



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 04:35 AM EDT

PDB ID : 5TAP
EMDB ID : EMD-8381
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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

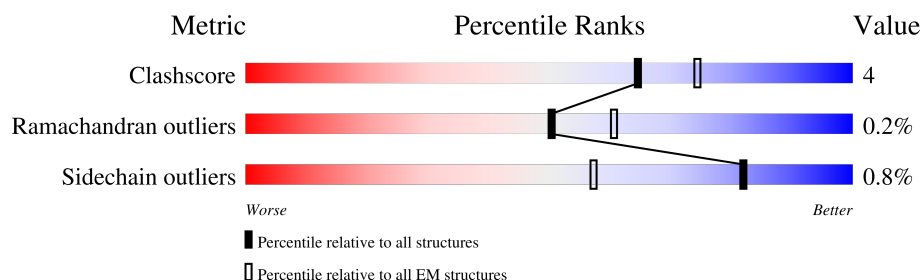
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

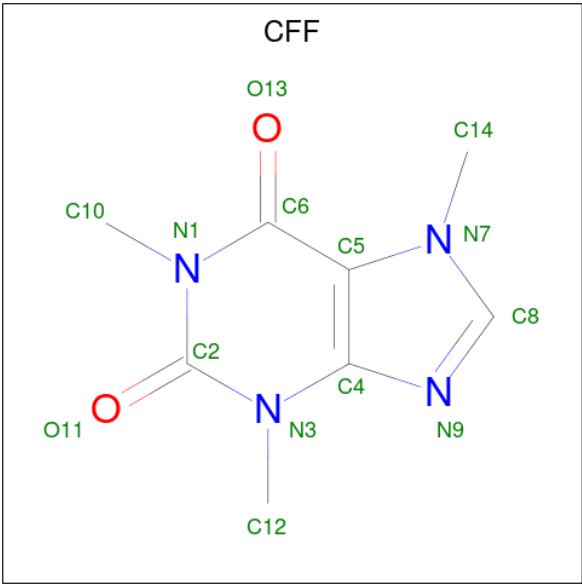
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

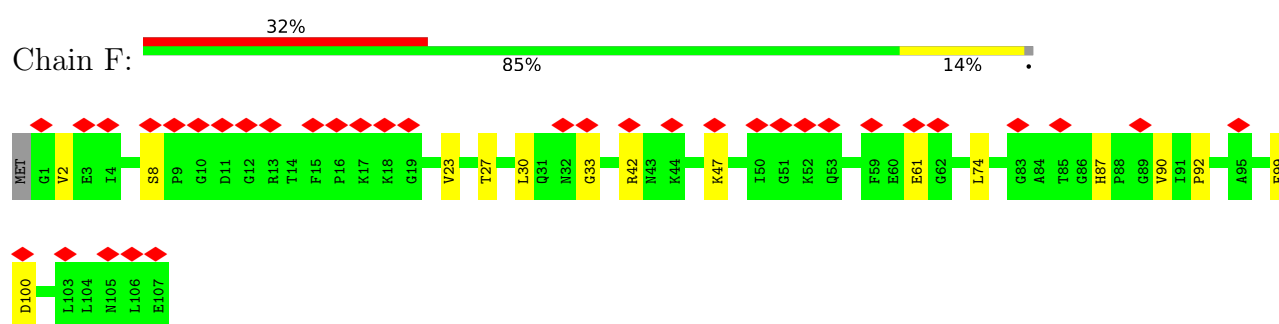
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

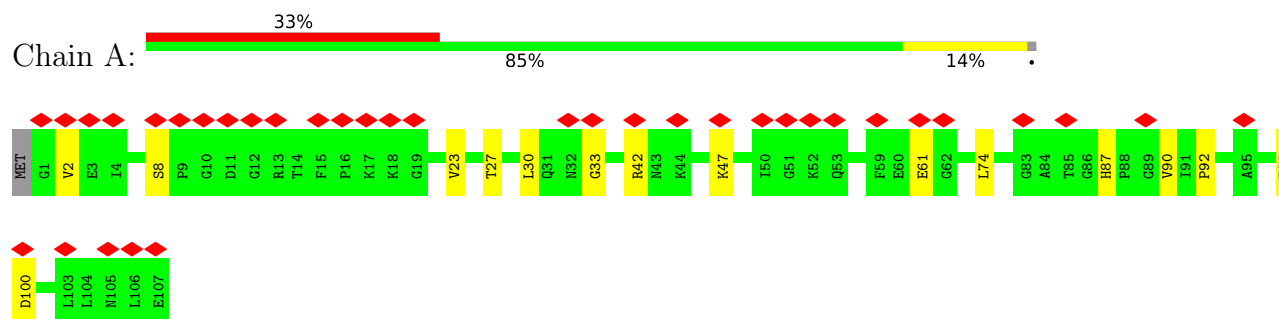
3 Residue-property plots [i](#)

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.

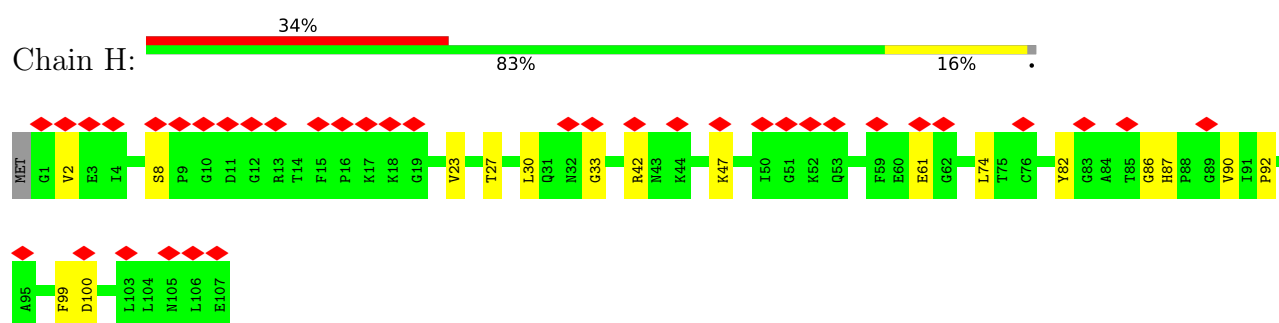
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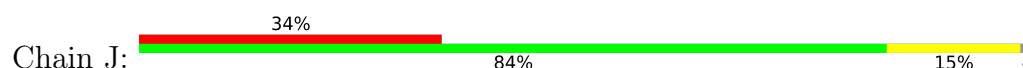
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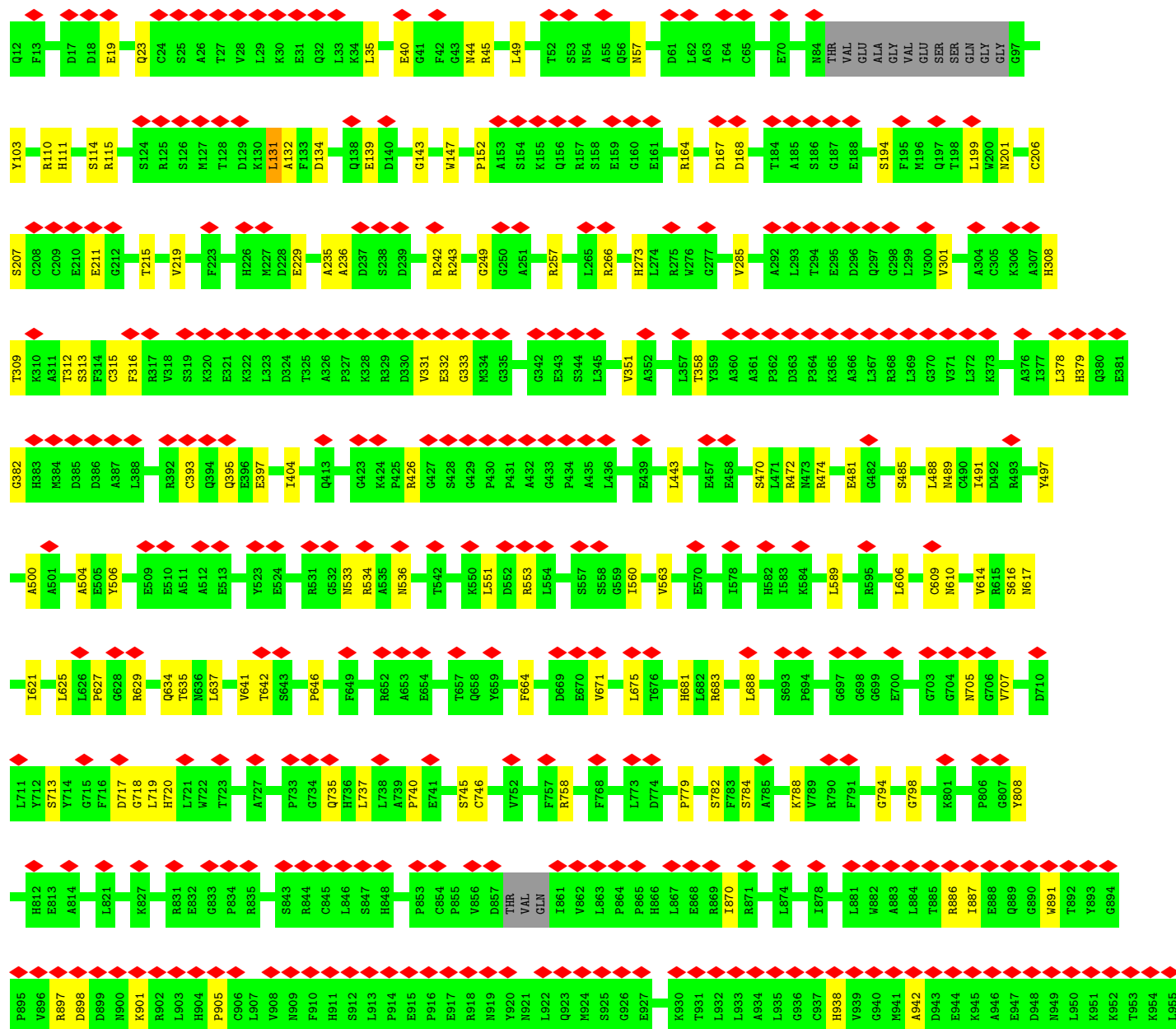
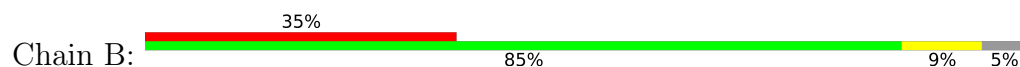
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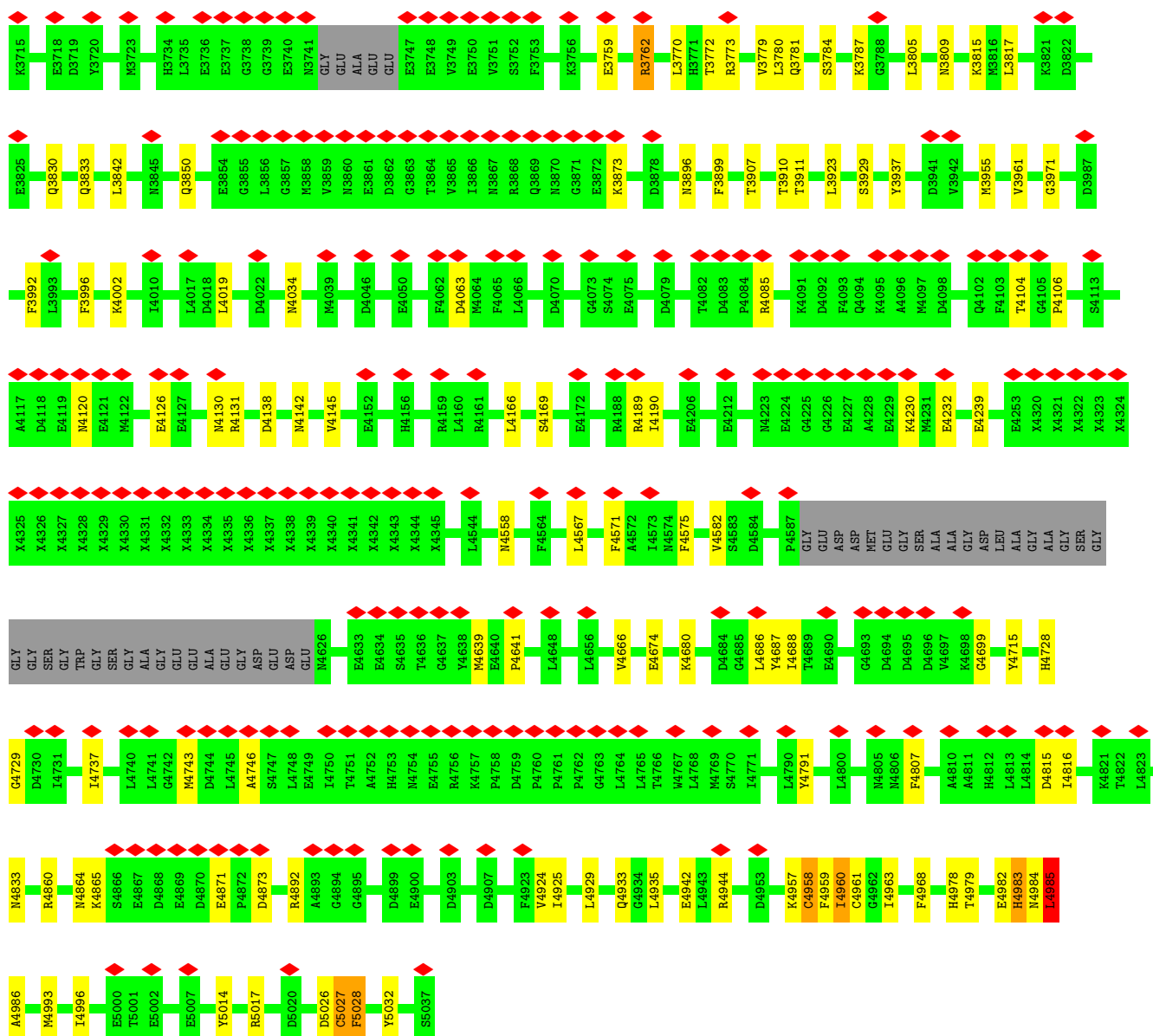


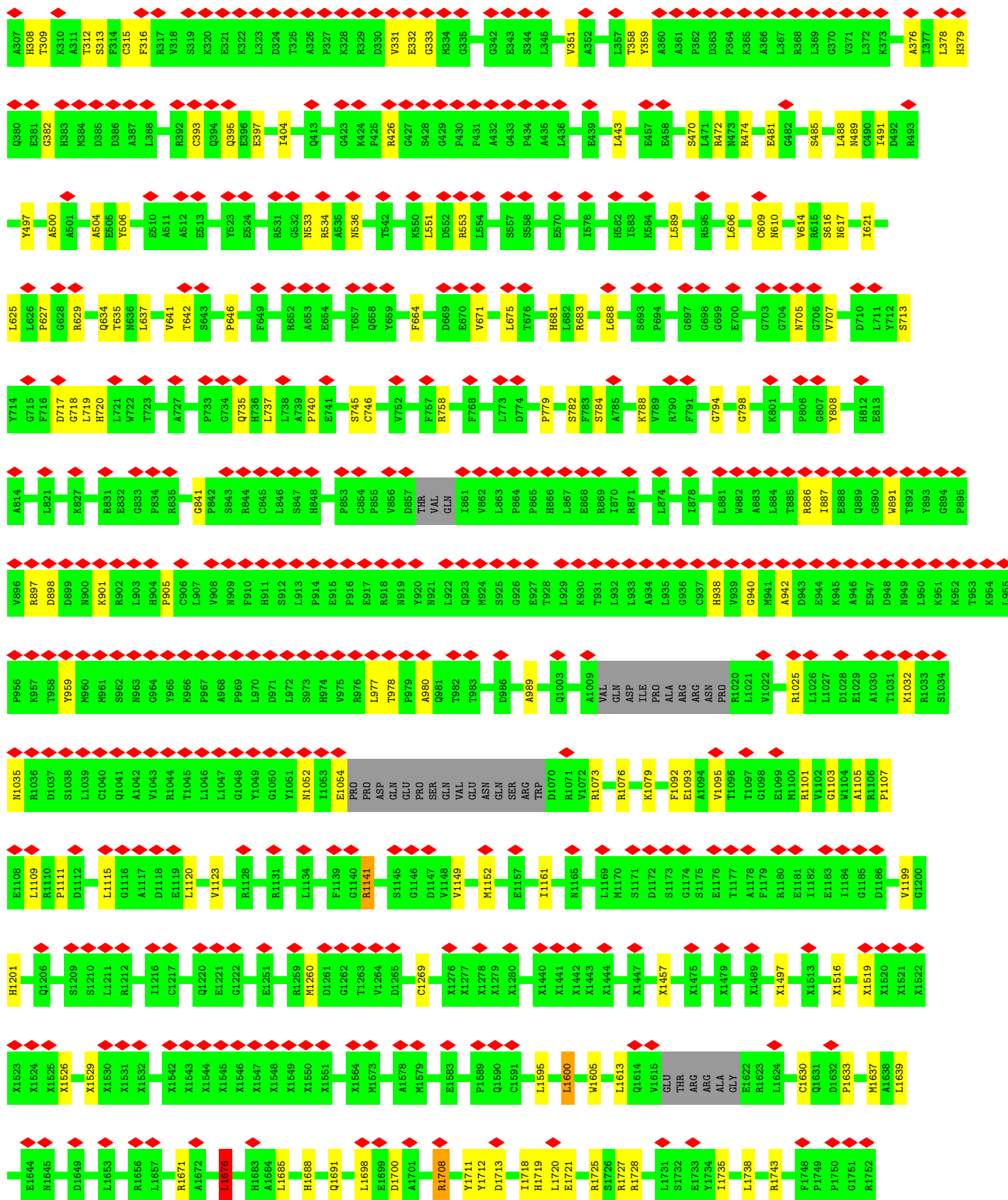
- Molecule 2: Ryanodine receptor 1





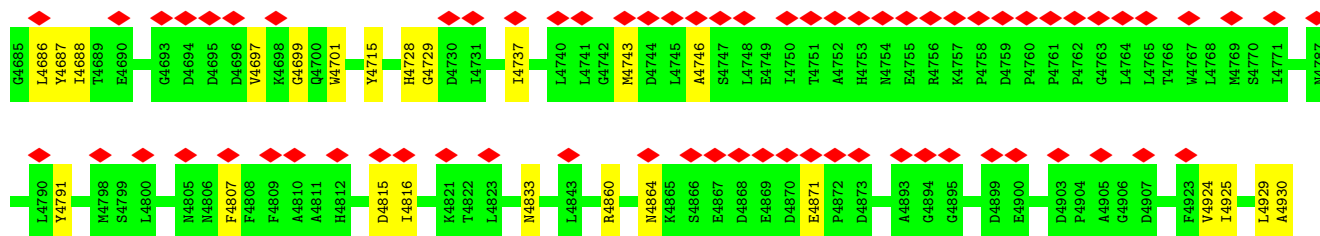




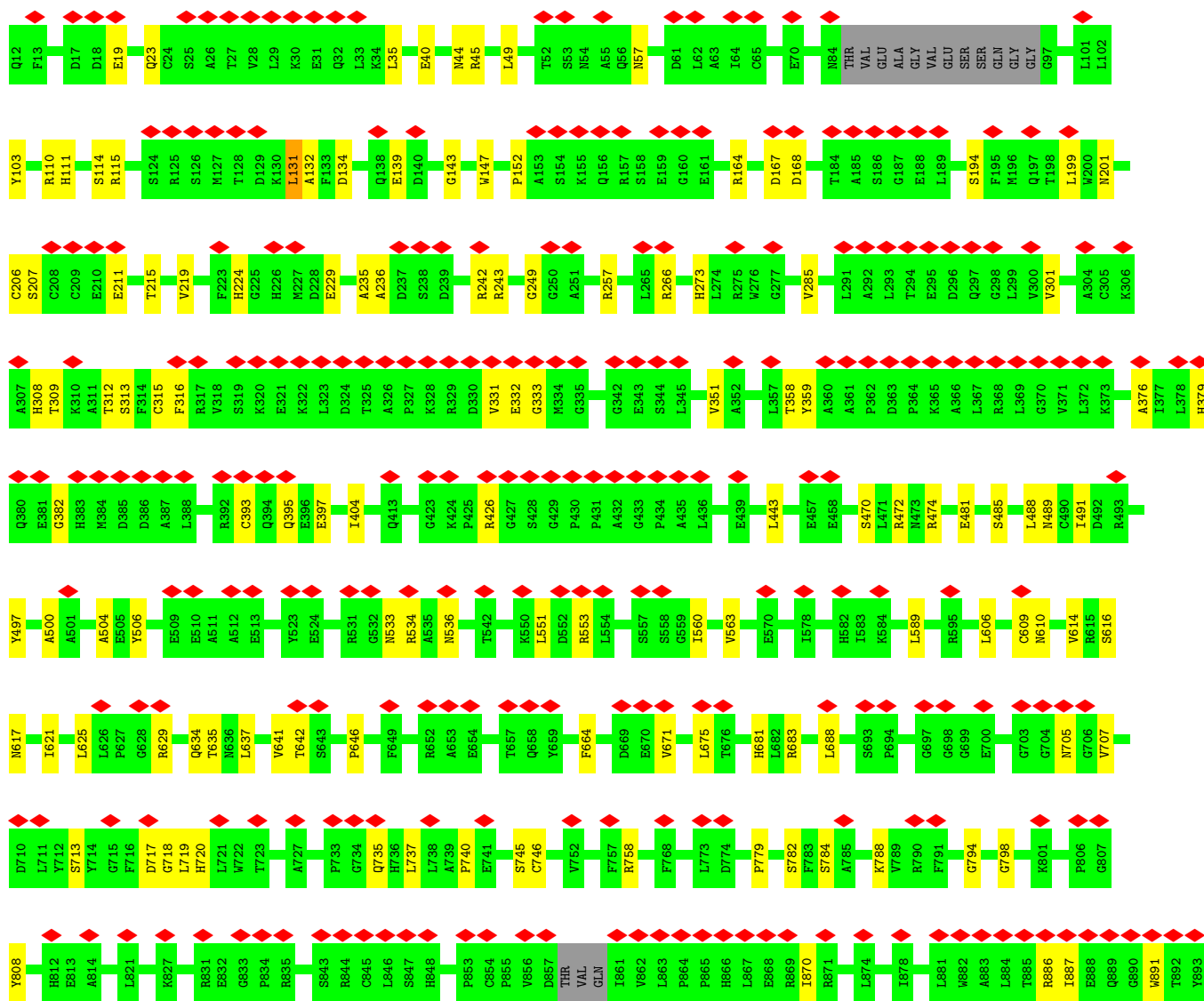
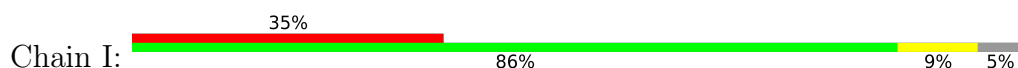




GLU	X3040	X3182	X3261	X3331	X3392	X3513	X3575	G3681	S3784	S3929	F4093	G4226	GLU
ASP	X3041	X3183	X3262	X3332	X3393	X3514	X3576	E3682	K3787	Y3937	Q4094	E4227	ASP
ASP	X3042	X3189	X3263	X3333	X3394	X3515	X3577	Q3683	G3788	Y3937	K4095	A4228	ASP
MET	X3043	X3191	X3264	X3334	X3395	X3516	X3578	E3684	L3805	D3941	A4096	A4229	GLY
GLU	X3044	X3192	X3265	X3335	X3396	X3517	X3579	E3685	L3805	V3942	M4097	K4230	GLY
SER	X3045	X3193	X3266	X3336	X3397	X3518	X3580	E3686	N3809	M3955	D4098	M4231	SER
ALA	X3046	X3194	X3267	X3337	X3398	X3519	X3581	E3687	N3809	M3955	D4098	E4232	ALA
ALA	X3047	X3195	X3268	X3338	X3399	X3520	X3582	E3688	M3815	V3961	Q4102	E4239	ALA
LEU	X3048	X3196	X3269	X3339	X3400	X3521	X3583	E3689	M3816	V3961	F4103	E4253	LEU
ALA	X3049	X3197	X3270	X3340	X3401	X3522	X3584	V3690	L3817	G3971	T4104	X4320	ALA
GLY	X3050	X3200	X3271	X3341	X3402	X3523	X3585	E3691	D3822	D3987	G4105	X4321	GLY
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GLY	X3143	X3223	X3290	X3360	X3433	X3542	X3608	GLU	T3864	E4050	V4145	X4340	GLY
GLY	X3144	X3224	X3291	X3361	X3434	X3543	X3609	ALA	V3865	F4062	E4152	X4341	GLY
GLY	X3145	X3225	X3292	X3362	X3435	X3544	X3610	GLU	L3866	D4063	H4156	X4342	GLY
GLY	X3146	X3226	X3293	X3363	X3436	X3545	X3611	GLU	N3867	M4064	R4159	X4343	GLY
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GLY	X3223	X3297	X3364	X3434	X3509	X3616	X3682						
GLY	X3224	X3298	X3365	X3435	X3510	X3617	X3683						
GLY	X3225	X3299	X3366	X3436	X3511	X3618	X3684						
GLY	X3226	X3300	X3367	X3437	X3512	X3619	X3685						
GLY	X3227	X3301	X3368	X3438	X3513	X3620	X3686						
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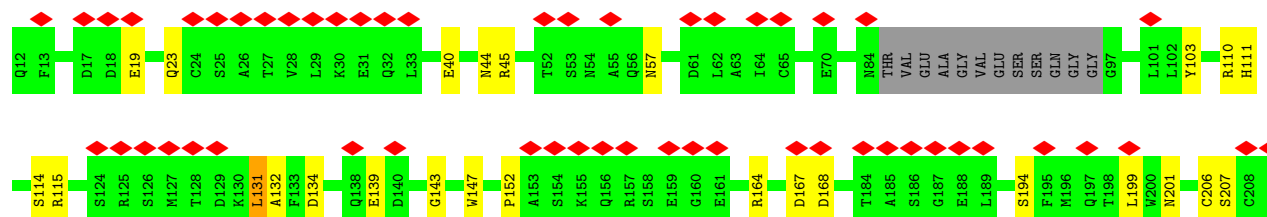


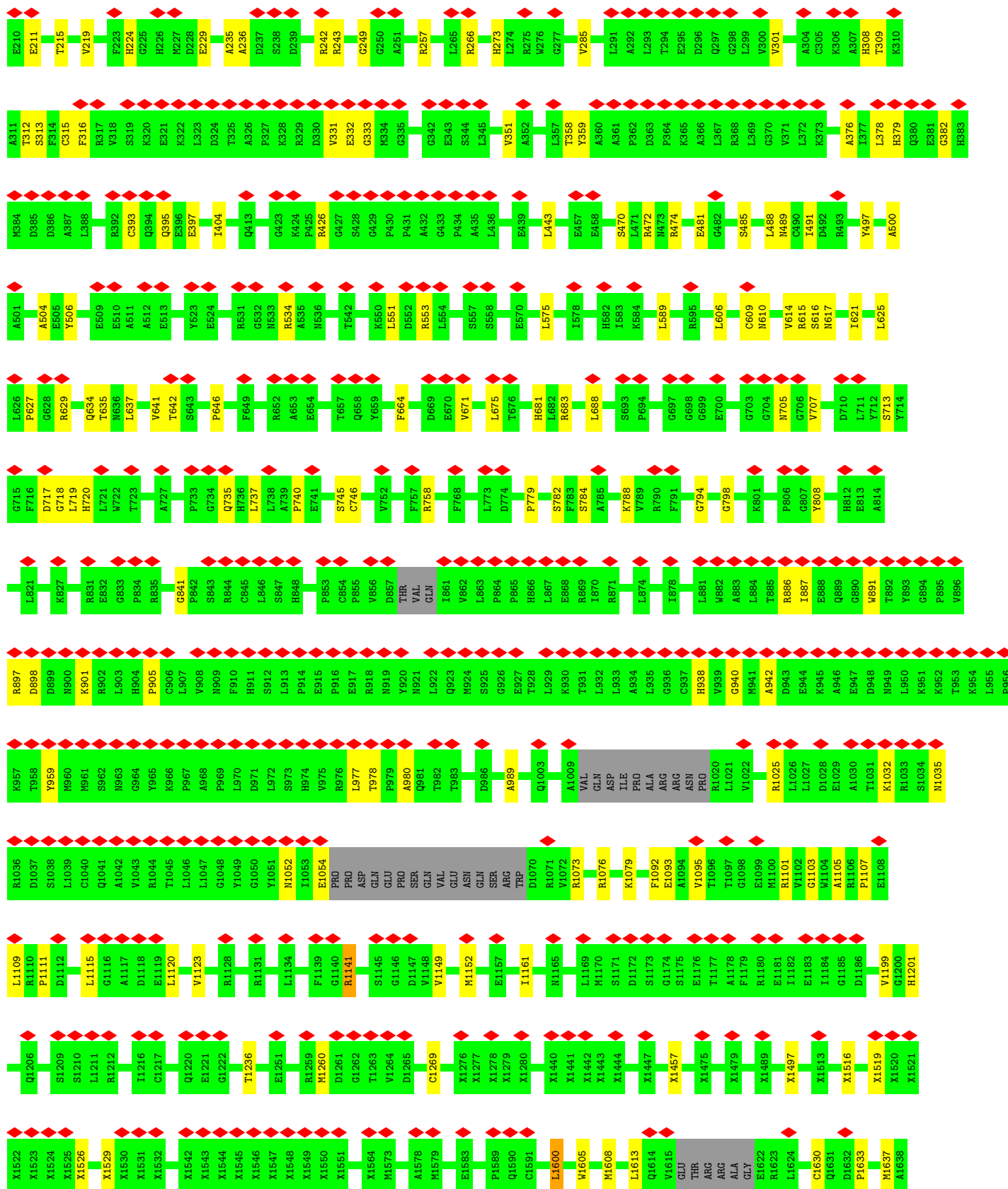
• Molecule 2: Ryanodine receptor 1





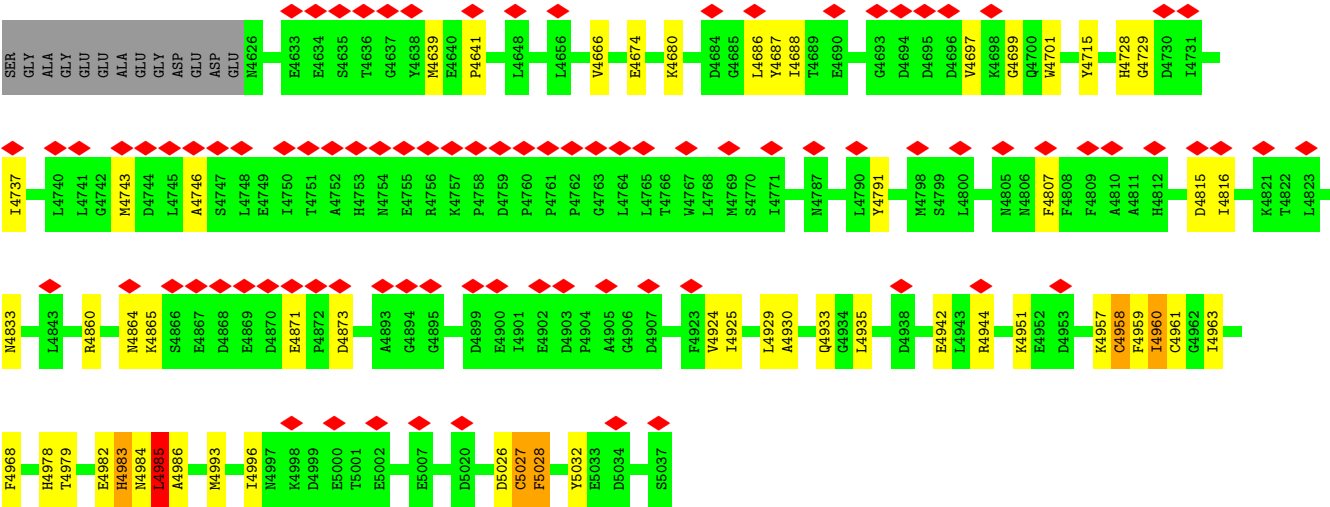






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P1749	P1750	G1751	R1752	K1753	G1754	G1755	N1756	A1757	R1758	G1764	V1765	G1766	V1767	T1768	L1771	R1772	A1773	P1774	H1775	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793	A1794	P1795	A1796	R1797	I1802	A1806	L1815	D1821	R1827	D1828	L1832	P1840	E1845	G1855	D1856	E1857	L1858	V1859	L1863	E1869																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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X4329	M4120	L3993	Q3830	S3714	X3588	X3526	X3405	X3344	X3274	X3201	X3050	X2951
X4330	E4121	K4002	Q3833	K3715	X3589	X3527	X3406	X3345	X3275	X3200	X3051	X2952
X4331	M4122		L3842	E3718	X3590	X3528	X3407	X3346	X3276	X3202	X3052	
X4332	Q4009	Q4010	N3845	D3719	X3591	X3529	X3408	X3347	X3277		X3053	
X4333	L4017		Q3850	Y3720	X3592	X3530	X3409	X3348	X3278	X3207		
X4334	L4018	L4019		M3723	X3595	X3531	X3410	X3349	X3279	X3208	X3057	X2964
X4335	L4019		E3854		X3596	X3532	X3411	X3350	X3280			X2965
X4336	D4022		G3855	H3734	X3597	X3533	X3412	X3351	X3281			X2966
X4337			L3856	L3735		X3534	X3413	X3352	X3282	X3211	X3061	X2967
X4338			G3857	E3736	X3600	X3535	X3414	X3353	X3283	X3212	X3062	X2968
X4339	M4034		G3857	E3737	X3601	X3536	X3415	X3354	X3284	X3213	X3063	X2969
X4340			M3858	G3738	X3602	X3537	X3416	X3355	X3285	X3214	X3064	X2970
X4341	V4145		V3859	G3738	X3603	X3538	X3422	X3356	X3286	X3215	X3065	X2971
X4342	X4343		G3739	E3740	X3604	X3539	X3423	X3357	X3287	X3216	X3066	X2972
X4343	X4343		V3860	E3740	X3605	X3540	X3427	X3358	X3288	X3217	X3067	X2973
X4344	D4046		E3861	M3741	X3606	X3541	X3432	X3359	X3289	X3218	X3068	X2974
X4345	E4050		D3862	GLY	X3607	X3542	X3432	X3360	X3290	X3219	X3069	X2975
			G3863	GLU	X3608	X3543	X3433	X3361	X3291	X3220	X3070	X2976
			V3864	ALA	X3609	X3544	X3433	X3362	X3292	X3221	X3071	X2977
			L3865	GLU	X3610	X3545	X3434	X3363	X3293	X3222	X3072	X2978
			L3866	GLU	X3611	X3546	X3435	X3364	X3294	X3223	X3073	X2979
			N3867	E3747	X3612	X3547	X3436	X3365	X3295	X3224	X3074	X2980
			R3868	E3748	X3613	X3548	X3437	X3366	X3296	X3225	X3075	X2981
			Q3869	V3749	X3639	X3549	X3438		X3297	X3226	X3076	X2982
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				V3751		X3551			X3299			X2984
				S3752		X3552	X3442		X3300			X2985
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	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	0.116	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	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: ATP, ZN, CFF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/834	0.51	0/1123
1	F	0.32	0/834	0.51	0/1123
1	H	0.32	0/834	0.51	0/1123
1	J	0.32	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.54	36/142628 (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	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	15
2	E	0	15
2	G	0	15
2	I	0	15
All	All	0	64

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2476	ILE	C-N	5.37	1.44	1.34
2	B	2476	ILE	C-N	5.34	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2476	ILE	C-N	5.33	1.44	1.34
2	G	2476	ILE	C-N	5.30	1.44	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.29	134.37	115.30
2	G	131	LEU	CA-CB-CG	8.28	134.35	115.30
2	B	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	E	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	G	1600	LEU	CA-CB-CG	7.05	131.52	115.30
2	I	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	E	1600	LEU	CA-CB-CG	7.03	131.48	115.30
2	I	1676	LEU	CA-CB-CG	6.55	130.37	115.30
2	B	1676	LEU	CA-CB-CG	6.54	130.33	115.30
2	G	1676	LEU	CA-CB-CG	6.52	130.31	115.30
2	E	1676	LEU	CA-CB-CG	6.51	130.28	115.30
2	I	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	G	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	B	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	E	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	G	977	LEU	CA-CB-CG	5.37	127.64	115.30
2	G	688	LEU	CA-CB-CG	5.36	127.63	115.30
2	B	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	688	LEU	CA-CB-CG	5.35	127.60	115.30
2	E	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	B	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	3770	LEU	CA-CB-CG	5.12	127.07	115.30
2	B	3770	LEU	CA-CB-CG	5.12	127.06	115.30
2	G	3770	LEU	CA-CB-CG	5.11	127.04	115.30
2	I	3770	LEU	CA-CB-CG	5.10	127.03	115.30
2	I	2290	LEU	CA-CB-CG	5.08	126.97	115.30
2	E	2290	LEU	CA-CB-CG	5.07	126.95	115.30
2	B	2290	LEU	CA-CB-CG	5.06	126.95	115.30
2	G	2290	LEU	CA-CB-CG	5.06	126.94	115.30
2	I	4639	MET	C-N-CA	5.05	134.32	121.70
2	G	4639	MET	C-N-CA	5.03	134.27	121.70
2	E	4639	MET	C-N-CA	5.03	134.27	121.70
2	B	4639	MET	C-N-CA	5.03	134.26	121.70

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	8	0
1	F	818	0	824	8	0
1	H	818	0	824	9	0
1	J	818	0	824	8	0
2	B	29499	0	24749	236	0
2	E	29499	0	24749	235	0
2	G	29499	0	24749	231	0
2	I	29499	0	24749	233	0
3	B	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102380	949	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (949) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.38	0.88
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.38	0.88
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.38	0.87
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.38	0.87
2:B:4983:HIS:CD2	2:B:4983:HIS:H	1.94	0.86
2:G:4983:HIS:CD2	2:G:4983:HIS:H	1.94	0.86
2:I:4983:HIS:H	2:I:4983:HIS:CD2	1.94	0.84
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	1.92	0.83
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	1.92	0.82
2:E:4983:HIS:CD2	2:E:4983:HIS:H	1.94	0.82
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	1.92	0.82
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.15	0.81
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	1.92	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.15	0.80
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.29	0.79
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.29	0.77
2:I:4983:HIS:H	2:I:4983:HIS:HD2	1.29	0.77
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.29	0.77
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.77	0.73
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.77	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.77	0.72
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.77	0.72
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.04	0.72
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.04	0.71
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.04	0.71
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.04	0.71
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.61	0.69
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.61	0.68
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.61	0.68
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.61	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.67
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.67
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.78	0.66
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.78	0.66
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.61	0.65
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.61	0.65
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.61	0.64
2:G:379:HIS:HD2	2:G:382:GLY:H	1.45	0.64
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.78	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.62	0.64
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.80	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.61	0.64
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.80	0.64
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.78	0.64
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.63	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.80	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.63
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.81	0.63
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.81	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.80	0.63
2:E:379:HIS:HD2	2:E:382:GLY:H	1.45	0.63
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.81	0.63
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.64	0.63
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.81	0.63
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.64	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.63	0.63
2:B:379:HIS:HD2	2:B:382:GLY:H	1.45	0.63
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.64	0.62
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.81	0.62
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.81	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.63	0.62
2:G:4982:GLU:HB3	2:G:4983:HIS:HD2	1.65	0.62
2:E:4982:GLU:HB3	2:E:4983:HIS:HD2	1.65	0.62
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.81	0.62
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.62
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.64	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:B:4982:GLU:HB3	2:B:4983:HIS:HD2	1.65	0.61
2:I:4982:GLU:HB3	2:I:4983:HIS:HD2	1.65	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.81	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.65	0.61
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.61
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.66	0.61
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	2.14	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.60
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.83	0.60
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	2.14	0.60
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.66	0.60
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.60
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.60
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.60
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.65	0.60
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	2.14	0.60
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	2.14	0.60
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.83	0.59
2:B:4979:THR:HG22	3:B:5101:ATP:H2	1.67	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4979:THR:HG22	3:I:5101:ATP:H2	1.67	0.59
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.65	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.83	0.59
2:B:132:ALA:HA	2:B:194:SER:HB2	1.84	0.59
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.67	0.59
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.85	0.59
2:E:132:ALA:HA	2:E:194:SER:HB2	1.84	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.85	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.85	0.59
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.85	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.58
2:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.24	0.58
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.22	0.58
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.22	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.85	0.58
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.58
2:G:4979:THR:HG22	3:G:5101:ATP:H2	1.67	0.58
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.22	0.58
2:E:4979:THR:HG22	3:E:5101:ATP:H2	1.67	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.58
2:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.24	0.58
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.24	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.57
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.86	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.85	0.57
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.57
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.57
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.22	0.57
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.86	0.57
2:G:132:ALA:HA	2:G:194:SER:HB2	1.84	0.57
2:G:4190:ILE:HD13	2:G:5026:ASP:CG	2.24	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.57
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.86	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.87	0.57
2:I:132:ALA:HA	2:I:194:SER:HB2	1.84	0.57
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.87	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.87	0.57
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.73	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.87	0.57
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.86	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.73	0.56
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.86	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.88	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.87	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.70	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.56
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.86	0.56
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.86	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.86	0.56
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.56
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.56
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	2.54	0.56
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.88	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.88	0.56
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.56
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.88	0.56
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.86	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.56
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.73	0.56
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.88	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.95	0.55
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.88	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.71	0.55
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.88	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.55
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	2.54	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.55
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.88	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.95	0.55
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.71	0.55
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	2.54	0.55
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.55
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.88	0.55
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.71	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.71	0.55
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	2.54	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.89	0.55
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.95	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.89	0.54
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.54
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.88	0.54
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.89	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.88	0.54
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.81	0.54
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.95	0.54
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.76	0.54
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.76	0.54
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.88	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.41	0.54
2:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.76	0.54
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.54
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.76	0.54
2:E:331:VAL:HG12	2:E:333:GLY:H	1.73	0.54
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.81	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.56	0.54
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.81	0.54
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.56	0.54
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.70	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.39	0.54
2:G:111:HIS:HD2	2:G:114:SER:H	1.56	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.26	0.53
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.26	0.53
2:G:794:GLY:H	2:G:798:GLY:HA3	1.73	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.90	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.53
2:I:794:GLY:H	2:I:798:GLY:HA3	1.73	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.53
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.91	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.73	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.56	0.53
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.41	0.53
2:B:794:GLY:H	2:B:798:GLY:HA3	1.73	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.91	0.53
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.90	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.53
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.53
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.73	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.91	0.53
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.26	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.53
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.74	0.53
2:E:794:GLY:H	2:E:798:GLY:HA3	1.74	0.53
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.73	0.53
2:G:331:VAL:HG12	2:G:333:GLY:H	1.73	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.26	0.53
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.92	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:B:2868:SER:O	2:B:2872:GLN:N	2.41	0.52
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.90	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.52
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.75	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.52
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.39	0.52
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.52
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.75	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.91	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.75	0.52
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.92	0.52
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.92	0.52
2:B:313:SER:HB3	2:B:351:VAL:HB	1.91	0.52
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.90	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.92	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.52
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.52
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.90	0.52
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.52
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:G:4979:THR:HG22	3:G:5101:ATP:C2	2.45	0.51
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.75	0.51
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.75	0.51
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.51
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.51
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:B:4979:THR:HG22	3:B:5101:ATP:C2	2.45	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.51
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.41	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.51
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.92	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.41	0.51
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.39	0.51
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.46	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.75	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.93	0.51
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.93	0.51
2:B:614:VAL:HG22	2:B:616:SER:H	1.75	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.51
2:E:4979:THR:HG22	3:E:5101:ATP:C2	2.45	0.51
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.93	0.51
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.75	0.51
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.46	0.50
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.50
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.45	0.50
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.93	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.45	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:I:4979:THR:HG22	3:I:5101:ATP:C2	2.45	0.50
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.94	0.50
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.50
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.50
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.94	0.50
2:I:614:VAL:HG22	2:I:616:SER:H	1.75	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.93	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.41	0.50
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.30	0.50
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.50
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.93	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.50
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.50
2:E:614:VAL:HG22	2:E:616:SER:H	1.75	0.50
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.50
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.50
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.93	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.41	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.49
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.93	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.30	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.49
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.94	0.49
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.95	0.49
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.30	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.94	0.49
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.49
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.94	0.49
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.93	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.49
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.95	0.49
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.94	0.49
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.94	0.49
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.95	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.49
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:I:642:THR:HG23	2:I:1613:LEU:HD12	1.95	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.95	0.49
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.95	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.95	0.49
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.45	0.49
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.95	0.49
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.46	0.49
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.49
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.41	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.45	0.49
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.95	0.49
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.94	0.49
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.45	0.49
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.31	0.49
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.46	0.49
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.94	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.48
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.48
2:G:3842:LEU:O	2:G:3929:SER:OG	2.31	0.48
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.95	0.48
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.95	0.48
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.31	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.41	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.45	0.48
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.45	0.48
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.96	0.48
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.48
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.95	0.48
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.93	0.48
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.46	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.32	0.48
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.95	0.48
2:G:642:THR:HG23	2:G:1613:LEU:HD12	1.95	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.30	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.46	0.48
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.96	0.48
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.96	0.48
2:I:3842:LEU:O	2:I:3929:SER:OG	2.31	0.48
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.95	0.48
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.96	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.45	0.48
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.94	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.48
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:HIS:CD2	2:G:114:SER:H	2.32	0.48
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.79	0.48
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.46	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.31	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.32	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.79	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.94	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.31	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.96	0.47
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.47
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.79	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.96	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.47
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.28	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.46	0.47
2:E:642:THR:HG23	2:E:1613:LEU:HD12	1.95	0.47
2:E:3842:LEU:O	2:E:3929:SER:OG	2.31	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.47
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.47
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.80	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.32	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.96	0.47
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.79	0.47
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.47
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.79	0.47
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.47
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.96	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.96	0.47
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.96	0.47
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.96	0.47
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.97	0.47
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.97	0.47
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.96	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.97	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.79	0.47
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.97	0.47
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.47
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.97	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:3676:ASP:HA	2:B:3679:LYS:HB3	1.97	0.47
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.97	0.47
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.96	0.47
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.96	0.47
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.79	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.96	0.47
2:I:3676:ASP:HA	2:I:3679:LYS:HB3	1.97	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.79	0.47
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.79	0.46
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.96	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.79	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.79	0.46
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.28	0.46
2:G:395:GLN:HG3	2:G:397:GLU:H	1.80	0.46
2:B:1738:LEU:HB3	2:B:2146:PRO:HG3	1.97	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.31	0.46
2:E:395:GLN:HG3	2:E:397:GLU:H	1.80	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.97	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.97	0.46
2:G:3676:ASP:HA	2:G:3679:LYS:HB3	1.97	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.79	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.96	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.97	0.46
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.46
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.97	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.97	0.46
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.46
2:B:134:ASP:OD1	2:B:134:ASP:N	2.48	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.46
2:G:1738:LEU:HB3	2:G:2146:PRO:HG3	1.97	0.46
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.98	0.46
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.46
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.46	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.97	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.97	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.96	0.46
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.46
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.97	0.46
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.98	0.46
2:E:1738:LEU:HB3	2:E:2146:PRO:HG3	1.97	0.46
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.46
2:I:1738:LEU:HB3	2:I:2146:PRO:HG3	1.97	0.46
2:E:134:ASP:N	2:E:134:ASP:OD1	2.48	0.46
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.98	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.34	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.80	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.79	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.97	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.98	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.43	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
2:B:621:ILE:O	2:B:625:LEU:N	2.48	0.45
2:I:395:GLN:HG3	2:I:397:GLU:H	1.80	0.45
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.48	0.45
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.98	0.45
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.45
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.97	0.45
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.45
2:E:3676:ASP:HA	2:E:3679:LYS:HB3	1.97	0.45
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.39	0.45
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.45
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.97	0.45
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	1.98	0.45
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.45
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.98	0.45
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.45
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.70	0.45
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.45
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:4571:PHE:O	2:B:4575:PHE:N	2.50	0.45
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.45
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.99	0.45
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.45
2:E:4571:PHE:O	2:E:4575:PHE:N	2.50	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:B:1516:UNK:N	2:B:1529:UNK:O	2.50	0.45
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.45
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.45
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.34	0.45
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.99	0.44
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.28	0.44
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.99	0.44
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.44
2:G:1516:UNK:N	2:G:1529:UNK:O	2.50	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.44
2:B:3910:THR:HG23	2:B:3911:THR:HG23	2.00	0.44
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.00	0.44
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.49	0.44
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.34	0.44
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.49	0.44
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.00	0.44
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.44
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.00	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.44
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.99	0.44
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.44
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.00	0.44
2:E:3910:THR:HG23	2:E:3911:THR:HG23	2.00	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.44
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	2.00	0.44
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.00	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.44
2:I:266:ARG:NH1	2:I:332:GLU:OE2	2.51	0.44
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
2:I:1516:UNK:N	2:I:1529:UNK:O	2.50	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.44
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.99	0.44
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.44
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.44
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.99	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.44
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.99	0.44
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.44
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.00	0.44
2:E:621:ILE:O	2:E:625:LEU:N	2.48	0.44
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.00	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.44
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.00	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.44
2:I:224:HIS:N	2:I:229:GLU:O	2.46	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.44
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.99	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.44
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.44
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.83	0.43
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.43
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.70	0.43
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.99	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.50	0.43
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.43
2:G:497:TYR:HB3	2:G:500:ALA:HB2	2.00	0.43
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.00	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.43
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.99	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	1.98	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.43
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.84	0.43
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.00	0.43
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.00	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.00	0.43
2:G:266:ARG:NH1	2:G:332:GLU:OE2	2.51	0.43
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.84	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.34	0.43
2:E:497:TYR:HB3	2:E:500:ALA:HB2	2.00	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	1.98	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.99	0.43
2:G:621:ILE:O	2:G:625:LEU:N	2.48	0.43
2:G:4571:PHE:O	2:G:4575:PHE:N	2.50	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.43
2:B:4933:GLN:HG2	2:I:4930:ALA:HB2	2.00	0.43
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.46	0.43
2:E:266:ARG:NH1	2:E:332:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.43
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.99	0.43
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.52	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	2.00	0.43
2:E:5028:PHE:O	2:E:5028:PHE:CG	2.70	0.43
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.84	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.00	0.43
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.43
2:I:4960:ILE:N	2:I:4960:ILE:CD1	2.73	0.43
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.50	0.43
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.43
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.52	0.43
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.67	0.43
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:4571:PHE:O	2:I:4575:PHE:N	2.50	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.43
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.52	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	2.00	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:E:2103:VAL:O	2:E:2107:GLN:N	2.46	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.51	0.42
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.01	0.42
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.01	0.42
2:B:266:ARG:NH1	2:B:332:GLU:OE2	2.51	0.42
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.42
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.01	0.42
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.52	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.42
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.67	0.42
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.52	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.00	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.42
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.42
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.50	0.42
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.42
2:G:224:HIS:N	2:G:229:GLU:O	2.46	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.46	0.42
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.50	0.42
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.52	0.42
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.99	0.42
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.42
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.42
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.42
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.51	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.53	0.42
2:I:4190:ILE:HD13	2:I:5026:ASP:OD2	2.19	0.42
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.01	0.42
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.42
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.53	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.42
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.01	0.42
2:B:3992:PHE:O	2:B:3996:PHE:N	2.42	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.02	0.42
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.53	0.42
2:I:621:ILE:O	2:I:625:LEU:N	2.48	0.42
2:B:206:CYS:SG	2:B:207:SER:N	2.93	0.41
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.83	0.41
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.41
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.02	0.41
2:E:4189:ARG:NH1	2:E:5032:TYR:OH	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.41
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.53	0.41
2:G:358:THR:HG21	2:G:382:GLY:HA2	2.02	0.41
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.49	0.41
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.53	0.41
2:G:2212:VAL:O	2:G:2216:GLY:N	2.45	0.41
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.41
2:B:4958:CYS:O	2:B:4958:CYS:SG	2.79	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.94	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:359:TYR:HA	2:E:376:ALA:HA	2.02	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:4958:CYS:O	2:E:4958:CYS:SG	2.79	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.03	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.41
2:E:206:CYS:SG	2:E:207:SER:N	2.93	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.03	0.41
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.47	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.36	0.41
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.36	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:B:4189:ARG:NH1	2:B:5032:TYR:OH	2.53	0.41
2:E:1595:LEU:HD23	2:E:1595:LEU:HA	1.96	0.41
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.02	0.41
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.03	0.41
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.52	0.41
2:G:206:CYS:SG	2:G:207:SER:N	2.93	0.41
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.54	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.86	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.03	0.41
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.02	0.41
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.03	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.70	0.41
2:G:378:LEU:HD23	2:G:378:LEU:HA	1.88	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.94	0.41
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.41
2:B:168:ASP:HB3	2:B:199:LEU:HD22	2.02	0.41
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.41
2:B:4865:LYS:HB2	2:B:4873:ASP:HB3	2.03	0.41
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.53	0.41
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.53	0.41
2:I:243:ARG:NH1	2:I:301:VAL:O	2.46	0.41
2:G:359:TYR:HA	2:G:376:ALA:HA	2.02	0.41
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	2.03	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.41
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.41
1:J:82:TYR:O	1:J:86:GLY:N	2.54	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.41
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	2.03	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.02	0.41
2:E:224:HIS:N	2:E:229:GLU:O	2.46	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.41
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.54	0.41
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.86	0.41
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.41
2:I:359:TYR:HA	2:I:376:ALA:HA	2.02	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.41
2:I:2543:UNK:O	2:I:2547:UNK:N	2.54	0.41
2:I:4958:CYS:O	2:I:4958:CYS:SG	2.79	0.41
2:I:4982:GLU:N	2:I:4982:GLU:OE1	2.54	0.41
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.03	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.41
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.35	0.41
2:G:4951:LYS:HE2	2:G:4951:LYS:HB3	1.96	0.41
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.88	0.41
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.94	0.41
2:B:2305:CYS:O	2:B:2324:ASN:ND2	2.54	0.41
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.03	0.41
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.49	0.41
2:E:2543:UNK:O	2:E:2547:UNK:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.41	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.53	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.41
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.03	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.50	0.41
2:G:4958:CYS:O	2:G:4958:CYS:SG	2.79	0.41
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.02	0.40
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.03	0.40
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	2.03	0.40
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.37	0.40
2:B:4982:GLU:OE1	2:B:4982:GLU:N	2.54	0.40
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.04	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.93	0.40
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	2.03	0.40
2:I:4933:GLN:HG2	2:G:4930:ALA:HB2	2.03	0.40
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.67	0.40
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.40
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.03	0.40
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.03	0.40
1:H:82:TYR:O	1:H:86:GLY:N	2.54	0.40
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.40
2:B:1865:MET:SD	2:B:1865:MET:N	2.95	0.40
2:B:4138:ASP:N	2:B:4138:ASP:OD1	2.52	0.40
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.40
2:E:4930:ALA:HB2	2:G:4933:GLN:HG2	2.03	0.40
2:I:1865:MET:N	2:I:1865:MET:SD	2.94	0.40
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.04	0.40
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.03	0.40
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.40
2:B:870:ILE:HD12	2:B:870:ILE:HA	1.92	0.40
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.40
2:E:378:LEU:HD23	2:E:378:LEU:HA	1.88	0.40
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.40
2:E:3992:PHE:O	2:E:3996:PHE:N	2.42	0.40
2:E:4982:GLU:OE1	2:E:4982:GLU:N	2.54	0.40
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.94	0.40
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.54	0.40
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.86	0.40
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.02	0.40
2:I:4697:VAL:O	2:I:4701:TRP:N	2.50	0.40
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.04	0.40
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.79	0.40
2:G:4865:LYS:HB2	2:G:4873:ASP:HB3	2.03	0.40
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.04	0.40
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.03	0.40
2:B:2543:UNK:O	2:B:2547:UNK:N	2.54	0.40
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.40
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.04	0.40
2:E:2212:VAL:O	2:E:2216:GLY:N	2.45	0.40
2:I:3992:PHE:O	2:I:3996:PHE:N	2.42	0.40
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.53	0.40
2:B:2212:VAL:O	2:B:2216:GLY:N	2.45	0.40
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.54	0.40
2:B:2880:GLU:O	2:B:2884:ASN:N	2.53	0.40
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.04	0.40
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.03	0.40
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.57	0.40
2:E:2305:CYS:O	2:E:2324:ASN:ND2	2.55	0.40
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.03	0.40
2:I:2305:CYS:O	2:I:2324:ASN:ND2	2.54	0.40
2:I:2780:ASN:O	2:I:2787:THR:OG1	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
2	E	3235/4416 (73%)	2908 (90%)	321 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	12010 (90%)	1326 (10%)	24 (0%)	50	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	4985	LEU
2	E	1708	ARG
2	E	4985	LEU
2	I	1708	ARG
2	I	4985	LEU
2	G	1708	ARG
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	PRO
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
2	E	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
2	G	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
All	All	10324/12444 (83%)	10240 (99%)	84 (1%)	82	89

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3762	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4166	LEU
2	B	4957	LYS
2	B	4958	CYS
2	B	4960	ILE

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Mol	Chain	Res	Type
2	B	4983	HIS
2	B	5027	CYS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3762	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4166	LEU
2	E	4957	LYS
2	E	4958	CYS
2	E	4960	ILE
2	E	4983	HIS
2	E	5027	CYS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3762	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4166	LEU
2	I	4957	LYS
2	I	4958	CYS
2	I	4960	ILE

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Mol	Chain	Res	Type
2	I	4983	HIS
2	I	5027	CYS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3762	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4166	LEU
2	G	4957	LYS
2	G	4958	CYS
2	G	4960	ILE
2	G	4983	HIS
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	582	HIS

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Mol	Chain	Res	Type
2	B	1041	GLN
2	B	1598	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2041	HIS
2	B	3809	ASN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4120	ASN
2	B	4806	ASN
2	B	4973	HIS
2	B	4983	HIS
2	E	57	ASN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	582	HIS
2	E	1041	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2041	HIS
2	E	3781	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN

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Mol	Chain	Res	Type
2	E	4034	ASN
2	E	4120	ASN
2	E	4806	ASN
2	E	4973	HIS
2	E	4983	HIS
2	I	57	ASN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	582	HIS
2	I	1041	GLN
2	I	1598	GLN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2041	HIS
2	I	2884	ASN
2	I	3809	ASN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4120	ASN
2	I	4806	ASN
2	I	4973	HIS
2	I	4983	HIS
2	G	57	ASN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	582	HIS
2	G	1041	GLN

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Mol	Chain	Res	Type
2	G	1598	GLN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2041	HIS
2	G	3781	GLN
2	G	3809	ASN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4120	ASN
2	G	4806	ASN
2	G	4973	HIS
2	G	4983	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	I	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.34	5 (16%)
4	CFF	E	5102	-	8,15,15	2.57	3 (37%)	8,23,23	1.43	2 (25%)
4	CFF	G	5102	-	8,15,15	2.59	3 (37%)	8,23,23	1.43	2 (25%)
3	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
3	ATP	B	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
4	CFF	B	5102	-	8,15,15	2.58	3 (37%)	8,23,23	1.42	2 (25%)
3	ATP	E	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
4	CFF	I	5102	-	8,15,15	2.59	3 (37%)	8,23,23	1.41	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C5-C4	-4.82	1.33	1.39
4	I	5102	CFF	C5-C4	-4.82	1.33	1.39
4	E	5102	CFF	C5-C4	-4.81	1.33	1.39
4	B	5102	CFF	C5-C4	-4.81	1.33	1.39
4	I	5102	CFF	C6-N1	-4.19	1.32	1.38
4	B	5102	CFF	C6-N1	-4.13	1.32	1.38
4	G	5102	CFF	C6-N1	-4.13	1.32	1.38
4	E	5102	CFF	C6-N1	-4.12	1.32	1.38
4	G	5102	CFF	O13-C6	-2.42	1.18	1.24
4	B	5102	CFF	O13-C6	-2.41	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	O13-C6	-2.41	1.18	1.24
4	E	5102	CFF	O13-C6	-2.38	1.18	1.24
3	E	5101	ATP	C5-C4	2.07	1.46	1.40
3	B	5101	ATP	C5-C4	2.04	1.46	1.40
3	G	5101	ATP	C5-C4	2.04	1.46	1.40
3	I	5101	ATP	C5-C4	2.02	1.46	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-3.25	123.60	128.68
3	E	5101	ATP	N3-C2-N1	-3.23	123.62	128.68
3	B	5101	ATP	N3-C2-N1	-3.22	123.64	128.68
3	I	5101	ATP	N3-C2-N1	-3.19	123.69	128.68
3	I	5101	ATP	PB-O3B-PG	-2.90	122.87	132.83
3	B	5101	ATP	PB-O3B-PG	-2.89	122.89	132.83
3	E	5101	ATP	PB-O3B-PG	-2.89	122.92	132.83
3	G	5101	ATP	PB-O3B-PG	-2.88	122.93	132.83
4	B	5102	CFF	C14-N7-C8	-2.77	112.09	125.43
4	I	5102	CFF	C14-N7-C8	-2.77	112.09	125.43
4	E	5102	CFF	C14-N7-C8	-2.77	112.11	125.43
4	G	5102	CFF	C14-N7-C8	-2.76	112.14	125.43
3	G	5101	ATP	PA-O3A-PB	-2.60	123.92	132.83
3	E	5101	ATP	PA-O3A-PB	-2.59	123.94	132.83
3	B	5101	ATP	PA-O3A-PB	-2.59	123.95	132.83
3	I	5101	ATP	PA-O3A-PB	-2.58	123.98	132.83
3	G	5101	ATP	C3'-C2'-C1'	2.44	104.65	100.98
3	B	5101	ATP	C3'-C2'-C1'	2.41	104.61	100.98
3	E	5101	ATP	C3'-C2'-C1'	2.40	104.60	100.98
3	I	5101	ATP	C3'-C2'-C1'	2.39	104.58	100.98
4	E	5102	CFF	C5-C6-N1	2.29	120.64	118.20
4	G	5102	CFF	C5-C6-N1	2.29	120.64	118.20
4	B	5102	CFF	C5-C6-N1	2.25	120.60	118.20
4	I	5102	CFF	C5-C6-N1	2.24	120.59	118.20
3	G	5101	ATP	C4-C5-N7	-2.21	107.10	109.40
3	E	5101	ATP	C4-C5-N7	-2.19	107.11	109.40
3	B	5101	ATP	C4-C5-N7	-2.17	107.14	109.40
3	I	5101	ATP	C4-C5-N7	-2.13	107.18	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

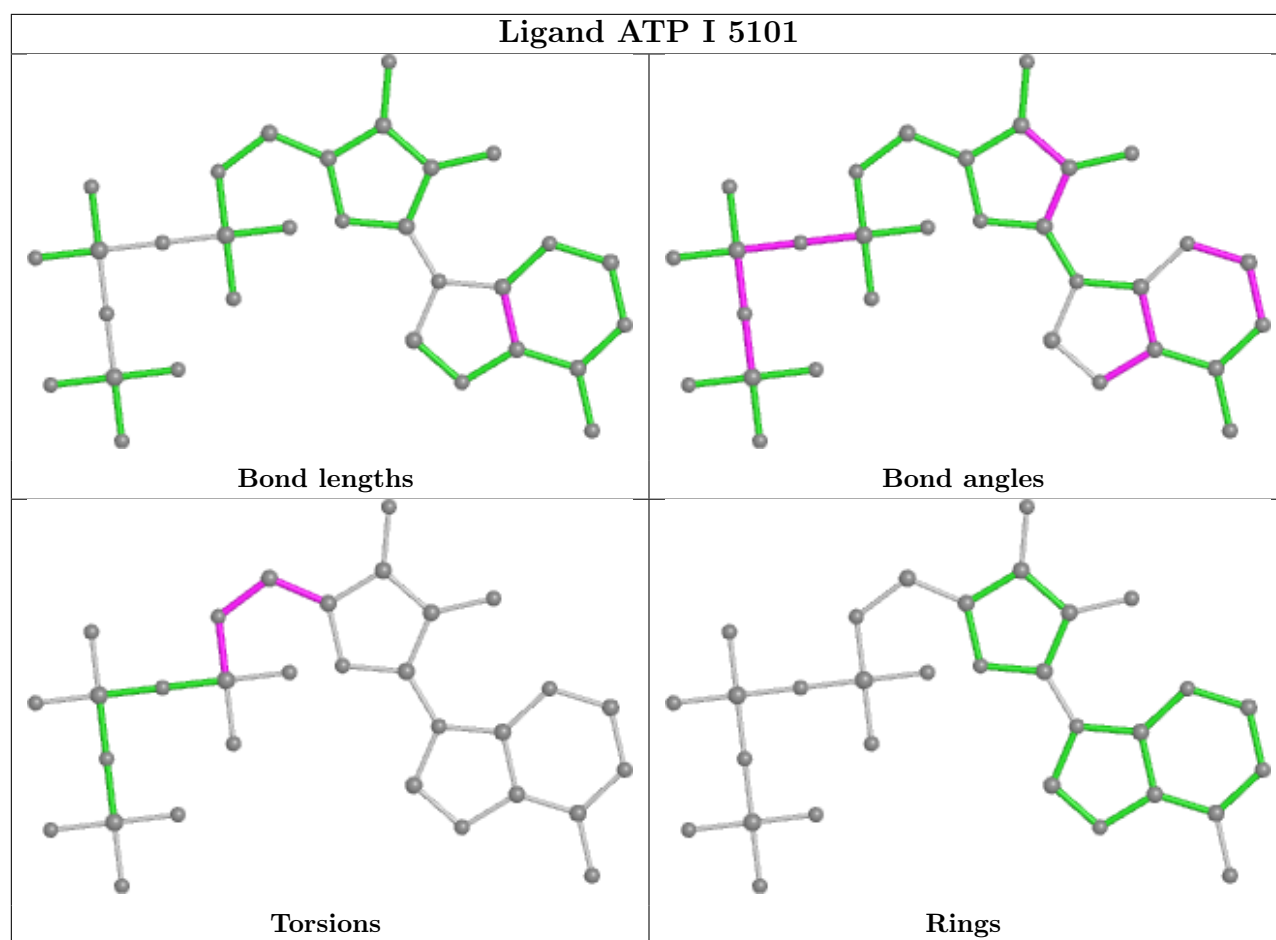
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C3'-C4'-C5'-O5'
3	E	5101	ATP	C3'-C4'-C5'-O5'
3	I	5101	ATP	C3'-C4'-C5'-O5'
3	G	5101	ATP	C3'-C4'-C5'-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A

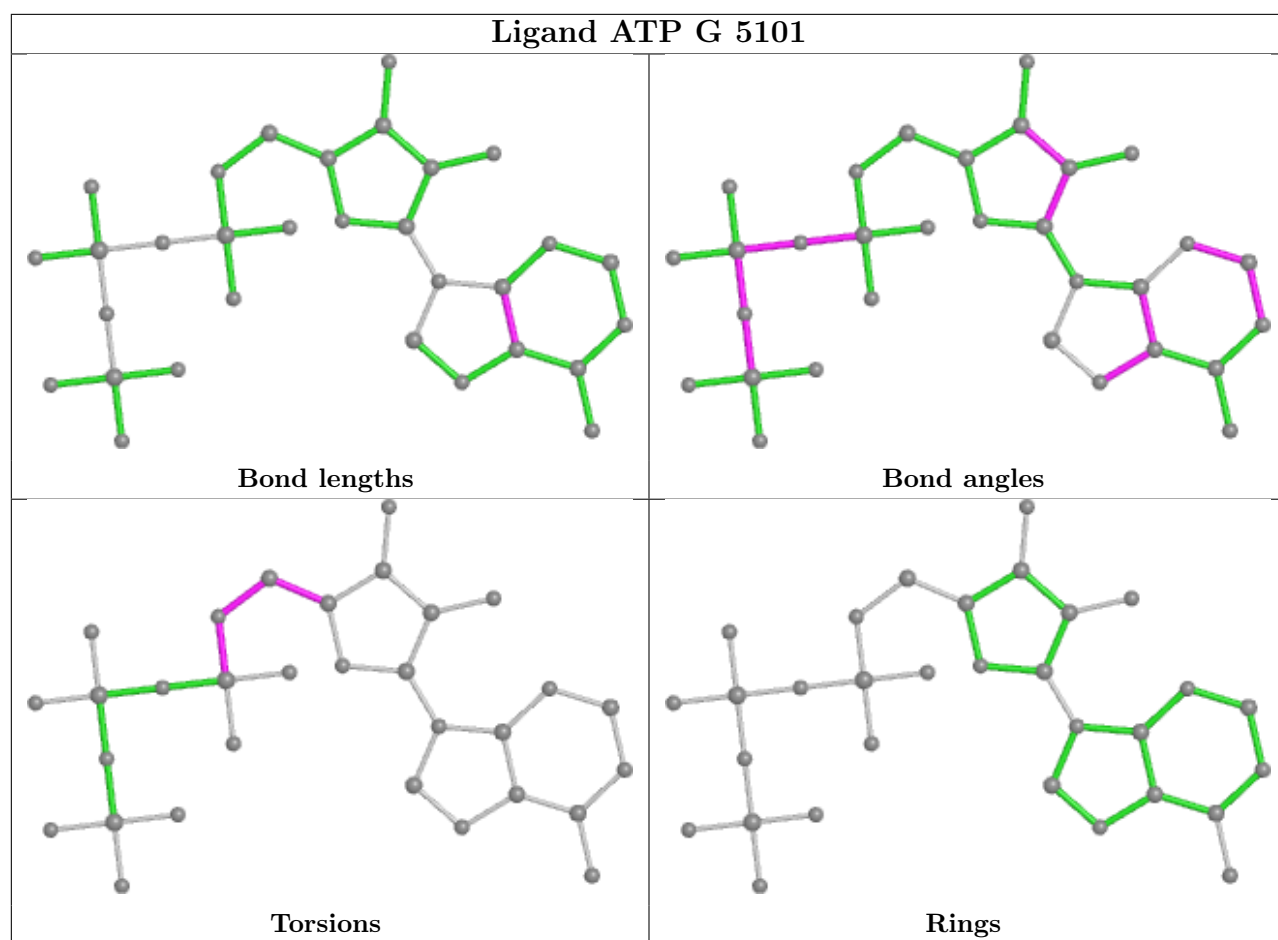
There are no ring outliers.

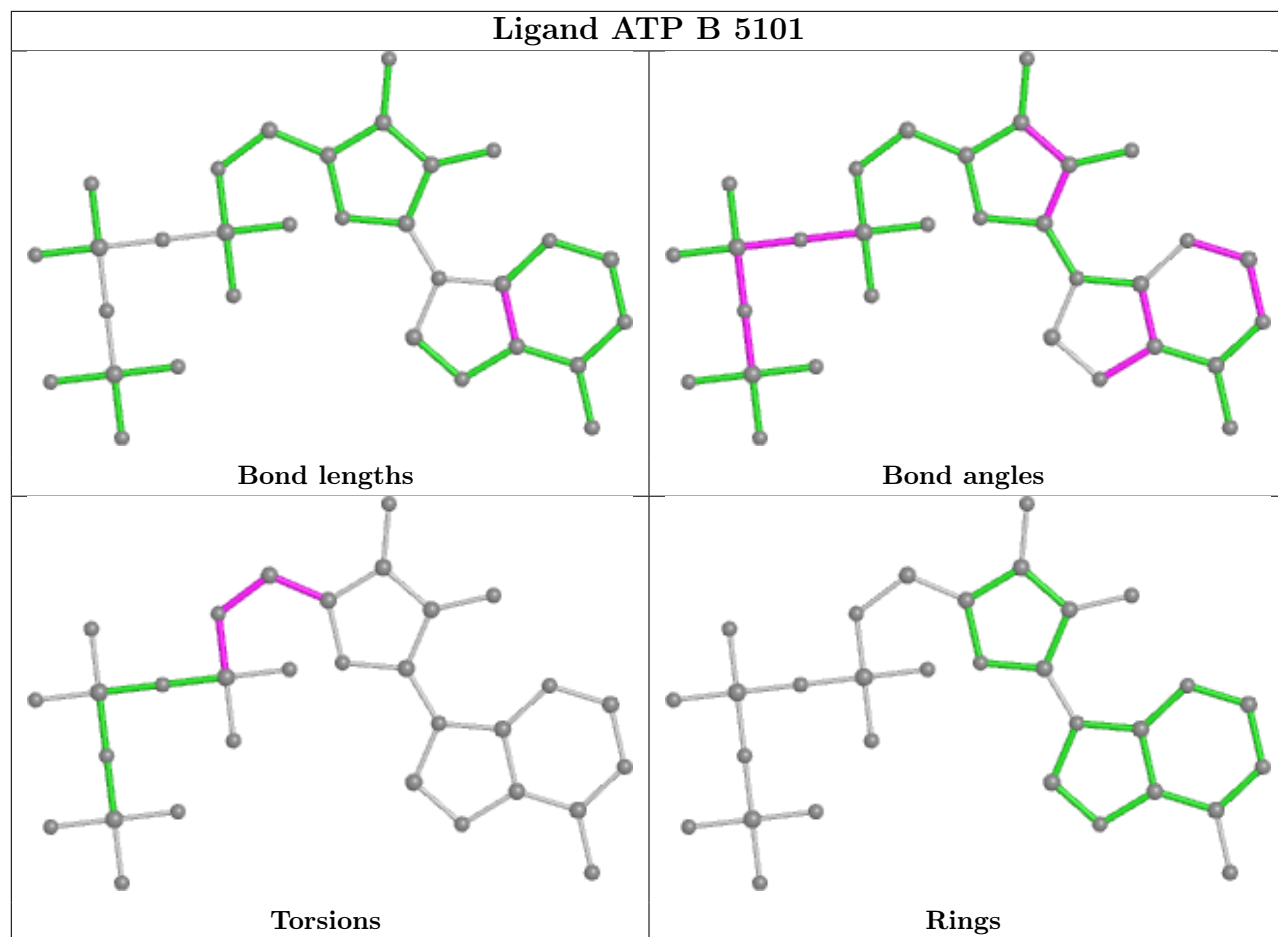
4 monomers are involved in 8 short contacts:

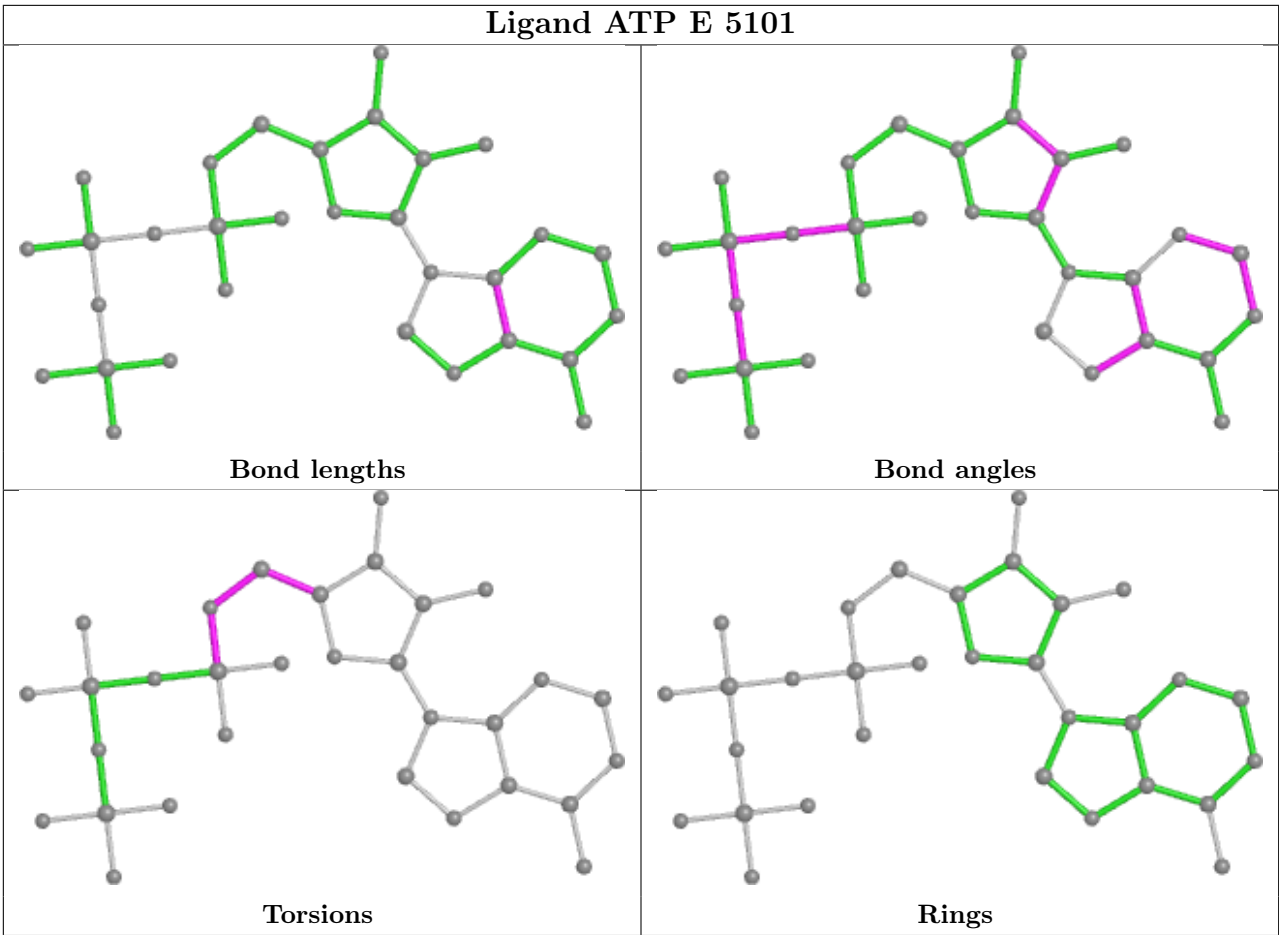
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	5101	ATP	2	0
3	G	5101	ATP	2	0
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.00
1	E	4345:UNK	C	4540:PHE	N	74.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	74.00
1	G	4345:UNK	C	4540:PHE	N	74.00
1	B	3613:UNK	C	3639:THR	N	43.80
1	E	3613:UNK	C	3639:THR	N	43.80
1	I	3613:UNK	C	3639:THR	N	43.80
1	G	3613:UNK	C	3639:THR	N	43.80
1	B	4253:GLU	C	4320:UNK	N	26.28
1	E	4253:GLU	C	4320:UNK	N	26.28
1	I	4253:GLU	C	4320:UNK	N	26.28
1	G	4253:GLU	C	4320:UNK	N	26.28
1	G	3163:UNK	C	3170:UNK	N	16.13
1	B	3163:UNK	C	3170:UNK	N	16.12
1	E	3163:UNK	C	3170:UNK	N	16.12
1	I	3163:UNK	C	3170:UNK	N	16.12
1	B	3063:UNK	C	3134:UNK	N	15.30
1	E	3063:UNK	C	3134:UNK	N	15.30
1	I	3063:UNK	C	3134:UNK	N	15.30
1	G	3063:UNK	C	3134:UNK	N	15.30
1	B	3468:UNK	C	3511:UNK	N	14.89
1	E	3468:UNK	C	3511:UNK	N	14.89
1	I	3468:UNK	C	3511:UNK	N	14.89
1	G	3468:UNK	C	3511:UNK	N	14.89
1	B	2703:UNK	C	2734:ASN	N	13.90
1	E	2703:UNK	C	2734:ASN	N	13.90
1	I	2703:UNK	C	2734:ASN	N	13.90
1	G	2703:UNK	C	2734:ASN	N	13.90
1	B	3236:UNK	C	3241:UNK	N	13.63
1	E	3236:UNK	C	3241:UNK	N	13.63
1	I	3236:UNK	C	3241:UNK	N	13.63
1	G	3236:UNK	C	3241:UNK	N	13.63
1	B	2976:UNK	C	2995:UNK	N	12.77
1	E	2976:UNK	C	2995:UNK	N	12.77
1	I	2976:UNK	C	2995:UNK	N	12.77
1	G	2976:UNK	C	2995:UNK	N	12.77
1	B	1564:UNK	C	1573:MET	N	12.33
1	E	1564:UNK	C	1573:MET	N	12.33
1	I	1564:UNK	C	1573:MET	N	12.33
1	G	1564:UNK	C	1573:MET	N	12.33
1	B	3254:UNK	C	3261:UNK	N	8.26
1	E	3254:UNK	C	3261:UNK	N	8.26
1	I	3254:UNK	C	3261:UNK	N	8.26
1	G	3254:UNK	C	3261:UNK	N	8.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1297:UNK	C	1430:UNK	N	6.06
1	G	1297:UNK	C	1430:UNK	N	6.06
1	B	1297:UNK	C	1430:UNK	N	6.05
1	I	1297:UNK	C	1430:UNK	N	6.05
1	B	2939:ARG	C	2942:UNK	N	3.63
1	E	2939:ARG	C	2942:UNK	N	3.63
1	I	2939:ARG	C	2942:UNK	N	3.63
1	G	2939:ARG	C	2942:UNK	N	3.63
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24

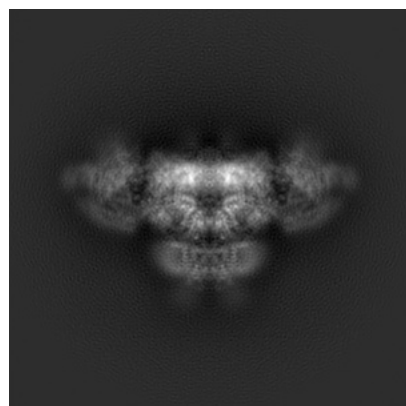
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8381. These allow visual inspection of the internal detail of the map and identification of artifacts.

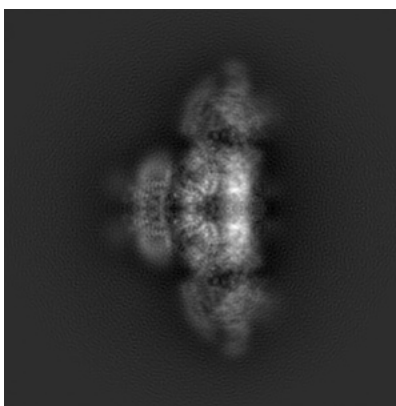
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

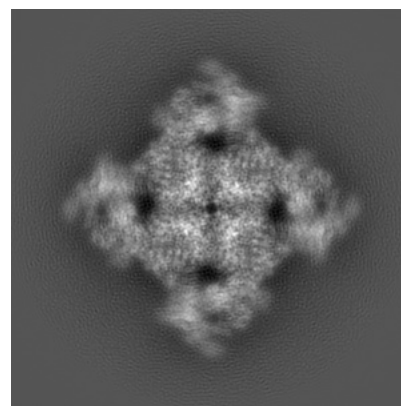
6.1.1 Primary map



X



Y

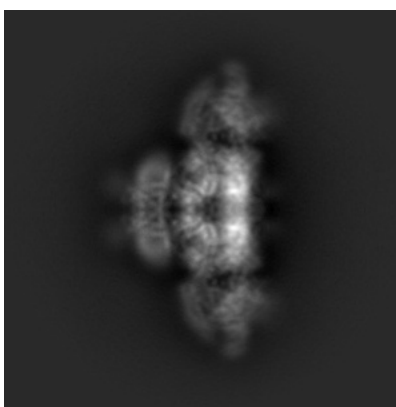


Z

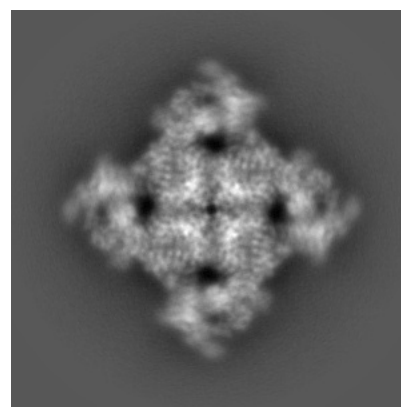
6.1.2 Raw map



X



Y

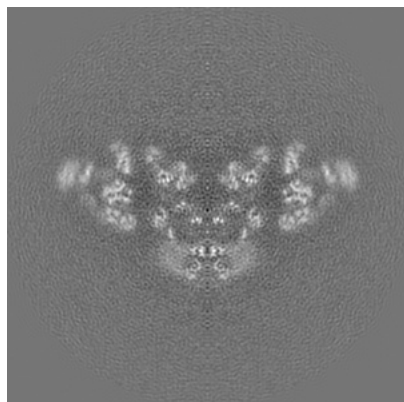


Z

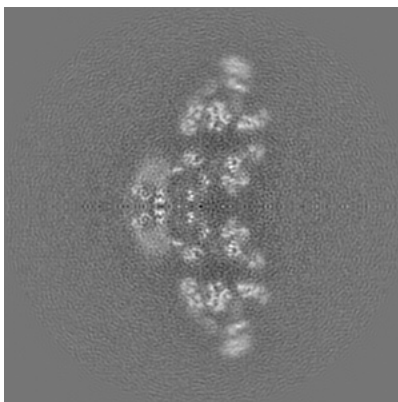
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

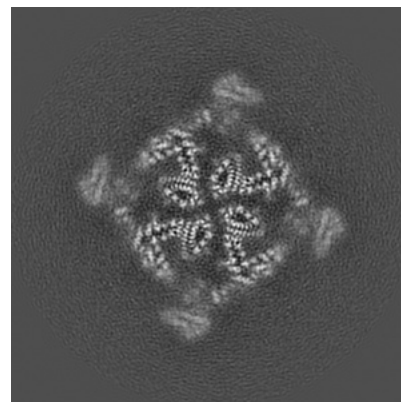
6.2.1 Primary map



X Index: 200

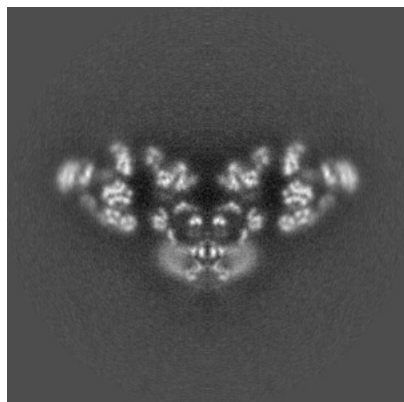


Y Index: 200

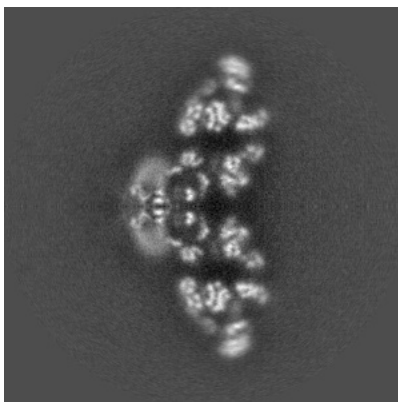


Z Index: 200

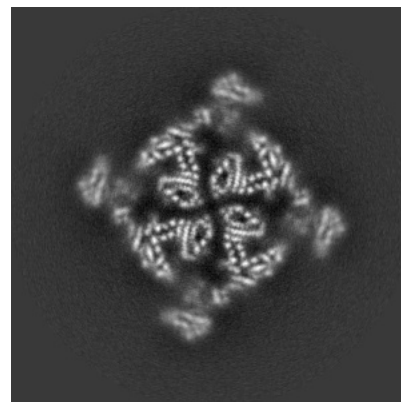
6.2.2 Raw map



X Index: 200



Y Index: 200

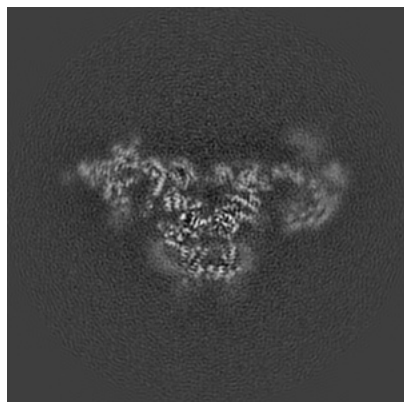


Z Index: 200

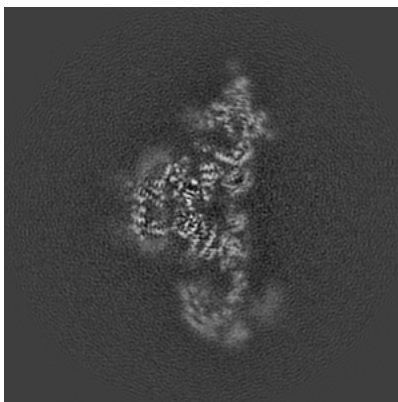
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

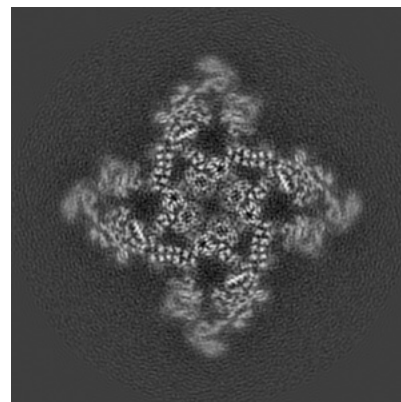
6.3.1 Primary map



X Index: 216

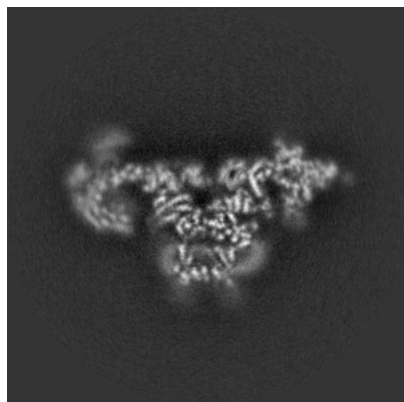


Y Index: 216

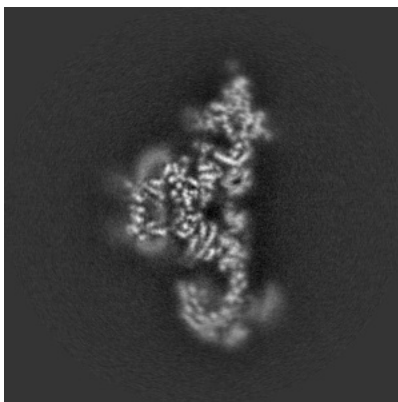


Z Index: 227

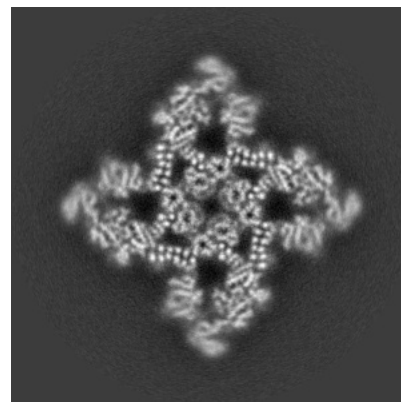
6.3.2 Raw map



X Index: 183



Y Index: 217

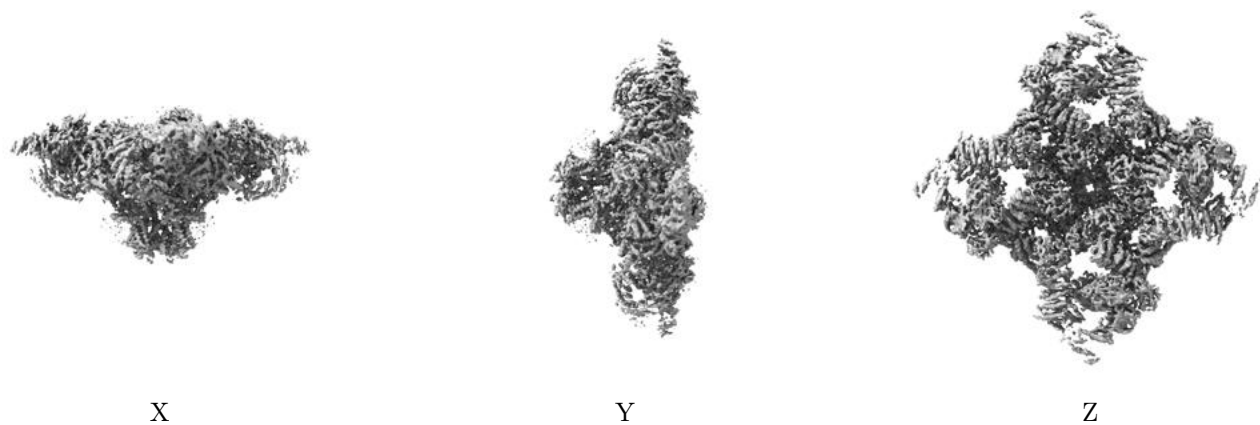


Z Index: 227

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



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

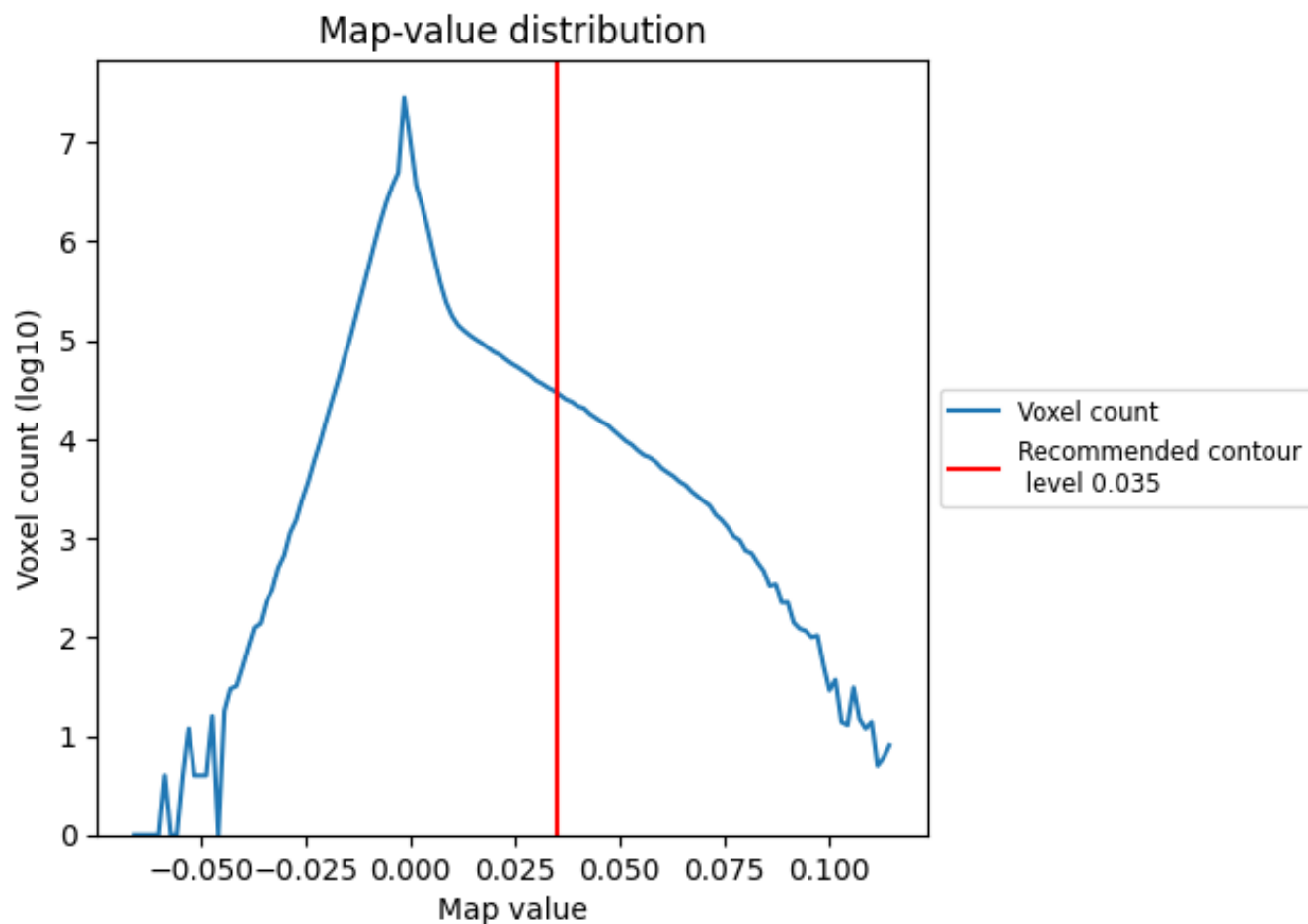
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

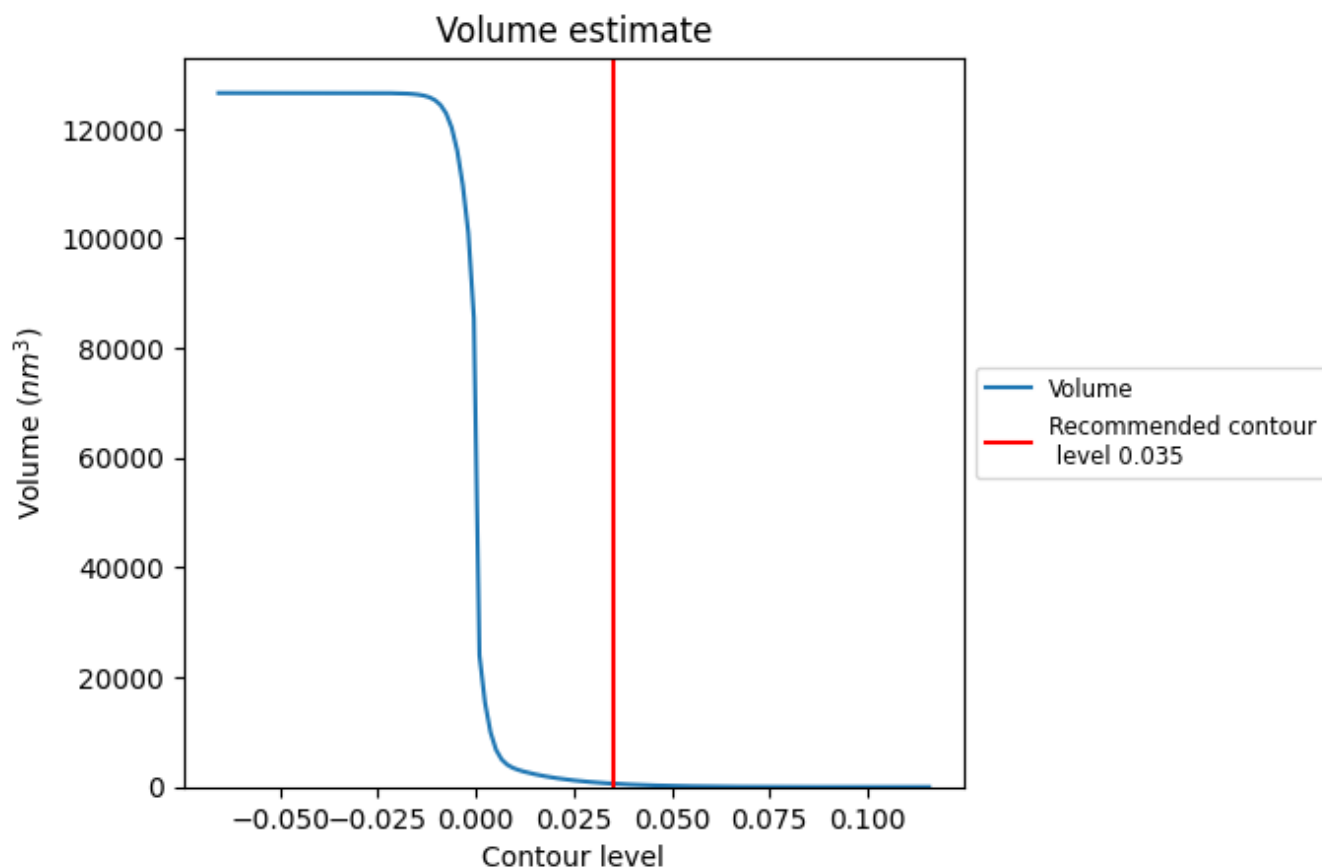
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

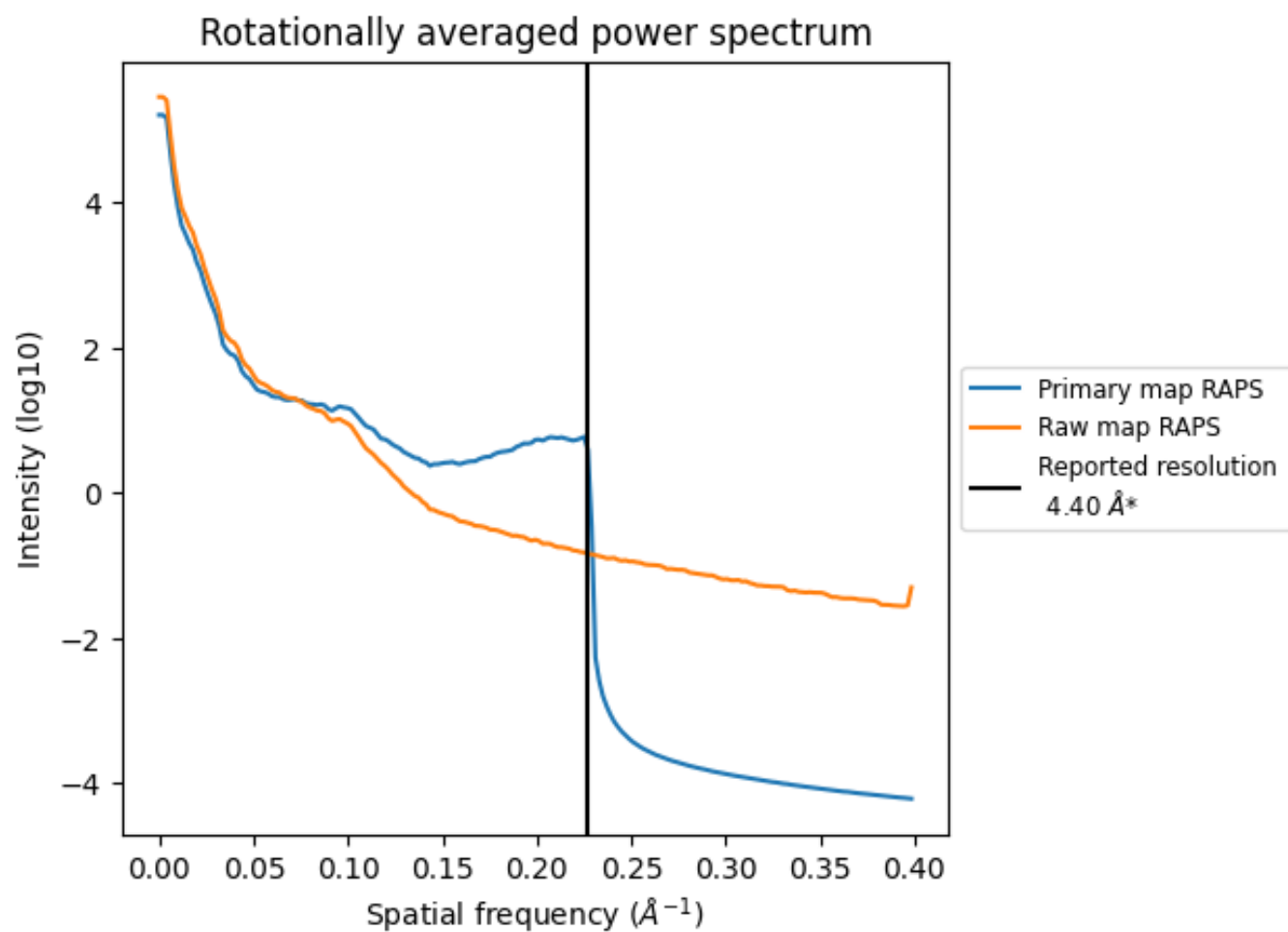
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 610 nm^3 ; this corresponds to an approximate mass of 551 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 ⓘ

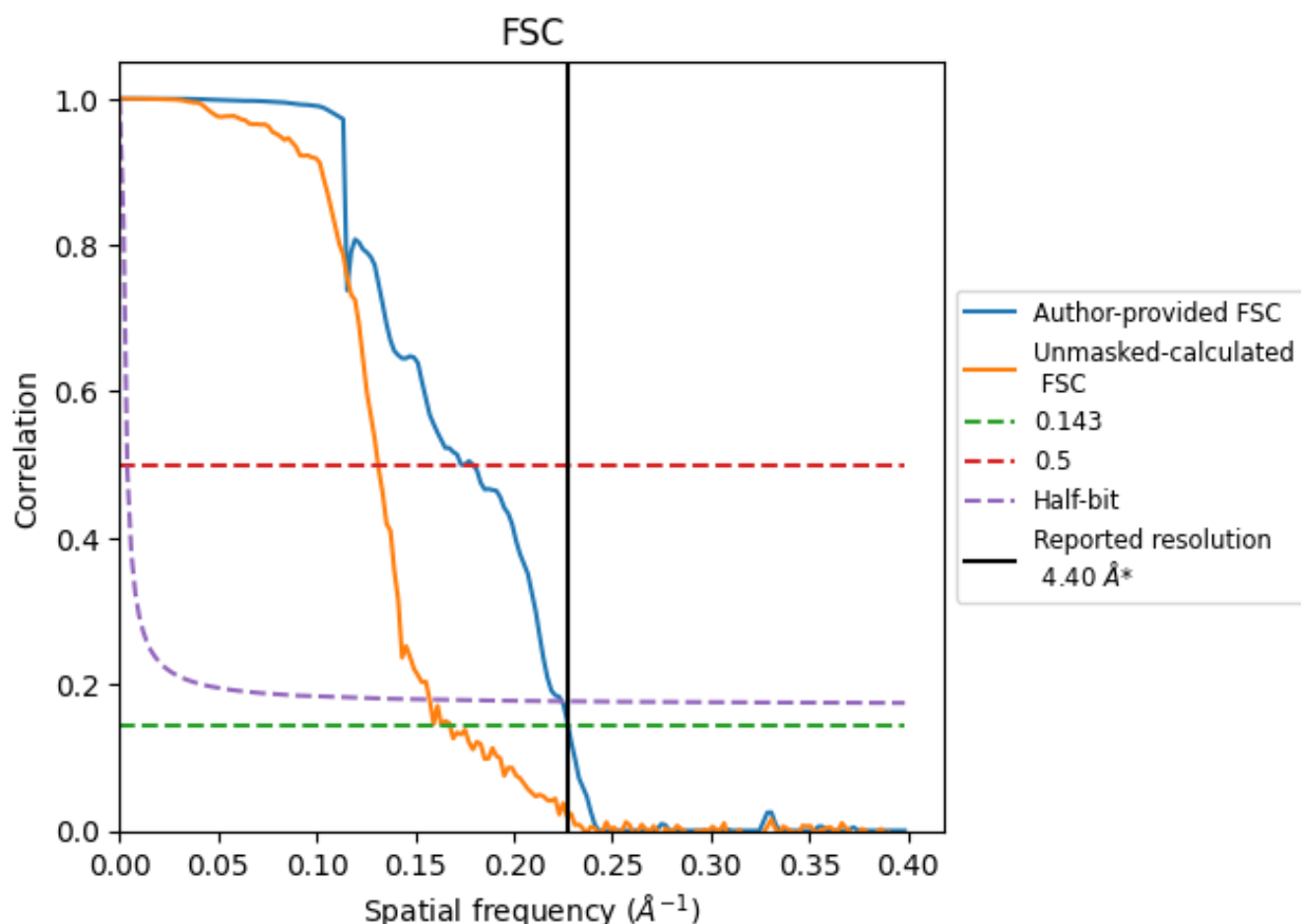


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

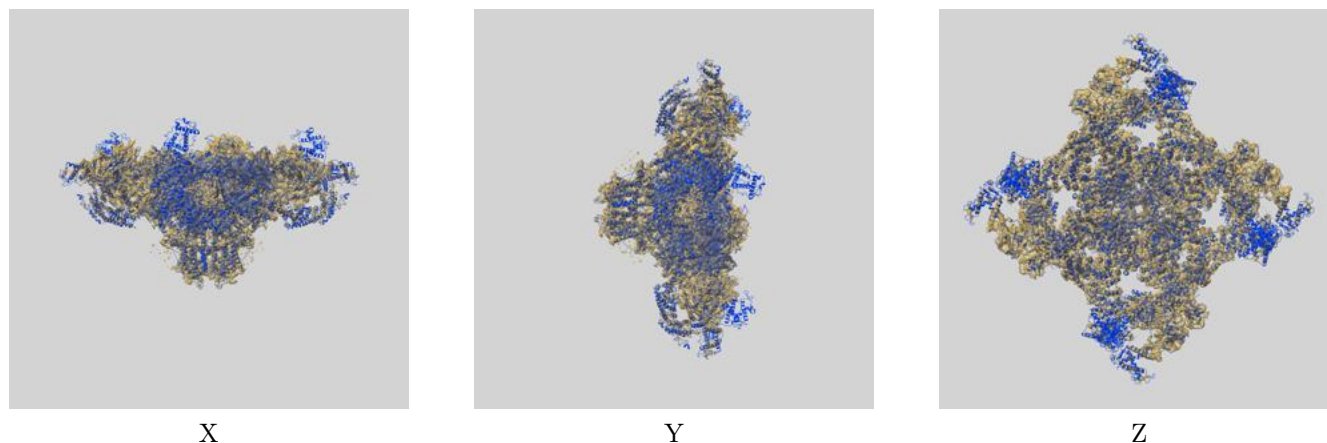
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.39	5.58	4.46
Unmasked-calculated*	5.96	7.62	6.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.96 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

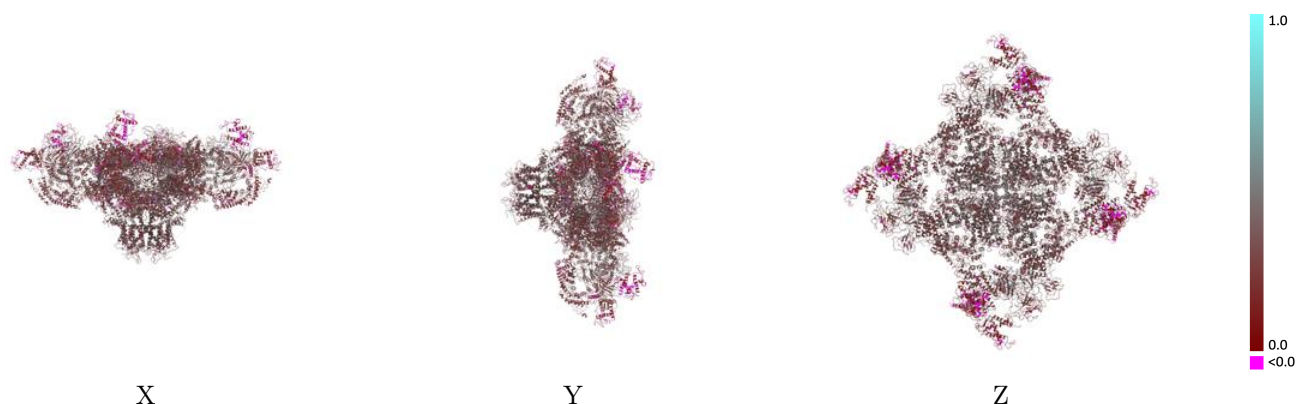
This section contains information regarding the fit between EMDB map EMD-8381 and PDB model 5TAP. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



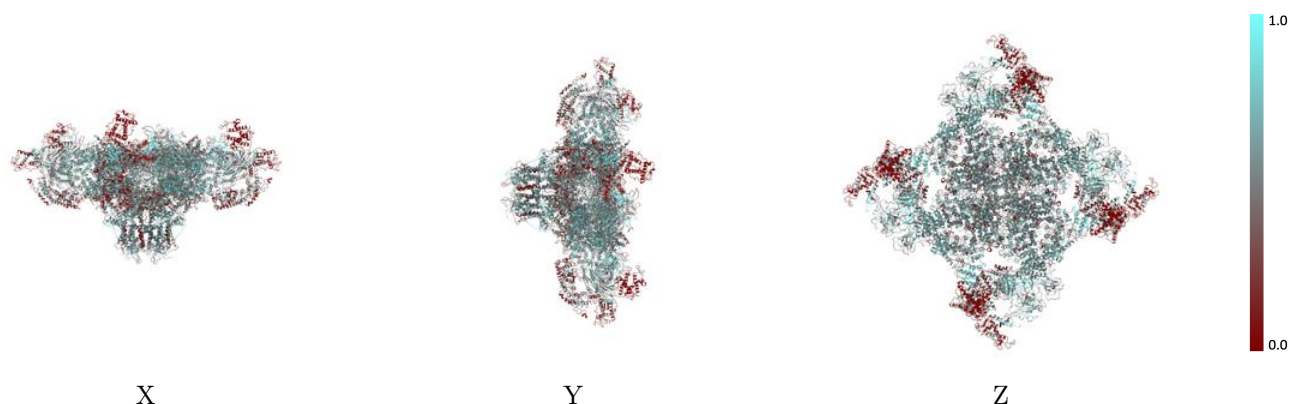
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



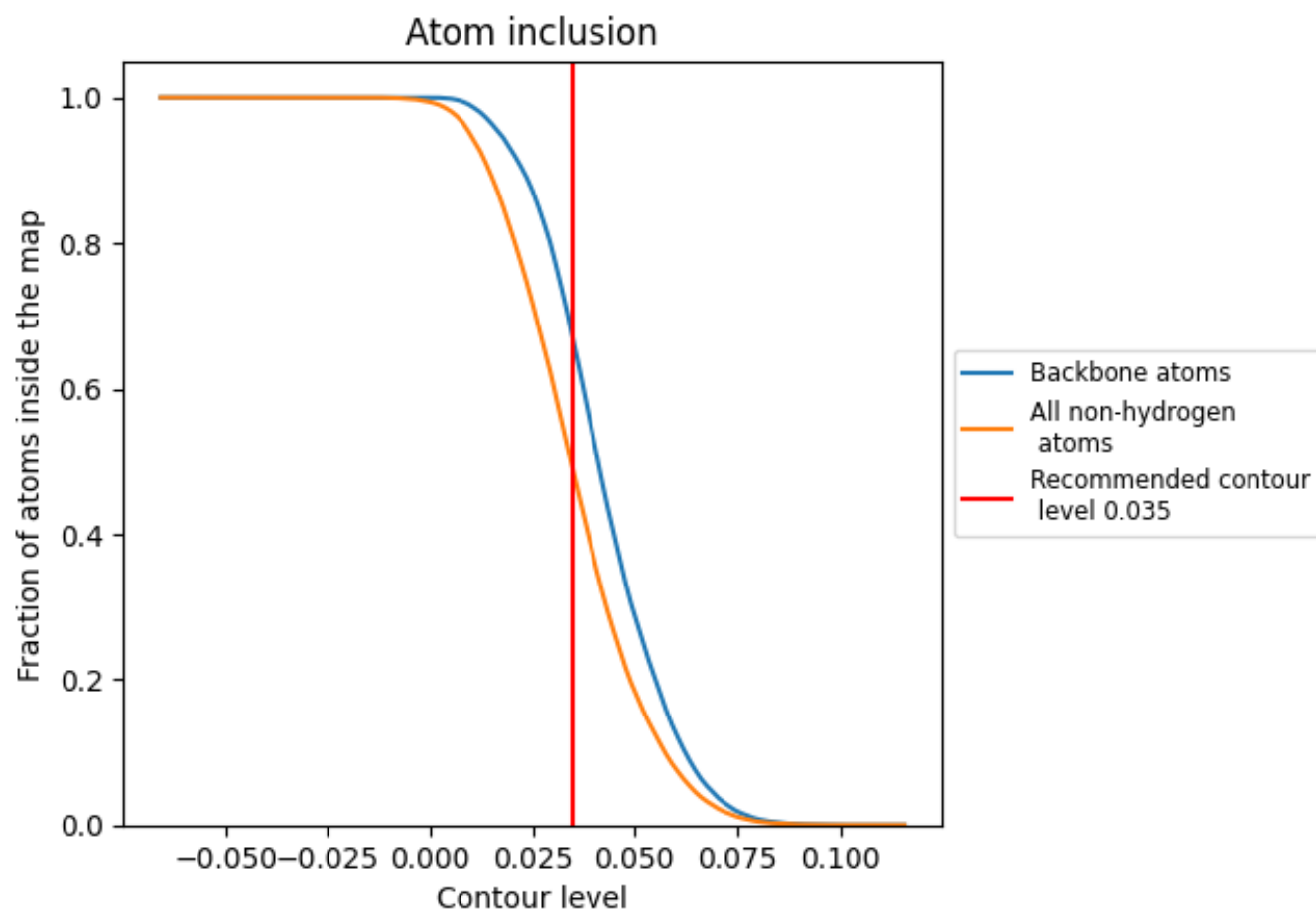
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 48% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.4836	<div><div></div></div> 0.2940
A	<div><div></div></div> 0.4901	<div><div></div></div> 0.3030
B	<div><div></div></div> 0.4838	<div><div></div></div> 0.2940
E	<div><div></div></div> 0.4839	<div><div></div></div> 0.2930
F	<div><div></div></div> 0.4938	<div><div></div></div> 0.3070
G	<div><div></div></div> 0.4833	<div><div></div></div> 0.2930
H	<div><div></div></div> 0.4888	<div><div></div></div> 0.3040
I	<div><div></div></div> 0.4826	<div><div></div></div> 0.2930
J	<div><div></div></div> 0.4901	<div><div></div></div> 0.3020

1.0

0.0

<0.0