I:3650:CYS:N	2.49	0.45
1:I:4674:GLU:HB3	1:I:4715:TYR:HB2	1.98	0.45
1:G:2813:LEU:HD21	1:G:2926:LEU:HD11	1.99	0.45
1:B:465:GLN:HG3	1:B:3710:LEU:HB3	1.99	0.45
1:B:2813:LEU:HD21	1:B:2926:LEU:HD11	1.98	0.45
1:E:395:GLN:HG3	1:E:397:GLU:H	1.81	0.45
1:E:1516:UNK:N	1:E:1529:UNK:O	2.49	0.45
1:E:3676:ASP:N	1:E:3676:ASP:OD1	2.48	0.45
1:E:4083:ASP:HA	1:E:4085:ARG:HH11	1.81	0.45
1:I:1708:ARG:HG2	1:I:1711:TYR:CE2	2.52	0.45
1:G:2764:GLU:HG3	1:G:2857:PRO:HB2	1.99	0.45
1:G:3890:LEU:HA	1:G:3893:GLU:HB2	1.97	0.45
1:G:3905:THR:HA	1:G:3912:THR:HG23	1.98	0.45
1:G:3963:ASN:O	1:G:3966:THR:OG1	2.29	0.45
1:B:983:THR:O	1:B:987:ARG:N	2.47	0.45
1:B:1973:GLN:HA	1:B:1976:ARG:HB3	1.98	0.45
1:B:4003:LEU:HB2	1:B:4013:LEU:HD13	1.99	0.45
1:B:4177:TYR:HA	1:B:4202:ARG:HH22	1.81	0.45
1:B:4571:PHE:O	1:B:4575:PHE:N	2.47	0.45
1:B:4735:GLU:HA	1:B:4738:ALA:HB3	1.98	0.45
1:E:2266:GLY:O	1:E:2330:ARG:NH2	2.50	0.45
1:E:2869:ARG:HH12	1:E:2945:UNK:C	2.29	0.45
1:E:3840:SER:OG	1:E:3875:MET:O	2.24	0.45
1:I:1973:GLN:HA	1:I:1976:ARG:HB3	1.98	0.45
1:I:2869:ARG:HH12	1:I:2945:UNK:C	2.29	0.45
1:I:4152:GLU:OE1	1:I:4194:TYR:OH	2.35	0.45
1:G:733:PRO:HD2	1:G:763:PRO:HD2	1.97	0.45
1:G:898:ASP:HB3	1:G:901:LYS:HB2	1.99	0.45
1:G:2868:SER:O	1:G:2872:GLN:N	2.47	0.45
1:G:4674:GLU:HB3	1:G:4715:TYR:HB2	1.98	0.45
1:B:235:ALA:HA	1:B:257:ARG:HD3	1.98	0.45
1:B:733:PRO:HD2	1:B:763:PRO:HD2	1.97	0.45
1:B:1708:ARG:HG2	1:B:1711:TYR:CE2	2.52	0.45
1:E:235:ALA:HA	1:E:257:ARG:HD3	1.98	0.45
1:E:2869:ARG:HA	1:E:2872:GLN:HB3	1.98	0.45
1:G:1684:ALA:HA	1:G:1782:PHE:HZ	1.81	0.45
1:G:3805:LEU:HA	1:G:3809:ASN:HB2	1.98	0.45
1:B:1203:ASN:ND2	1:B:1210:SER:O	2.49	0.45
1:E:898:ASP:HB3	1:E:901:LYS:HB2	1.99	0.45
1:E:3832:ILE:O	1:E:3836:MET:N	2.47	0.45
1:I:838:HIS:CE1	1:I:1201:HIS:HD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1639:LEU:HD12	1:I:1653:LEU:HD21	1.97	0.45
1:I:3676:ASP:OD1	1:I:3676:ASP:N	2.48	0.45
1:G:1103:GLY:HA3	1:G:1123:VAL:HA	1.99	0.45
1:G:4003:LEU:HB2	1:G:4013:LEU:HD13	1.99	0.45
1:G:4152:GLU:OE1	1:G:4194:TYR:OH	2.35	0.45
1:G:4826:ILE:HG23	1:G:4940:PHE:HZ	1.81	0.45
2:A:76:CYS:HB2	2:A:97:LEU:HB2	1.97	0.45
1:B:215:THR:HG22	1:B:273:HIS:HA	1.98	0.45
1:B:1076:ARG:HD3	1:B:1237:TRP:HB2	1.99	0.45
1:B:4024:VAL:HG23	1:B:4027:LEU:HD12	1.99	0.45
1:E:266:ARG:NH2	1:E:269:TRP:O	2.50	0.45
1:E:1099:GLU:OE2	1:E:1127:HIS:ND1	2.40	0.45
1:E:1659:LEU:O	1:E:1663:HIS:N	2.43	0.45
1:E:3805:LEU:HA	1:E:3809:ASN:HB2	1.98	0.45
1:E:4152:GLU:OE1	1:E:4194:TYR:OH	2.35	0.45
1:I:4003:LEU:HB2	1:I:4013:LEU:HD13	1.99	0.45
1:G:331:VAL:HG12	1:G:333:GLY:H	1.82	0.45
1:G:1076:ARG:HD3	1:G:1237:TRP:HB2	1.99	0.45
1:G:3646:THR:O	1:G:3650:CYS:N	2.49	0.45
1:E:1203:ASN:ND2	1:E:1210:SER:O	2.49	0.45
1:E:1684:ALA:HA	1:E:1782:PHE:HZ	1.81	0.45
1:I:4735:GLU:HA	1:I:4738:ALA:HB3	1.98	0.45
1:G:835:ARG:HD3	1:G:1210:SER:HA	1.98	0.45
1:G:4560:TYR:O	1:G:4564:PHE:N	2.41	0.45
1:G:4688:ILE:HG21	1:G:4728:HIS:HB3	1.99	0.45
1:E:465:GLN:HG3	1:E:3710:LEU:HB3	1.99	0.44
1:E:4735:GLU:HA	1:E:4738:ALA:HB3	1.98	0.44
1:I:1076:ARG:HD3	1:I:1237:TRP:HB2	1.99	0.44
2:F:76:CYS:HB2	2:F:97:LEU:HB2	1.97	0.44
2:J:91:ILE:HD12	2:J:97:LEU:HD11	1.99	0.44
1:B:1286:UNK:HA	1:B:1461:UNK:HA	1.99	0.44
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.35	0.44
1:B:4177:TYR:HE1	1:B:4199:GLU:HB2	1.81	0.44
1:E:1076:ARG:HD3	1:E:1237:TRP:HB2	1.99	0.44
1:E:4024:VAL:HG23	1:E:4027:LEU:HD12	1.99	0.44
1:G:4177:TYR:HE1	1:G:4199:GLU:HB2	1.81	0.44
2:F:57:LYS:HB2	2:F:80:VAL:HB	2.00	0.44
1:B:1103:GLY:HA3	1:B:1123:VAL:HA	1.99	0.44
1:B:3930:ILE:HG23	1:B:3951:PHE:HE1	1.83	0.44
1:E:870:ILE:HD12	1:E:870:ILE:HA	1.88	0.44
1:I:395:GLN:HG3	1:I:397:GLU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4142:ASN:HA	1:I:4145:VAL:HG12	1.99	0.44
1:G:1708:ARG:HG2	1:G:1711:TYR:CE2	2.52	0.44
1:B:1096:THR:HG23	1:B:1199:VAL:HG22	1.99	0.44
1:B:4688:ILE:HG21	1:B:4728:HIS:HB3	1.99	0.44
1:E:1936:LYS:O	1:E:1940:CYS:N	2.45	0.44
1:E:2265:LEU:HD22	1:E:2330:ARG:HB3	1.99	0.44
1:E:4782:VAL:O	1:E:4785:THR:OG1	2.29	0.44
1:I:266:ARG:NH2	1:I:269:TRP:O	2.50	0.44
1:G:1659:LEU:O	1:G:1663:HIS:N	2.43	0.44
1:G:2265:LEU:HD22	1:G:2330:ARG:HB3	1.99	0.44
1:G:4142:ASN:HA	1:G:4145:VAL:HG12	1.99	0.44
1:G:4980:LEU:O	1:G:4984:ASN:ND2	2.43	0.44
2:H:91:ILE:HD12	2:H:97:LEU:HD11	1.99	0.44
1:B:4083:ASP:HA	1:B:4085:ARG:HH11	1.82	0.44
1:B:4763:GLY:O	1:B:4766:THR:OG1	2.31	0.44
1:E:1718:ILE:HG13	1:E:1719:HIS:CD2	2.53	0.44
1:I:1096:THR:HG23	1:I:1199:VAL:HG22	2.00	0.44
1:I:1099:GLU:OE2	1:I:1127:HIS:ND1	2.40	0.44
1:I:2778:GLY:HA3	1:I:2787:THR:HB	1.99	0.44
1:I:4204:GLN:NE2	1:I:4245:MET:SD	2.88	0.44
1:G:1244:GLN:HB3	1:G:1646:ARG:HH12	1.83	0.44
1:G:3930:ILE:HG23	1:G:3951:PHE:HE1	1.83	0.44
1:B:331:VAL:HG12	1:B:333:GLY:H	1.82	0.44
1:B:794:GLY:H	1:B:798:GLY:HA3	1.83	0.44
1:B:2266:GLY:O	1:B:2330:ARG:NH2	2.50	0.44
1:B:3676:ASP:OD1	1:B:3676:ASP:N	2.48	0.44
1:B:4069:LYS:HD2	1:B:4133:GLN:HG3	2.00	0.44
1:B:4204:GLN:NE2	1:B:4245:MET:SD	2.88	0.44
1:E:218:HIS:HB3	1:E:392:ARG:HD3	2.00	0.44
1:E:4688:ILE:HG21	1:E:4728:HIS:HB3	1.99	0.44
1:I:342:GLY:HA2	1:I:389:PHE:HD2	1.83	0.44
1:I:1103:GLY:HA3	1:I:1123:VAL:HA	1.99	0.44
1:I:1854:PHE:HD1	1:I:1858:ASP:HB3	1.83	0.44
1:I:3930:ILE:HG23	1:I:3951:PHE:HE1	1.83	0.44
2:J:57:LYS:HB2	2:J:80:VAL:HB	1.99	0.44
1:B:45:ARG:NH2	1:B:447:ASP:OD1	2.45	0.44
1:B:4147:LEU:O	1:B:4151:SER:OG	2.32	0.44
1:E:1244:GLN:HB3	1:E:1646:ARG:HH12	1.83	0.44
1:E:4826:ILE:O	1:E:4829:SER:OG	2.29	0.44
1:I:794:GLY:H	1:I:798:GLY:HA3	1.83	0.44
2:F:91:ILE:HD12	2:F:97:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:TYR:N	1:B:1224:GLU:O	2.51	0.44
1:B:2265:LEU:HD22	1:B:2330:ARG:HB3	1.99	0.44
1:E:3930:ILE:HG23	1:E:3951:PHE:HE1	1.83	0.44
1:I:21:VAL:HG12	1:I:66:CYS:HA	2.00	0.44
1:I:465:GLN:HG3	1:I:3710:LEU:HB3	1.99	0.44
1:I:898:ASP:HB3	1:I:901:LYS:HB2	1.99	0.44
1:G:266:ARG:NH2	1:G:269:TRP:O	2.50	0.44
1:G:794:GLY:H	1:G:798:GLY:HA3	1.82	0.44
2:H:57:LYS:HB2	2:H:80:VAL:HB	1.99	0.44
1:B:898:ASP:HB3	1:B:901:LYS:HB2	1.99	0.44
1:B:1865:MET:SD	1:B:1865:MET:N	2.91	0.44
1:E:1103:GLY:HA3	1:E:1123:VAL:HA	1.99	0.44
1:I:4743:MET:HB3	1:I:4746:ALA:HB3	2.00	0.44
1:G:1854:PHE:HD1	1:G:1858:ASP:HB3	1.83	0.44
1:G:4125:PHE:HA	1:G:4128:PHE:HB3	2.00	0.44
1:B:1718:ILE:HG13	1:B:1719:HIS:CD2	2.53	0.43
1:B:3992:PHE:O	1:B:3996:PHE:N	2.43	0.43
1:E:663:TYR:HB2	1:E:808:TYR:HB3	2.00	0.43
1:E:750:LEU:HD21	1:E:777:PHE:HE2	1.83	0.43
1:I:1865:MET:SD	1:I:1865:MET:N	2.91	0.43
1:I:3994:HIS:O	1:I:3998:HIS:ND1	2.45	0.43
1:G:45:ARG:NH2	1:G:447:ASP:OD1	2.45	0.43
1:G:465:GLN:HG3	1:G:3710:LEU:HB3	1.99	0.43
1:G:4735:GLU:HA	1:G:4738:ALA:HB3	1.98	0.43
1:B:1090:PHE:HD2	1:B:1202:LEU:HD11	1.84	0.43
1:B:4125:PHE:HA	1:B:4128:PHE:HB3	2.00	0.43
1:B:4826:ILE:O	1:B:4829:SER:OG	2.29	0.43
1:E:342:GLY:HA2	1:E:389:PHE:HD2	1.83	0.43
1:E:4142:ASN:HA	1:E:4145:VAL:HG12	1.99	0.43
1:I:4024:VAL:HG23	1:I:4027:LEU:HD12	1.99	0.43
1:G:218:HIS:HB3	1:G:392:ARG:HD3	2.00	0.43
1:G:4069:LYS:HD2	1:G:4133:GLN:HG3	2.00	0.43
1:B:4142:ASN:HA	1:B:4145:VAL:HG12	1.99	0.43
1:E:794:GLY:H	1:E:798:GLY:HA3	1.83	0.43
1:E:1854:PHE:HD1	1:E:1858:ASP:HB3	1.83	0.43
1:E:2318:TYR:OH	1:E:2414:ASN:N	2.52	0.43
1:E:4104:THR:HG22	1:E:4106:PRO:HD2	2.01	0.43
1:E:4125:PHE:HA	1:E:4128:PHE:HB3	2.00	0.43
1:E:4743:MET:HB3	1:E:4746:ALA:HB3	2.00	0.43
1:I:2121:PHE:O	1:I:3725:TYR:OH	2.35	0.43
1:I:4671:PHE:HE1	1:I:4715:TYR:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:VAL:HG12	1:G:66:CYS:HA	2.00	0.43
1:G:750:LEU:HD21	1:G:777:PHE:HE2	1.83	0.43
1:G:1863:LEU:HB3	1:G:1870:VAL:HG11	2.01	0.43
1:G:2121:PHE:O	1:G:3725:TYR:OH	2.35	0.43
1:G:3832:ILE:O	1:G:3836:MET:N	2.47	0.43
2:A:7:ILE:N	2:A:71:ARG:O	2.44	0.43
1:B:218:HIS:HB3	1:B:392:ARG:HD3	2.00	0.43
1:B:342:GLY:HA2	1:B:389:PHE:HD2	1.83	0.43
1:E:1090:PHE:HD2	1:E:1202:LEU:HD11	1.84	0.43
1:E:4671:PHE:HE1	1:E:4715:TYR:HA	1.84	0.43
1:I:1244:GLN:HB3	1:I:1646:ARG:HH12	1.83	0.43
1:I:1730:MET:O	1:I:1772:ARG:NH1	2.51	0.43
1:I:2265:LEU:HD22	1:I:2330:ARG:HB3	1.99	0.43
1:I:4125:PHE:HA	1:I:4128:PHE:HB3	2.00	0.43
1:I:4937:ILE:HD11	1:G:4933:GLN:HE22	1.83	0.43
1:G:685:GLY:N	1:G:780:VAL:O	2.39	0.43
1:G:2326:CYS:SG	1:G:2327:GLY:N	2.92	0.43
2:A:57:LYS:HB2	2:A:80:VAL:HB	1.99	0.43
2:A:91:ILE:HD12	2:A:97:LEU:HD11	1.99	0.43
1:B:750:LEU:HD21	1:B:777:PHE:HE2	1.83	0.43
1:B:864:PRO:HD2	1:B:867:LEU:HD12	2.00	0.43
1:I:45:ARG:HG2	1:I:443:LEU:HD21	2.00	0.43
1:I:663:TYR:HB2	1:I:808:TYR:HB3	2.00	0.43
1:G:342:GLY:HA2	1:G:389:PHE:HD2	1.83	0.43
1:G:4104:THR:HG22	1:G:4106:PRO:HD2	2.01	0.43
1:B:232:THR:HB	1:B:252:VAL:HG11	2.01	0.43
1:B:1863:LEU:HB3	1:B:1870:VAL:HG11	2.01	0.43
1:B:2778:GLY:HA3	1:B:2787:THR:HB	1.99	0.43
1:B:4144:ALA:HB2	1:B:4170:ILE:HG22	2.01	0.43
1:B:4671:PHE:HE1	1:B:4715:TYR:HA	1.84	0.43
1:E:345:LEU:HD23	1:E:389:PHE:HB3	2.01	0.43
1:E:488:LEU:HD23	1:E:491:ILE:HD12	2.00	0.43
1:E:1730:MET:O	1:E:1772:ARG:NH1	2.51	0.43
1:E:2326:CYS:SG	1:E:2327:GLY:N	2.92	0.43
1:E:2778:GLY:HA3	1:E:2787:THR:HB	1.99	0.43
1:E:4069:LYS:HD2	1:E:4133:GLN:HG3	2.00	0.43
1:E:4144:ALA:HB2	1:E:4170:ILE:HG22	2.01	0.43
1:E:4719:PHE:HD1	1:E:4722:ARG:HD3	1.84	0.43
1:I:331:VAL:HG12	1:I:333:GLY:H	1.82	0.43
1:I:1089:TYR:N	1:I:1224:GLU:O	2.51	0.43
1:I:4719:PHE:HD1	1:I:4722:ARG:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:HIS:N	1:G:116:MET:O	2.44	0.43
1:G:283:ARG:NH2	1:G:402:ARG:HH12	2.17	0.43
1:G:488:LEU:HD23	1:G:491:ILE:HD12	2.00	0.43
1:G:1952:GLN:HA	1:G:1955:VAL:HG12	2.01	0.43
1:G:4719:PHE:HD1	1:G:4722:ARG:HD3	1.84	0.43
2:F:90:VAL:HG12	2:F:91:ILE:HG12	2.00	0.43
1:B:2326:CYS:SG	1:B:2327:GLY:N	2.92	0.43
1:B:3927:GLN:O	1:B:3931:SER:N	2.49	0.43
1:E:1089:TYR:N	1:E:1224:GLU:O	2.51	0.43
1:E:3713:LYS:HG2	1:E:3715:LYS:H	1.84	0.43
1:E:3889:GLN:HE22	1:E:3963:ASN:HB3	1.84	0.43
1:I:283:ARG:NH2	1:I:402:ARG:HH12	2.17	0.43
1:I:1679:ASN:O	1:I:1683:HIS:ND1	2.37	0.43
1:I:2326:CYS:SG	1:I:2327:GLY:N	2.92	0.43
1:G:494:LEU:HD22	1:G:515:TRP:HE1	1.84	0.43
1:G:864:PRO:HD2	1:G:867:LEU:HD12	2.00	0.43
1:G:983:THR:O	1:G:987:ARG:N	2.47	0.43
1:G:2778:GLY:HA3	1:G:2787:THR:HB	1.99	0.43
1:G:3713:LYS:HG2	1:G:3715:LYS:H	1.84	0.43
1:G:3889:GLN:HE22	1:G:3963:ASN:HB3	1.84	0.43
1:G:4024:VAL:HG23	1:G:4027:LEU:HD12	1.99	0.43
1:G:4144:ALA:HB2	1:G:4170:ILE:HG22	2.01	0.43
1:G:4743:MET:HB3	1:G:4746:ALA:HB3	2.00	0.43
1:B:110:ARG:HA	1:B:117:TYR:HA	2.01	0.43
1:B:2102:VAL:HB	1:B:2124:LEU:HD12	2.01	0.43
1:E:1096:THR:HG23	1:E:1199:VAL:HG22	1.99	0.43
1:E:1952:GLN:HA	1:E:1955:VAL:HG12	2.01	0.43
1:I:494:LEU:HD22	1:I:515:TRP:HE1	1.84	0.43
1:I:1090:PHE:HD2	1:I:1202:LEU:HD11	1.83	0.43
1:I:1718:ILE:HG13	1:I:1719:HIS:CD2	2.53	0.43
1:I:4688:ILE:HG21	1:I:4728:HIS:HB3	1.99	0.43
1:G:345:LEU:HD23	1:G:389:PHE:HB3	2.01	0.43
2:J:90:VAL:HG12	2:J:91:ILE:HG12	2.00	0.43
1:B:4719:PHE:HD1	1:B:4722:ARG:HD3	1.84	0.43
1:B:4782:VAL:O	1:B:4785:THR:OG1	2.28	0.43
1:E:232:THR:HB	1:E:252:VAL:HG11	2.01	0.43
1:E:3927:GLN:O	1:E:3931:SER:N	2.49	0.43
1:I:218:HIS:HB3	1:I:392:ARG:HD3	2.00	0.43
1:I:349:GLN:HE21	1:I:354:GLY:HA2	1.84	0.43
1:I:864:PRO:HD2	1:I:867:LEU:HD12	2.00	0.43
1:I:1841:VAL:HA	1:I:1844:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1936:LYS:O	1:G:1940:CYS:N	2.45	0.43
1:B:494:LEU:HD22	1:B:515:TRP:HE1	1.84	0.43
1:B:1679:ASN:O	1:B:1683:HIS:ND1	2.37	0.43
1:B:3646:THR:O	1:B:3650:CYS:N	2.49	0.43
1:B:3829:PHE:HA	1:B:3832:ILE:HD12	2.00	0.43
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	2.01	0.43
1:E:21:VAL:HG12	1:E:66:CYS:HA	2.00	0.43
1:E:2102:VAL:HB	1:E:2124:LEU:HD12	2.01	0.43
1:I:2102:VAL:HB	1:I:2124:LEU:HD12	2.01	0.43
1:I:2751:LEU:HD11	1:I:2823:ILE:HG21	2.01	0.43
1:I:4144:ALA:HB2	1:I:4170:ILE:HG22	2.01	0.43
1:I:4702:ASP:HA	1:I:4778:TRP:HE1	1.84	0.43
1:G:349:GLN:HE21	1:G:354:GLY:HA2	1.84	0.43
1:G:1089:TYR:N	1:G:1224:GLU:O	2.51	0.43
1:G:1096:THR:HG23	1:G:1199:VAL:HG22	2.00	0.43
1:G:1865:MET:SD	1:G:1865:MET:N	2.91	0.43
1:G:2102:VAL:HB	1:G:2124:LEU:HD12	2.01	0.43
1:G:4702:ASP:HA	1:G:4778:TRP:HE1	1.84	0.43
1:B:345:LEU:HD23	1:B:389:PHE:HB3	2.01	0.42
1:B:876:GLU:O	1:B:880:GLU:N	2.51	0.42
1:B:1244:GLN:HB3	1:B:1646:ARG:HH12	1.83	0.42
1:B:2318:TYR:OH	1:B:2414:ASN:N	2.52	0.42
1:B:4049:VAL:HG21	1:B:4159:ARG:HD2	2.01	0.42
1:B:4743:MET:HB3	1:B:4746:ALA:HB3	2.00	0.42
1:E:494:LEU:HD22	1:E:515:TRP:HE1	1.84	0.42
1:E:864:PRO:HD2	1:E:867:LEU:HD12	2.00	0.42
1:E:1865:MET:SD	1:E:1865:MET:N	2.91	0.42
1:E:4049:VAL:HG21	1:E:4159:ARG:HD2	2.01	0.42
1:I:345:LEU:HD23	1:I:389:PHE:HB3	2.01	0.42
1:I:488:LEU:HD23	1:I:491:ILE:HD12	2.00	0.42
1:I:2247:GLN:O	1:I:2279:SER:OG	2.37	0.42
1:G:1718:ILE:HG13	1:G:1719:HIS:CD2	2.53	0.42
1:G:1848:LEU:HD22	1:G:1853:ILE:HG13	2.01	0.42
1:G:2517:UNK:O	1:G:2521:UNK:N	2.52	0.42
1:G:2869:ARG:HH12	1:G:2945:UNK:C	2.31	0.42
1:B:349:GLN:HE21	1:B:354:GLY:HA2	1.84	0.42
1:B:1854:PHE:HD1	1:B:1858:ASP:HB3	1.83	0.42
1:B:2021:CYS:HA	1:B:2022:PRO:HD3	1.93	0.42
1:E:23:GLN:HE21	1:E:34:LYS:HB3	1.84	0.42
1:E:349:GLN:HE21	1:E:354:GLY:HA2	1.84	0.42
1:E:615:ARG:NH1	1:E:1677:GLY:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1848:LEU:HD22	1:E:1853:ILE:HG13	2.01	0.42
1:I:23:GLN:HE21	1:I:34:LYS:HB3	1.84	0.42
1:I:983:THR:O	1:I:987:ARG:N	2.47	0.42
1:I:3829:PHE:HA	1:I:3832:ILE:HD12	2.00	0.42
1:I:4069:LYS:HD2	1:I:4133:GLN:HG3	2.00	0.42
1:G:663:TYR:HB2	1:G:808:TYR:HB3	2.01	0.42
1:G:4229:GLU:HA	1:G:4232:GLU:HB3	2.01	0.42
1:B:21:VAL:HG12	1:B:66:CYS:HA	2.00	0.42
1:B:4229:GLU:HA	1:B:4232:GLU:HB3	2.02	0.42
1:E:1863:LEU:HB3	1:E:1870:VAL:HG11	2.01	0.42
1:E:3754:GLU:HA	1:E:3757:GLU:HG2	2.01	0.42
1:I:627:PRO:HB2	2:J:92:PRO:HD3	2.00	0.42
1:I:750:LEU:HD21	1:I:777:PHE:HE2	1.83	0.42
1:I:1516:UNK:N	1:I:1529:UNK:O	2.52	0.42
1:I:1668:ARG:HA	1:I:1671:ARG:HH11	1.84	0.42
1:I:1838:PHE:HB3	1:I:1842:LEU:HD11	2.02	0.42
1:I:1848:LEU:HD22	1:I:1853:ILE:HG13	2.01	0.42
1:I:1952:GLN:HA	1:I:1955:VAL:HG12	2.01	0.42
1:I:4229:GLU:HA	1:I:4232:GLU:HB3	2.01	0.42
1:B:379:HIS:CD2	1:B:381:GLU:H	2.38	0.42
1:B:635:THR:HB	1:B:1639:LEU:HD23	2.02	0.42
1:B:1685:LEU:HD22	1:B:1718:ILE:HD13	2.01	0.42
1:B:1841:VAL:HA	1:B:1844:LEU:HB3	2.01	0.42
1:B:3889:GLN:HE22	1:B:3963:ASN:HB3	1.84	0.42
1:E:247:TYR:HB2	1:E:374:LYS:HB2	2.02	0.42
1:E:1841:VAL:HA	1:E:1844:LEU:HB3	2.01	0.42
1:E:2286:LEU:HA	1:E:2289:ALA:HB3	2.01	0.42
1:E:3829:PHE:HA	1:E:3832:ILE:HD12	2.00	0.42
1:I:1269:CYS:HA	1:I:1473:UNK:HA	2.01	0.42
1:I:2517:UNK:O	1:I:2521:UNK:N	2.52	0.42
1:I:3889:GLN:HE22	1:I:3963:ASN:HB3	1.84	0.42
1:G:232:THR:HB	1:G:252:VAL:HG11	2.01	0.42
1:G:1778:SER:N	1:G:1799:SER:O	2.52	0.42
1:G:2247:GLN:O	1:G:2279:SER:OG	2.37	0.42
1:G:3927:GLN:O	1:G:3931:SER:N	2.49	0.42
1:G:4671:PHE:HE1	1:G:4715:TYR:HA	1.84	0.42
1:G:4822:THR:O	1:G:4825:THR:OG1	2.30	0.42
1:G:5012:LYS:O	1:G:5016:GLU:N	2.49	0.42
2:A:90:VAL:HG12	2:A:91:ILE:HG12	2.00	0.42
2:H:90:VAL:HG12	2:H:91:ILE:HG12	2.00	0.42
1:B:621:ILE:O	1:B:625:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1099:GLU:OE2	1:B:1127:HIS:ND1	2.40	0.42
1:B:1668:ARG:HA	1:B:1671:ARG:HH11	1.84	0.42
1:B:1778:SER:N	1:B:1799:SER:O	2.52	0.42
1:B:1952:GLN:HA	1:B:1955:VAL:HG12	2.01	0.42
1:B:2247:GLN:O	1:B:2279:SER:OG	2.37	0.42
1:E:110:ARG:HA	1:E:117:TYR:HA	2.01	0.42
1:E:932:LEU:HD23	1:E:935:LEU:HD12	2.02	0.42
1:E:1668:ARG:HA	1:E:1671:ARG:HH11	1.84	0.42
1:E:1778:SER:N	1:E:1799:SER:O	2.52	0.42
1:E:1796:ALA:HB1	1:E:1797:ARG:HH21	1.85	0.42
1:I:668:VAL:HG22	1:I:789:VAL:HG23	2.01	0.42
1:I:4176:PRO:O	1:I:4202:ARG:NH2	2.52	0.42
1:G:1090:PHE:HD2	1:G:1202:LEU:HD11	1.83	0.42
1:B:23:GLN:HE21	1:B:34:LYS:HB3	1.85	0.42
1:B:488:LEU:HD23	1:B:491:ILE:HD12	2.00	0.42
1:B:1848:LEU:HD22	1:B:1853:ILE:HG13	2.01	0.42
1:B:2121:PHE:O	1:B:3725:TYR:OH	2.35	0.42
1:E:283:ARG:NH2	1:E:402:ARG:HH12	2.17	0.42
1:E:299:LEU:HD13	1:E:378:LEU:HG	2.02	0.42
1:E:379:HIS:CD2	1:E:381:GLU:H	2.38	0.42
1:E:2121:PHE:O	1:E:3725:TYR:OH	2.35	0.42
1:E:2517:UNK:O	1:E:2521:UNK:N	2.53	0.42
1:E:4571:PHE:O	1:E:4575:PHE:N	2.47	0.42
1:E:4823:LEU:HD13	1:E:4826:ILE:HD12	2.01	0.42
1:E:4942:GLU:O	1:E:4946:GLN:N	2.45	0.42
1:I:2318:TYR:OH	1:I:2414:ASN:N	2.52	0.42
1:G:20:VAL:HA	1:G:205:ILE:H	1.85	0.42
1:G:932:LEU:HD23	1:G:935:LEU:HD12	2.02	0.42
1:G:1668:ARG:HA	1:G:1671:ARG:HH11	1.84	0.42
1:G:3829:PHE:HA	1:G:3832:ILE:HD12	2.00	0.42
1:B:283:ARG:NH2	1:B:402:ARG:HH12	2.17	0.42
1:B:1838:PHE:HB3	1:B:1842:LEU:HD11	2.02	0.42
1:B:2235:PHE:HA	1:B:2238:TYR:HD2	1.84	0.42
1:B:4702:ASP:HA	1:B:4778:TRP:HE1	1.84	0.42
1:B:4822:THR:O	1:B:4825:THR:OG1	2.30	0.42
1:E:45:ARG:HG2	1:E:443:LEU:HD21	2.00	0.42
1:E:1685:LEU:HD22	1:E:1718:ILE:HD13	2.01	0.42
1:E:2751:LEU:HD11	1:E:2823:ILE:HG21	2.01	0.42
1:E:4229:GLU:HA	1:E:4232:GLU:HB3	2.02	0.42
1:I:110:ARG:HA	1:I:117:TYR:HA	2.01	0.42
1:I:247:TYR:HB2	1:I:374:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:299:LEU:HD13	1:I:378:LEU:HG	2.02	0.42
1:I:4104:THR:HG22	1:I:4106:PRO:HD2	2.01	0.42
1:G:173:SER:OG	1:G:174:VAL:N	2.53	0.42
1:G:4705:VAL:HB	1:G:4778:TRP:CG	2.55	0.42
1:B:45:ARG:HG2	1:B:443:LEU:HD21	2.00	0.42
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.51	0.42
1:B:2286:LEU:HA	1:B:2289:ALA:HB3	2.01	0.42
1:B:3754:GLU:HA	1:B:3757:GLU:HG2	2.01	0.42
1:E:20:VAL:HA	1:E:205:ILE:H	1.85	0.42
1:E:2247:GLN:O	1:E:2279:SER:OG	2.37	0.42
1:E:4736:ARG:O	1:E:4740:LEU:N	2.51	0.42
1:I:232:THR:HB	1:I:252:VAL:HG11	2.01	0.42
1:I:1863:LEU:HB3	1:I:1870:VAL:HG11	2.01	0.42
1:I:3713:LYS:HG2	1:I:3715:LYS:H	1.84	0.42
1:I:4049:VAL:HG21	1:I:4159:ARG:HD2	2.01	0.42
1:I:5012:LYS:O	1:I:5016:GLU:N	2.49	0.42
1:G:23:GLN:HE21	1:G:34:LYS:HB3	1.84	0.42
1:G:247:TYR:HB2	1:G:374:LYS:HB2	2.02	0.42
1:B:173:SER:OG	1:B:174:VAL:N	2.53	0.42
1:B:3713:LYS:HG2	1:B:3715:LYS:H	1.84	0.42
1:I:211:GLU:OE2	1:I:3907:THR:OG1	2.38	0.42
1:I:1778:SER:N	1:I:1799:SER:O	2.52	0.42
1:I:2235:PHE:HA	1:I:2238:TYR:HD2	1.85	0.42
1:G:45:ARG:HG2	1:G:443:LEU:HD21	2.00	0.42
1:G:110:ARG:HA	1:G:117:TYR:HA	2.01	0.42
1:G:299:LEU:HD13	1:G:378:LEU:HG	2.02	0.42
1:G:635:THR:HB	1:G:1639:LEU:HD23	2.02	0.42
1:G:1838:PHE:HB3	1:G:1842:LEU:HD11	2.02	0.42
1:G:4049:VAL:HG21	1:G:4159:ARG:HD2	2.01	0.42
1:G:4863:TYR:HA	1:G:4901:ILE:HG23	2.02	0.42
1:G:4987:ASN:OD1	1:G:4987:ASN:N	2.53	0.42
1:B:1663:HIS:O	1:B:1667:LEU:N	2.51	0.42
1:B:1796:ALA:HB1	1:B:1797:ARG:HH21	1.85	0.42
1:B:2871:LEU:HD22	1:B:2927:LEU:HD22	2.02	0.42
1:B:4823:LEU:HD13	1:B:4826:ILE:HD12	2.01	0.42
1:E:173:SER:OG	1:E:174:VAL:N	2.53	0.42
1:E:3646:THR:O	1:E:3650:CYS:N	2.49	0.42
1:I:629:ARG:NH2	2:J:89:GLY:O	2.53	0.42
1:I:793:LEU:HG	1:I:1625:GLY:HA2	2.02	0.42
1:I:1685:LEU:HD22	1:I:1718:ILE:HD13	2.01	0.42
1:I:4863:TYR:HA	1:I:4901:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1679:ASN:O	1:G:1683:HIS:ND1	2.37	0.42
1:B:247:TYR:HB2	1:B:374:LYS:HB2	2.02	0.41
1:B:2751:LEU:HD11	1:B:2823:ILE:HG21	2.01	0.41
1:E:467:LYS:O	1:E:471:LEU:N	2.53	0.41
1:E:2272:PRO:HA	1:E:2275:VAL:HG12	2.02	0.41
1:E:4961:CYS:HB3	1:E:4983:HIS:HE1	1.85	0.41
1:I:467:LYS:O	1:I:471:LEU:N	2.53	0.41
1:I:1687:SER:OG	2:J:90:VAL:HG22	2.20	0.41
1:G:379:HIS:CD2	1:G:381:GLU:H	2.38	0.41
1:G:707:VAL:HG23	1:G:713:SER:HB2	2.02	0.41
1:G:4176:PRO:O	1:G:4202:ARG:NH2	2.53	0.41
1:B:233:ILE:HD12	1:B:242:ARG:HB3	2.02	0.41
1:B:793:LEU:HD12	1:B:797:HIS:HB2	2.02	0.41
1:B:2517:UNK:O	1:B:2521:UNK:N	2.53	0.41
1:B:2869:ARG:HH12	1:B:2945:UNK:C	2.33	0.41
1:B:4176:PRO:O	1:B:4202:ARG:NH2	2.52	0.41
1:E:233:ILE:HD12	1:E:242:ARG:HB3	2.02	0.41
1:E:635:THR:HB	1:E:1639:LEU:HD23	2.01	0.41
1:E:793:LEU:HD12	1:E:797:HIS:HB2	2.02	0.41
1:E:1154:ASP:O	1:E:1158:ASN:N	2.53	0.41
1:E:2235:PHE:HA	1:E:2238:TYR:HD2	1.84	0.41
1:E:3779:VAL:HG23	1:E:3780:LEU:HD12	2.02	0.41
1:E:4176:PRO:O	1:E:4202:ARG:NH2	2.53	0.41
1:E:4702:ASP:HA	1:E:4778:TRP:HE1	1.84	0.41
1:I:233:ILE:HD12	1:I:242:ARG:HB3	2.02	0.41
1:I:793:LEU:HD12	1:I:797:HIS:HB2	2.02	0.41
1:I:2286:LEU:HA	1:I:2289:ALA:HB3	2.01	0.41
1:I:3754:GLU:HA	1:I:3757:GLU:HG2	2.01	0.41
1:I:4987:ASN:OD1	1:I:4987:ASN:N	2.53	0.41
1:G:463:GLU:O	1:G:466:SER:OG	2.31	0.41
1:G:500:ALA:HA	1:G:503:PHE:HB3	2.02	0.41
1:G:793:LEU:HD12	1:G:797:HIS:HB2	2.02	0.41
1:G:876:GLU:O	1:G:880:GLU:N	2.51	0.41
1:G:1841:VAL:HA	1:G:1844:LEU:HB3	2.01	0.41
2:F:55:VAL:HG23	2:F:60:GLU:HB2	2.02	0.41
1:B:33:LEU:HD12	1:B:53:SER:HB2	2.03	0.41
1:B:4705:VAL:HB	1:B:4778:TRP:CG	2.55	0.41
1:B:4987:ASN:OD1	1:B:4987:ASN:N	2.53	0.41
1:E:4044:MET:HA	1:E:4047:MET:HG2	2.03	0.41
1:E:4705:VAL:HB	1:E:4778:TRP:CG	2.55	0.41
1:E:4863:TYR:HA	1:E:4901:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:SER:OG	1:I:174:VAL:N	2.53	0.41
1:I:932:LEU:HD23	1:I:935:LEU:HD12	2.01	0.41
1:I:2871:LEU:HD22	1:I:2927:LEU:HD22	2.02	0.41
1:I:4823:LEU:HD13	1:I:4826:ILE:HD12	2.01	0.41
1:G:414:PHE:HE1	1:G:436:LEU:HB3	1.86	0.41
1:G:668:VAL:HG22	1:G:789:VAL:HG23	2.01	0.41
1:G:731:THR:OG1	1:G:1520:UNK:O	2.38	0.41
1:G:1796:ALA:HB1	1:G:1797:ARG:HH21	1.85	0.41
1:G:2297:LYS:O	1:G:2301:TYR:N	2.51	0.41
1:G:2318:TYR:OH	1:G:2414:ASN:N	2.52	0.41
1:G:2751:LEU:HD11	1:G:2823:ILE:HG21	2.01	0.41
1:G:4736:ARG:O	1:G:4740:LEU:N	2.51	0.41
1:B:299:LEU:HD13	1:B:378:LEU:HG	2.02	0.41
1:B:663:TYR:HB2	1:B:808:TYR:HB3	2.00	0.41
1:B:4044:MET:HA	1:B:4047:MET:HG2	2.03	0.41
1:E:243:ARG:HA	1:E:301:VAL:HB	2.02	0.41
1:E:668:VAL:HG22	1:E:789:VAL:HG23	2.01	0.41
1:E:4987:ASN:OD1	1:E:4987:ASN:N	2.53	0.41
1:I:500:ALA:HA	1:I:503:PHE:HB3	2.02	0.41
1:I:870:ILE:HD12	1:I:870:ILE:HA	1.88	0.41
1:I:1931:LEU:HD22	1:I:1935:VAL:HG11	2.03	0.41
1:I:2430:ILE:HG21	1:I:2502:UNK:HA	2.02	0.41
1:I:4961:CYS:HB3	1:I:4983:HIS:HE1	1.85	0.41
1:G:410:LEU:HD21	1:G:441:VAL:HA	2.03	0.41
1:G:2286:LEU:HA	1:G:2289:ALA:HB3	2.01	0.41
1:G:4044:MET:HA	1:G:4047:MET:HG2	2.03	0.41
1:B:467:LYS:O	1:B:471:LEU:N	2.53	0.41
1:B:1931:LEU:HD22	1:B:1935:VAL:HG11	2.03	0.41
1:B:2104:ARG:HA	1:B:2107:GLN:HB3	2.03	0.41
1:B:3779:VAL:HG23	1:B:3780:LEU:HD12	2.02	0.41
1:B:4184:MET:HE1	1:B:4188:ARG:HA	2.03	0.41
1:E:533:ASN:ND2	1:E:536:ASN:OD1	2.47	0.41
1:E:876:GLU:O	1:E:880:GLU:N	2.51	0.41
1:E:2297:LYS:O	1:E:2301:TYR:N	2.51	0.41
1:E:4105:GLY:HA2	1:E:4108:ILE:HD12	2.02	0.41
1:I:379:HIS:CD2	1:I:381:GLU:H	2.38	0.41
1:I:707:VAL:HG23	1:I:713:SER:HB2	2.02	0.41
1:I:1796:ALA:HB1	1:I:1797:ARG:HH21	1.85	0.41
1:G:211:GLU:OE2	1:G:3907:THR:OG1	2.38	0.41
1:G:1685:LEU:HD22	1:G:1718:ILE:HD13	2.01	0.41
1:G:2104:ARG:HA	1:G:2107:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4823:LEU:HD13	1:G:4826:ILE:HD12	2.01	0.41
2:A:55:VAL:HG23	2:A:60:GLU:HB2	2.02	0.41
1:B:20:VAL:HA	1:B:205:ILE:H	1.85	0.41
1:B:668:VAL:HG22	1:B:789:VAL:HG23	2.01	0.41
1:B:1936:LYS:O	1:B:1940:CYS:N	2.45	0.41
1:B:4568:PHE:HA	1:B:4571:PHE:HD2	1.86	0.41
1:E:211:GLU:OE2	1:E:3907:THR:OG1	2.38	0.41
1:E:711:LEU:HD13	1:E:1513:UNK:HA	2.02	0.41
1:I:243:ARG:HA	1:I:301:VAL:HB	2.02	0.41
1:I:3832:ILE:O	1:I:3836:MET:N	2.47	0.41
1:G:1099:GLU:OE2	1:G:1127:HIS:ND1	2.40	0.41
1:G:1235:THR:OG1	1:G:1607:ARG:NE	2.54	0.41
1:G:2272:PRO:HA	1:G:2275:VAL:HG12	2.02	0.41
1:G:4568:PHE:HA	1:G:4571:PHE:HD2	1.86	0.41
1:G:4833:ASN:ND2	1:G:4935:LEU:O	2.54	0.41
1:B:181:HIS:ND1	1:B:195:PHE:HB2	2.36	0.41
1:B:243:ARG:HA	1:B:301:VAL:HB	2.02	0.41
1:B:932:LEU:HD23	1:B:935:LEU:HD12	2.01	0.41
1:B:4863:TYR:HA	1:B:4901:ILE:HG23	2.02	0.41
1:E:257:ARG:O	1:E:284:HIS:NE2	2.44	0.41
1:E:793:LEU:HG	1:E:1625:GLY:HA2	2.02	0.41
1:E:1838:PHE:HB3	1:E:1842:LEU:HD11	2.02	0.41
1:E:2104:ARG:HA	1:E:2107:GLN:HB3	2.03	0.41
1:E:3915:ILE:H	1:E:3915:ILE:HG13	1.71	0.41
1:I:33:LEU:HD12	1:I:53:SER:HB2	2.03	0.41
1:G:1663:HIS:O	1:G:1667:LEU:N	2.50	0.41
1:G:3552:UNK:O	1:G:3556:UNK:N	2.54	0.41
1:G:3754:GLU:HA	1:G:3757:GLU:HG2	2.01	0.41
1:G:4961:CYS:HB3	1:G:4983:HIS:HE1	1.85	0.41
1:B:500:ALA:HA	1:B:503:PHE:HB3	2.02	0.41
1:E:153:ALA:HA	1:E:170:ILE:HG12	2.03	0.41
1:E:181:HIS:ND1	1:E:195:PHE:HB2	2.36	0.41
1:E:621:ILE:O	1:E:625:LEU:N	2.53	0.41
1:I:4044:MET:HA	1:I:4047:MET:HG2	2.03	0.41
1:G:233:ILE:HD12	1:G:242:ARG:HB3	2.02	0.41
1:G:533:ASN:ND2	1:G:536:ASN:OD1	2.47	0.41
1:G:2235:PHE:HA	1:G:2238:TYR:HD2	1.85	0.41
2:H:55:VAL:HG23	2:H:60:GLU:HB2	2.02	0.41
1:B:153:ALA:HA	1:B:170:ILE:HG12	2.03	0.41
1:B:211:GLU:OE2	1:B:3907:THR:OG1	2.38	0.41
1:B:793:LEU:HG	1:B:1625:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1235:THR:OG1	1:B:1607:ARG:NE	2.54	0.41
1:B:1284:UNK:HA	1:B:1463:UNK:HA	2.03	0.41
1:B:3994:HIS:O	1:B:3998:HIS:ND1	2.45	0.41
1:B:4961:CYS:HB3	1:B:4983:HIS:HE1	1.84	0.41
1:E:414:PHE:HE1	1:E:436:LEU:HB3	1.86	0.41
1:E:2788:HIS:CE1	1:E:2790:MET:HB2	2.56	0.41
1:E:2871:LEU:HD22	1:E:2927:LEU:HD22	2.02	0.41
1:E:3992:PHE:O	1:E:3996:PHE:N	2.43	0.41
1:I:533:ASN:ND2	1:I:536:ASN:OD1	2.48	0.41
1:I:3552:UNK:O	1:I:3556:UNK:N	2.54	0.41
1:I:4147:LEU:O	1:I:4151:SER:OG	2.32	0.41
1:G:1730:MET:O	1:G:1772:ARG:NH1	2.51	0.41
1:G:2871:LEU:HD22	1:G:2927:LEU:HD22	2.02	0.41
1:G:3994:HIS:O	1:G:3998:HIS:ND1	2.45	0.41
1:G:4208:PRO:HA	1:G:4211:LYS:HB3	2.03	0.41
2:F:23:VAL:HB	2:F:105:ASN:HA	2.03	0.41
2:A:23:VAL:HB	2:A:105:ASN:HA	2.03	0.41
2:H:83:GLY:HA2	2:H:94:ASN:H	1.86	0.41
2:J:83:GLY:HA2	2:J:94:ASN:H	1.86	0.41
1:B:707:VAL:HG23	1:B:713:SER:HB2	2.02	0.41
1:B:2788:HIS:CE1	1:B:2790:MET:HB2	2.56	0.41
1:B:4860:ARG:HD2	1:E:4582:VAL:HG11	2.03	0.41
1:E:410:LEU:HD21	1:E:441:VAL:HA	2.03	0.41
1:E:3552:UNK:O	1:E:3556:UNK:N	2.54	0.41
1:I:410:LEU:HD21	1:I:441:VAL:HA	2.03	0.41
1:I:550:LYS:HD3	1:I:550:LYS:HA	1.91	0.41
1:I:3779:VAL:HG23	1:I:3780:LEU:HD12	2.02	0.41
1:I:4105:GLY:HA2	1:I:4108:ILE:HD12	2.02	0.41
1:I:4705:VAL:HB	1:I:4778:TRP:CG	2.55	0.41
1:G:181:HIS:ND1	1:G:195:PHE:HB2	2.36	0.41
1:G:2287:ALA:HA	1:G:2290:LEU:HD13	2.03	0.41
1:G:4105:GLY:HA2	1:G:4108:ILE:HD12	2.02	0.41
1:G:4782:VAL:O	1:G:4785:THR:OG1	2.29	0.41
1:B:18:ASP:HB2	1:B:69:LEU:HD12	2.03	0.40
1:B:414:PHE:HE1	1:B:436:LEU:HB3	1.86	0.40
1:B:4208:PRO:HA	1:B:4211:LYS:HB3	2.03	0.40
1:E:33:LEU:HD12	1:E:53:SER:HB2	2.03	0.40
1:E:157:ARG:HH21	1:E:164:ARG:HD2	1.86	0.40
1:E:3994:HIS:O	1:E:3998:HIS:ND1	2.45	0.40
1:I:18:ASP:HB2	1:I:69:LEU:HD12	2.03	0.40
1:I:736:HIS:HB2	2:J:7:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1235:THR:OG1	1:I:1607:ARG:NE	2.54	0.40
1:I:2104:ARG:HA	1:I:2107:GLN:HB3	2.03	0.40
1:I:4055:VAL:O	1:I:4059:LEU:N	2.54	0.40
1:I:4961:CYS:HB2	1:I:4963:ILE:HD12	2.03	0.40
1:G:157:ARG:HH21	1:G:164:ARG:HD2	1.86	0.40
1:G:793:LEU:HG	1:G:1625:GLY:HA2	2.02	0.40
1:G:2788:HIS:CE1	1:G:2790:MET:HB2	2.56	0.40
1:G:4561:THR:O	1:G:4565:LEU:N	2.54	0.40
1:B:2039:LEU:HA	1:B:2042:CYS:HB3	2.04	0.40
1:B:2272:PRO:HA	1:B:2275:VAL:HG12	2.02	0.40
1:B:3552:UNK:O	1:B:3556:UNK:N	2.54	0.40
1:B:4105:GLY:HA2	1:B:4108:ILE:HD12	2.02	0.40
1:B:4736:ARG:O	1:B:4740:LEU:N	2.51	0.40
1:I:711:LEU:HD13	1:I:1513:UNK:HA	2.02	0.40
1:I:1154:ASP:O	1:I:1158:ASN:N	2.53	0.40
1:I:4208:PRO:HA	1:I:4211:LYS:HB3	2.04	0.40
1:G:1154:ASP:O	1:G:1158:ASN:N	2.53	0.40
1:G:3694:LYS:HA	1:G:3695:PRO:HD3	1.96	0.40
1:G:3779:VAL:HG23	1:G:3780:LEU:HD12	2.02	0.40
2:A:83:GLY:HA2	2:A:94:ASN:H	1.86	0.40
1:B:1092:PHE:N	1:B:1149:VAL:O	2.38	0.40
1:E:71:GLN:O	1:E:108:LEU:N	2.54	0.40
1:I:20:VAL:HA	1:I:205:ILE:H	1.85	0.40
1:I:181:HIS:ND1	1:I:195:PHE:HB2	2.36	0.40
1:I:635:THR:HB	1:I:1639:LEU:HD23	2.01	0.40
1:I:2297:LYS:O	1:I:2301:TYR:N	2.51	0.40
1:G:467:LYS:O	1:G:471:LEU:N	2.53	0.40
1:G:1931:LEU:HD22	1:G:1935:VAL:HG11	2.03	0.40
1:G:2039:LEU:HA	1:G:2042:CYS:HB3	2.03	0.40
1:G:4961:CYS:HB2	1:G:4963:ILE:HD12	2.03	0.40
1:B:157:ARG:HH21	1:B:164:ARG:HD2	1.86	0.40
1:B:1497:UNK:HA	1:B:1535:UNK:HA	2.03	0.40
1:B:4961:CYS:HB2	1:B:4963:ILE:HD12	2.03	0.40
1:E:4208:PRO:HA	1:E:4211:LYS:HB3	2.03	0.40
1:E:4958:CYS:SG	1:E:4959:PHE:N	2.95	0.40
1:I:1970:GLN:HA	1:I:3641:LEU:HG	2.03	0.40
1:I:2212:VAL:O	1:I:2216:GLY:N	2.51	0.40
1:I:4833:ASN:ND2	1:I:4935:LEU:O	2.54	0.40
1:G:1970:GLN:HA	1:G:3641:LEU:HG	2.04	0.40
1:G:2212:VAL:O	1:G:2216:GLY:N	2.51	0.40
1:G:3362:UNK:O	1:G:3366:UNK:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:HIS:N	1:B:116:MET:O	2.44	0.40
1:B:410:LEU:HD21	1:B:441:VAL:HA	2.03	0.40
1:B:2287:ALA:HA	1:B:2290:LEU:HD13	2.04	0.40
1:E:25:SER:HA	1:E:34:LYS:HA	2.04	0.40
1:E:500:ALA:HA	1:E:503:PHE:HB3	2.02	0.40
1:E:3663:LEU:H	1:E:3663:LEU:HG	1.64	0.40
1:E:4183:ILE:O	1:E:4191:GLU:N	2.38	0.40
1:E:4833:ASN:ND2	1:E:4935:LEU:O	2.54	0.40
1:I:71:GLN:O	1:I:108:LEU:N	2.54	0.40
1:I:153:ALA:HA	1:I:170:ILE:HG12	2.03	0.40
1:I:3663:LEU:H	1:I:3663:LEU:HG	1.64	0.40
1:G:621:ILE:O	1:G:625:LEU:N	2.53	0.40
2:J:23:VAL:HB	2:J:105:ASN:HA	2.03	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	B	3235/4687 (69%)	2897 (90%)	334 (10%)	4 (0%)	51	85
1	E	3235/4687 (69%)	2895 (90%)	336 (10%)	4 (0%)	51	85
1	G	3235/4687 (69%)	2896 (90%)	335 (10%)	4 (0%)	51	85
1	I	3235/4687 (69%)	2895 (90%)	336 (10%)	4 (0%)	51	85
2	A	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	J	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
All	All	13360/19176 (70%)	11963 (90%)	1381 (10%)	16 (0%)	54	85

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1708	ARG
1	E	1708	ARG
1	I	1708	ARG
1	G	1708	ARG
1	B	1932	PRO
1	E	1932	PRO
1	I	1932	PRO
1	G	1932	PRO
1	B	1840	PRO
1	B	4667	PRO
1	E	1840	PRO
1	E	4667	PRO
1	I	1840	PRO
1	I	4667	PRO
1	G	1840	PRO
1	G	4667	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
1	E	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
1	G	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
1	I	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
2	A	88/88 (100%)	88 (100%)	0	100	100
2	F	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
2	J	88/88 (100%)	88 (100%)	0	100	100
All	All	10324/13188 (78%)	10244 (99%)	80 (1%)	82	89

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	534	ARG
1	B	553	ARG
1	B	978	THR
1	B	1076	ARG
1	B	1141	ARG
1	B	1964	ARG
1	B	3663	LEU
1	B	3770	LEU
1	B	3787	LYS
1	B	3805	LEU
1	B	3896	ASN
1	B	4034	ASN
1	B	4063	ASP
1	B	4085	ARG
1	B	4120	ASN
1	B	4137	ARG
1	B	4175	ARG
1	B	4189	ARG
1	B	4821	LYS
1	B	4985	LEU
1	E	534	ARG
1	E	553	ARG
1	E	978	THR
1	E	1076	ARG
1	E	1141	ARG
1	E	1964	ARG
1	E	3663	LEU
1	E	3770	LEU
1	E	3787	LYS
1	E	3805	LEU
1	E	3896	ASN
1	E	4034	ASN
1	E	4063	ASP
1	E	4085	ARG
1	E	4120	ASN
1	E	4137	ARG
1	E	4175	ARG
1	E	4189	ARG
1	E	4821	LYS
1	E	4985	LEU
1	I	534	ARG
1	I	553	ARG
1	I	978	THR

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Mol	Chain	Res	Type
1	I	1076	ARG
1	I	1141	ARG
1	I	1964	ARG
1	I	3663	LEU
1	I	3770	LEU
1	I	3787	LYS
1	I	3805	LEU
1	I	3896	ASN
1	I	4034	ASN
1	I	4063	ASP
1	I	4085	ARG
1	I	4120	ASN
1	I	4137	ARG
1	I	4175	ARG
1	I	4189	ARG
1	I	4821	LYS
1	I	4985	LEU
1	G	534	ARG
1	G	553	ARG
1	G	978	THR
1	G	1076	ARG
1	G	1141	ARG
1	G	1964	ARG
1	G	3663	LEU
1	G	3770	LEU
1	G	3787	LYS
1	G	3805	LEU
1	G	3896	ASN
1	G	4034	ASN
1	G	4063	ASP
1	G	4085	ARG
1	G	4120	ASN
1	G	4137	ARG
1	G	4175	ARG
1	G	4189	ARG
1	G	4821	LYS
1	G	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	GLN

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Mol	Chain	Res	Type
1	B	57	ASN
1	B	105	HIS
1	B	111	HIS
1	B	113	HIS
1	B	203	ASN
1	B	273	HIS
1	B	379	HIS
1	B	383	HIS
1	B	395	GLN
1	B	413	GLN
1	B	479	GLN
1	B	838	HIS
1	B	1035	ASN
1	B	1158	ASN
1	B	1598	GLN
1	B	1679	ASN
1	B	1691	GLN
1	B	1719	HIS
1	B	1775	HIS
1	B	1973	GLN
1	B	2005	GLN
1	B	2127	GLN
1	B	3771	HIS
1	B	3889	GLN
1	B	3896	ASN
1	B	3946	GLN
1	B	3950	ASN
1	B	3960	GLN
1	B	3976	ASN
1	B	4120	ASN
1	B	4142	ASN
1	B	4201	ASN
1	B	4553	ASN
1	B	4714	ASN
1	B	4728	HIS
1	B	4933	GLN
1	E	23	GLN
1	E	57	ASN
1	E	105	HIS
1	E	111	HIS
1	E	113	HIS
1	E	203	ASN

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Mol	Chain	Res	Type
1	E	273	HIS
1	E	379	HIS
1	E	383	HIS
1	E	395	GLN
1	E	413	GLN
1	E	479	GLN
1	E	797	HIS
1	E	838	HIS
1	E	1035	ASN
1	E	1158	ASN
1	E	1598	GLN
1	E	1679	ASN
1	E	1691	GLN
1	E	1719	HIS
1	E	1775	HIS
1	E	1973	GLN
1	E	2005	GLN
1	E	2127	GLN
1	E	3771	HIS
1	E	3889	GLN
1	E	3896	ASN
1	E	3946	GLN
1	E	3950	ASN
1	E	3960	GLN
1	E	3976	ASN
1	E	4120	ASN
1	E	4142	ASN
1	E	4201	ASN
1	E	4553	ASN
1	E	4714	ASN
1	E	4728	HIS
1	E	4933	GLN
1	I	23	GLN
1	I	57	ASN
1	I	105	HIS
1	I	111	HIS
1	I	113	HIS
1	I	203	ASN
1	I	273	HIS
1	I	379	HIS
1	I	383	HIS
1	I	395	GLN

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Mol	Chain	Res	Type
1	I	413	GLN
1	I	479	GLN
1	I	797	HIS
1	I	838	HIS
1	I	1035	ASN
1	I	1158	ASN
1	I	1598	GLN
1	I	1679	ASN
1	I	1691	GLN
1	I	1719	HIS
1	I	1775	HIS
1	I	1973	GLN
1	I	2005	GLN
1	I	2127	GLN
1	I	3771	HIS
1	I	3889	GLN
1	I	3896	ASN
1	I	3946	GLN
1	I	3950	ASN
1	I	3960	GLN
1	I	3976	ASN
1	I	4120	ASN
1	I	4142	ASN
1	I	4201	ASN
1	I	4553	ASN
1	I	4714	ASN
1	I	4728	HIS
1	I	4933	GLN
1	G	23	GLN
1	G	57	ASN
1	G	105	HIS
1	G	111	HIS
1	G	113	HIS
1	G	203	ASN
1	G	273	HIS
1	G	379	HIS
1	G	383	HIS
1	G	395	GLN
1	G	413	GLN
1	G	479	GLN
1	G	838	HIS
1	G	1035	ASN

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Mol	Chain	Res	Type
1	G	1158	ASN
1	G	1598	GLN
1	G	1679	ASN
1	G	1691	GLN
1	G	1719	HIS
1	G	1775	HIS
1	G	1973	GLN
1	G	2005	GLN
1	G	2127	GLN
1	G	3771	HIS
1	G	3889	GLN
1	G	3896	ASN
1	G	3946	GLN
1	G	3950	ASN
1	G	3960	GLN
1	G	3976	ASN
1	G	4120	ASN
1	G	4142	ASN
1	G	4201	ASN
1	G	4553	ASN
1	G	4714	ASN
1	G	4728	HIS
1	G	4933	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	12
1	I	12
1	E	12
1	B	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	3613:UNK	C	3639:THR	N	45.09
1	I	3613:UNK	C	3639:THR	N	45.04
1	E	3613:UNK	C	3639:THR	N	45.01
1	B	3613:UNK	C	3639:THR	N	44.86
1	G	3163:UNK	C	3170:UNK	N	16.51
1	E	3163:UNK	C	3170:UNK	N	16.50
1	I	3163:UNK	C	3170:UNK	N	16.49
1	B	3163:UNK	C	3170:UNK	N	16.48
1	B	3468:UNK	C	3511:UNK	N	14.92
1	E	3468:UNK	C	3511:UNK	N	14.89
1	I	3468:UNK	C	3511:UNK	N	14.87
1	G	3468:UNK	C	3511:UNK	N	14.84
1	E	3063:UNK	C	3134:UNK	N	14.77
1	B	3063:UNK	C	3134:UNK	N	14.76
1	I	3063:UNK	C	3134:UNK	N	14.74
1	G	3063:UNK	C	3134:UNK	N	14.74
1	G	2703:UNK	C	2734:ASN	N	14.44
1	B	2703:UNK	C	2734:ASN	N	14.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2703:UNK	C	2734:ASN	N	14.36
1	I	2703:UNK	C	2734:ASN	N	14.33
1	B	3236:UNK	C	3241:UNK	N	13.36
1	E	3236:UNK	C	3241:UNK	N	13.36
1	I	3236:UNK	C	3241:UNK	N	13.36
1	G	3236:UNK	C	3241:UNK	N	13.34
1	I	1564:UNK	C	1573:MET	N	12.87
1	G	1564:UNK	C	1573:MET	N	12.87
1	E	1564:UNK	C	1573:MET	N	12.84
1	B	1564:UNK	C	1573:MET	N	12.70
1	G	2976:UNK	C	2995:UNK	N	12.39
1	E	2976:UNK	C	2995:UNK	N	12.38
1	I	2976:UNK	C	2995:UNK	N	12.38
1	B	2976:UNK	C	2995:UNK	N	12.37
1	I	3254:UNK	C	3261:UNK	N	8.68
1	G	3254:UNK	C	3261:UNK	N	8.67
1	B	3254:UNK	C	3261:UNK	N	8.65
1	E	3254:UNK	C	3261:UNK	N	8.65
1	E	1297:UNK	C	1430:UNK	N	5.75
1	I	1297:UNK	C	1430:UNK	N	5.75
1	B	1297:UNK	C	1430:UNK	N	5.71
1	G	1297:UNK	C	1430:UNK	N	5.67
1	I	2939:ARG	C	2942:UNK	N	3.79
1	G	2479:LEU	C	2487:UNK	N	3.78
1	E	2939:ARG	C	2942:UNK	N	3.76
1	G	2939:ARG	C	2942:UNK	N	3.74
1	B	2939:ARG	C	2942:UNK	N	3.64
1	I	2479:LEU	C	2487:UNK	N	3.64
1	B	2479:LEU	C	2487:UNK	N	3.61
1	E	2479:LEU	C	2487:UNK	N	3.60

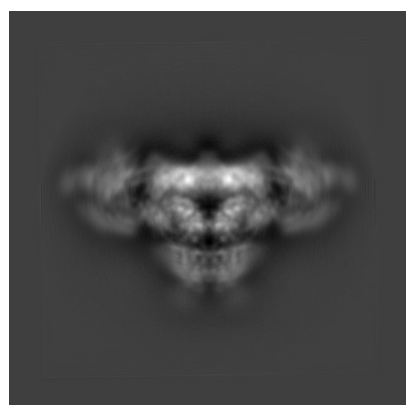
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22393. These allow visual inspection of the internal detail of the map and identification of artifacts.

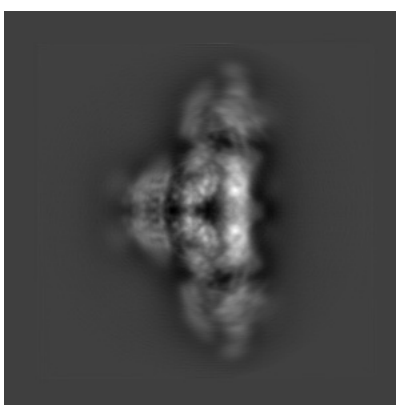
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

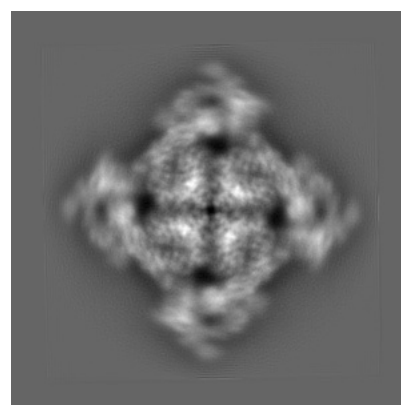
6.1.1 Primary map



X



Y

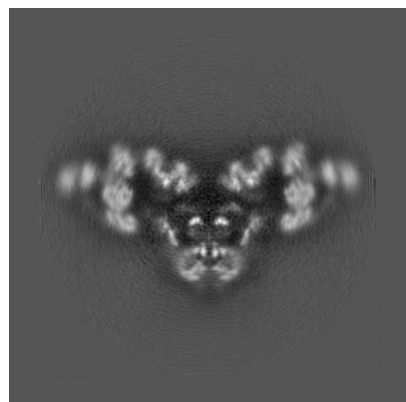


Z

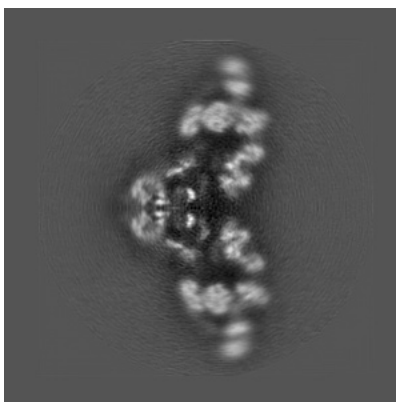
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

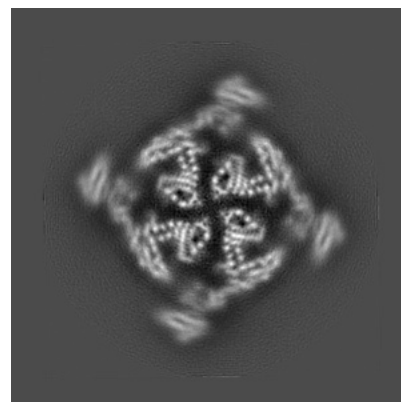
6.2.1 Primary map



X Index: 200



Y Index: 200

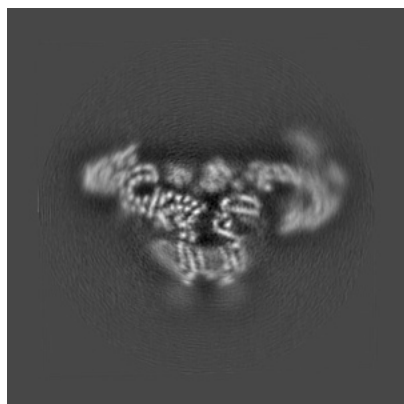


Z Index: 200

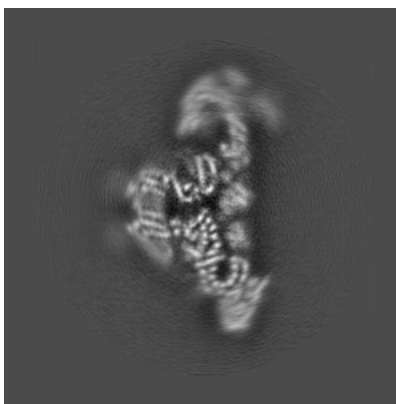
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

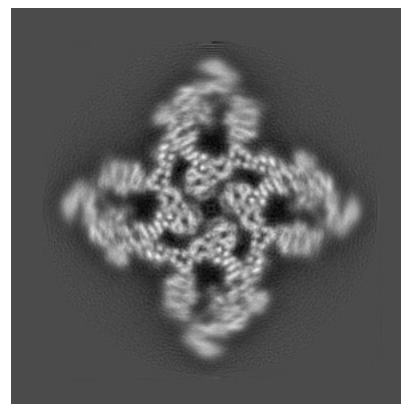
6.3.1 Primary map



X Index: 222



Y Index: 177



Z Index: 230

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

6.4 Orthogonal surface views [i](#)

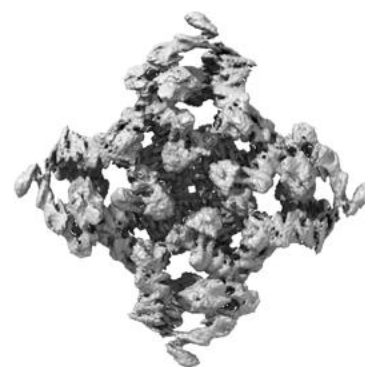
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

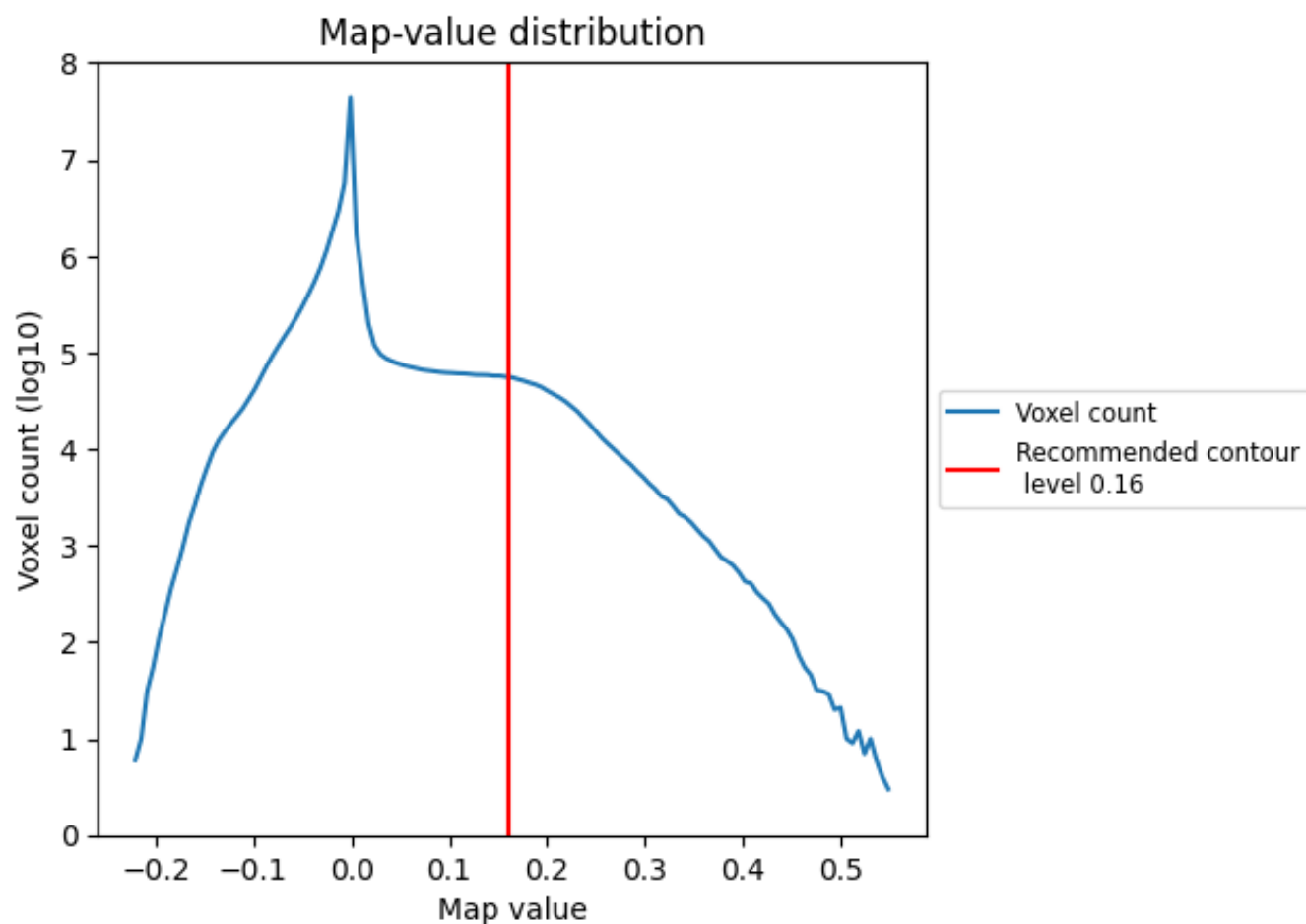
6.5 Mask visualisation

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

7 Map analysis [i](#)

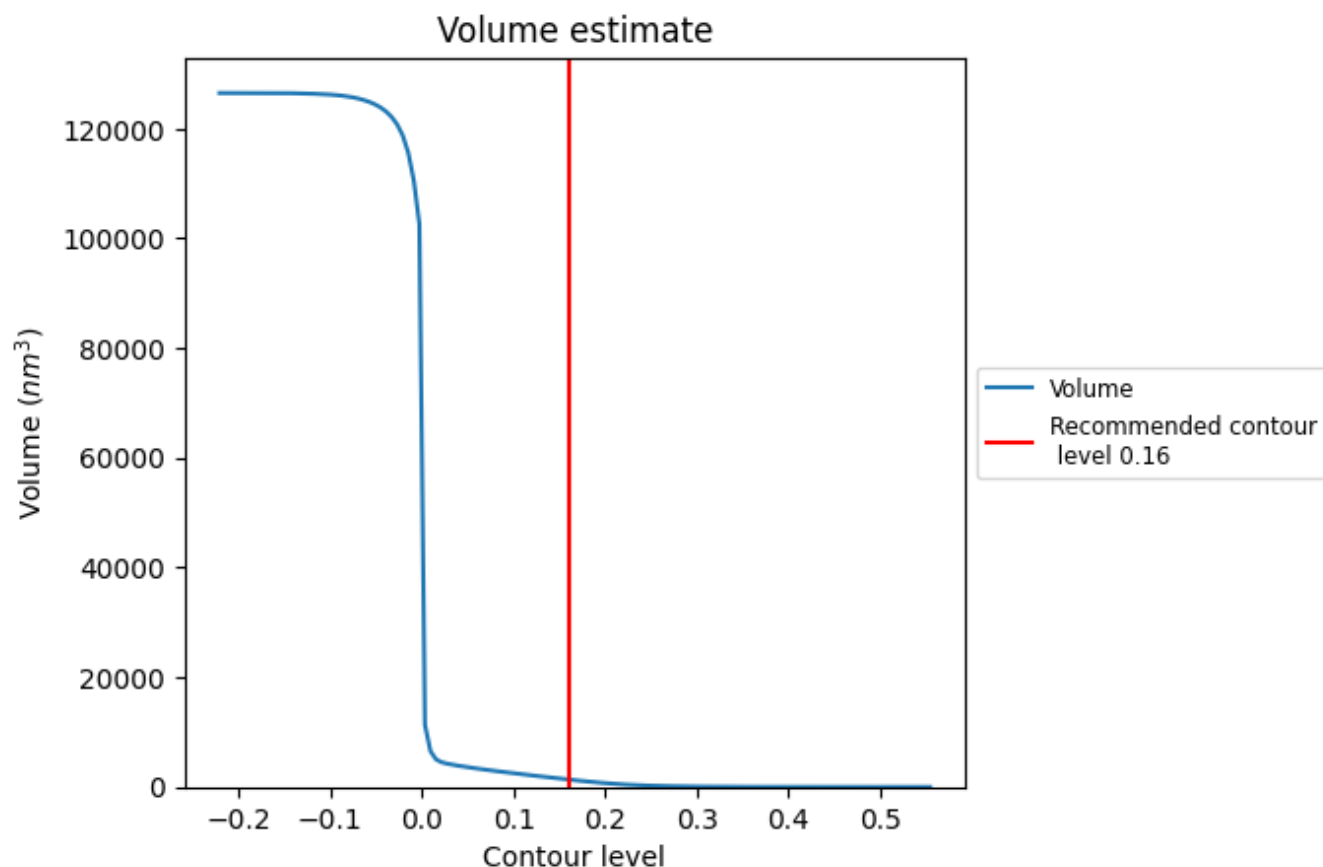
This section contains the results of statistical analysis of the map.

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.

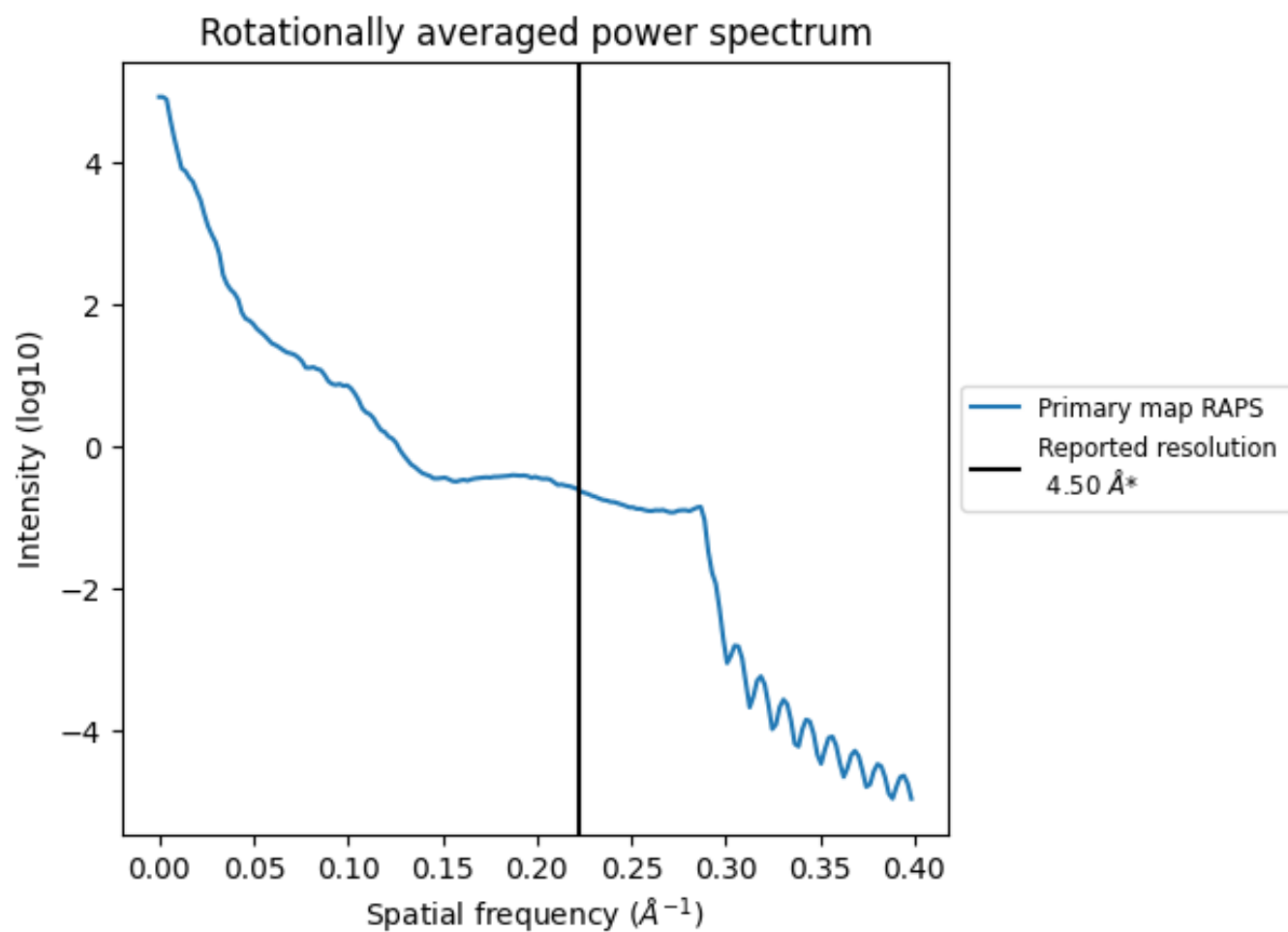
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1358 nm³; this corresponds to an approximate mass of 1227 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 0.222 Å⁻¹

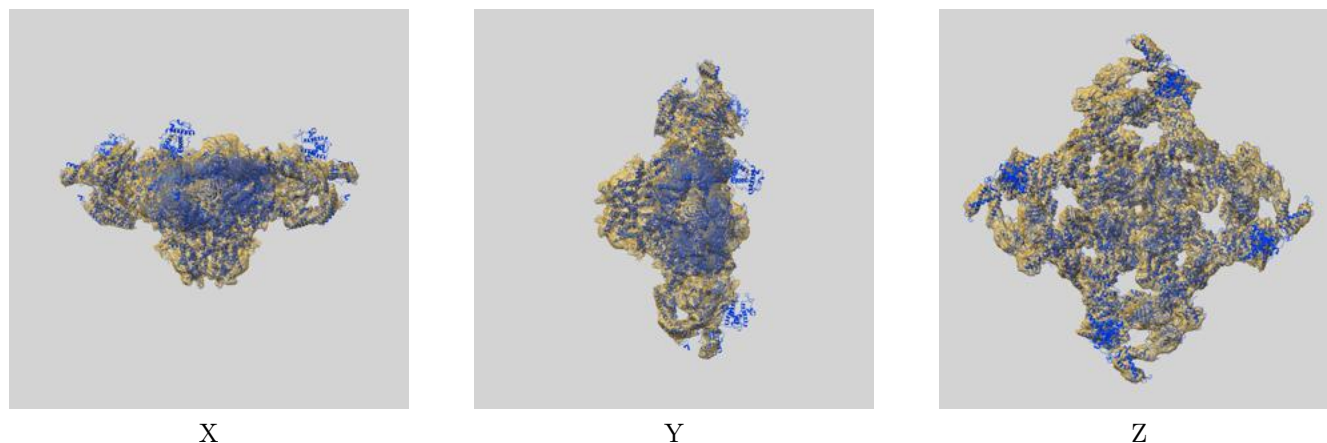
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

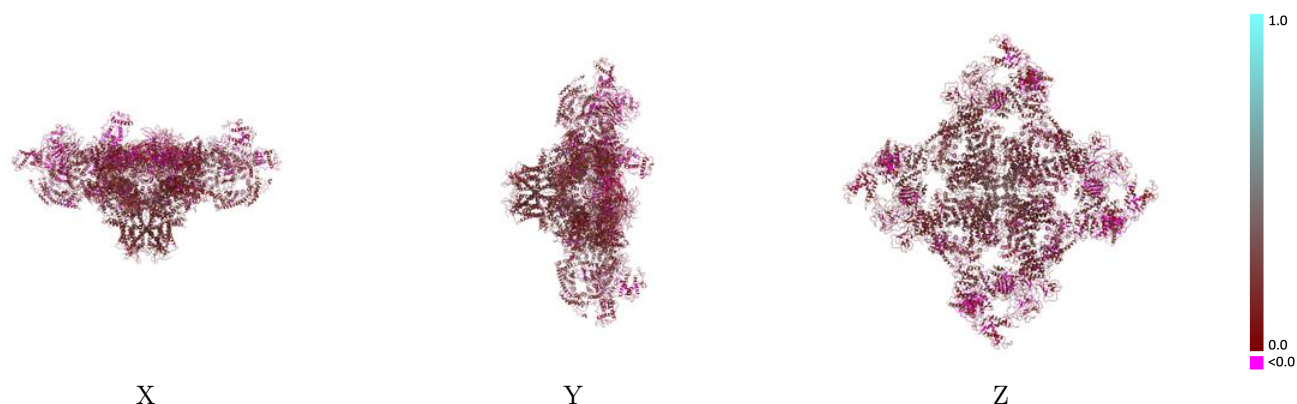
This section contains information regarding the fit between EMDB map EMD-22393 and PDB model 7JMG. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



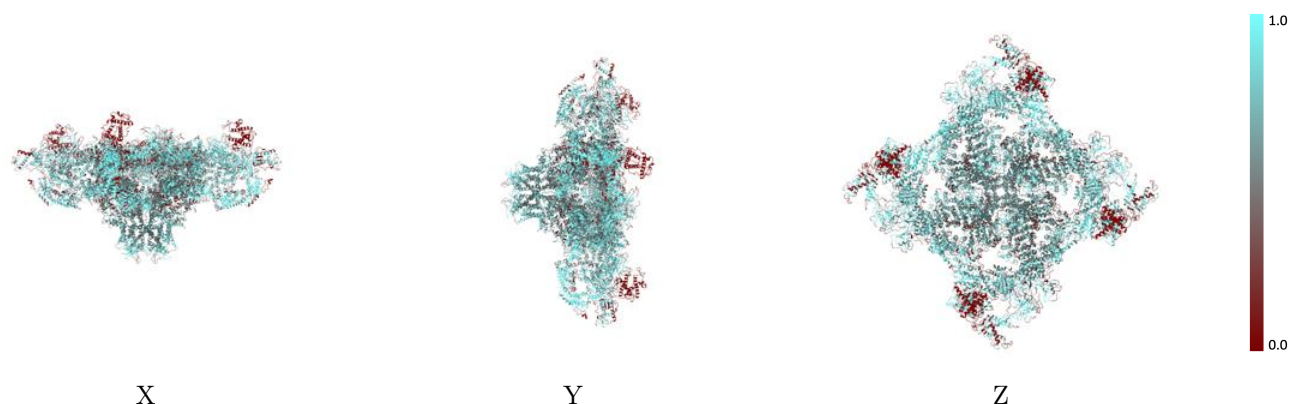
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



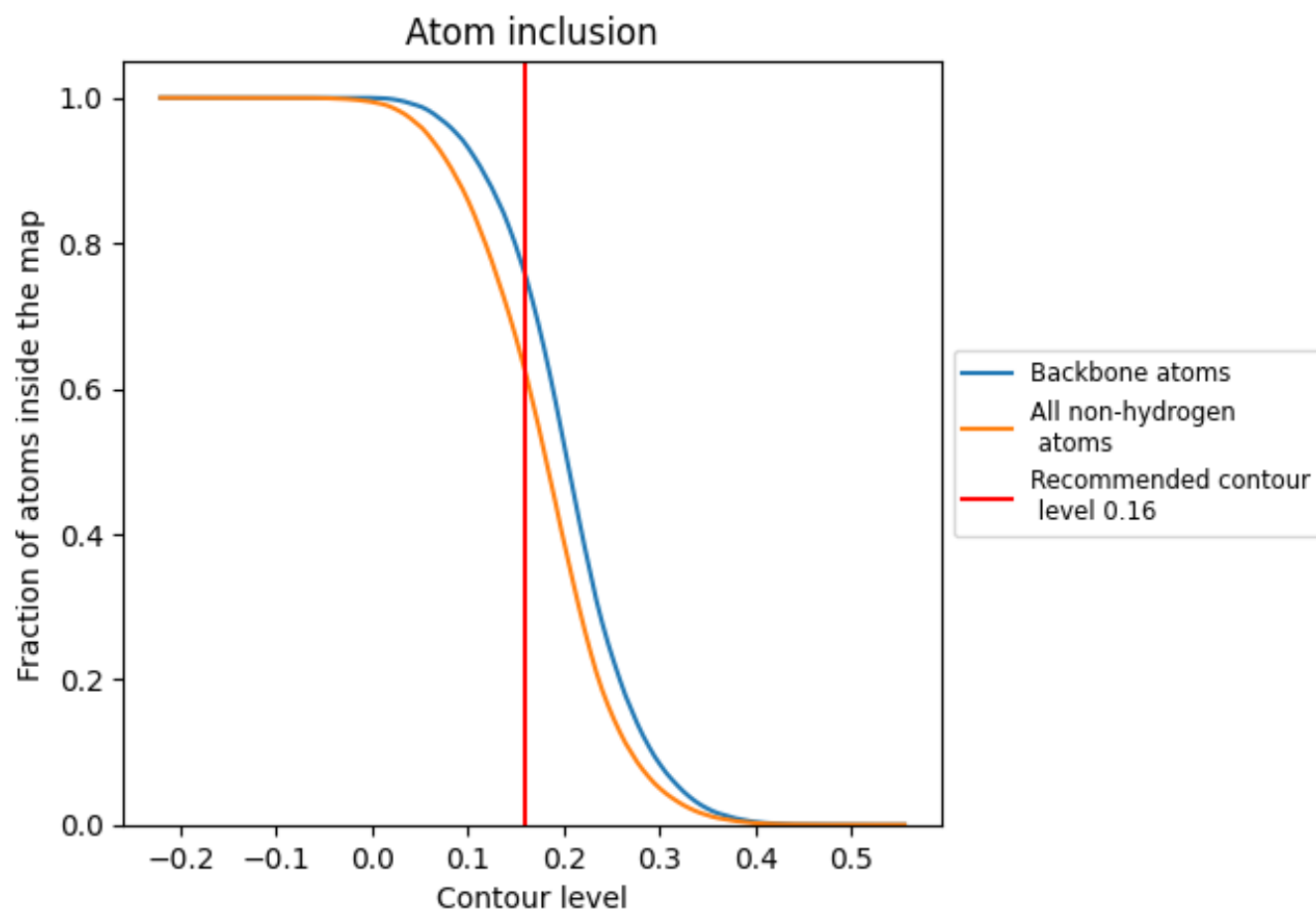
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 62% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6216	<div><div></div></div> 0.1550
A	<div><div></div></div> 0.7060	<div><div></div></div> 0.1500
B	<div><div></div></div> 0.6410	<div><div></div></div> 0.1760
E	<div><div></div></div> 0.6130	<div><div></div></div> 0.1450
F	<div><div></div></div> 0.6576	<div><div></div></div> 0.1250
G	<div><div></div></div> 0.6064	<div><div></div></div> 0.1410
H	<div><div></div></div> 0.6154	<div><div></div></div> 0.1140
I	<div><div></div></div> 0.6216	<div><div></div></div> 0.1600
J	<div><div></div></div> 0.6737	<div><div></div></div> 0.1360

1.0

0.0

<0.0