



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:56 AM UTC

PDB ID : 8XJI / pdb_00008xji
EMDB ID : EMD-38398
Title : Structure of chimeric RyR complex with flubendiamide
Authors : Lin, L.; Wang, C.; Wang, W.; Jiang, H.; Yuchi, Z.
Deposited on : 2023-12-21
Resolution : 3.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

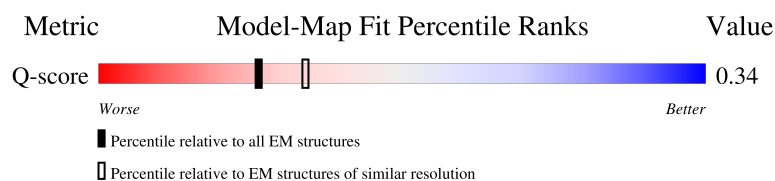
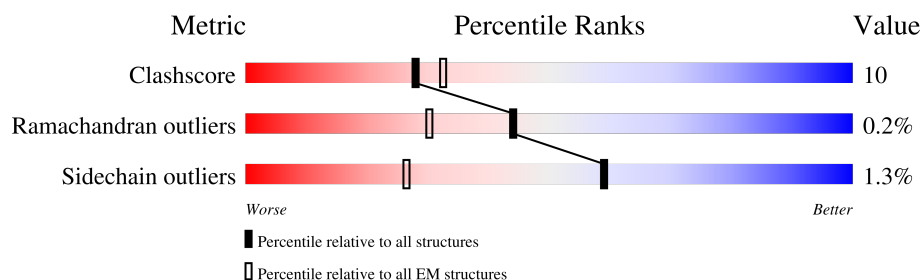
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7920 (3.41 - 4.41)

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	E	107	
1	F	107	
1	G	107	
1	H	107	

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Mol	Chain	Length	Quality of chain
2	I	148	39%69%25%6%
2	J	148	39%70%24%6%
2	K	148	39%68%26%6%
2	L	148	39%68%26%6%
3	A	5037	17%64%14%•22%
3	B	5037	17%64%14%•22%
3	C	5037	17%64%14%•22%
3	D	5037	16%64%14%•22%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 119704 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	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	G	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	K	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	J	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	I	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23
K	32	ALA	GLU	engineered mutation	UNP P0DP23
K	68	ALA	GLU	engineered mutation	UNP P0DP23
K	105	ALA	GLU	engineered mutation	UNP P0DP23
K	141	ALA	GLU	engineered mutation	UNP P0DP23
J	32	ALA	GLU	engineered mutation	UNP P0DP23

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Chain	Residue	Modelled	Actual	Comment	Reference
J	68	ALA	GLU	engineered mutation	UNP P0DP23
J	105	ALA	GLU	engineered mutation	UNP P0DP23
J	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23

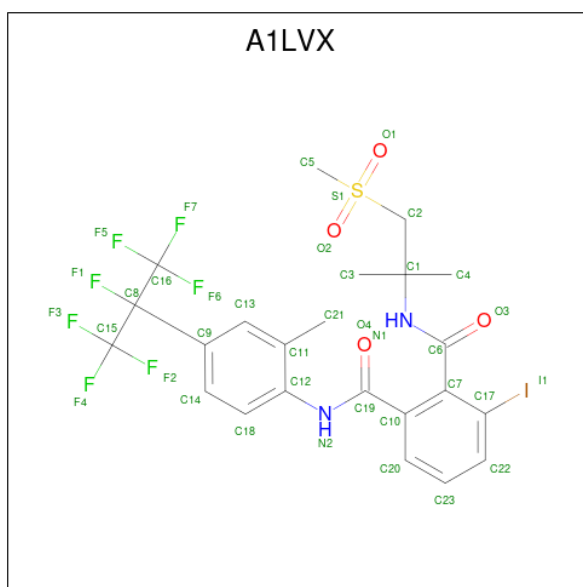
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		
3	A	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		
3	B	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		
3	C	3928	Total	C	N	O	S	1	0
			27995	17849	4984	4987	175		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	4563	LYS	ARG	engineered mutation	UNP P11716
D	4564	TYR	PHE	engineered mutation	UNP P11716
D	4657	ILE	CYS	engineered mutation	UNP P11716
D	4792	SER	LEU	engineered mutation	UNP P11716
A	4563	LYS	ARG	engineered mutation	UNP P11716
A	4564	TYR	PHE	engineered mutation	UNP P11716
A	4657	ILE	CYS	engineered mutation	UNP P11716
A	4792	SER	LEU	engineered mutation	UNP P11716
B	4563	LYS	ARG	engineered mutation	UNP P11716
B	4564	TYR	PHE	engineered mutation	UNP P11716
B	4657	ILE	CYS	engineered mutation	UNP P11716
B	4792	SER	LEU	engineered mutation	UNP P11716
C	4563	LYS	ARG	engineered mutation	UNP P11716
C	4564	TYR	PHE	engineered mutation	UNP P11716
C	4657	ILE	CYS	engineered mutation	UNP P11716
C	4792	SER	LEU	engineered mutation	UNP P11716

- Molecule 4 is Flubendiamide (CCD ID: A1LVX) (formula: $C_{23}H_{22}F_7IN_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
4	D	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	
4	A	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	
4	B	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	
4	C	1	Total	C	F	I	N	O	S	0
			38	23	7	1	2	4	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

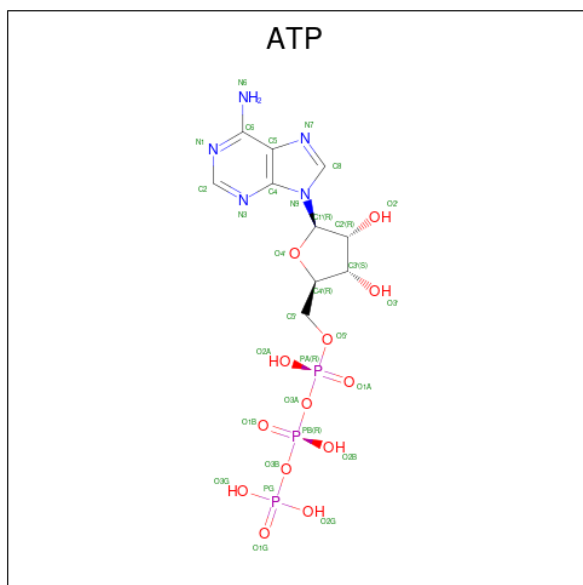
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	

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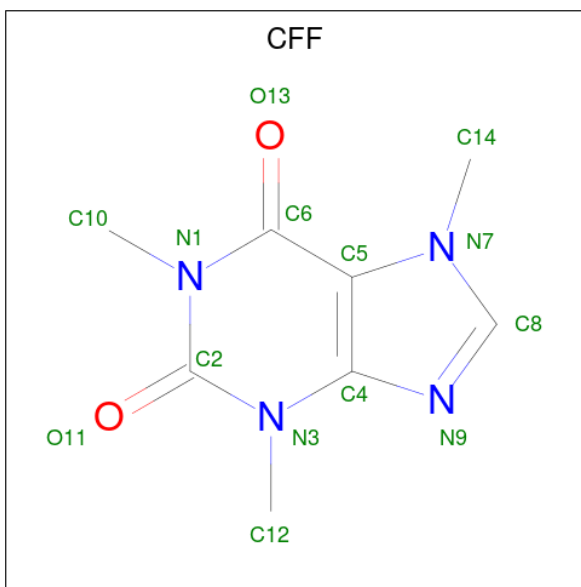
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 8 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).

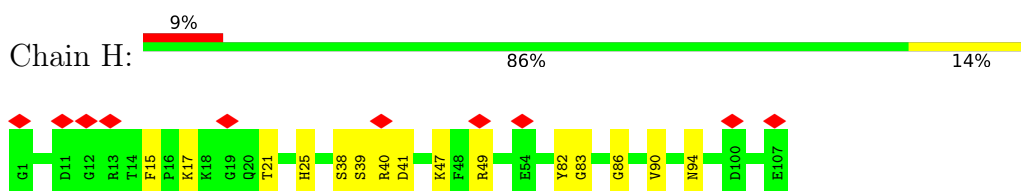


Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			14	8	4	2	
8	A	1	Total	C	N	O	0
			14	8	4	2	
8	B	1	Total	C	N	O	0
			14	8	4	2	
8	C	1	Total	C	N	O	0
			14	8	4	2	

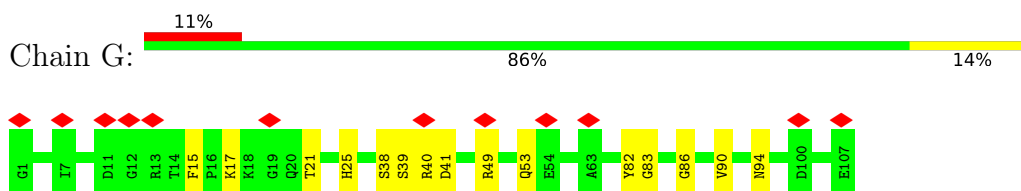
3 Residue-property plots

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.

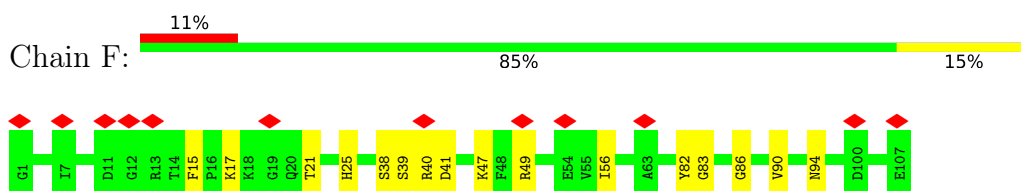
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



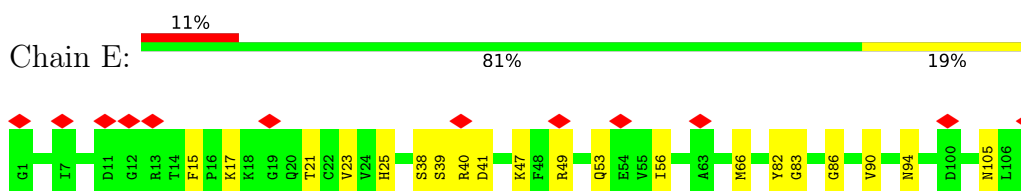
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



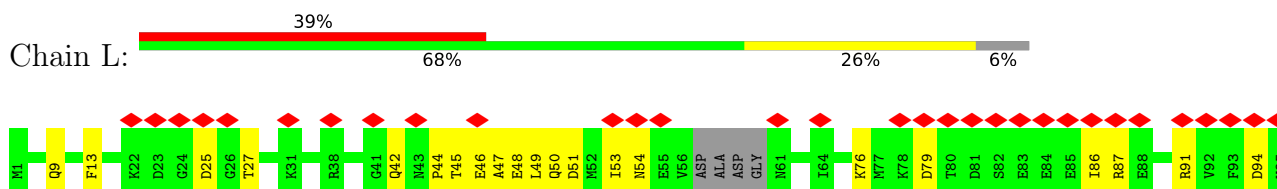
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

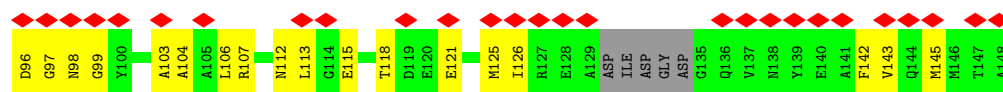


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

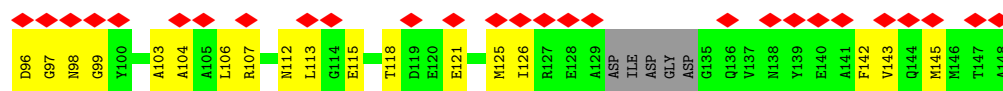
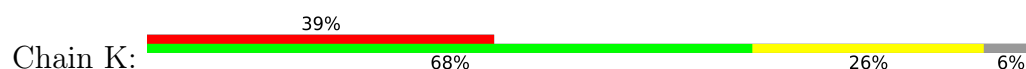


- Molecule 2: Calmodulin-1

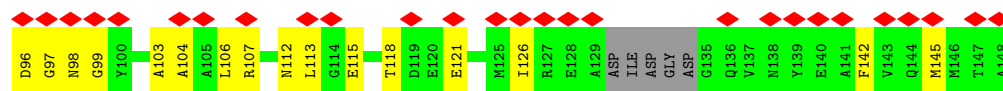
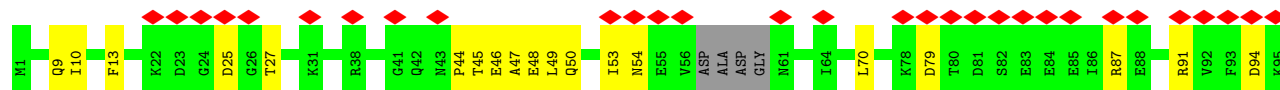
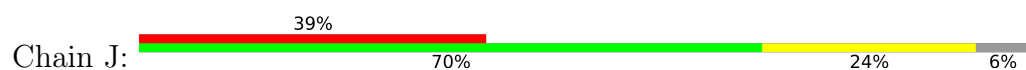




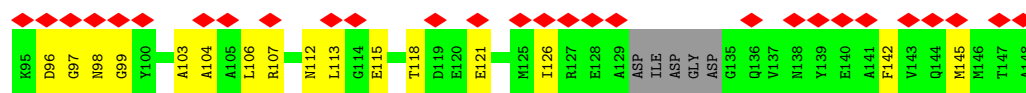
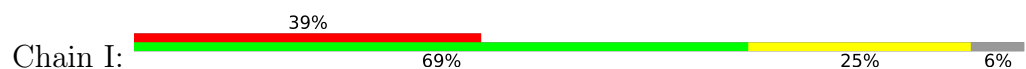
• Molecule 2: Calmodulin-1



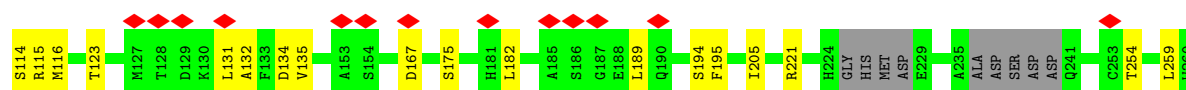
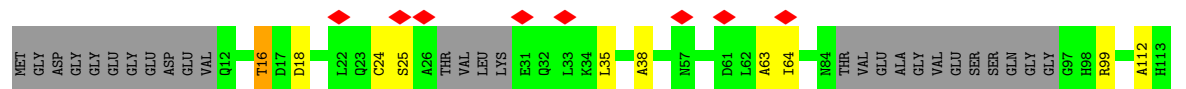
• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



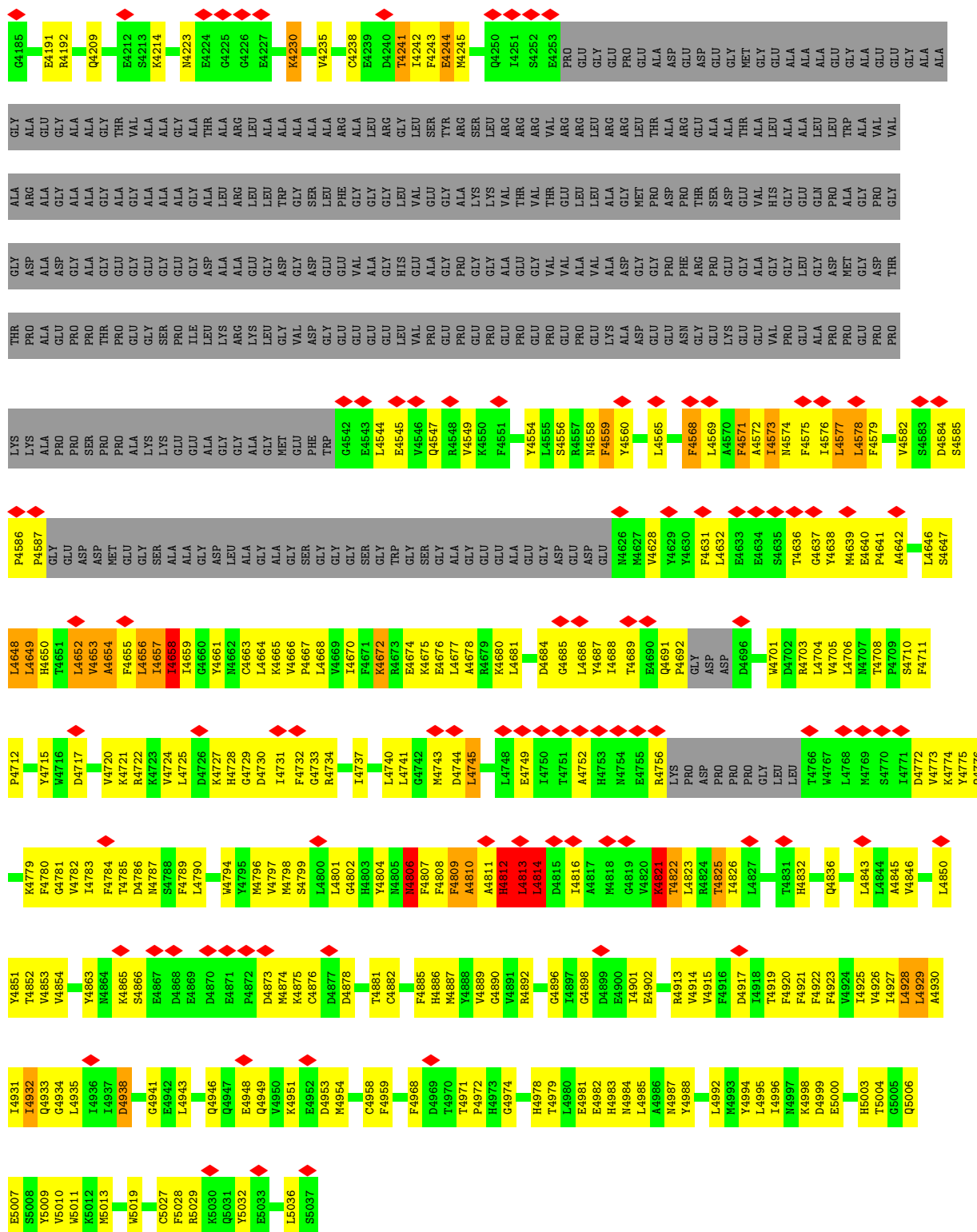
• Molecule 3: Ryanodine receptor 1







M4026	L4027	L4028	S4029	L4030	V4036	M4039	D4046	V4049	M4054	V4055	E4056	M4057	L4058	L4059	F4065	S4074	E4075	A4076	F4077	D4078	D4079	Y4080	P4084	R4085	T4104	G4105	I4108	A4117	D4118	E4121	Q4133	D4138	D4157	P4158	E4165	E4172	R4175	R4180	I4181																	
R3849	K3852	N3860	H3734	E3861	D3862	R3868	Q3869	N3870	G3871	V3874	D3878	F3885	R3886	F3887	L3888	Q3889	D3898	F3899	Q3900	L3903	R3904	N3914	I3915	I3916	T3919	S3929	K3940	Q3946	R3949	N3950	T3966	E3967	Y3968	I3969	Q3970	N3976	Q3977	D3987	M4000	V4024	V4025															
M3729	S3732	C3733	H3734	L3735	E3736	E3737	GLY	GLY	GLU	ASN	GLY	ALA	GLU	GLU	VAL	E3750	V3751	S3752	F3753	Q3766	Q3767	S3768	R3769	L3770	H3771	T3772	R3773	L3780	Q3781	V3794	T3797	L3800	I3804	L3805	M3816	D3818	Y3819	G3827	F3828	F3829	L3842	D3843	A3846													
P3527	T3528	D3529	GLN	ASP	LEU	ILE	M3534	L3535	A3536	A3541	L3542	K3543	E3547	VAL	GLU	ARG	GLU	GLU	PHE	L3553	Q3554	N3555	N3556	L3557	H3558	L3559	GLY	LYS	VAL	GLU	ARG	GLY	GLY	ASP	ARG	TYR	SER	VAL	GLN	VAL	GLU	GLU	ASP	PRO	E3590	V3596	V3599	L3606	E3610	HIS						
R3380	A3383	K3384	A3385	E3386	A3387	E3388	GLU	GLY	GLU	LEU	LEU	VAL	R3395	D3396	E3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	N3418	N3419	R3420	A3421	P3427	N3430	ALA	GLU	GLU	LEU	F3435	V3438	I3441	W3445	S3446	K3452	ARG	GLU	GLU	Q3456	N3457						
F3302	P3303	A3306	V3307	T3308	S3309	ASP	HIS	LEU	ASN	SER	LEU	L3316	V3324	L3327	D3330	E3331	A3332	T3333	TRP	MET	LYS	ARG	LEU	ALA	V3340	F3341	A3342	Q3343	P3344	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	SER	PHE	P3360	T3361	L3365	A3369	V3373	E3376									
GLU	MET	CYS	PRO	ASP	ILE	PRO	VAL	LEU	ASP	ARG	ALA	ILE	GLY	GLY	LEU	ALA	GLU	SER	GLY	ALA	TYR	THR	MET	PRO	HIS	V3269	I3270	E3271	P3275	M3276	Y3280	L3281	P3282	R3283	W3284	W3285	GLU	ARG	GLY	PRO	GLU	ALA	PRO	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301				
TYR	ARG	THR	L3169	C3170	S3171	T3172	I3173	S3174	L3175	G3176	T3177	T3178	E3184	P3188	A3189	LEU	GLY	GLU	CYS	LEU	ALA	VAL	GLN	ASN	VAL	VAL	ASN	CYS	TYR	THR	THR	I3210	N3211	E3212	ASN	ALA	CYS	SER	VAL	TYR	T3221	K3222	S3223	R3225	E3226	R3227	A3228	I3229	L3230	G3231	LEU	PRO	ASN	SER	VAL	GLU
VAL	L3025	A3031	K3034	E3035	M3038	L3042	PHE	CYS	LYS	LEU	ALA	ALA	L3049	H3052	R3053	T3059	D3060	A3061	P3062	VAL	VAL	VAL	VAL	ASN	LEU	THR	TYR	THR	THR	VAL	ALA	LEU	ARG	SER	LEU	ASP	ALA	ARG	THR	VAL	MET	LYS	VAL	L3013	C3014	L3015	TYR	PHE	LEU	THR	PRO	ALA	LYS			
F2955	A2956	F2959	L2960	Q2961	Q2962	W2966	W2967	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	LEU	GLU	ALA	VAL	VAL	SER	SER	GLY	ARG	VAL	VAL	VAL	GLU	GLY	ILE	K2996	F2997	F2998	I3001	L3002	L3003	P3004	L3005	Y3009	H3013	C3014	L3015	TYR	PHE	LEU	THR	PRO	ALA	LYS								



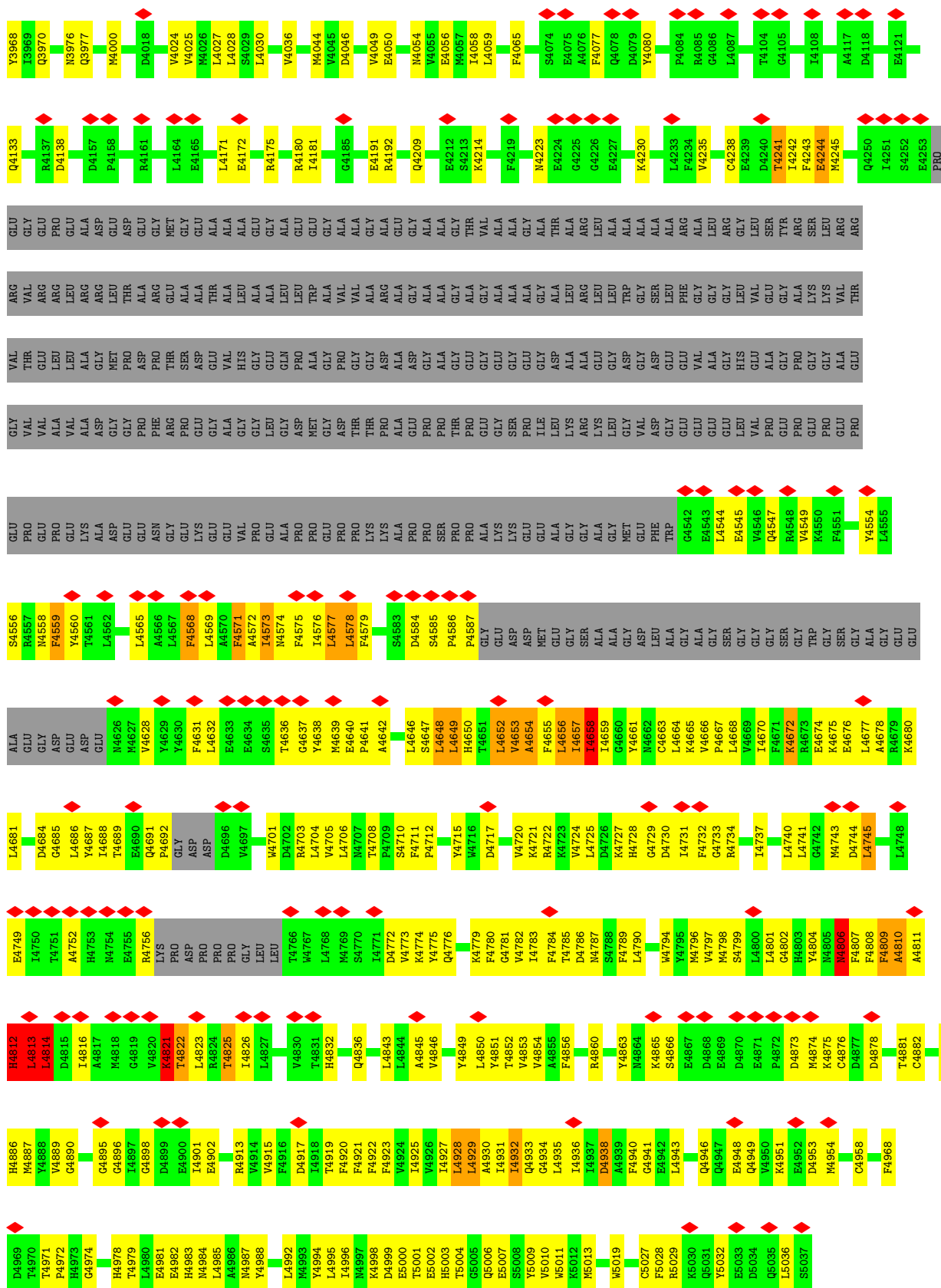
• Molecule 3: Ryanodine receptor 1

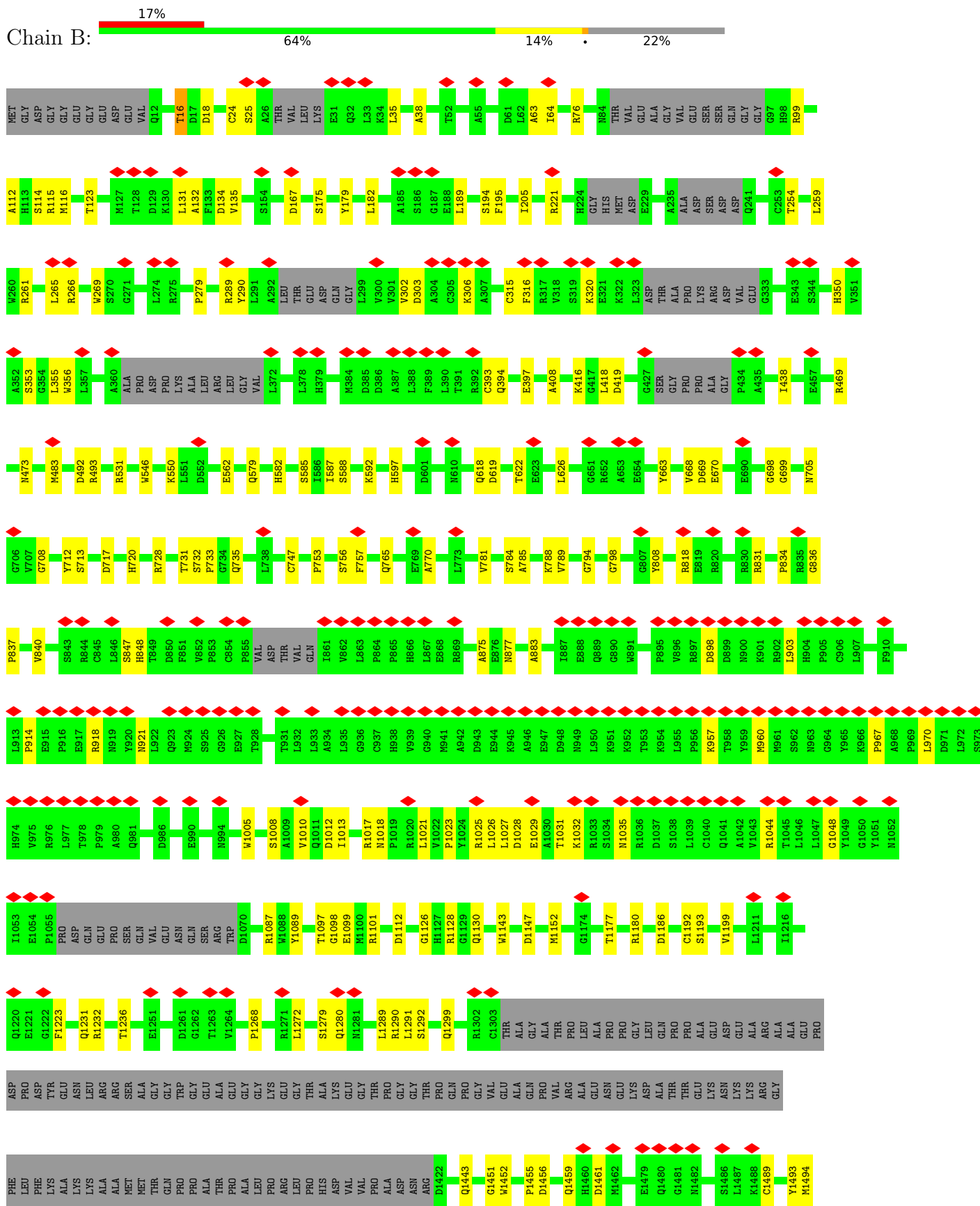


















Chain C: 17% 64% 14% 22%











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35721	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.185	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, A1LVX, ZN, CFF, 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	E	0.38	0/820	0.56	0/1105
1	F	0.38	0/820	0.56	0/1105
1	G	0.38	0/820	0.56	0/1105
1	H	0.37	0/820	0.56	0/1105
2	I	0.24	0/1052	0.53	0/1416
2	J	0.25	0/1052	0.53	0/1416
2	K	0.25	0/1052	0.53	0/1416
2	L	0.24	0/1052	0.53	0/1416
3	A	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
3	B	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
3	C	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
3	D	0.38	3/28526 (0.0%)	0.65	41/38845 (0.1%)
All	All	0.37	12/121592 (0.0%)	0.64	164/165464 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1268	PRO	N-CD	-28.10	1.47	2.03
3	B	1268	PRO	N-CD	-28.10	1.47	2.03
3	C	1268	PRO	N-CD	-28.10	1.47	2.03
3	D	1268	PRO	N-CD	-28.10	1.47	2.03
3	D	4813	LEU	CA-C	-5.38	1.45	1.52
3	A	4813	LEU	CA-C	-5.37	1.45	1.52
3	B	4813	LEU	CA-C	-5.37	1.45	1.52
3	C	4813	LEU	CA-C	-5.37	1.45	1.52
3	B	4806	ASN	C-O	5.33	1.30	1.24
3	D	4806	ASN	C-O	5.30	1.30	1.24
3	A	4806	ASN	C-O	5.26	1.30	1.24
3	C	4806	ASN	C-O	5.26	1.30	1.24

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	836	GLY	CA-C-N	12.15	135.02	119.84
3	C	836	GLY	C-N-CA	12.15	135.02	119.84
3	D	836	GLY	CA-C-N	12.14	135.01	119.84
3	D	836	GLY	C-N-CA	12.14	135.01	119.84
3	A	836	GLY	CA-C-N	12.11	134.98	119.84
3	A	836	GLY	C-N-CA	12.11	134.98	119.84
3	B	836	GLY	CA-C-N	12.10	134.96	119.84
3	B	836	GLY	C-N-CA	12.10	134.96	119.84
3	B	4658	ILE	N-CA-C	-9.49	102.62	111.45
3	C	4658	ILE	N-CA-C	-9.49	102.62	111.45
3	D	4658	ILE	N-CA-C	-9.49	102.63	111.45
3	A	4658	ILE	N-CA-C	-9.46	102.65	111.45
3	C	4654	ALA	N-CA-C	-9.10	99.66	112.13
3	D	4654	ALA	N-CA-C	-9.09	99.67	112.13
3	B	4654	ALA	N-CA-C	-9.09	99.67	112.13
3	A	4654	ALA	N-CA-C	-9.09	99.68	112.13
3	B	3294	PRO	N-CA-CB	7.98	110.88	103.46
3	D	3294	PRO	N-CA-CB	7.93	110.84	103.46
3	A	3294	PRO	N-CA-CB	7.92	110.83	103.46
3	C	3294	PRO	N-CA-CB	7.90	110.81	103.46
3	C	4656	LEU	CA-C-N	7.82	132.01	122.16
3	C	4656	LEU	C-N-CA	7.82	132.01	122.16
3	A	3527	PRO	N-CA-CB	7.82	110.62	103.20
3	D	3527	PRO	N-CA-CB	7.81	110.62	103.20
3	D	4656	LEU	CA-C-N	7.80	131.99	122.16
3	D	4656	LEU	C-N-CA	7.80	131.99	122.16
3	A	4656	LEU	CA-C-N	7.80	131.98	122.16
3	A	4656	LEU	C-N-CA	7.80	131.98	122.16
3	C	3527	PRO	N-CA-CB	7.79	110.60	103.20
3	B	3527	PRO	N-CA-CB	7.79	110.60	103.20
3	C	3302	PRO	N-CA-CB	7.79	110.63	103.08
3	D	3302	PRO	N-CA-CB	7.77	110.62	103.08
3	A	3302	PRO	N-CA-CB	7.77	110.61	103.08
3	B	4656	LEU	CA-C-N	7.76	131.94	122.16
3	B	4656	LEU	C-N-CA	7.76	131.94	122.16
3	B	3302	PRO	N-CA-CB	7.73	110.58	103.08
3	A	4809	PHE	N-CA-C	-7.68	104.33	112.93
3	D	4809	PHE	N-CA-C	-7.66	104.35	112.93
3	B	4809	PHE	N-CA-C	-7.64	104.37	112.93
3	C	4809	PHE	N-CA-C	-7.64	104.37	112.93
3	B	3188	PRO	N-CA-CB	7.49	110.70	103.51
3	D	3188	PRO	N-CA-CB	7.49	110.70	103.51
3	A	3301	PRO	N-CA-CB	7.49	110.34	103.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3301	PRO	N-CA-CB	7.49	110.34	103.08
3	D	3301	PRO	N-CA-CB	7.49	110.34	103.08
3	A	3188	PRO	N-CA-CB	7.48	110.69	103.51
3	C	3188	PRO	N-CA-CB	7.48	110.69	103.51
3	D	3344	PRO	N-CA-CB	7.48	110.69	103.51
3	B	3344	PRO	N-CA-CB	7.47	110.68	103.51
3	C	3301	PRO	N-CA-CB	7.46	110.32	103.08
3	A	3344	PRO	N-CA-CB	7.45	110.66	103.51
3	C	3344	PRO	N-CA-CB	7.45	110.66	103.51
3	A	3275	PRO	N-CA-CB	7.37	110.58	103.51
3	B	3275	PRO	N-CA-CB	7.35	110.57	103.51
3	C	3275	PRO	N-CA-CB	7.34	110.56	103.51
3	D	3275	PRO	N-CA-CB	7.34	110.56	103.51
3	B	3519	PRO	N-CA-CB	7.32	110.54	103.51
3	D	3519	PRO	N-CA-CB	7.32	110.53	103.51
3	A	3519	PRO	N-CA-CB	7.29	110.51	103.51
3	C	3519	PRO	N-CA-CB	7.29	110.51	103.51
3	C	3293	PRO	N-CA-CB	7.12	110.84	103.00
3	A	3293	PRO	N-CA-CB	7.11	110.82	103.00
3	D	3293	PRO	N-CA-CB	7.10	110.81	103.00
3	B	3293	PRO	N-CA-CB	7.08	110.78	103.00
3	D	2640	PRO	N-CA-CB	7.07	110.30	103.51
3	B	2640	PRO	N-CA-CB	7.04	110.27	103.51
3	A	2640	PRO	N-CA-CB	7.03	110.26	103.51
3	C	2640	PRO	N-CA-CB	7.03	110.26	103.51
3	C	4657	ILE	N-CA-C	-6.99	105.81	113.43
3	B	4657	ILE	N-CA-C	-6.98	105.82	113.43
3	B	3282	PRO	N-CA-CB	6.95	110.89	103.52
3	A	3224	PRO	N-CA-CB	6.95	110.88	103.52
3	B	3303	PRO	N-CA-CB	6.94	110.88	103.52
3	D	4657	ILE	N-CA-C	-6.94	105.87	113.43
3	D	3303	PRO	N-CA-CB	6.94	110.87	103.52
3	D	3282	PRO	N-CA-CB	6.93	110.87	103.52
3	C	3224	PRO	N-CA-CB	6.93	110.87	103.52
3	A	3303	PRO	N-CA-CB	6.93	110.87	103.52
3	A	3360	PRO	N-CA-CB	6.93	110.86	103.52
3	B	3224	PRO	N-CA-CB	6.93	110.86	103.52
3	D	3224	PRO	N-CA-CB	6.92	110.85	103.52
3	C	3282	PRO	N-CA-CB	6.92	110.85	103.52
3	C	3303	PRO	N-CA-CB	6.91	110.85	103.52
3	B	3360	PRO	N-CA-CB	6.91	110.85	103.52
3	C	3297	PRO	N-CA-CB	6.91	110.50	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4657	ILE	N-CA-C	-6.90	105.91	113.43
3	A	3282	PRO	N-CA-CB	6.89	110.82	103.52
3	D	3360	PRO	N-CA-CB	6.89	110.82	103.52
3	C	3360	PRO	N-CA-CB	6.89	110.82	103.52
3	D	3297	PRO	N-CA-CB	6.88	110.48	103.25
3	B	3297	PRO	N-CA-CB	6.88	110.47	103.25
3	D	4559	PHE	O-C-N	-6.86	113.47	122.59
3	A	3297	PRO	N-CA-CB	6.86	110.45	103.25
3	B	4559	PHE	O-C-N	-6.85	113.47	122.59
3	A	4559	PHE	O-C-N	-6.84	113.49	122.59
3	C	3004	PRO	N-CA-CB	6.83	110.42	103.25
3	C	4559	PHE	O-C-N	-6.81	113.53	122.59
3	C	3062	PRO	N-CA-CB	6.81	110.49	103.00
3	D	3004	PRO	N-CA-CB	6.80	110.39	103.25
3	B	3208	PRO	N-CA-CB	6.80	110.73	103.52
3	A	3004	PRO	N-CA-CB	6.80	110.39	103.25
3	D	3062	PRO	N-CA-CB	6.79	110.47	103.00
3	A	3062	PRO	N-CA-CB	6.79	110.47	103.00
3	B	3062	PRO	N-CA-CB	6.79	110.47	103.00
3	C	3208	PRO	N-CA-CB	6.79	110.71	103.52
3	D	3208	PRO	N-CA-CB	6.78	110.70	103.52
3	B	3004	PRO	N-CA-CB	6.76	110.35	103.25
3	A	3208	PRO	N-CA-CB	6.75	110.67	103.52
3	D	3410	PRO	N-CA-CB	6.66	110.58	103.52
3	C	3410	PRO	N-CA-CB	6.65	110.57	103.52
3	B	3410	PRO	N-CA-CB	6.65	110.56	103.52
3	A	3410	PRO	N-CA-CB	6.63	110.54	103.52
3	B	3427	PRO	N-CA-CB	6.59	110.82	103.44
3	C	3427	PRO	N-CA-CB	6.59	110.82	103.44
3	A	3427	PRO	N-CA-CB	6.56	110.79	103.44
3	D	3427	PRO	N-CA-CB	6.55	110.78	103.44
3	D	4814	LEU	N-CA-C	6.52	121.07	113.18
3	A	4814	LEU	N-CA-C	6.52	121.07	113.18
3	B	4814	LEU	N-CA-C	6.49	121.04	113.18
3	C	4814	LEU	N-CA-C	6.49	121.04	113.18
3	B	3202	PRO	N-CA-CB	6.42	110.62	103.44
3	C	3202	PRO	N-CA-CB	6.41	110.62	103.44
3	A	4812	HIS	N-CA-C	-6.40	103.82	111.69
3	D	3202	PRO	N-CA-CB	6.40	110.61	103.44
3	A	3202	PRO	N-CA-CB	6.40	110.61	103.44
3	B	4812	HIS	N-CA-C	-6.39	103.83	111.69
3	D	4812	HIS	N-CA-C	-6.38	103.85	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4812	HIS	N-CA-C	-6.37	103.86	111.69
3	B	3351	PRO	N-CA-CB	6.32	110.22	103.52
3	A	3351	PRO	N-CA-CB	6.31	110.20	103.52
3	C	3351	PRO	N-CA-CB	6.30	110.19	103.52
3	D	3351	PRO	N-CA-CB	6.29	110.19	103.52
3	B	4821	LYS	CA-C-N	6.04	129.19	120.38
3	B	4821	LYS	C-N-CA	6.04	129.19	120.38
3	D	4821	LYS	CA-C-N	6.03	129.19	120.38
3	D	4821	LYS	C-N-CA	6.03	129.19	120.38
3	C	4821	LYS	CA-C-N	6.03	129.18	120.38
3	C	4821	LYS	C-N-CA	6.03	129.18	120.38
3	A	4821	LYS	CA-C-N	5.99	129.13	120.38
3	A	4821	LYS	C-N-CA	5.99	129.13	120.38
3	D	836	GLY	C-N-CD	-5.69	101.67	125.00
3	A	836	GLY	C-N-CD	-5.69	101.68	125.00
3	B	836	GLY	C-N-CD	-5.69	101.68	125.00
3	C	836	GLY	C-N-CD	-5.67	101.73	125.00
3	D	4560	TYR	N-CA-C	5.52	118.00	111.33
3	A	4560	TYR	N-CA-C	5.50	117.99	111.33
3	B	4560	TYR	N-CA-C	5.50	117.98	111.33
3	C	4560	TYR	N-CA-C	5.50	117.98	111.33
3	C	4656	LEU	O-C-N	-5.42	113.70	122.42
3	B	4656	LEU	O-C-N	-5.40	113.73	122.42
3	D	4656	LEU	O-C-N	-5.39	113.74	122.42
3	A	4656	LEU	O-C-N	-5.38	113.75	122.42
3	B	4806	ASN	O-C-N	-5.27	115.58	122.59
3	D	4806	ASN	O-C-N	-5.26	115.60	122.59
3	A	4806	ASN	O-C-N	-5.25	115.61	122.59
3	C	4806	ASN	O-C-N	-5.25	115.61	122.59
3	A	4811	ALA	N-CA-C	-5.16	107.15	113.50
3	D	4811	ALA	N-CA-C	-5.15	107.17	113.50
3	B	4811	ALA	N-CA-C	-5.14	107.18	113.50
3	A	4810	ALA	N-CA-C	-5.14	105.69	112.94
3	C	4810	ALA	N-CA-C	-5.12	105.72	112.94
3	B	4810	ALA	N-CA-C	-5.12	105.72	112.94
3	C	4811	ALA	N-CA-C	-5.12	107.20	113.50
3	D	4810	ALA	N-CA-C	-5.11	105.73	112.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	804	0	812	13	0
1	F	804	0	812	10	0
1	G	804	0	812	9	0
1	H	804	0	812	9	0
2	I	1042	0	972	25	0
2	J	1042	0	972	25	0
2	K	1042	0	972	25	0
2	L	1042	0	972	25	0
3	A	27995	0	25202	517	0
3	B	27995	0	25202	524	0
3	C	27995	0	25202	532	0
3	D	27995	0	25202	534	0
4	A	38	0	0	0	0
4	B	38	0	0	0	0
4	C	38	0	0	0	0
4	D	38	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	31	0	12	2	0
7	B	31	0	12	2	0
7	C	31	0	12	2	0
7	D	31	0	12	2	0
8	A	14	0	10	0	0
8	B	14	0	10	0	0
8	C	14	0	10	0	0
8	D	14	0	10	0	0
All	All	119704	0	108032	2193	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 10.

All (2193) 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)
3:A:4802:GLY:HA2	3:A:4808:PHE:HB2	1.52	0.90
3:D:4578:LEU:CD1	3:A:4849:TYR:HE2	1.84	0.90
3:C:4802:GLY:HA2	3:C:4808:PHE:HB2	1.52	0.90
3:D:4802:GLY:HA2	3:D:4808:PHE:HB2	1.52	0.89
3:B:4802:GLY:HA2	3:B:4808:PHE:HB2	1.52	0.89
3:C:4874:MET:HA	3:C:4874:MET:HE3	1.56	0.88
3:D:4874:MET:HA	3:D:4874:MET:HE3	1.56	0.87
3:B:4874:MET:HA	3:B:4874:MET:HE3	1.56	0.87
3:A:4874:MET:HA	3:A:4874:MET:HE3	1.56	0.85
3:C:4655:PHE:HB2	3:C:4796:MET:HE1	1.59	0.85
3:B:4655:PHE:HB2	3:B:4796:MET:HE1	1.59	0.83
3:D:4655:PHE:HB2	3:D:4796:MET:HE1	1.59	0.83
3:A:4655:PHE:HB2	3:A:4796:MET:HE1	1.59	0.83
3:C:4577:LEU:HD21	3:C:4807:PHE:HE1	1.43	0.82
3:D:4577:LEU:HD21	3:D:4807:PHE:HE1	1.43	0.82
3:A:4577:LEU:HD21	3:A:4807:PHE:HE1	1.43	0.82
3:B:4577:LEU:HD21	3:B:4807:PHE:HE1	1.43	0.82
3:A:4554:TYR:O	3:A:4558:ASN:ND2	2.14	0.80
3:D:4554:TYR:O	3:D:4558:ASN:ND2	2.14	0.80
3:C:4554:TYR:O	3:C:4558:ASN:ND2	2.14	0.79
3:B:4554:TYR:O	3:B:4558:ASN:ND2	2.14	0.79
3:D:4578:LEU:HD13	3:A:4849:TYR:HE2	1.46	0.78
3:D:4786:ASP:O	3:D:4790:LEU:HD23	1.84	0.78
3:B:4786:ASP:O	3:B:4790:LEU:HD23	1.84	0.78
3:C:4786:ASP:O	3:C:4790:LEU:HD23	1.84	0.77
3:C:4577:LEU:HD21	3:C:4807:PHE:CE1	2.19	0.77
3:A:4786:ASP:O	3:A:4790:LEU:HD23	1.84	0.77
3:B:4577:LEU:HD21	3:B:4807:PHE:CE1	2.19	0.77
3:D:4577:LEU:HD21	3:D:4807:PHE:CE1	2.19	0.76
3:A:4577:LEU:HD21	3:A:4807:PHE:CE1	2.19	0.76
3:C:4235:VAL:HG21	3:C:5019:TRP:CH2	2.22	0.75
3:D:4235:VAL:HG21	3:D:5019:TRP:CH2	2.22	0.75
3:A:4992:LEU:O	3:A:4996:ILE:HG13	1.88	0.74
3:B:4992:LEU:O	3:B:4996:ILE:HG13	1.88	0.74
3:C:4992:LEU:O	3:C:4996:ILE:HG13	1.88	0.74
3:B:4235:VAL:HG21	3:B:5019:TRP:CH2	2.22	0.74
3:D:4992:LEU:O	3:D:4996:ILE:HG13	1.88	0.74
3:A:4235:VAL:HG21	3:A:5019:TRP:CH2	2.22	0.74
3:D:4577:LEU:C	3:D:4579:PHE:H	1.97	0.73
3:A:4845:ALA:HA	3:A:4887:MET:HE1	1.71	0.73
3:A:4577:LEU:C	3:A:4579:PHE:H	1.97	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4845:ALA:HA	3:D:4887:MET:HE1	1.71	0.72
3:D:4722:ARG:HA	3:D:4743:MET:HE1	1.71	0.72
3:C:4577:LEU:C	3:C:4579:PHE:H	1.97	0.72
3:D:4927:ILE:HD12	3:C:4936:ILE:HG13	1.72	0.72
3:C:4845:ALA:HA	3:C:4887:MET:HE1	1.71	0.72
3:D:4927:ILE:HG23	3:C:4936:ILE:HG21	1.69	0.72
3:C:4722:ARG:HA	3:C:4743:MET:HE1	1.71	0.71
3:B:4845:ALA:HA	3:B:4887:MET:HE1	1.71	0.71
3:B:4722:ARG:HA	3:B:4743:MET:HE1	1.71	0.71
3:A:4722:ARG:HA	3:A:4743:MET:HE1	1.71	0.71
3:C:4636:THR:HG22	3:C:4637:GLY:H	1.56	0.71
3:A:4783:ILE:HG13	3:A:4784:PHE:HD1	1.56	0.70
3:B:4577:LEU:C	3:B:4579:PHE:H	1.97	0.70
3:B:4783:ILE:HG13	3:B:4784:PHE:HD1	1.56	0.70
3:D:4822:THR:HG21	3:A:4836:GLN:CB	2.21	0.70
3:A:4585:SER:O	3:A:4587:PRO:HD3	1.91	0.70
3:A:4636:THR:HG22	3:A:4637:GLY:H	1.56	0.70
3:C:4585:SER:O	3:C:4587:PRO:HD3	1.91	0.70
3:D:4927:ILE:CD1	3:C:4936:ILE:HG13	2.22	0.70
3:B:4585:SER:O	3:B:4587:PRO:HD3	1.91	0.70
3:D:4585:SER:O	3:D:4587:PRO:HD3	1.91	0.69
3:B:4636:THR:HG22	3:B:4637:GLY:H	1.56	0.69
3:D:4569:LEU:HD21	3:D:4649:LEU:HB3	1.74	0.69
3:C:4783:ILE:HG13	3:C:4784:PHE:HD1	1.56	0.69
3:D:4578:LEU:CD1	3:A:4849:TYR:CE2	2.73	0.69
3:A:4181:ILE:HD11	3:A:4988:TYR:CG	2.28	0.69
3:A:4569:LEU:HD21	3:A:4649:LEU:HB3	1.74	0.69
3:D:4783:ILE:HG13	3:D:4784:PHE:HD1	1.56	0.69
3:B:4181:ILE:HD11	3:B:4988:TYR:CG	2.28	0.69
3:C:4181:ILE:HD11	3:C:4988:TYR:CG	2.28	0.69
3:C:4223:ASN:HD21	3:C:4946:GLN:HB3	1.58	0.68
3:B:4223:ASN:HD21	3:B:4946:GLN:HB3	1.59	0.68
3:C:4569:LEU:HD21	3:C:4649:LEU:HB3	1.74	0.68
3:A:4752:ALA:O	3:A:4756:ARG:N	2.26	0.68
3:B:4569:LEU:HD21	3:B:4649:LEU:HB3	1.74	0.68
3:D:4181:ILE:HD11	3:D:4988:TYR:CG	2.28	0.68
3:D:4223:ASN:HD21	3:D:4946:GLN:HB3	1.59	0.68
3:D:4636:THR:HG22	3:D:4637:GLY:H	1.56	0.68
3:A:4223:ASN:HD21	3:A:4946:GLN:HB3	1.59	0.68
3:C:4752:ALA:O	3:C:4756:ARG:N	2.26	0.67
3:D:4708:THR:HG21	3:D:4775:TYR:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4926:VAL:O	3:C:4933:GLN:HG3	1.94	0.67
3:D:4752:ALA:O	3:D:4756:ARG:N	2.26	0.67
3:C:4708:THR:HG21	3:C:4775:TYR:HB2	1.76	0.67
3:A:4708:THR:HG21	3:A:4775:TYR:HB2	1.76	0.66
3:B:4708:THR:HG21	3:B:4775:TYR:HB2	1.76	0.66
3:C:4958:CYS:O	7:C:5104:ATP:N6	2.29	0.66
1:G:82:TYR:HB3	1:G:86:GLY:HA2	1.78	0.66
3:A:4578:LEU:CD1	3:B:4849:TYR:HE2	2.09	0.66
3:A:4958:CYS:O	7:A:5104:ATP:N6	2.29	0.65
3:B:4958:CYS:O	7:B:5104:ATP:N6	2.29	0.65
3:D:4958:CYS:O	7:D:5104:ATP:N6	2.29	0.65
1:F:82:TYR:HB3	1:F:86:GLY:HA2	1.78	0.65
3:B:728:ARG:NH2	3:B:1489:CYS:SG	2.69	0.65
3:C:728:ARG:NH2	3:C:1489:CYS:SG	2.69	0.65
3:A:4994:TYR:OH	3:A:4998:LYS:NZ	2.24	0.65
3:A:728:ARG:NH2	3:A:1489:CYS:SG	2.69	0.65
3:D:4668:LEU:HD23	3:D:4668:LEU:O	1.97	0.65
3:B:2368:LEU:HD11	3:B:2376:LEU:HD13	1.79	0.65
3:D:4927:ILE:HD12	3:C:4936:ILE:HG21	1.79	0.64
3:A:4568:PHE:O	3:A:4569:LEU:C	2.40	0.64
3:D:1292:SER:HB3	3:D:1598:GLN:HE21	1.63	0.64
3:B:4568:PHE:O	3:B:4569:LEU:C	2.40	0.64
3:C:4668:LEU:O	3:C:4668:LEU:HD23	1.97	0.64
1:E:82:TYR:HB3	1:E:86:GLY:HA2	1.78	0.64
3:D:728:ARG:NH2	3:D:1489:CYS:SG	2.69	0.64
3:A:2368:LEU:HD11	3:A:2376:LEU:HD13	1.79	0.64
3:B:4578:LEU:CD1	3:C:4849:TYR:HE2	2.10	0.64
3:A:4578:LEU:HD13	3:B:4849:TYR:HE2	1.61	0.64
3:B:393:CYS:SG	3:B:394:GLN:N	2.68	0.64
3:A:4640:GLU:HB2	3:A:4641:PRO:HD3	1.79	0.64
3:B:5000:GLU:HA	3:B:5003:HIS:CE1	2.33	0.64
1:H:82:TYR:HB3	1:H:86:GLY:HA2	1.78	0.64
3:D:2368:LEU:HD11	3:D:2376:LEU:HD13	1.79	0.64
3:B:4578:LEU:HD13	3:C:4849:TYR:HE2	1.62	0.64
3:B:4780:PHE:HA	3:B:4783:ILE:HG12	1.80	0.64
3:A:5000:GLU:HA	3:A:5003:HIS:CE1	2.33	0.64
3:C:2368:LEU:HD11	3:C:2376:LEU:HD13	1.79	0.64
3:D:4568:PHE:O	3:D:4569:LEU:C	2.40	0.63
3:B:1292:SER:HB3	3:B:1598:GLN:HE21	1.63	0.63
3:C:1292:SER:HB3	3:C:1598:GLN:HE21	1.63	0.63
3:B:4668:LEU:O	3:B:4668:LEU:HD23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4780:PHE:HA	3:A:4783:ILE:HG12	1.80	0.63
3:B:4691:GLN:OE1	3:B:4692:PRO:HD2	1.99	0.63
3:C:4568:PHE:O	3:C:4569:LEU:C	2.40	0.63
3:C:5000:GLU:HA	3:C:5003:HIS:CE1	2.33	0.63
3:A:4668:LEU:HD23	3:A:4668:LEU:O	1.97	0.63
3:A:4691:GLN:OE1	3:A:4692:PRO:HD2	1.99	0.63
3:C:4691:GLN:OE1	3:C:4692:PRO:HD2	1.99	0.63
3:D:393:CYS:SG	3:D:394:GLN:N	2.68	0.63
3:D:4722:ARG:HH22	3:D:4749:GLU:HA	1.64	0.63
3:B:4715:TYR:CE2	3:B:4717:ASP:HB3	2.34	0.63
3:C:4640:GLU:HB2	3:C:4641:PRO:HD3	1.79	0.63
3:D:5000:GLU:HA	3:D:5003:HIS:CE1	2.33	0.63
3:C:4901:ILE:HB	3:C:4913:ARG:NH2	2.14	0.63
3:A:1954:ARG:NH1	3:A:2042:CYS:SG	2.72	0.63
3:B:4640:GLU:HB2	3:B:4641:PRO:HD3	1.79	0.63
3:C:1954:ARG:NH1	3:C:2042:CYS:SG	2.72	0.63
3:A:4675:LYS:HG3	3:A:4715:TYR:CE1	2.34	0.63
3:A:4715:TYR:CE2	3:A:4717:ASP:HB3	2.34	0.63
3:D:1739:THR:HG23	3:D:1742:THR:H	1.64	0.62
3:B:4901:ILE:HB	3:B:4913:ARG:NH2	2.14	0.62
3:D:4640:GLU:HB2	3:D:4641:PRO:HD3	1.79	0.62
3:D:4691:GLN:OE1	3:D:4692:PRO:HD2	1.99	0.62
3:B:4577:LEU:C	3:B:4579:PHE:N	2.57	0.62
3:C:4722:ARG:HH22	3:C:4749:GLU:HA	1.64	0.62
3:A:1292:SER:HB3	3:A:1598:GLN:HE21	1.63	0.62
3:B:4675:LYS:HG3	3:B:4715:TYR:CE1	2.34	0.62
3:D:4901:ILE:HB	3:D:4913:ARG:NH2	2.14	0.62
3:D:4675:LYS:HG3	3:D:4715:TYR:CE1	2.34	0.62
3:D:4784:PHE:O	3:D:4790:LEU:HD21	2.00	0.62
3:A:4703:ARG:O	3:A:4704:LEU:HD12	2.00	0.62
3:B:4545:GLU:O	3:B:4549:VAL:HG23	2.00	0.62
3:B:4722:ARG:HH22	3:B:4749:GLU:HA	1.64	0.62
3:D:4715:TYR:CE2	3:D:4717:ASP:HB3	2.34	0.62
3:A:4722:ARG:HH22	3:A:4749:GLU:HA	1.64	0.62
3:B:4850:LEU:O	3:B:4853:VAL:HG12	2.00	0.62
3:A:1739:THR:HG23	3:A:1742:THR:H	1.64	0.62
3:C:4703:ARG:O	3:C:4704:LEU:HD12	2.00	0.62
3:D:4703:ARG:O	3:D:4704:LEU:HD12	2.00	0.62
3:D:4780:PHE:HA	3:D:4783:ILE:HG12	1.80	0.62
3:D:4874:MET:HA	3:D:4874:MET:CE	2.30	0.62
3:C:4715:TYR:CE2	3:C:4717:ASP:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1954:ARG:NH1	3:D:2042:CYS:SG	2.72	0.62
3:A:4545:GLU:O	3:A:4549:VAL:HG23	2.00	0.62
3:B:1954:ARG:NH1	3:B:2042:CYS:SG	2.72	0.62
3:D:4689:THR:HG22	3:D:4732:PHE:CE1	2.35	0.62
3:A:4689:THR:HG22	3:A:4732:PHE:CE1	2.35	0.62
3:A:4850:LEU:O	3:A:4853:VAL:HG12	2.00	0.62
3:C:4675:LYS:HG3	3:C:4715:TYR:CE1	2.34	0.62
3:C:4784:PHE:O	3:C:4790:LEU:HD21	2.00	0.62
3:C:4850:LEU:O	3:C:4853:VAL:HG12	2.00	0.62
3:B:4784:PHE:O	3:B:4790:LEU:HD21	2.00	0.61
3:C:4780:PHE:HA	3:C:4783:ILE:HG12	1.80	0.61
3:C:1739:THR:HG23	3:C:1742:THR:H	1.64	0.61
3:C:4874:MET:HA	3:C:4874:MET:CE	2.30	0.61
3:D:2452:ARG:HH11	3:A:175:SER:HA	1.65	0.61
3:A:4901:ILE:HB	3:A:4913:ARG:NH2	2.14	0.61
3:B:1739:THR:HG23	3:B:1742:THR:H	1.64	0.61
3:B:4703:ARG:O	3:B:4704:LEU:HD12	2.00	0.61
3:C:4545:GLU:O	3:C:4549:VAL:HG23	2.00	0.61
3:C:4876:CYS:HA	3:C:4882:CYS:HB2	1.83	0.61
3:D:4545:GLU:O	3:D:4549:VAL:HG23	2.00	0.61
3:D:4850:LEU:O	3:D:4853:VAL:HG12	2.00	0.61
3:A:4865:LYS:HB3	3:A:4875:LYS:HE2	1.83	0.61
3:B:4901:ILE:HG22	3:B:4902:GLU:H	1.66	0.61
3:C:4689:THR:HG22	3:C:4732:PHE:CE1	2.35	0.61
3:D:1192:CYS:SG	3:D:1193:SER:N	2.74	0.61
3:B:1192:CYS:SG	3:B:1193:SER:N	2.74	0.61
3:B:4752:ALA:O	3:B:4756:ARG:N	2.26	0.61
3:D:4556:SER:OG	3:D:4663:CYS:SG	2.59	0.61
3:D:4981:GLU:OE1	3:D:4981:GLU:HA	2.00	0.61
3:A:4577:LEU:C	3:A:4579:PHE:N	2.57	0.61
3:A:4784:PHE:O	3:A:4790:LEU:HD21	2.00	0.61
3:C:4577:LEU:C	3:C:4579:PHE:N	2.57	0.61
3:D:4876:CYS:HA	3:D:4882:CYS:HB2	1.83	0.61
3:C:1192:CYS:SG	3:C:1193:SER:N	2.74	0.61
3:C:4994:TYR:OH	3:C:4998:LYS:NZ	2.24	0.61
3:B:4865:LYS:HB3	3:B:4875:LYS:HE2	1.83	0.60
3:B:4981:GLU:OE1	3:B:4981:GLU:HA	2.00	0.60
3:C:4192:ARG:HD3	3:C:5028:PHE:CE2	2.37	0.60
3:C:4798:MET:C	3:C:4812:HIS:HE1	2.10	0.60
3:A:898:ASP:H	3:A:903:LEU:HB2	1.67	0.60
3:B:4689:THR:HG22	3:B:4732:PHE:CE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3904:ARG:HB3	3:C:3916:ILE:HD12	1.83	0.60
3:C:4981:GLU:OE1	3:C:4981:GLU:HA	2.00	0.60
3:A:4655:PHE:HD2	3:A:4656:LEU:HD12	1.67	0.60
3:A:4779:LYS:O	3:A:4782:VAL:HG12	2.01	0.60
3:A:4799:SER:HA	3:A:4812:HIS:NE2	2.16	0.60
3:A:4901:ILE:HG22	3:A:4902:GLU:H	1.66	0.60
3:A:4981:GLU:OE1	3:A:4981:GLU:HA	2.00	0.60
3:B:4556:SER:OG	3:B:4663:CYS:SG	2.59	0.60
3:D:4192:ARG:HD3	3:D:5028:PHE:CE2	2.37	0.60
3:A:4556:SER:OG	3:A:4663:CYS:SG	2.59	0.60
3:C:4556:SER:OG	3:C:4663:CYS:SG	2.59	0.60
3:C:4865:LYS:HB3	3:C:4875:LYS:HE2	1.83	0.60
3:B:4655:PHE:HD2	3:B:4656:LEU:HD12	1.67	0.60
3:D:4901:ILE:HG22	3:D:4902:GLU:H	1.66	0.60
3:B:1619:ARG:HA	3:B:1626:TRP:HA	1.84	0.60
3:A:733:PRO:HD3	3:A:765:GLN:HE22	1.67	0.60
3:A:3904:ARG:HB3	3:A:3916:ILE:HD12	1.83	0.60
3:C:4887:MET:HG3	3:C:4887:MET:O	2.02	0.60
3:D:24:CYS:SG	3:D:25:SER:N	2.75	0.60
3:D:4798:MET:C	3:D:4812:HIS:HE1	2.10	0.60
3:D:4865:LYS:HB3	3:D:4875:LYS:HE2	1.83	0.60
3:A:4192:ARG:HD3	3:A:5028:PHE:CE2	2.37	0.60
3:B:4799:SER:HA	3:B:4812:HIS:NE2	2.16	0.60
3:C:24:CYS:SG	3:C:25:SER:N	2.75	0.60
3:C:898:ASP:H	3:C:903:LEU:HB2	1.66	0.59
3:D:4994:TYR:OH	3:D:4998:LYS:NZ	2.24	0.59
3:A:4823:LEU:HA	3:A:4826:ILE:HD12	1.85	0.59
3:B:4192:ARG:HD3	3:B:5028:PHE:CE2	2.37	0.59
3:B:4573:ILE:HD11	3:B:4647:SER:N	2.17	0.59
3:B:4786:ASP:OD1	3:B:4787:ASN:N	2.35	0.59
3:C:4799:SER:HA	3:C:4812:HIS:NE2	2.16	0.59
2:J:87:ARG:NH1	2:J:87:ARG:O	2.36	0.59
3:D:898:ASP:H	3:D:903:LEU:HB2	1.67	0.59
3:D:4779:LYS:O	3:D:4782:VAL:HG12	2.01	0.59
3:A:24:CYS:SG	3:A:25:SER:N	2.75	0.59
3:A:393:CYS:SG	3:A:394:GLN:N	2.68	0.59
3:A:4573:ILE:HD11	3:A:4647:SER:N	2.17	0.59
3:B:4772:ASP:O	3:B:4776:GLN:HG2	2.03	0.59
3:B:4798:MET:C	3:B:4812:HIS:HE1	2.10	0.59
3:B:4876:CYS:HA	3:B:4882:CYS:HB2	1.83	0.59
3:D:4786:ASP:OD1	3:D:4787:ASN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4823:LEU:HA	3:B:4826:ILE:HD12	1.85	0.59
3:B:4887:MET:HG3	3:B:4887:MET:O	2.02	0.59
3:C:4901:ILE:HG22	3:C:4902:GLU:H	1.66	0.59
3:A:2437:ALA:O	3:A:2508:ARG:NH2	2.36	0.59
3:B:3904:ARG:HB3	3:B:3916:ILE:HD12	1.83	0.59
3:A:1192:CYS:SG	3:A:1193:SER:N	2.74	0.59
3:A:4772:ASP:O	3:A:4776:GLN:HG2	2.03	0.59
3:B:898:ASP:H	3:B:903:LEU:HB2	1.66	0.59
3:B:4779:LYS:O	3:B:4782:VAL:HG12	2.01	0.59
2:I:87:ARG:NH1	2:I:87:ARG:O	2.36	0.59
3:D:733:PRO:HD3	3:D:765:GLN:HE22	1.67	0.59
3:D:4655:PHE:HD2	3:D:4656:LEU:HD12	1.67	0.59
3:D:4799:SER:HA	3:D:4812:HIS:NE2	2.16	0.59
3:A:4786:ASP:OD1	3:A:4787:ASN:N	2.35	0.59
3:A:4876:CYS:HA	3:A:4882:CYS:HB2	1.83	0.59
3:A:4887:MET:O	3:A:4887:MET:HG3	2.02	0.59
3:C:733:PRO:HD3	3:C:765:GLN:HE22	1.67	0.59
3:C:4655:PHE:HD2	3:C:4656:LEU:HD12	1.67	0.59
3:C:4772:ASP:O	3:C:4776:GLN:HG2	2.03	0.59
3:D:4823:LEU:HA	3:D:4826:ILE:HD12	1.85	0.59
3:B:733:PRO:HD3	3:B:765:GLN:HE22	1.67	0.59
3:C:4573:ILE:HD11	3:C:4647:SER:N	2.17	0.59
3:D:3904:ARG:HB3	3:D:3916:ILE:HD12	1.83	0.59
3:A:1619:ARG:HA	3:A:1626:TRP:HA	1.84	0.59
3:D:4573:ILE:HD11	3:D:4647:SER:N	2.17	0.59
3:C:2437:ALA:O	3:C:2508:ARG:NH2	2.36	0.59
3:C:4786:ASP:OD1	3:C:4787:ASN:N	2.35	0.59
3:D:4577:LEU:C	3:D:4579:PHE:N	2.57	0.58
3:B:24:CYS:SG	3:B:25:SER:N	2.75	0.58
3:B:4953:ASP:OD1	3:B:4954:MET:N	2.36	0.58
3:B:4994:TYR:OH	3:B:4998:LYS:NZ	2.24	0.58
3:C:4676:GLU:OE1	3:C:4680:LYS:HE3	2.03	0.58
3:C:4779:LYS:O	3:C:4782:VAL:HG12	2.01	0.58
3:C:4823:LEU:HA	3:C:4826:ILE:HD12	1.85	0.58
3:D:4565:LEU:HD22	3:D:4653:VAL:HG11	1.85	0.58
3:A:4565:LEU:HD22	3:A:4653:VAL:HG11	1.86	0.58
3:B:4676:GLU:OE1	3:B:4680:LYS:HE3	2.04	0.58
3:C:4046:ASP:HA	3:C:4049:VAL:HG22	1.85	0.58
2:K:87:ARG:NH1	2:K:87:ARG:O	2.36	0.58
3:D:2437:ALA:O	3:D:2508:ARG:NH2	2.36	0.58
3:D:4772:ASP:O	3:D:4776:GLN:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4887:MET:HG3	3:D:4887:MET:O	2.02	0.58
3:A:4798:MET:C	3:A:4812:HIS:HE1	2.10	0.58
3:A:4898:GLY:HA3	3:A:4917:ASP:OD2	2.03	0.58
3:B:4046:ASP:HA	3:B:4049:VAL:HG22	1.85	0.58
3:C:1619:ARG:HA	3:C:1626:TRP:HA	1.84	0.58
3:C:4898:GLY:HA3	3:C:4917:ASP:OD2	2.03	0.58
3:A:2271:THR:HG23	3:A:2274:ASP:H	1.69	0.58
3:A:4676:GLU:OE1	3:A:4680:LYS:HE3	2.03	0.58
3:A:4953:ASP:OD1	3:A:4954:MET:N	2.36	0.58
2:J:50:GLN:O	2:J:54:ASN:ND2	2.36	0.58
3:D:4676:GLU:OE1	3:D:4680:LYS:HE3	2.03	0.58
3:D:4953:ASP:OD1	3:D:4954:MET:N	2.36	0.58
3:B:2437:ALA:O	3:B:2508:ARG:NH2	2.36	0.58
3:B:4242:ILE:HA	3:B:4245:MET:HE3	1.85	0.58
3:C:4565:LEU:HD22	3:C:4653:VAL:HG11	1.85	0.58
3:C:4953:ASP:OD1	3:C:4954:MET:N	2.36	0.58
2:K:50:GLN:O	2:K:54:ASN:ND2	2.36	0.58
3:D:4780:PHE:HD1	3:D:4783:ILE:HD11	1.68	0.58
3:A:4780:PHE:HD1	3:A:4783:ILE:HD11	1.68	0.58
3:B:4565:LEU:HD22	3:B:4653:VAL:HG11	1.85	0.58
3:C:4242:ILE:HA	3:C:4245:MET:HE3	1.85	0.58
3:A:315:CYS:SG	3:A:316:PHE:N	2.77	0.58
3:B:4681:LEU:HD21	3:B:4724:VAL:HG21	1.86	0.58
3:D:4687:TYR:HE2	3:D:4703:ARG:HB2	1.69	0.57
3:A:4812:HIS:O	3:A:4813:LEU:C	2.47	0.57
3:C:289:ARG:NH1	3:C:303:ASP:OD1	2.37	0.57
3:D:289:ARG:NH1	3:D:303:ASP:OD1	2.37	0.57
3:D:315:CYS:SG	3:D:316:PHE:N	2.77	0.57
3:D:1619:ARG:HA	3:D:1626:TRP:HA	1.84	0.57
3:B:2271:THR:HG23	3:B:2274:ASP:H	1.69	0.57
3:B:4812:HIS:O	3:B:4813:LEU:C	2.47	0.57
3:C:4681:LEU:HD21	3:C:4724:VAL:HG21	1.86	0.57
2:L:50:GLN:O	2:L:54:ASN:ND2	2.36	0.57
3:D:4046:ASP:HA	3:D:4049:VAL:HG22	1.85	0.57
3:D:4898:GLY:HA3	3:D:4917:ASP:OD2	2.03	0.57
3:B:4822:THR:HG21	3:C:4836:GLN:CB	2.34	0.57
3:B:4898:GLY:HA3	3:B:4917:ASP:OD2	2.03	0.57
3:C:315:CYS:SG	3:C:316:PHE:N	2.77	0.57
3:C:4780:PHE:HD1	3:C:4783:ILE:HD11	1.68	0.57
3:B:315:CYS:SG	3:B:316:PHE:N	2.77	0.57
3:D:1012:ASP:H	3:D:1017:ARG:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4242:ILE:HA	3:D:4245:MET:HE3	1.85	0.57
3:A:4794:TRP:HA	3:A:4797:VAL:HG12	1.86	0.57
3:B:4687:TYR:HE2	3:B:4703:ARG:HB2	1.69	0.57
3:B:4780:PHE:HD1	3:B:4783:ILE:HD11	1.69	0.57
3:C:2271:THR:HG23	3:C:2274:ASP:H	1.69	0.57
2:L:87:ARG:NH1	2:L:87:ARG:O	2.36	0.57
2:L:91:ARG:NH1	2:L:91:ARG:O	2.37	0.57
2:K:142:PHE:HA	2:K:145:MET:HG2	1.86	0.57
2:I:50:GLN:O	2:I:54:ASN:ND2	2.36	0.57
3:D:818:ARG:NH2	3:D:1027:LEU:O	2.38	0.57
3:A:4046:ASP:HA	3:A:4049:VAL:HG22	1.85	0.57
3:A:4866:SER:HB3	3:A:4873:ASP:OD2	2.05	0.57
3:C:818:ARG:NH2	3:C:1027:LEU:O	2.38	0.57
3:D:546:TRP:O	3:D:550:LYS:NZ	2.37	0.57
3:D:1023:PRO:HG2	3:D:1026:LEU:HD13	1.87	0.57
3:A:4822:THR:HG21	3:B:4836:GLN:CB	2.34	0.57
2:K:103:ALA:O	2:K:107:ARG:NH1	2.38	0.57
2:J:103:ALA:O	2:J:107:ARG:NH1	2.38	0.57
3:D:4902:GLU:OE1	3:D:4902:GLU:N	2.36	0.57
3:A:546:TRP:O	3:A:550:LYS:NZ	2.38	0.57
2:I:91:ARG:NH1	2:I:91:ARG:O	2.37	0.57
3:D:4866:SER:HB3	3:D:4873:ASP:OD2	2.05	0.57
3:A:4242:ILE:HA	3:A:4245:MET:HE3	1.85	0.57
3:B:818:ARG:NH2	3:B:1027:LEU:O	2.38	0.57
3:B:4866:SER:HB3	3:B:4873:ASP:OD2	2.05	0.57
3:C:4687:TYR:HE2	3:C:4703:ARG:HB2	1.69	0.57
2:J:142:PHE:HA	2:J:145:MET:HG2	1.86	0.57
3:A:818:ARG:NH2	3:A:1027:LEU:O	2.38	0.57
3:A:4878:ASP:O	3:A:4881:THR:N	2.35	0.57
3:B:546:TRP:O	3:B:550:LYS:NZ	2.37	0.57
3:B:1012:ASP:H	3:B:1017:ARG:HB2	1.70	0.57
3:C:4866:SER:HB3	3:C:4873:ASP:OD2	2.05	0.57
3:C:4902:GLU:N	3:C:4902:GLU:OE1	2.36	0.57
2:J:91:ARG:NH1	2:J:91:ARG:O	2.37	0.56
2:I:142:PHE:HA	2:I:145:MET:HG2	1.86	0.56
3:D:1632:ASP:OD1	3:D:1632:ASP:N	2.38	0.56
3:C:4915:VAL:O	3:C:4919:THR:HG22	2.05	0.56
1:G:21:THR:HG22	1:G:49:ARG:HG2	1.88	0.56
3:D:831:ARG:HH21	3:D:840:VAL:HG11	1.70	0.56
3:A:1023:PRO:HG2	3:A:1026:LEU:HD13	1.87	0.56
3:B:4579:PHE:HB2	3:B:4631:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:831:ARG:HH21	3:C:840:VAL:HG11	1.70	0.56
3:C:1023:PRO:HG2	3:C:1026:LEU:HD13	1.87	0.56
3:C:1128:ARG:HH21	3:C:1130:GLN:HE21	1.53	0.56
2:L:103:ALA:O	2:L:107:ARG:NH1	2.38	0.56
2:K:91:ARG:NH1	2:K:91:ARG:O	2.37	0.56
1:E:15:PHE:O	1:E:17:LYS:NZ	2.39	0.56
1:E:21:THR:HG22	1:E:49:ARG:HG2	1.88	0.56
3:D:2271:THR:HG23	3:D:2274:ASP:H	1.69	0.56
3:A:831:ARG:HH21	3:A:840:VAL:HG11	1.70	0.56
3:A:2270:SER:OG	3:A:2271:THR:N	2.38	0.56
3:A:4579:PHE:HB2	3:A:4631:PHE:CE1	2.41	0.56
3:A:4951:LYS:HB2	3:A:4951:LYS:HZ3	1.70	0.56
3:B:289:ARG:NH1	3:B:303:ASP:OD1	2.37	0.56
3:C:546:TRP:O	3:C:550:LYS:NZ	2.37	0.56
3:C:1632:ASP:N	3:C:1632:ASP:OD1	2.38	0.56
3:C:4675:LYS:HG3	3:C:4715:TYR:HE1	1.71	0.56
2:L:142:PHE:HA	2:L:145:MET:HG2	1.86	0.56
3:A:18:ASP:OD1	3:A:18:ASP:N	2.39	0.56
3:A:1012:ASP:H	3:A:1017:ARG:HB2	1.70	0.56
3:A:4687:TYR:HE2	3:A:4703:ARG:HB2	1.69	0.56
3:A:4885:PHE:CE1	3:A:4889:VAL:HG21	2.41	0.56
3:B:712:TYR:OH	3:B:1459:GLN:NE2	2.39	0.56
3:B:831:ARG:HH21	3:B:840:VAL:HG11	1.70	0.56
3:B:4885:PHE:CE1	3:B:4889:VAL:HG21	2.41	0.56
3:B:4949:GLN:OE1	3:B:4949:GLN:HA	2.06	0.56
1:F:15:PHE:O	1:F:17:LYS:NZ	2.39	0.56
2:I:103:ALA:O	2:I:107:ARG:NH1	2.38	0.56
3:D:4915:VAL:O	3:D:4919:THR:HG22	2.05	0.56
3:A:1632:ASP:OD1	3:A:1632:ASP:N	2.38	0.56
3:C:4794:TRP:HA	3:C:4797:VAL:HG12	1.86	0.56
3:C:4885:PHE:CE1	3:C:4889:VAL:HG21	2.41	0.56
1:H:21:THR:HG22	1:H:49:ARG:HG2	1.88	0.56
1:F:21:THR:HG22	1:F:49:ARG:HG2	1.88	0.56
3:D:2516:ASP:OD1	3:D:2516:ASP:N	2.39	0.56
3:D:4885:PHE:CE1	3:D:4889:VAL:HG21	2.41	0.56
3:D:4949:GLN:OE1	3:D:4949:GLN:HA	2.06	0.56
3:B:4794:TRP:HA	3:B:4797:VAL:HG12	1.87	0.56
3:C:4949:GLN:OE1	3:C:4949:GLN:HA	2.06	0.56
1:G:15:PHE:O	1:G:17:LYS:NZ	2.39	0.56
3:D:712:TYR:OH	3:D:1459:GLN:NE2	2.39	0.56
3:D:2358:ILE:HD12	3:A:195:PHE:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:289:ARG:NH1	3:A:303:ASP:OD1	2.37	0.56
3:A:4666:VAL:HB	3:A:4667:PRO:HD3	1.88	0.56
3:B:4638:TYR:C	3:B:4641:PRO:HD2	2.31	0.56
3:C:1012:ASP:H	3:C:1017:ARG:HB2	1.70	0.56
3:D:4579:PHE:HB2	3:D:4631:PHE:CE1	2.41	0.56
3:A:2208:MET:SD	3:A:2253:HIS:ND1	2.79	0.56
3:B:4663:CYS:O	3:B:4664:LEU:HD23	2.06	0.56
3:C:3843:ASP:OD2	3:C:3846:ALA:N	2.35	0.56
3:C:4638:TYR:C	3:C:4641:PRO:HD2	2.31	0.56
3:C:4812:HIS:O	3:C:4813:LEU:C	2.47	0.56
3:A:4638:TYR:C	3:A:4641:PRO:HD2	2.31	0.56
3:A:4681:LEU:HD21	3:A:4724:VAL:HG21	1.86	0.56
3:B:1023:PRO:HG2	3:B:1026:LEU:HD13	1.87	0.56
3:B:1128:ARG:HH21	3:B:1130:GLN:HE21	1.53	0.56
3:B:4878:ASP:O	3:B:4881:THR:N	2.35	0.56
3:C:2288:LEU:O	3:C:3849:ARG:NH1	2.39	0.56
3:A:4688:ILE:HG13	3:A:4689:THR:HG23	1.88	0.55
3:B:2516:ASP:N	3:B:2516:ASP:OD1	2.39	0.55
3:C:712:TYR:OH	3:C:1459:GLN:NE2	2.39	0.55
3:C:2516:ASP:OD1	3:C:2516:ASP:N	2.39	0.55
3:D:35:LEU:HD12	3:D:182:LEU:HD11	1.88	0.55
3:D:4675:LYS:HG3	3:D:4715:TYR:HE1	1.71	0.55
3:A:35:LEU:HD12	3:A:182:LEU:HD11	1.88	0.55
3:B:2288:LEU:O	3:B:3849:ARG:NH1	2.39	0.55
3:B:4902:GLU:OE1	3:B:4902:GLU:N	2.36	0.55
3:C:2208:MET:SD	3:C:2253:HIS:ND1	2.79	0.55
3:D:18:ASP:OD1	3:D:18:ASP:N	2.39	0.55
3:D:1456:ASP:OD1	3:D:1456:ASP:N	2.39	0.55
3:D:4681:LEU:HD21	3:D:4724:VAL:HG21	1.86	0.55
3:D:4914:VAL:HG11	3:C:4884:LEU:HD11	1.89	0.55
3:A:4663:CYS:O	3:A:4664:LEU:HD23	2.06	0.55
3:B:4915:VAL:O	3:B:4919:THR:HG22	2.05	0.55
3:C:4579:PHE:HB2	3:C:4631:PHE:CE1	2.41	0.55
1:H:15:PHE:O	1:H:17:LYS:NZ	2.39	0.55
2:I:113:LEU:HD12	2:I:115:GLU:H	1.72	0.55
3:D:221:ARG:NH2	3:D:397:GLU:OE2	2.40	0.55
3:D:669:ASP:N	3:D:669:ASP:OD1	2.38	0.55
3:D:4794:TRP:HA	3:D:4797:VAL:HG12	1.87	0.55
3:A:669:ASP:N	3:A:669:ASP:OD1	2.38	0.55
3:A:712:TYR:OH	3:A:1459:GLN:NE2	2.39	0.55
3:A:2288:LEU:O	3:A:3849:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:670:GLU:HB3	3:B:788:LYS:HB3	1.88	0.55
3:B:1236:THR:OG1	3:B:1608:MET:SD	2.64	0.55
3:B:4577:LEU:O	3:B:4579:PHE:N	2.40	0.55
3:B:4928:LEU:C	3:B:4930:ALA:H	2.14	0.55
3:C:3946:GLN:HA	3:C:3949:ARG:HE	1.71	0.55
3:C:4577:LEU:O	3:C:4579:PHE:N	2.40	0.55
3:D:1128:ARG:HH21	3:D:1130:GLN:HE21	1.53	0.55
3:D:2288:LEU:O	3:D:3849:ARG:NH1	2.39	0.55
3:D:3843:ASP:OD2	3:D:3846:ALA:N	2.35	0.55
3:D:4865:LYS:O	3:D:4865:LYS:HG3	2.07	0.55
3:A:221:ARG:NH2	3:A:397:GLU:OE2	2.40	0.55
3:B:1232:ARG:NH1	3:B:1828:ASP:O	2.40	0.55
3:B:1857:GLU:HA	3:B:1860:LYS:HD3	1.89	0.55
3:B:3843:ASP:OD2	3:B:3846:ALA:N	2.35	0.55
3:B:3946:GLN:HA	3:B:3949:ARG:HE	1.71	0.55
3:B:4666:VAL:HB	3:B:4667:PRO:HD3	1.88	0.55
3:D:4812:HIS:O	3:D:4813:LEU:C	2.47	0.55
3:A:4577:LEU:O	3:A:4579:PHE:N	2.40	0.55
3:A:4915:VAL:O	3:A:4919:THR:HG22	2.05	0.55
3:B:2208:MET:SD	3:B:2253:HIS:ND1	2.79	0.55
3:D:4638:TYR:C	3:D:4641:PRO:HD2	2.31	0.55
3:A:1031:THR:O	3:A:1035:ASN:ND2	2.40	0.55
3:A:1232:ARG:NH1	3:A:1828:ASP:O	2.40	0.55
3:A:1857:GLU:HA	3:A:1860:LYS:HD3	1.89	0.55
3:C:731:THR:O	3:C:765:GLN:NE2	2.40	0.55
3:A:818:ARG:NH2	3:A:1025:ARG:O	2.40	0.55
3:C:4663:CYS:O	3:C:4664:LEU:HD23	2.06	0.55
3:C:4978:HIS:HA	3:C:4982:GLU:HG2	1.89	0.55
2:J:113:LEU:HD12	2:J:115:GLU:H	1.71	0.55
3:D:731:THR:O	3:D:765:GLN:NE2	2.40	0.55
3:D:2208:MET:SD	3:D:2253:HIS:ND1	2.79	0.55
3:A:670:GLU:HB3	3:A:788:LYS:HB3	1.88	0.55
3:B:731:THR:O	3:B:765:GLN:NE2	2.40	0.55
3:B:4688:ILE:HG13	3:B:4689:THR:HG23	1.88	0.55
3:B:4865:LYS:HG3	3:B:4865:LYS:O	2.07	0.55
1:F:41:ASP:OD1	1:F:41:ASP:N	2.39	0.55
3:D:3946:GLN:HA	3:D:3949:ARG:HE	1.71	0.55
3:D:4181:ILE:CD1	3:D:4988:TYR:HA	2.37	0.55
3:A:4652:LEU:C	3:A:4654:ALA:H	2.15	0.55
3:B:818:ARG:NH2	3:B:1025:ARG:O	2.40	0.55
3:B:4951:LYS:HZ3	3:B:4951:LYS:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:ARG:NH2	3:C:397:GLU:OE2	2.40	0.55
3:C:670:GLU:HB3	3:C:788:LYS:HB3	1.88	0.55
3:D:670:GLU:HB3	3:D:788:LYS:HB3	1.88	0.54
3:D:4663:CYS:O	3:D:4664:LEU:HD23	2.06	0.54
3:D:4799:SER:HA	3:D:4812:HIS:CE1	2.43	0.54
3:D:4812:HIS:C	3:D:4814:LEU:N	2.65	0.54
3:D:4978:HIS:HA	3:D:4982:GLU:HG2	1.89	0.54
3:A:4675:LYS:HG3	3:A:4715:TYR:HE1	1.71	0.54
3:A:4874:MET:HA	3:A:4874:MET:CE	2.30	0.54
3:A:4949:GLN:OE1	3:A:4949:GLN:HA	2.06	0.54
3:B:669:ASP:N	3:B:669:ASP:OD1	2.38	0.54
3:C:3676:ASP:HA	3:C:3679:LYS:HG2	1.89	0.54
3:C:4652:LEU:C	3:C:4654:ALA:H	2.15	0.54
3:C:4865:LYS:HG3	3:C:4865:LYS:O	2.07	0.54
3:C:4928:LEU:C	3:C:4930:ALA:H	2.14	0.54
3:D:4938:ASP:O	3:D:4941:GLY:N	2.40	0.54
3:A:4181:ILE:CD1	3:A:4988:TYR:HA	2.38	0.54
3:B:4655:PHE:CD2	3:B:4656:LEU:HD12	2.42	0.54
3:C:393:CYS:SG	3:C:394:GLN:N	2.68	0.54
3:C:4181:ILE:CD1	3:C:4988:TYR:HA	2.37	0.54
3:C:4711:PHE:HB3	3:C:4712:PRO:HD3	1.90	0.54
3:D:818:ARG:NH2	3:D:1025:ARG:O	2.40	0.54
3:D:4577:LEU:O	3:D:4579:PHE:N	2.40	0.54
3:A:731:THR:O	3:A:765:GLN:NE2	2.40	0.54
3:A:3946:GLN:HA	3:A:3949:ARG:HE	1.71	0.54
3:B:1031:THR:O	3:B:1035:ASN:ND2	2.40	0.54
3:B:4711:PHE:HB3	3:B:4712:PRO:HD3	1.90	0.54
3:C:1857:GLU:HA	3:C:1860:LYS:HD3	1.89	0.54
3:C:4666:VAL:HB	3:C:4667:PRO:HD3	1.88	0.54
3:C:4688:ILE:HG13	3:C:4689:THR:HG23	1.88	0.54
1:H:41:ASP:N	1:H:41:ASP:OD1	2.39	0.54
1:E:41:ASP:N	1:E:41:ASP:OD1	2.39	0.54
3:D:4666:VAL:HB	3:D:4667:PRO:HD3	1.88	0.54
3:D:4928:LEU:C	3:D:4930:ALA:H	2.14	0.54
3:A:1128:ARG:HH21	3:A:1130:GLN:HE21	1.53	0.54
3:A:4678:ALA:HB1	3:A:4720:VAL:HG21	1.90	0.54
3:B:35:LEU:HD12	3:B:182:LEU:HD11	1.88	0.54
3:C:4812:HIS:C	3:C:4814:LEU:N	2.65	0.54
3:A:4928:LEU:C	3:A:4930:ALA:H	2.14	0.54
3:C:1291:LEU:HB2	3:C:1550:PRO:HG2	1.90	0.54
3:C:2548:LEU:HD21	3:C:2594:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:104:ALA:HA	2:L:107:ARG:HH22	1.73	0.54
2:I:104:ALA:HA	2:I:107:ARG:HH22	1.73	0.54
3:D:1031:THR:O	3:D:1035:ASN:ND2	2.40	0.54
3:A:4655:PHE:CD2	3:A:4656:LEU:HD12	2.42	0.54
3:B:1008:SER:HB3	3:B:1017:ARG:HH11	1.72	0.54
3:B:4678:ALA:HB1	3:B:4720:VAL:HG21	1.90	0.54
3:D:732:SER:HB3	3:D:735:GLN:HB3	1.89	0.54
3:D:1857:GLU:HA	3:D:1860:LYS:HD3	1.89	0.54
3:D:4652:LEU:C	3:D:4654:ALA:H	2.15	0.54
3:D:4688:ILE:HG13	3:D:4689:THR:HG23	1.88	0.54
3:A:4865:LYS:O	3:A:4865:LYS:HG3	2.07	0.54
3:A:4978:HIS:HA	3:A:4982:GLU:HG2	1.89	0.54
3:B:18:ASP:N	3:B:18:ASP:OD1	2.39	0.54
3:B:2548:LEU:HD21	3:B:2594:SER:HB2	1.90	0.54
3:B:3676:ASP:HA	3:B:3679:LYS:HG2	1.89	0.54
3:B:4181:ILE:CD1	3:B:4988:TYR:HA	2.38	0.54
3:B:4675:LYS:HG3	3:B:4715:TYR:HE1	1.71	0.54
3:C:1008:SER:HB3	3:C:1017:ARG:HH11	1.72	0.54
3:C:1031:THR:O	3:C:1035:ASN:ND2	2.40	0.54
3:C:4655:PHE:CD2	3:C:4656:LEU:HD12	2.42	0.54
3:D:1008:SER:HB3	3:D:1017:ARG:HH11	1.72	0.54
3:D:1232:ARG:NH1	3:D:1828:ASP:O	2.40	0.54
3:D:1291:LEU:HB2	3:D:1550:PRO:HG2	1.90	0.54
3:D:3676:ASP:HA	3:D:3679:LYS:HG2	1.89	0.54
3:A:1008:SER:HB3	3:A:1017:ARG:HH11	1.72	0.54
3:B:4799:SER:HA	3:B:4812:HIS:CE1	2.43	0.54
3:C:818:ARG:NH2	3:C:1025:ARG:O	2.40	0.54
2:L:113:LEU:HD12	2:L:115:GLU:H	1.71	0.54
3:A:4938:ASP:O	3:A:4941:GLY:N	2.40	0.54
3:B:1676:LEU:HD12	3:B:2167:ILE:HD12	1.90	0.54
3:B:3818:ASP:N	3:B:3818:ASP:OD1	2.41	0.54
3:C:35:LEU:HD12	3:C:182:LEU:HD11	1.88	0.54
3:C:669:ASP:OD1	3:C:669:ASP:N	2.38	0.54
3:C:1676:LEU:HD12	3:C:2167:ILE:HD12	1.90	0.54
3:C:4678:ALA:HB1	3:C:4720:VAL:HG21	1.90	0.54
3:C:4799:SER:HA	3:C:4812:HIS:CE1	2.42	0.54
3:D:4678:ALA:HB1	3:D:4720:VAL:HG21	1.90	0.54
3:D:4780:PHE:CD1	3:D:4783:ILE:HD11	2.43	0.54
3:A:1099:GLU:OE2	3:A:1101:ARG:NH1	2.41	0.54
3:A:2377:LEU:HD22	3:A:2468:GLY:HA3	1.90	0.54
3:C:18:ASP:OD1	3:C:18:ASP:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:113:LEU:HD12	2:K:115:GLU:H	1.72	0.53
3:D:4655:PHE:CD2	3:D:4656:LEU:HD12	2.42	0.53
3:A:4799:SER:HA	3:A:4812:HIS:CE1	2.42	0.53
3:B:1099:GLU:OE2	3:B:1101:ARG:NH1	2.41	0.53
3:B:2179:ILE:HD11	3:B:2228:MET:HA	1.90	0.53
3:B:2270:SER:OG	3:B:2271:THR:N	2.38	0.53
3:B:4209:GLN:HE21	3:B:4665:LYS:NZ	2.07	0.53
3:B:4874:MET:HA	3:B:4874:MET:CE	2.30	0.53
3:C:1099:GLU:OE2	3:C:1101:ARG:NH1	2.41	0.53
3:C:3818:ASP:N	3:C:3818:ASP:OD1	2.41	0.53
3:A:1291:LEU:HB2	3:A:1550:PRO:HG2	1.90	0.53
3:A:4902:GLU:OE1	3:A:4902:GLU:N	2.36	0.53
3:B:1927:LEU:HD22	3:B:2101:MET:HE2	1.90	0.53
3:B:2377:LEU:HD22	3:B:2468:GLY:HA3	1.90	0.53
3:C:4687:TYR:CE2	3:C:4703:ARG:HB2	2.44	0.53
3:D:4181:ILE:HD11	3:D:4988:TYR:HA	1.90	0.53
3:D:4711:PHE:HB3	3:D:4712:PRO:HD3	1.90	0.53
3:A:732:SER:HB3	3:A:735:GLN:HB3	1.89	0.53
3:A:2179:ILE:HD11	3:A:2228:MET:HA	1.90	0.53
3:C:4181:ILE:HD11	3:C:4988:TYR:HA	1.90	0.53
3:C:4780:PHE:CD1	3:C:4783:ILE:HD11	2.43	0.53
3:D:2377:LEU:HD22	3:D:2468:GLY:HA3	1.90	0.53
3:A:1948:ASP:OD1	3:A:2126:ARG:NH2	2.42	0.53
3:A:4556:SER:OG	3:A:4664:LEU:HD21	2.09	0.53
3:B:221:ARG:NH2	3:B:397:GLU:OE2	2.40	0.53
3:B:732:SER:HB3	3:B:735:GLN:HB3	1.89	0.53
3:B:4978:HIS:HA	3:B:4982:GLU:HG2	1.89	0.53
3:C:1232:ARG:NH1	3:C:1828:ASP:O	2.40	0.53
3:C:2148:SER:O	3:C:2152:THR:OG1	2.26	0.53
3:C:4209:GLN:HE21	3:C:4665:LYS:NZ	2.07	0.53
2:K:104:ALA:HA	2:K:107:ARG:HH22	1.73	0.53
2:J:104:ALA:HA	2:J:107:ARG:HH22	1.73	0.53
3:D:1948:ASP:OD1	3:D:2126:ARG:NH2	2.42	0.53
3:D:2548:LEU:HD21	3:D:2594:SER:HB2	1.90	0.53
3:A:4568:PHE:O	3:A:4571:PHE:N	2.42	0.53
3:A:4711:PHE:HB3	3:A:4712:PRO:HD3	1.90	0.53
3:B:1948:ASP:OD1	3:B:2126:ARG:NH2	2.42	0.53
3:B:4652:LEU:C	3:B:4654:ALA:H	2.15	0.53
3:B:4780:PHE:CD1	3:B:4783:ILE:HD11	2.43	0.53
3:C:1948:ASP:OD1	3:C:2126:ARG:NH2	2.42	0.53
3:D:1099:GLU:OE2	3:D:1101:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3818:ASP:OD1	3:D:3818:ASP:N	2.41	0.53
3:A:1299:GLN:OE1	3:A:1545:ASN:ND2	2.42	0.53
3:A:4209:GLN:HE21	3:A:4665:LYS:NZ	2.07	0.53
3:B:1456:ASP:OD1	3:B:1456:ASP:N	2.39	0.53
3:B:4687:TYR:CE2	3:B:4703:ARG:HB2	2.44	0.53
3:C:2478:THR:O	3:C:2486:VAL:N	2.42	0.53
3:D:1236:THR:OG1	3:D:1608:MET:SD	2.64	0.53
3:D:2478:THR:O	3:D:2486:VAL:N	2.42	0.53
3:D:4209:GLN:HE21	3:D:4665:LYS:NZ	2.07	0.53
3:D:4773:VAL:HG23	3:D:4774:LYS:N	2.24	0.53
3:A:2516:ASP:OD1	3:A:2516:ASP:N	2.39	0.53
3:A:2548:LEU:HD21	3:A:2594:SER:HB2	1.90	0.53
3:B:4568:PHE:O	3:B:4571:PHE:N	2.42	0.53
3:C:4688:ILE:HD11	3:C:4728:HIS:CG	2.44	0.53
3:D:1299:GLN:OE1	3:D:1545:ASN:ND2	2.42	0.53
3:D:2359:ARG:HD3	3:A:179:TYR:OH	2.09	0.53
3:D:4688:ILE:HD11	3:D:4728:HIS:CG	2.44	0.53
3:C:1299:GLN:OE1	3:C:1545:ASN:ND2	2.42	0.53
3:C:3680:ALA:HB3	3:C:3697:PRO:HG2	1.91	0.53
3:D:4556:SER:OG	3:D:4664:LEU:HD21	2.09	0.53
3:D:4636:THR:HG22	3:D:4637:GLY:N	2.23	0.53
3:D:4892:ARG:NH1	3:A:4895:GLY:O	2.42	0.53
3:A:3676:ASP:HA	3:A:3679:LYS:HG2	1.89	0.53
3:A:4780:PHE:CD1	3:A:4783:ILE:HD11	2.43	0.53
3:B:1291:LEU:HB2	3:B:1550:PRO:HG2	1.89	0.53
3:B:4938:ASP:O	3:B:4941:GLY:N	2.40	0.53
3:C:4773:VAL:HG23	3:C:4774:LYS:N	2.24	0.53
1:G:41:ASP:OD1	1:G:41:ASP:N	2.39	0.53
3:D:4721:LYS:HB3	3:D:4743:MET:HE3	1.91	0.53
3:A:1456:ASP:OD1	3:A:1456:ASP:N	2.39	0.53
3:B:1087:ARG:HG3	3:B:1223:PHE:HA	1.91	0.53
3:C:2377:LEU:HD22	3:C:2468:GLY:HA3	1.90	0.53
3:C:4138:ASP:N	3:C:4138:ASP:OD1	2.42	0.53
3:C:4721:LYS:HB3	3:C:4743:MET:HE3	1.91	0.53
3:C:4886:HIS:O	3:C:4890:GLY:N	2.42	0.53
3:D:2358:ILE:HD12	3:A:195:PHE:CE1	2.43	0.52
3:D:4687:TYR:CE2	3:D:4703:ARG:HB2	2.44	0.52
3:A:1927:LEU:HD22	3:A:2101:MET:HE2	1.90	0.52
3:A:2478:THR:O	3:A:2486:VAL:N	2.42	0.52
3:A:4688:ILE:HD11	3:A:4728:HIS:CG	2.44	0.52
3:B:4181:ILE:HD11	3:B:4988:TYR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:732:SER:HB3	3:C:735:GLN:HB3	1.89	0.52
3:D:2288:LEU:HD21	3:D:3852:LYS:HE2	1.91	0.52
3:D:4568:PHE:O	3:D:4571:PHE:N	2.42	0.52
3:A:1676:LEU:HD12	3:A:2167:ILE:HD12	1.90	0.52
3:A:4721:LYS:HB3	3:A:4743:MET:HE3	1.91	0.52
3:A:4773:VAL:HG23	3:A:4774:LYS:N	2.24	0.52
3:B:2503:VAL:HG11	3:B:2557:ALA:HB1	1.92	0.52
3:B:4688:ILE:HD11	3:B:4728:HIS:CG	2.44	0.52
3:D:2179:ILE:HD11	3:D:2228:MET:HA	1.90	0.52
3:A:1087:ARG:HG3	3:A:1223:PHE:HA	1.91	0.52
3:A:3680:ALA:HB3	3:A:3697:PRO:HG2	1.91	0.52
3:A:4731:ILE:HG23	3:A:4732:PHE:HD1	1.75	0.52
3:B:4812:HIS:C	3:B:4814:LEU:N	2.65	0.52
3:C:3752:SER:OG	3:C:3753:PHE:N	2.43	0.52
3:D:1676:LEU:HD12	3:D:2167:ILE:HD12	1.90	0.52
3:D:3752:SER:OG	3:D:3753:PHE:N	2.43	0.52
3:A:2288:LEU:HD21	3:A:3852:LYS:HE2	1.91	0.52
3:A:2503:VAL:HG11	3:A:2557:ALA:HB1	1.91	0.52
3:A:4687:TYR:CE2	3:A:4703:ARG:HB2	2.44	0.52
3:B:4556:SER:OG	3:B:4664:LEU:HD21	2.09	0.52
3:D:1927:LEU:HD22	3:D:2101:MET:HE2	1.90	0.52
3:D:3717:ASP:OD1	3:D:3717:ASP:N	2.42	0.52
3:A:4181:ILE:HD11	3:A:4988:TYR:HA	1.90	0.52
3:B:663:TYR:HB2	3:B:808:TYR:HB3	1.92	0.52
3:B:1299:GLN:OE1	3:B:1545:ASN:ND2	2.42	0.52
3:C:4556:SER:OG	3:C:4664:LEU:HD21	2.09	0.52
3:C:4878:ASP:O	3:C:4881:THR:N	2.35	0.52
3:D:1008:SER:OG	3:D:1010:VAL:O	2.28	0.52
3:D:2503:VAL:HG11	3:D:2557:ALA:HB1	1.92	0.52
3:A:4636:THR:HG22	3:A:4637:GLY:N	2.23	0.52
3:A:4725:LEU:O	3:A:4729:GLY:N	2.43	0.52
3:B:2478:THR:O	3:B:2486:VAL:N	2.42	0.52
3:C:2179:ILE:HD11	3:C:2228:MET:HA	1.90	0.52
1:H:83:GLY:O	1:H:94:ASN:ND2	2.43	0.52
2:L:96:ASP:OD2	2:L:98:ASN:ND2	2.43	0.52
3:D:1186:ASP:OD1	3:D:1186:ASP:N	2.42	0.52
3:A:132:ALA:HA	3:A:194:SER:HB2	1.92	0.52
3:A:875:ALA:O	3:A:921:ASN:ND2	2.43	0.52
3:A:1008:SER:OG	3:A:1010:VAL:O	2.28	0.52
3:B:708:GLY:H	3:B:713:SER:HG	1.55	0.52
3:B:3752:SER:OG	3:B:3753:PHE:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:875:ALA:O	3:C:921:ASN:ND2	2.43	0.52
3:C:4568:PHE:O	3:C:4571:PHE:N	2.42	0.52
3:C:4938:ASP:O	3:C:4941:GLY:N	2.40	0.52
2:J:112:ASN:HD22	3:B:1991:THR:HG23	1.75	0.52
3:D:875:ALA:O	3:D:921:ASN:ND2	2.43	0.52
3:D:1087:ARG:HG3	3:D:1223:PHE:HA	1.91	0.52
3:A:1629:GLN:OE1	3:A:1631:GLN:NE2	2.43	0.52
3:B:4636:THR:HG22	3:B:4637:GLY:N	2.23	0.52
3:C:1087:ARG:HG3	3:C:1223:PHE:HA	1.91	0.52
3:C:1236:THR:OG1	3:C:1608:MET:SD	2.64	0.52
3:C:1629:GLN:OE1	3:C:1631:GLN:NE2	2.43	0.52
3:C:1927:LEU:HD22	3:C:2101:MET:HE2	1.90	0.52
2:K:96:ASP:OD2	2:K:98:ASN:ND2	2.43	0.52
2:I:112:ASN:HD22	3:C:1991:THR:HG23	1.75	0.52
3:D:2023:LEU:O	3:D:2028:ARG:NH2	2.43	0.52
3:A:1186:ASP:OD1	3:A:1186:ASP:N	2.42	0.52
3:A:1596:GLU:OE1	3:A:1598:GLN:NE2	2.43	0.52
3:B:4721:LYS:HB3	3:B:4743:MET:HE3	1.91	0.52
3:B:4731:ILE:HG23	3:B:4732:PHE:HD1	1.75	0.52
3:B:4773:VAL:HG23	3:B:4774:LYS:N	2.24	0.52
3:C:1008:SER:OG	3:C:1010:VAL:O	2.28	0.52
3:C:2288:LEU:HD21	3:C:3852:LYS:HE2	1.91	0.52
3:C:2503:VAL:HG11	3:C:2557:ALA:HB1	1.92	0.52
3:C:3977:GLN:NE2	3:C:4030:LEU:O	2.43	0.52
3:D:1629:GLN:OE1	3:D:1631:GLN:NE2	2.43	0.52
3:B:3680:ALA:HB3	3:B:3697:PRO:HG2	1.91	0.52
3:C:2025:GLU:HA	3:C:2028:ARG:HG2	1.92	0.52
3:C:4544:LEU:HA	3:C:4547:GLN:NE2	2.25	0.52
2:I:96:ASP:OD2	2:I:98:ASN:ND2	2.43	0.51
3:D:3680:ALA:HB3	3:D:3697:PRO:HG2	1.91	0.51
3:A:2025:GLU:HA	3:A:2028:ARG:HG2	1.92	0.51
3:B:875:ALA:O	3:B:921:ASN:ND2	2.43	0.51
3:B:1186:ASP:OD1	3:B:1186:ASP:N	2.42	0.51
3:B:1691:GLN:HE21	3:B:1802:ILE:HG13	1.76	0.51
3:B:4138:ASP:OD1	3:B:4138:ASP:N	2.42	0.51
3:C:663:TYR:HB2	3:C:808:TYR:HB3	1.92	0.51
3:C:1596:GLU:OE1	3:C:1598:GLN:NE2	2.43	0.51
3:D:3889:GLN:HG3	3:D:3967:GLU:HG3	1.92	0.51
3:A:3717:ASP:OD1	3:A:3717:ASP:N	2.42	0.51
3:A:3843:ASP:OD2	3:A:3846:ALA:N	2.35	0.51
3:A:3977:GLN:NE2	3:A:4030:LEU:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4544:LEU:HA	3:A:4547:GLN:NE2	2.25	0.51
3:B:132:ALA:HA	3:B:194:SER:HB2	1.92	0.51
3:B:3977:GLN:NE2	3:B:4030:LEU:O	2.43	0.51
3:B:4725:LEU:O	3:B:4729:GLY:N	2.43	0.51
2:J:96:ASP:OD2	2:J:98:ASN:ND2	2.43	0.51
3:D:4574:ASN:O	3:D:4575:PHE:C	2.54	0.51
3:A:2442:LEU:HD22	3:A:2447:LYS:HG3	1.92	0.51
3:A:3752:SER:OG	3:A:3753:PHE:N	2.43	0.51
3:A:5001:THR:OG1	3:A:5002:GLU:OE2	2.20	0.51
3:B:1596:GLU:OE1	3:B:1598:GLN:NE2	2.43	0.51
3:C:4725:LEU:O	3:C:4729:GLY:N	2.43	0.51
2:L:112:ASN:HD22	3:D:1991:THR:HG23	1.75	0.51
1:G:83:GLY:O	1:G:94:ASN:ND2	2.43	0.51
3:D:4677:LEU:HD23	3:D:4711:PHE:CE1	2.46	0.51
3:A:2023:LEU:O	3:A:2028:ARG:NH2	2.43	0.51
3:A:3818:ASP:OD1	3:A:3818:ASP:N	2.41	0.51
3:B:1629:GLN:OE1	3:B:1631:GLN:NE2	2.43	0.51
3:B:2023:LEU:O	3:B:2028:ARG:NH2	2.43	0.51
3:C:194:SER:OG	3:C:195:PHE:N	2.44	0.51
2:K:94:ASP:OD1	2:K:94:ASP:N	2.44	0.51
3:D:1596:GLU:OE1	3:D:1598:GLN:NE2	2.43	0.51
3:D:2025:GLU:HA	3:D:2028:ARG:HG2	1.92	0.51
3:D:3977:GLN:NE2	3:D:4030:LEU:O	2.43	0.51
3:A:4138:ASP:OD1	3:A:4138:ASP:N	2.42	0.51
3:A:4655:PHE:HD2	3:A:4656:LEU:CD1	2.24	0.51
3:B:2442:LEU:HD22	3:B:2447:LYS:HG3	1.92	0.51
2:J:94:ASP:OD1	2:J:94:ASP:N	2.44	0.51
3:D:1089:TYR:HD1	3:D:1152:MET:HB3	1.76	0.51
3:D:2270:SER:OG	3:D:2271:THR:N	2.38	0.51
3:D:4065:PHE:O	3:D:4133:GLN:NE2	2.44	0.51
3:A:4812:HIS:C	3:A:4814:LEU:N	2.65	0.51
3:B:1008:SER:OG	3:B:1010:VAL:O	2.28	0.51
1:E:83:GLY:O	1:E:94:ASN:ND2	2.43	0.51
3:A:4065:PHE:O	3:A:4133:GLN:NE2	2.44	0.51
3:B:2534:ALA:HB1	3:B:2588:ARG:HD2	1.93	0.51
3:C:1089:TYR:HD1	3:C:1152:MET:HB3	1.76	0.51
3:C:3889:GLN:HG3	3:C:3967:GLU:HG3	1.92	0.51
3:C:4731:ILE:HG23	3:C:4732:PHE:HD1	1.75	0.51
3:C:4808:PHE:C	3:C:4810:ALA:H	2.19	0.51
2:K:112:ASN:HD22	3:A:1991:THR:HG23	1.75	0.51
1:F:83:GLY:O	1:F:94:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4648:LEU:O	3:D:4649:LEU:C	2.53	0.51
3:D:4655:PHE:HD2	3:D:4656:LEU:CD1	2.24	0.51
3:D:4725:LEU:O	3:D:4729:GLY:N	2.43	0.51
3:D:4731:ILE:HG23	3:D:4732:PHE:HD1	1.75	0.51
3:A:1089:TYR:HD1	3:A:1152:MET:HB3	1.76	0.51
3:B:1089:TYR:HD1	3:B:1152:MET:HB3	1.76	0.51
3:B:4544:LEU:HA	3:B:4547:GLN:NE2	2.25	0.51
3:B:4886:HIS:O	3:B:4890:GLY:N	2.42	0.51
3:C:132:ALA:HA	3:C:194:SER:HB2	1.92	0.51
3:C:4648:LEU:O	3:C:4649:LEU:C	2.53	0.51
3:C:4677:LEU:HD23	3:C:4711:PHE:CE1	2.46	0.51
3:D:4544:LEU:HA	3:D:4547:GLN:NE2	2.25	0.51
3:D:4565:LEU:CD2	3:D:4653:VAL:HG21	2.41	0.51
3:D:4901:ILE:HG22	3:D:4902:GLU:N	2.25	0.51
3:B:4655:PHE:HD2	3:B:4656:LEU:CD1	2.24	0.51
3:C:2023:LEU:O	3:C:2028:ARG:NH2	2.43	0.51
3:C:4065:PHE:O	3:C:4133:GLN:NE2	2.44	0.51
3:C:4655:PHE:HD2	3:C:4656:LEU:CD1	2.24	0.51
3:C:4901:ILE:HG22	3:C:4902:GLU:N	2.25	0.51
3:D:663:TYR:HB2	3:D:808:TYR:HB3	1.92	0.51
3:C:2442:LEU:HD22	3:C:2447:LYS:HG3	1.92	0.51
3:C:2534:ALA:HB1	3:C:2588:ARG:HD2	1.93	0.51
3:C:4565:LEU:CD2	3:C:4653:VAL:HG21	2.41	0.51
3:D:4558:ASN:O	3:D:4559:PHE:C	2.54	0.50
3:A:4708:THR:HG22	3:A:4710:SER:H	1.76	0.50
3:B:1126:GLY:HA3	3:B:1143:TRP:CE2	2.47	0.50
3:B:2025:GLU:HA	3:B:2028:ARG:HG2	1.92	0.50
3:B:2288:LEU:HD21	3:B:3852:LYS:HE2	1.91	0.50
3:B:2359:ARG:HD3	3:C:179:TYR:OH	2.11	0.50
3:B:3717:ASP:N	3:B:3717:ASP:OD1	2.42	0.50
3:B:4556:SER:CB	3:B:4664:LEU:HD21	2.42	0.50
3:B:4565:LEU:CD2	3:B:4653:VAL:HG21	2.41	0.50
3:B:4843:LEU:HA	3:B:4846:VAL:HG22	1.93	0.50
3:C:2270:SER:OG	3:C:2271:THR:N	2.38	0.50
3:C:4636:THR:HG22	3:C:4637:GLY:N	2.23	0.50
3:C:4843:LEU:HA	3:C:4846:VAL:HG22	1.93	0.50
3:D:469:ARG:O	3:D:473:ASN:ND2	2.45	0.50
3:D:2442:LEU:HD22	3:D:2447:LYS:HG3	1.92	0.50
3:D:4138:ASP:OD1	3:D:4138:ASP:N	2.42	0.50
3:D:4658:ILE:HG22	3:D:4659:ILE:N	2.26	0.50
3:B:4677:LEU:HD23	3:B:4711:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:469:ARG:O	3:C:473:ASN:ND2	2.45	0.50
3:C:3968:TYR:O	3:C:3976:ASN:ND2	2.45	0.50
3:C:4054:ASN:OD1	3:C:4054:ASN:N	2.44	0.50
3:C:4556:SER:CB	3:C:4664:LEU:HD21	2.42	0.50
3:D:132:ALA:HA	3:D:194:SER:HB2	1.92	0.50
3:D:1126:GLY:HA3	3:D:1143:TRP:CE2	2.47	0.50
3:D:2003:GLN:HE21	3:D:2007:ASN:HD21	1.60	0.50
3:A:1691:GLN:HE21	3:A:1802:ILE:HG13	1.76	0.50
3:B:1833:SER:OG	3:B:1834:VAL:N	2.45	0.50
3:B:3889:GLN:HG3	3:B:3967:GLU:HG3	1.92	0.50
3:B:4648:LEU:O	3:B:4649:LEU:C	2.53	0.50
3:C:4708:THR:HG22	3:C:4710:SER:H	1.76	0.50
3:D:1691:GLN:HE21	3:D:1802:ILE:HG13	1.75	0.50
3:D:3829:PHE:HD1	3:D:3915:ILE:HD11	1.76	0.50
3:A:2148:SER:O	3:A:2152:THR:OG1	2.26	0.50
3:A:3829:PHE:HD1	3:A:3915:ILE:HD11	1.77	0.50
3:A:4565:LEU:CD2	3:A:4653:VAL:HG21	2.41	0.50
3:A:4574:ASN:O	3:A:4575:PHE:C	2.54	0.50
3:B:2189:LYS:O	3:B:2193:GLN:NE2	2.45	0.50
3:B:4885:PHE:O	3:B:4889:VAL:HG22	2.11	0.50
3:B:5032:TYR:O	3:B:5036:LEU:HG	2.12	0.50
3:C:182:LEU:HD21	3:C:189:LEU:HB3	1.94	0.50
3:C:4658:ILE:HG22	3:C:4659:ILE:N	2.26	0.50
3:C:5032:TYR:O	3:C:5036:LEU:HG	2.12	0.50
3:D:2534:ALA:HB1	3:D:2588:ARG:HD2	1.93	0.50
3:D:3732:SER:OG	3:D:3769:ARG:NH2	2.45	0.50
3:A:469:ARG:O	3:A:473:ASN:ND2	2.45	0.50
3:A:663:TYR:HB2	3:A:808:TYR:HB3	1.92	0.50
3:A:2003:GLN:HE21	3:A:2007:ASN:HD21	1.60	0.50
3:A:4677:LEU:HD23	3:A:4711:PHE:CE1	2.46	0.50
3:B:2452:ARG:HE	3:C:175:SER:HA	1.77	0.50
3:D:4808:PHE:C	3:D:4810:ALA:H	2.19	0.50
3:A:3732:SER:OG	3:A:3769:ARG:NH2	2.45	0.50
3:A:3889:GLN:HG3	3:A:3967:GLU:HG3	1.92	0.50
3:A:4658:ILE:HG22	3:A:4659:ILE:N	2.26	0.50
3:A:4901:ILE:HG22	3:A:4902:GLU:N	2.25	0.50
3:B:4558:ASN:O	3:B:4559:PHE:C	2.54	0.50
3:C:708:GLY:H	3:C:713:SER:HG	1.57	0.50
3:C:1177:THR:OG1	3:C:1180:ARG:NH1	2.40	0.50
3:D:182:LEU:HD21	3:D:189:LEU:HB3	1.94	0.50
3:D:747:CYS:HB2	3:D:756:SER:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:708:GLY:H	3:A:713:SER:HG	1.56	0.50
3:A:2189:LYS:O	3:A:2193:GLN:NE2	2.45	0.50
3:C:1126:GLY:HA3	3:C:1143:TRP:CE2	2.46	0.50
3:A:582:HIS:O	3:A:585:SER:OG	2.29	0.50
3:A:5032:TYR:O	3:A:5036:LEU:HG	2.12	0.50
3:B:4982:GLU:OE1	3:B:4982:GLU:HA	2.12	0.50
3:B:5004:THR:OG1	3:B:5007:GLU:HG3	2.12	0.50
3:C:753:PRO:HB2	3:C:770:ALA:H	1.77	0.50
3:C:3717:ASP:N	3:C:3717:ASP:OD1	2.42	0.50
3:C:4982:GLU:OE1	3:C:4982:GLU:HA	2.12	0.50
3:D:1833:SER:OG	3:D:1834:VAL:N	2.45	0.50
3:A:1126:GLY:HA3	3:A:1143:TRP:CE2	2.47	0.50
3:A:4885:PHE:O	3:A:4889:VAL:HG22	2.11	0.50
3:A:4982:GLU:HA	3:A:4982:GLU:OE1	2.12	0.50
3:B:3732:SER:OG	3:B:3769:ARG:NH2	2.45	0.50
3:B:3968:TYR:O	3:B:3976:ASN:ND2	2.45	0.50
3:C:1147:ASP:OD1	3:C:1147:ASP:N	2.40	0.50
3:C:3829:PHE:HD1	3:C:3915:ILE:HD11	1.76	0.50
3:C:4574:ASN:O	3:C:4575:PHE:C	2.54	0.50
3:C:4885:PHE:O	3:C:4889:VAL:HG22	2.11	0.50
2:J:87:ARG:NH2	2:J:97:GLY:O	2.45	0.49
3:D:753:PRO:HB2	3:D:770:ALA:H	1.77	0.49
3:A:1236:THR:OG1	3:A:1608:MET:SD	2.64	0.49
3:A:2359:ARG:HD3	3:B:179:TYR:OH	2.12	0.49
3:A:4928:LEU:C	3:A:4930:ALA:N	2.69	0.49
3:A:5004:THR:OG1	3:A:5007:GLU:HG3	2.12	0.49
3:B:753:PRO:HB2	3:B:770:ALA:H	1.77	0.49
3:B:4813:LEU:O	3:B:4813:LEU:HD22	2.12	0.49
3:B:4901:ILE:HG22	3:B:4902:GLU:N	2.25	0.49
3:C:1186:ASP:N	3:C:1186:ASP:OD1	2.42	0.49
3:C:1691:GLN:HE21	3:C:1802:ILE:HG13	1.76	0.49
3:C:1833:SER:OG	3:C:1834:VAL:N	2.45	0.49
3:C:3732:SER:OG	3:C:3769:ARG:NH2	2.45	0.49
2:I:87:ARG:NH2	2:I:97:GLY:O	2.45	0.49
3:D:1147:ASP:OD1	3:D:1147:ASP:N	2.40	0.49
3:D:4192:ARG:HD3	3:D:5028:PHE:CD2	2.47	0.49
3:D:4843:LEU:HA	3:D:4846:VAL:HG22	1.93	0.49
3:D:4885:PHE:O	3:D:4889:VAL:HG22	2.11	0.49
3:D:5032:TYR:O	3:D:5036:LEU:HG	2.12	0.49
3:A:16:THR:OG1	3:A:99:ARG:O	2.31	0.49
3:A:112:ALA:O	3:A:115:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:303:ASP:OD2	3:A:306:LYS:NZ	2.44	0.49
3:A:2536:LEU:HD13	3:A:2544:THR:HG21	1.94	0.49
3:A:4843:LEU:HA	3:A:4846:VAL:HG22	1.93	0.49
3:B:182:LEU:HD21	3:B:189:LEU:HB3	1.94	0.49
3:B:2536:LEU:HD13	3:B:2544:THR:HG21	1.94	0.49
3:C:2003:GLN:HE21	3:C:2007:ASN:HD21	1.60	0.49
3:C:4650:HIS:CE1	3:C:4812:HIS:CD2	3.00	0.49
3:D:303:ASP:OD2	3:D:306:LYS:NZ	2.44	0.49
3:D:1496:TRP:CD1	3:D:1498:GLY:H	2.30	0.49
3:A:2214:VAL:HG21	3:A:2228:MET:HE2	1.94	0.49
3:A:2434:GLY:O	3:A:2508:ARG:NE	2.37	0.49
3:A:4813:LEU:O	3:A:4813:LEU:HD22	2.12	0.49
3:A:4886:HIS:O	3:A:4890:GLY:N	2.42	0.49
3:B:2003:GLN:HE21	3:B:2007:ASN:HD21	1.60	0.49
3:C:4558:ASN:O	3:C:4559:PHE:C	2.54	0.49
2:K:87:ARG:NH2	2:K:97:GLY:O	2.45	0.49
3:D:2189:LYS:O	3:D:2193:GLN:NE2	2.45	0.49
3:D:4556:SER:CB	3:D:4664:LEU:HD21	2.42	0.49
3:D:4813:LEU:O	3:D:4813:LEU:HD22	2.12	0.49
3:D:4982:GLU:OE1	3:D:4982:GLU:HA	2.12	0.49
3:D:4995:LEU:HD13	3:D:5011:TRP:HB2	1.95	0.49
3:A:747:CYS:HB2	3:A:756:SER:HB3	1.94	0.49
3:A:2534:ALA:HB1	3:A:2588:ARG:HD2	1.93	0.49
3:B:194:SER:OG	3:B:195:PHE:N	2.44	0.49
3:B:1861:GLN:HG2	3:B:1865:MET:HE2	1.94	0.49
3:B:3829:PHE:HD1	3:B:3915:ILE:HD11	1.76	0.49
3:B:4808:PHE:C	3:B:4810:ALA:H	2.19	0.49
3:C:303:ASP:OD2	3:C:306:LYS:NZ	2.44	0.49
3:C:2536:LEU:HD13	3:C:2544:THR:HG21	1.95	0.49
3:C:4631:PHE:CE2	3:C:4639:MET:HB2	2.48	0.49
3:D:3781:GLN:NE2	3:D:3819:TYR:OH	2.45	0.49
3:A:3794:VAL:HA	3:A:3797:THR:HG22	1.94	0.49
3:B:4631:PHE:CE2	3:B:4639:MET:HB2	2.48	0.49
3:C:588:SER:OG	3:C:592:LYS:NZ	2.46	0.49
3:C:2189:LYS:O	3:C:2193:GLN:NE2	2.45	0.49
3:C:3781:GLN:NE2	3:C:3819:TYR:OH	2.45	0.49
3:C:4192:ARG:HD3	3:C:5028:PHE:CD2	2.47	0.49
3:C:4898:GLY:HA3	3:C:4917:ASP:CG	2.37	0.49
3:C:5004:THR:OG1	3:C:5007:GLU:HG3	2.12	0.49
2:L:87:ARG:NH2	2:L:97:GLY:O	2.45	0.49
2:I:46:GLU:HA	2:I:49:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4898:GLY:HA3	3:D:4917:ASP:CG	2.37	0.49
3:D:4928:LEU:C	3:D:4930:ALA:N	2.69	0.49
3:A:194:SER:OG	3:A:195:PHE:N	2.44	0.49
3:A:1861:GLN:HG2	3:A:1865:MET:HE2	1.95	0.49
3:A:4631:PHE:CE2	3:A:4639:MET:HB2	2.48	0.49
3:A:4648:LEU:O	3:A:4649:LEU:C	2.53	0.49
3:A:4898:GLY:HA3	3:A:4917:ASP:CG	2.37	0.49
3:B:16:THR:OG1	3:B:99:ARG:O	2.31	0.49
3:B:3781:GLN:NE2	3:B:3819:TYR:OH	2.45	0.49
3:C:4670:ILE:HG21	3:C:4779:LYS:HG3	1.94	0.49
3:D:2214:VAL:HG21	3:D:2228:MET:HE2	1.95	0.49
3:D:5004:THR:OG1	3:D:5007:GLU:HG3	2.12	0.49
3:A:4556:SER:CB	3:A:4664:LEU:HD21	2.42	0.49
3:B:4658:ILE:HG22	3:B:4659:ILE:N	2.26	0.49
3:C:2314:LEU:HD21	3:C:2320:ASP:HA	1.95	0.49
3:C:4813:LEU:O	3:C:4813:LEU:HD22	2.13	0.49
3:C:4928:LEU:C	3:C:4930:ALA:N	2.69	0.49
3:C:4995:LEU:HD13	3:C:5011:TRP:HB2	1.95	0.49
3:D:16:THR:OG1	3:D:99:ARG:O	2.31	0.49
3:D:2148:SER:O	3:D:2152:THR:OG1	2.26	0.49
3:A:3781:GLN:NE2	3:A:3819:TYR:OH	2.45	0.49
3:A:4191:GLU:HG3	3:A:5006:GLN:OE1	2.13	0.49
3:A:4808:PHE:C	3:A:4810:ALA:H	2.19	0.49
3:A:4999:ASP:O	3:A:5003:HIS:NE2	2.46	0.49
3:B:469:ARG:O	3:B:473:ASN:ND2	2.45	0.49
3:B:2148:SER:O	3:B:2152:THR:OG1	2.26	0.49
3:B:4650:HIS:CE1	3:B:4812:HIS:CD2	3.00	0.49
3:B:4708:THR:HG22	3:B:4710:SER:H	1.76	0.49
3:B:4999:ASP:O	3:B:5003:HIS:NE2	2.46	0.49
3:C:4954:MET:HE2	3:C:4954:MET:HA	1.95	0.49
2:L:118:THR:N	2:L:121:GLU:OE1	2.46	0.49
3:D:2314:LEU:HD21	3:D:2320:ASP:HA	1.95	0.49
3:D:4650:HIS:CE1	3:D:4812:HIS:CD2	3.00	0.49
3:D:4670:ILE:HG21	3:D:4779:LYS:HG3	1.94	0.49
3:D:4999:ASP:O	3:D:5003:HIS:NE2	2.46	0.49
3:A:1496:TRP:CD1	3:A:1498:GLY:H	2.30	0.49
3:A:1833:SER:OG	3:A:1834:VAL:N	2.45	0.49
3:A:2314:LEU:HD21	3:A:2320:ASP:HA	1.95	0.49
3:A:4642:ALA:O	3:A:4646:LEU:HD13	2.13	0.49
3:A:4954:MET:HA	3:A:4954:MET:HE2	1.95	0.49
3:B:134:ASP:OD1	3:B:134:ASP:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2214:VAL:HG21	3:B:2228:MET:HE2	1.94	0.49
3:B:4192:ARG:HD3	3:B:5028:PHE:CD2	2.47	0.49
3:B:4948:GLU:OE1	3:B:4948:GLU:HA	2.13	0.49
3:C:847:SER:OG	3:C:848:HIS:N	2.46	0.49
3:C:4948:GLU:HA	3:C:4948:GLU:OE1	2.13	0.49
3:D:1452:TRP:N	3:D:1493:TYR:O	2.42	0.49
3:D:1861:GLN:HG2	3:D:1865:MET:HE2	1.94	0.49
3:D:4642:ALA:O	3:D:4646:LEU:HD13	2.13	0.49
3:D:5027:CYS:O	3:D:5029:ARG:N	2.46	0.49
3:A:4631:PHE:HZ	3:A:4639:MET:SD	2.36	0.49
3:B:619:ASP:OD2	3:B:1680:ARG:NH2	2.46	0.49
3:B:1496:TRP:CD1	3:B:1498:GLY:H	2.30	0.49
3:B:4928:LEU:C	3:B:4930:ALA:N	2.69	0.49
3:B:4954:MET:HE2	3:B:4954:MET:HA	1.95	0.49
3:C:619:ASP:OD2	3:C:1680:ARG:NH2	2.46	0.49
3:C:1496:TRP:CD1	3:C:1498:GLY:H	2.30	0.49
2:I:94:ASP:OD1	2:I:94:ASP:N	2.44	0.48
3:D:2536:LEU:HD13	3:D:2544:THR:HG21	1.94	0.48
3:A:182:LEU:HD21	3:A:189:LEU:HB3	1.94	0.48
3:A:4653:VAL:O	3:A:4653:VAL:HG12	2.13	0.48
3:B:705:ASN:N	3:B:705:ASN:OD1	2.46	0.48
3:B:1451:GLY:HA3	3:B:1494:MET:HA	1.94	0.48
3:B:4065:PHE:O	3:B:4133:GLN:NE2	2.44	0.48
3:B:4191:GLU:HG3	3:B:5006:GLN:OE1	2.13	0.48
3:B:5027:CYS:O	3:B:5029:ARG:N	2.46	0.48
3:C:2532:ALA:O	3:C:2535:SER:OG	2.31	0.48
3:C:4999:ASP:O	3:C:5003:HIS:NE2	2.46	0.48
3:D:4238:CYS:O	3:D:4242:ILE:HD13	2.14	0.48
3:D:4708:THR:HG22	3:D:4710:SER:H	1.76	0.48
3:D:4851:TYR:HD2	3:D:4920:PHE:HD2	1.60	0.48
3:A:114:SER:HB2	3:A:116:MET:HE3	1.96	0.48
3:A:619:ASP:OD2	3:A:1680:ARG:NH2	2.46	0.48
3:A:1177:THR:OG1	3:A:1180:ARG:NH1	2.40	0.48
3:A:2452:ARG:HE	3:B:175:SER:HA	1.78	0.48
3:A:4238:CYS:O	3:A:4242:ILE:HD13	2.14	0.48
3:A:4670:ILE:HG21	3:A:4779:LYS:HG3	1.94	0.48
3:A:4851:TYR:HD2	3:A:4920:PHE:HD2	1.60	0.48
3:A:5007:GLU:O	3:A:5010:VAL:HG12	2.13	0.48
3:B:3794:VAL:HA	3:B:3797:THR:HG22	1.94	0.48
3:B:4574:ASN:O	3:B:4575:PHE:C	2.54	0.48
3:B:4898:GLY:HA3	3:B:4917:ASP:CG	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:SER:HB2	3:C:116:MET:HE3	1.96	0.48
3:C:747:CYS:HB2	3:C:756:SER:HB3	1.94	0.48
3:C:5001:THR:OG1	3:C:5002:GLU:OE2	2.20	0.48
2:J:46:GLU:HA	2:J:49:LEU:HB2	1.94	0.48
3:D:134:ASP:OD1	3:D:134:ASP:N	2.40	0.48
3:D:705:ASN:N	3:D:705:ASN:OD1	2.46	0.48
3:D:4578:LEU:HD13	3:A:4849:TYR:CE2	2.37	0.48
3:A:847:SER:OG	3:A:848:HIS:N	2.46	0.48
3:A:3968:TYR:O	3:A:3976:ASN:ND2	2.45	0.48
3:A:4650:HIS:CE1	3:A:4812:HIS:CD2	3.00	0.48
3:B:4722:ARG:NH2	3:B:4749:GLU:HA	2.28	0.48
3:C:914:PRO:O	3:C:918:ARG:N	2.46	0.48
3:C:5027:CYS:O	3:C:5029:ARG:N	2.46	0.48
2:K:25:ASP:HB3	2:K:27:THR:HG22	1.96	0.48
2:K:46:GLU:HA	2:K:49:LEU:HB2	1.94	0.48
3:D:1451:GLY:HA3	3:D:1494:MET:HA	1.94	0.48
3:D:3794:VAL:HA	3:D:3797:THR:HG22	1.94	0.48
3:D:4631:PHE:CE2	3:D:4639:MET:HB2	2.48	0.48
3:A:753:PRO:HB2	3:A:770:ALA:H	1.77	0.48
3:A:1856:ASP:N	3:A:1856:ASP:OD1	2.46	0.48
3:A:4192:ARG:HD3	3:A:5028:PHE:CD2	2.47	0.48
3:B:588:SER:OG	3:B:592:LYS:NZ	2.46	0.48
3:B:4642:ALA:O	3:B:4646:LEU:HD13	2.13	0.48
3:B:4670:ILE:HG21	3:B:4779:LYS:HG3	1.94	0.48
3:C:16:THR:OG1	3:C:99:ARG:O	2.31	0.48
3:D:114:SER:HB2	3:D:116:MET:HE3	1.95	0.48
3:D:4836:GLN:CB	3:C:4822:THR:HG21	2.44	0.48
3:A:588:SER:OG	3:A:592:LYS:NZ	2.46	0.48
3:A:4558:ASN:O	3:A:4559:PHE:C	2.54	0.48
3:B:747:CYS:HB2	3:B:756:SER:HB3	1.94	0.48
3:B:1637:MET:HE1	3:B:1697:ALA:HB2	1.96	0.48
3:B:4936:ILE:HG21	3:C:4927:ILE:HG23	1.96	0.48
3:B:4995:LEU:HD13	3:B:5011:TRP:HB2	1.95	0.48
3:C:1452:TRP:N	3:C:1493:TYR:O	2.42	0.48
3:C:2204:HIS:HB2	3:C:2250:MET:HE1	1.96	0.48
3:C:3878:ASP:N	3:C:3878:ASP:OD1	2.46	0.48
1:H:38:SER:OG	1:H:39:SER:N	2.47	0.48
2:L:46:GLU:HA	2:L:49:LEU:HB2	1.94	0.48
2:I:118:THR:N	2:I:121:GLU:OE1	2.46	0.48
3:D:588:SER:OG	3:D:592:LYS:NZ	2.46	0.48
3:D:619:ASP:OD2	3:D:1680:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:708:GLY:H	3:D:713:SER:HG	1.58	0.48
3:D:4948:GLU:OE1	3:D:4948:GLU:HA	2.13	0.48
3:A:1028:ASP:OD1	3:A:1028:ASP:N	2.47	0.48
3:C:4642:ALA:O	3:C:4646:LEU:HD13	2.13	0.48
3:C:4851:TYR:HD2	3:C:4920:PHE:HD2	1.60	0.48
2:L:25:ASP:HB3	2:L:27:THR:HG22	1.96	0.48
1:G:38:SER:OG	1:G:39:SER:N	2.47	0.48
2:J:118:THR:N	2:J:121:GLU:OE1	2.46	0.48
2:I:25:ASP:HB3	2:I:27:THR:HG22	1.96	0.48
3:D:847:SER:OG	3:D:848:HIS:N	2.46	0.48
3:D:4565:LEU:CD2	3:D:4653:VAL:HG11	2.44	0.48
3:D:4886:HIS:O	3:D:4890:GLY:N	2.42	0.48
3:A:266:ARG:NH1	3:A:269:TRP:O	2.44	0.48
3:A:4948:GLU:OE1	3:A:4948:GLU:HA	2.13	0.48
3:A:5027:CYS:O	3:A:5029:ARG:N	2.46	0.48
3:C:2030:ASP:N	3:C:2030:ASP:OD1	2.46	0.48
3:C:3794:VAL:HA	3:C:3797:THR:HG22	1.94	0.48
3:C:4077:PHE:HA	3:C:4080:TYR:HB2	1.95	0.48
2:L:9:GLN:O	2:L:13:PHE:N	2.43	0.48
3:D:4631:PHE:HZ	3:D:4639:MET:SD	2.36	0.48
3:A:705:ASN:OD1	3:A:705:ASN:N	2.46	0.48
3:A:1451:GLY:HA3	3:A:1494:MET:HA	1.94	0.48
3:A:4731:ILE:HG13	3:A:4732:PHE:CD1	2.49	0.48
3:B:4077:PHE:HA	3:B:4080:TYR:HB2	1.95	0.48
3:B:4631:PHE:HZ	3:B:4639:MET:SD	2.36	0.48
3:B:5007:GLU:O	3:B:5010:VAL:HG12	2.13	0.48
3:C:784:SER:OG	3:C:785:ALA:N	2.47	0.48
3:C:1861:GLN:HG2	3:C:1865:MET:HE2	1.94	0.48
3:C:3842:LEU:O	3:C:3929:SER:OG	2.32	0.48
3:C:4191:GLU:HG3	3:C:5006:GLN:OE1	2.13	0.48
3:D:877:ASN:HD22	3:D:970:LEU:H	1.62	0.48
3:D:2333:ASP:N	3:D:2333:ASP:OD1	2.46	0.48
3:D:3878:ASP:N	3:D:3878:ASP:OD1	2.46	0.48
3:D:4582:VAL:HG13	3:A:4856:PHE:CZ	2.48	0.48
3:D:4653:VAL:O	3:D:4653:VAL:HG12	2.13	0.48
3:D:4681:LEU:CD2	3:D:4724:VAL:HG21	2.44	0.48
3:A:4995:LEU:HD13	3:A:5011:TRP:HB2	1.95	0.48
3:B:114:SER:HB2	3:B:116:MET:HE3	1.95	0.48
3:B:588:SER:O	3:B:592:LYS:NZ	2.43	0.48
3:B:2030:ASP:OD1	3:B:2030:ASP:N	2.46	0.48
3:B:2375:GLY:O	3:B:2379:ALA:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4653:VAL:O	3:B:4653:VAL:HG12	2.14	0.48
3:C:2214:VAL:HG21	3:C:2228:MET:HE2	1.94	0.48
3:C:4681:LEU:CD2	3:C:4724:VAL:HG21	2.44	0.48
3:C:4731:ILE:HG13	3:C:4732:PHE:CD1	2.49	0.48
3:D:4191:GLU:HG3	3:D:5006:GLN:OE1	2.13	0.48
3:D:4241:THR:HA	3:D:4244:GLU:CG	2.44	0.48
3:D:4721:LYS:CB	3:D:4743:MET:HE3	2.44	0.48
3:D:5007:GLU:O	3:D:5010:VAL:HG12	2.13	0.48
3:A:784:SER:OG	3:A:785:ALA:N	2.47	0.48
3:A:2204:HIS:HB2	3:A:2250:MET:HE1	1.96	0.48
3:A:4668:LEU:HD23	3:A:4672:LYS:HZ2	1.79	0.48
3:A:4730:ASP:O	3:A:4731:ILE:C	2.56	0.48
3:B:2314:LEU:HD21	3:B:2320:ASP:HA	1.95	0.48
3:B:4730:ASP:O	3:B:4731:ILE:C	2.57	0.48
3:C:582:HIS:O	3:C:585:SER:OG	2.29	0.48
3:C:698:GLY:H	3:C:1636:MET:HE1	1.79	0.48
3:C:836:GLY:HA3	3:C:837:PRO:HD2	1.78	0.48
3:C:1451:GLY:HA3	3:C:1494:MET:HA	1.94	0.48
3:D:4722:ARG:NH2	3:D:4749:GLU:HA	2.28	0.47
3:D:4951:LYS:HB2	3:D:4951:LYS:HZ3	1.79	0.47
3:D:4954:MET:HE2	3:D:4954:MET:HA	1.95	0.47
3:A:877:ASN:HD22	3:A:970:LEU:H	1.62	0.47
3:B:4851:TYR:HD2	3:B:4920:PHE:HD2	1.60	0.47
3:B:4901:ILE:HD12	3:B:4913:ARG:NH2	2.30	0.47
3:C:4722:ARG:HD3	3:C:4743:MET:HE2	1.96	0.47
2:J:25:ASP:HB3	2:J:27:THR:HG22	1.96	0.47
3:D:698:GLY:H	3:D:1636:MET:HE1	1.79	0.47
3:D:4731:ILE:HG13	3:D:4732:PHE:CD1	2.49	0.47
3:A:3842:LEU:O	3:A:3929:SER:OG	2.32	0.47
3:A:4681:LEU:CD2	3:A:4724:VAL:HG21	2.44	0.47
3:B:2333:ASP:OD1	3:B:2333:ASP:N	2.46	0.47
3:B:4722:ARG:HD3	3:B:4743:MET:HE2	1.96	0.47
3:B:4802:GLY:CA	3:B:4808:PHE:HB2	2.36	0.47
3:C:1443:GLN:OE1	3:C:1557:THR:N	2.47	0.47
3:C:4631:PHE:HZ	3:C:4639:MET:SD	2.36	0.47
2:K:79:ASP:OD1	2:K:79:ASP:N	2.47	0.47
3:D:3946:GLN:O	3:D:3950:ASN:ND2	2.43	0.47
3:D:3968:TYR:O	3:D:3976:ASN:ND2	2.45	0.47
3:A:698:GLY:H	3:A:1636:MET:HE1	1.79	0.47
3:A:4901:ILE:HD12	3:A:4913:ARG:NH2	2.30	0.47
3:B:784:SER:OG	3:B:785:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1147:ASP:OD1	3:B:1147:ASP:N	2.40	0.47
3:B:4686:LEU:HD23	3:B:4687:TYR:CE1	2.49	0.47
3:B:4721:LYS:CB	3:B:4743:MET:HE3	2.44	0.47
3:C:408:ALA:HB2	3:C:483:MET:HE1	1.97	0.47
3:C:2596:THR:OG1	3:C:2597:LYS:N	2.48	0.47
3:C:4653:VAL:O	3:C:4653:VAL:HG12	2.13	0.47
3:C:4686:LEU:HD23	3:C:4687:TYR:CE1	2.49	0.47
3:C:4721:LYS:CB	3:C:4743:MET:HE3	2.44	0.47
3:D:622:THR:HG23	3:D:626:LEU:HD12	1.97	0.47
3:D:1861:GLN:HA	3:D:1864:LYS:HD3	1.96	0.47
3:A:622:THR:HG23	3:A:626:LEU:HD12	1.97	0.47
3:A:836:GLY:HA3	3:A:837:PRO:HD2	1.78	0.47
3:B:112:ALA:O	3:B:115:ARG:NH2	2.44	0.47
3:B:2596:THR:OG1	3:B:2597:LYS:N	2.48	0.47
3:B:4238:CYS:O	3:B:4242:ILE:HD13	2.14	0.47
3:C:622:THR:HG23	3:C:626:LEU:HD12	1.97	0.47
3:C:4722:ARG:NH2	3:C:4749:GLU:HA	2.28	0.47
3:D:668:VAL:HA	3:D:789:VAL:HG23	1.97	0.47
3:D:3842:LEU:O	3:D:3929:SER:OG	2.32	0.47
3:D:4685:GLY:O	3:D:4689:THR:OG1	2.32	0.47
3:D:4901:ILE:HD12	3:D:4913:ARG:NH2	2.30	0.47
3:A:2375:GLY:O	3:A:2379:ALA:N	2.45	0.47
3:A:4077:PHE:HA	3:A:4080:TYR:HB2	1.95	0.47
3:A:4686:LEU:HD23	3:A:4687:TYR:CE1	2.49	0.47
3:B:668:VAL:HA	3:B:789:VAL:HG23	1.97	0.47
3:B:847:SER:OG	3:B:848:HIS:N	2.46	0.47
3:B:1028:ASP:N	3:B:1028:ASP:OD1	2.47	0.47
3:B:4681:LEU:CD2	3:B:4724:VAL:HG21	2.44	0.47
3:B:4731:ILE:HG13	3:B:4732:PHE:CD1	2.49	0.47
3:B:4794:TRP:O	3:B:4797:VAL:HG12	2.15	0.47
3:B:5009:TYR:OH	3:B:5013:MET:HE1	2.14	0.47
3:C:4565:LEU:CD2	3:C:4653:VAL:HG11	2.44	0.47
3:C:4685:GLY:O	3:C:4689:THR:OG1	2.32	0.47
3:C:4863:TYR:OH	3:C:4886:HIS:NE2	2.46	0.47
3:D:408:ALA:HB2	3:D:483:MET:HE1	1.97	0.47
3:D:4794:TRP:O	3:D:4797:VAL:HG12	2.15	0.47
3:A:2030:ASP:N	3:A:2030:ASP:OD1	2.46	0.47
3:A:4241:THR:HA	3:A:4244:GLU:CG	2.44	0.47
3:B:408:ALA:HB2	3:B:483:MET:HE1	1.97	0.47
3:C:2578:MET:HB3	3:C:2578:MET:HE2	1.81	0.47
3:C:4238:CYS:O	3:C:4242:ILE:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4794:TRP:O	3:C:4797:VAL:HG12	2.15	0.47
3:C:4901:ILE:HD12	3:C:4913:ARG:NH2	2.30	0.47
1:H:25:HIS:CE1	1:H:40:ARG:HG2	2.49	0.47
2:L:79:ASP:N	2:L:79:ASP:OD1	2.47	0.47
1:G:25:HIS:CE1	1:G:40:ARG:HG2	2.49	0.47
2:J:79:ASP:OD1	2:J:79:ASP:N	2.47	0.47
1:E:38:SER:OG	1:E:39:SER:N	2.47	0.47
3:D:914:PRO:O	3:D:918:ARG:N	2.46	0.47
3:D:2030:ASP:N	3:D:2030:ASP:OD1	2.46	0.47
3:D:4077:PHE:HA	3:D:4080:TYR:HB2	1.95	0.47
3:D:4686:LEU:HD23	3:D:4687:TYR:CE1	2.49	0.47
3:D:5009:TYR:OH	3:D:5013:MET:HE1	2.14	0.47
3:A:408:ALA:HB2	3:A:483:MET:HE1	1.97	0.47
3:A:4241:THR:HA	3:A:4244:GLU:HG2	1.97	0.47
3:A:4722:ARG:NH2	3:A:4749:GLU:HA	2.28	0.47
3:A:5009:TYR:OH	3:A:5013:MET:HE1	2.14	0.47
3:B:698:GLY:H	3:B:1636:MET:HE1	1.79	0.47
3:B:3898:ASP:OD1	3:B:3898:ASP:N	2.46	0.47
3:B:4241:THR:HA	3:B:4244:GLU:HG2	1.97	0.47
3:B:4685:GLY:O	3:B:4689:THR:OG1	2.32	0.47
3:B:5001:THR:OG1	3:B:5002:GLU:OE2	2.20	0.47
3:C:1868:PRO:O	3:C:1872:THR:OG1	2.29	0.47
3:C:4241:THR:HA	3:C:4244:GLU:CG	2.44	0.47
3:C:4556:SER:HB3	3:C:4664:LEU:HD21	1.96	0.47
3:C:5007:GLU:O	3:C:5010:VAL:HG12	2.13	0.47
3:C:5009:TYR:OH	3:C:5013:MET:HE1	2.14	0.47
3:D:175:SER:HA	3:C:2452:ARG:HE	1.80	0.47
3:D:1537:ASN:OD1	3:D:1537:ASN:N	2.48	0.47
3:D:2204:HIS:HB2	3:D:2250:MET:HE1	1.96	0.47
3:A:4685:GLY:O	3:A:4689:THR:OG1	2.32	0.47
3:A:4721:LYS:CB	3:A:4743:MET:HE3	2.44	0.47
3:A:4794:TRP:O	3:A:4797:VAL:HG12	2.15	0.47
3:B:582:HIS:O	3:B:585:SER:OG	2.29	0.47
3:B:622:THR:HG23	3:B:626:LEU:HD12	1.97	0.47
3:C:668:VAL:HA	3:C:789:VAL:HG23	1.97	0.47
3:C:1101:ARG:HB2	3:C:1193:SER:HB3	1.97	0.47
3:C:3804:ILE:HG22	3:C:3805:LEU:HD12	1.97	0.47
1:E:25:HIS:CE1	1:E:40:ARG:HG2	2.49	0.47
3:D:1279:SER:OG	3:D:1280:GLN:N	2.48	0.47
3:D:2578:MET:HB3	3:D:2578:MET:HE2	1.81	0.47
3:A:134:ASP:OD1	3:A:134:ASP:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1637:MET:HE1	3:A:1697:ALA:HB2	1.96	0.47
3:A:4675:LYS:HA	3:A:4715:TYR:CD1	2.50	0.47
3:B:1101:ARG:HB2	3:B:1193:SER:HB3	1.97	0.47
3:B:4556:SER:HB3	3:B:4664:LEU:HD21	1.96	0.47
3:B:4565:LEU:CD2	3:B:4653:VAL:HG11	2.44	0.47
3:C:2616:PRO:HA	3:C:2619:LEU:HD13	1.97	0.47
2:K:118:THR:N	2:K:121:GLU:OE1	2.46	0.47
3:D:582:HIS:O	3:D:585:SER:OG	2.29	0.47
3:D:3804:ILE:HG22	3:D:3805:LEU:HD12	1.97	0.47
3:A:668:VAL:HA	3:A:789:VAL:HG23	1.97	0.47
3:A:1279:SER:OG	3:A:1280:GLN:N	2.48	0.47
3:A:1727:ARG:HE	3:A:1775:HIS:CE1	2.33	0.47
3:A:4565:LEU:CD2	3:A:4653:VAL:HG11	2.44	0.47
3:B:2616:PRO:HA	3:B:2619:LEU:HD13	1.97	0.47
3:B:3878:ASP:OD1	3:B:3878:ASP:N	2.46	0.47
3:C:4951:LYS:HZ3	3:C:4951:LYS:HB2	1.79	0.47
3:D:1637:MET:HE1	3:D:1697:ALA:HB2	1.96	0.46
3:D:4722:ARG:HD3	3:D:4743:MET:HE2	1.96	0.46
3:A:1537:ASN:N	3:A:1537:ASN:OD1	2.48	0.46
3:A:4680:LYS:HG2	3:A:4680:LYS:O	2.15	0.46
3:B:3842:LEU:O	3:B:3929:SER:OG	2.32	0.46
3:C:877:ASN:HD22	3:C:970:LEU:H	1.62	0.46
3:C:1637:MET:HE1	3:C:1697:ALA:HB2	1.96	0.46
3:C:1856:ASP:N	3:C:1856:ASP:OD1	2.46	0.46
1:F:38:SER:OG	1:F:39:SER:N	2.47	0.46
3:D:4799:SER:N	3:D:4812:HIS:CE1	2.84	0.46
3:A:794:GLY:O	3:A:798:GLY:N	2.49	0.46
3:A:2333:ASP:N	3:A:2333:ASP:OD1	2.46	0.46
3:A:4814:LEU:O	3:A:4814:LEU:HD22	2.15	0.46
3:C:4209:GLN:HE21	3:C:4665:LYS:HZ1	1.61	0.46
3:C:4680:LYS:HG2	3:C:4680:LYS:O	2.15	0.46
2:K:45:THR:N	2:K:48:GLU:OE1	2.49	0.46
2:J:45:THR:N	2:J:48:GLU:OE1	2.49	0.46
3:D:2359:ARG:NH1	3:A:179:TYR:OH	2.34	0.46
3:D:3766:GLN:HG2	3:D:3769:ARG:HH12	1.80	0.46
3:D:4680:LYS:O	3:D:4680:LYS:HG2	2.15	0.46
3:A:4054:ASN:OD1	3:A:4054:ASN:N	2.44	0.46
3:B:794:GLY:O	3:B:798:GLY:N	2.49	0.46
3:B:877:ASN:HD22	3:B:970:LEU:H	1.62	0.46
3:B:1727:ARG:HE	3:B:1775:HIS:CE1	2.33	0.46
3:B:4241:THR:HA	3:B:4244:GLU:CG	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4674:GLU:OE2	3:B:4775:TYR:OH	2.29	0.46
3:C:794:GLY:O	3:C:798:GLY:N	2.49	0.46
3:C:1537:ASN:OD1	3:C:1537:ASN:N	2.48	0.46
3:C:4584:ASP:O	3:C:4586:PRO:HD3	2.16	0.46
3:D:1290:ARG:HH21	3:D:1598:GLN:HG3	1.81	0.46
3:D:2616:PRO:HA	3:D:2619:LEU:HD13	1.97	0.46
3:D:4724:VAL:HG13	3:D:4725:LEU:N	2.31	0.46
3:D:4878:ASP:O	3:D:4881:THR:N	2.35	0.46
3:A:2616:PRO:HA	3:A:2619:LEU:HD13	1.97	0.46
3:A:3804:ILE:HG22	3:A:3805:LEU:HD12	1.97	0.46
3:B:3766:GLN:HG2	3:B:3769:ARG:HH12	1.80	0.46
3:C:123:THR:OG1	3:C:134:ASP:OD2	2.34	0.46
3:C:1861:GLN:HA	3:C:1864:LYS:HD3	1.97	0.46
3:C:3898:ASP:N	3:C:3898:ASP:OD1	2.46	0.46
3:C:4801:LEU:O	3:C:4804:TYR:HB3	2.16	0.46
3:D:4556:SER:HB3	3:D:4664:LEU:HD21	1.96	0.46
3:D:4632:LEU:HD23	3:D:4632:LEU:C	2.41	0.46
3:A:1290:ARG:HH21	3:A:1598:GLN:HG3	1.81	0.46
3:A:1861:GLN:HA	3:A:1864:LYS:HD3	1.96	0.46
3:A:4556:SER:HB3	3:A:4664:LEU:HD21	1.96	0.46
3:A:4724:VAL:HG13	3:A:4725:LEU:N	2.31	0.46
3:B:303:ASP:OD2	3:B:306:LYS:NZ	2.44	0.46
3:B:3804:ILE:HG22	3:B:3805:LEU:HD12	1.97	0.46
3:B:4054:ASN:OD1	3:B:4054:ASN:N	2.44	0.46
3:B:4724:VAL:HG13	3:B:4725:LEU:N	2.31	0.46
3:B:4801:LEU:O	3:B:4804:TYR:HB3	2.16	0.46
1:F:25:HIS:CE1	1:F:40:ARG:HG2	2.49	0.46
3:D:2186:MET:O	3:D:2192:TYR:OH	2.32	0.46
3:D:4801:LEU:O	3:D:4804:TYR:HB3	2.16	0.46
3:A:588:SER:O	3:A:592:LYS:NZ	2.43	0.46
3:A:1443:GLN:OE1	3:A:1557:THR:N	2.47	0.46
3:A:3898:ASP:OD1	3:A:3898:ASP:N	2.46	0.46
3:A:4936:ILE:HG21	3:B:4927:ILE:HG23	1.97	0.46
3:B:4814:LEU:O	3:B:4814:LEU:HD22	2.15	0.46
3:C:1810:LYS:HG2	3:C:1814:MET:HE2	1.97	0.46
3:D:2596:THR:OG1	3:D:2597:LYS:N	2.48	0.46
3:D:4241:THR:HA	3:D:4244:GLU:HG2	1.97	0.46
3:D:4802:GLY:CA	3:D:4808:PHE:HB2	2.36	0.46
3:A:4632:LEU:HD23	3:A:4632:LEU:C	2.41	0.46
3:A:4799:SER:N	3:A:4812:HIS:CE1	2.84	0.46
3:A:4801:LEU:O	3:A:4804:TYR:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1290:ARG:HH21	3:B:1598:GLN:HG3	1.81	0.46
3:B:1856:ASP:OD1	3:B:1856:ASP:N	2.46	0.46
3:C:112:ALA:O	3:C:115:ARG:NH2	2.44	0.46
3:C:4632:LEU:HD23	3:C:4632:LEU:C	2.41	0.46
3:D:1101:ARG:HB2	3:D:1193:SER:HB3	1.97	0.46
3:D:4814:LEU:O	3:D:4814:LEU:HD22	2.15	0.46
3:A:4571:PHE:HD1	3:A:4571:PHE:HA	1.70	0.46
3:B:1861:GLN:HA	3:B:1864:LYS:HD3	1.96	0.46
3:C:1727:ARG:HE	3:C:1775:HIS:CE1	2.33	0.46
3:C:1738:LEU:HB2	3:C:2146:PRO:HD3	1.98	0.46
3:C:2333:ASP:OD1	3:C:2333:ASP:N	2.46	0.46
3:C:4799:SER:N	3:C:4812:HIS:CE1	2.84	0.46
2:K:9:GLN:O	2:K:13:PHE:N	2.43	0.46
2:I:45:THR:N	2:I:48:GLU:OE1	2.49	0.46
3:D:123:THR:OG1	3:D:134:ASP:OD2	2.34	0.46
3:D:4863:TYR:OH	3:D:4886:HIS:NE2	2.46	0.46
3:B:2204:HIS:HB2	3:B:2250:MET:HE1	1.96	0.46
3:C:266:ARG:NH1	3:C:269:TRP:O	2.44	0.46
3:C:1290:ARG:HH21	3:C:1598:GLN:HG3	1.81	0.46
3:C:4783:ILE:HG13	3:C:4784:PHE:CD1	2.45	0.46
2:L:45:THR:N	2:L:48:GLU:OE1	2.49	0.46
2:J:9:GLN:O	2:J:13:PHE:N	2.43	0.46
3:D:1461:ASP:OD1	3:D:1461:ASP:N	2.49	0.46
3:D:1727:ARG:HE	3:D:1775:HIS:CE1	2.33	0.46
3:D:4675:LYS:HA	3:D:4715:TYR:CD1	2.50	0.46
3:A:4655:PHE:CB	3:A:4796:MET:HE1	2.39	0.46
3:B:1653:LEU:HA	3:B:1656:ARG:HB2	1.98	0.46
3:B:2527:LEU:HD11	3:B:2582:MET:HB2	1.98	0.46
3:C:2375:GLY:O	3:C:2379:ALA:N	2.45	0.46
3:D:4584:ASP:O	3:D:4586:PRO:HD3	2.16	0.45
3:D:4798:MET:C	3:D:4812:HIS:CE1	2.93	0.45
3:A:1452:TRP:N	3:A:1493:TYR:O	2.42	0.45
3:A:1653:LEU:HA	3:A:1656:ARG:HB2	1.98	0.45
3:A:3766:GLN:HG2	3:A:3769:ARG:HH12	1.80	0.45
3:A:4243:PHE:O	3:A:4244:GLU:C	2.59	0.45
3:A:4722:ARG:HD3	3:A:4743:MET:HE2	1.96	0.45
3:B:1537:ASN:OD1	3:B:1537:ASN:N	2.48	0.45
3:B:1810:LYS:HG2	3:B:1814:MET:HE2	1.97	0.45
3:C:1044:ARG:O	3:C:1048:GLY:N	2.49	0.45
3:C:4243:PHE:O	3:C:4244:GLU:C	2.59	0.45
3:C:4675:LYS:HA	3:C:4715:TYR:CD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:112:ALA:O	3:D:115:ARG:NH2	2.44	0.45
3:D:1028:ASP:OD1	3:D:1028:ASP:N	2.47	0.45
3:D:1810:LYS:HG2	3:D:1814:MET:HE2	1.97	0.45
3:A:3878:ASP:N	3:A:3878:ASP:OD1	2.46	0.45
3:B:4632:LEU:C	3:B:4632:LEU:HD23	2.41	0.45
3:C:1461:ASP:OD1	3:C:1461:ASP:N	2.49	0.45
3:C:4724:VAL:HG13	3:C:4725:LEU:N	2.31	0.45
3:D:4638:TYR:CB	3:D:4641:PRO:HG2	2.47	0.45
3:A:2596:THR:OG1	3:A:2597:LYS:N	2.48	0.45
3:B:883:ALA:HB3	3:B:967:PRO:HG3	1.99	0.45
3:B:4799:SER:N	3:B:4812:HIS:CE1	2.84	0.45
3:C:788:LYS:HG3	3:C:1629:GLN:HB3	1.98	0.45
3:C:3766:GLN:HG2	3:C:3769:ARG:HH12	1.80	0.45
3:C:4241:THR:HA	3:C:4244:GLU:HG2	1.97	0.45
3:C:4780:PHE:HA	3:C:4783:ILE:CG1	2.46	0.45
3:D:4730:ASP:O	3:D:4731:ILE:C	2.57	0.45
3:A:1101:ARG:HB2	3:A:1193:SER:HB3	1.97	0.45
3:A:1839:VAL:HG23	3:A:1935:VAL:HG22	1.98	0.45
3:A:4931:ILE:O	3:A:4932:ILE:C	2.60	0.45
3:C:1279:SER:OG	3:C:1280:GLN:N	2.48	0.45
3:C:2527:LEU:HD11	3:C:2582:MET:HB2	1.98	0.45
3:C:4730:ASP:O	3:C:4731:ILE:C	2.57	0.45
3:D:531:ARG:NH2	3:D:562:GLU:OE1	2.43	0.45
3:D:1653:LEU:HA	3:D:1656:ARG:HB2	1.98	0.45
3:D:2527:LEU:HD11	3:D:2582:MET:HB2	1.98	0.45
3:A:1738:LEU:HB2	3:A:2146:PRO:HD3	1.98	0.45
3:A:4584:ASP:O	3:A:4586:PRO:HD3	2.16	0.45
3:A:4638:TYR:CB	3:A:4641:PRO:HG2	2.47	0.45
3:B:699:GLY:HA3	3:B:705:ASN:HD21	1.81	0.45
3:B:3900:GLN:NE2	3:B:3967:GLU:O	2.50	0.45
3:B:4728:HIS:O	3:B:4729:GLY:C	2.60	0.45
3:B:4929:LEU:HD13	3:B:4929:LEU:HA	1.72	0.45
3:C:531:ARG:NH2	3:C:562:GLU:OE1	2.43	0.45
3:C:1839:VAL:HG23	3:C:1935:VAL:HG22	1.98	0.45
3:C:4814:LEU:O	3:C:4814:LEU:HD22	2.15	0.45
2:L:94:ASP:N	2:L:94:ASP:OD1	2.44	0.45
2:I:9:GLN:O	2:I:13:PHE:N	2.43	0.45
3:D:699:GLY:HA3	3:D:705:ASN:HD21	1.81	0.45
3:D:4931:ILE:O	3:D:4932:ILE:C	2.60	0.45
3:A:468:LEU:HD23	3:A:468:LEU:HA	1.84	0.45
3:A:4798:MET:C	3:A:4812:HIS:CE1	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:579:GLN:OE1	3:B:582:HIS:NE2	2.50	0.45
3:B:1044:ARG:O	3:B:1048:GLY:N	2.48	0.45
3:B:1279:SER:OG	3:B:1280:GLN:N	2.48	0.45
3:B:1452:TRP:N	3:B:1493:TYR:O	2.42	0.45
3:B:4243:PHE:O	3:B:4244:GLU:C	2.59	0.45
3:B:4584:ASP:O	3:B:4586:PRO:HD3	2.16	0.45
3:C:699:GLY:HA3	3:C:705:ASN:HD21	1.81	0.45
3:C:3900:GLN:NE2	3:C:3967:GLU:O	2.50	0.45
3:C:4638:TYR:CB	3:C:4641:PRO:HG2	2.47	0.45
3:C:4652:LEU:O	3:C:4654:ALA:N	2.50	0.45
3:D:266:ARG:NH1	3:D:269:TRP:O	2.44	0.45
3:D:618:GLN:OE1	3:D:1678:ASN:ND2	2.35	0.45
3:D:794:GLY:O	3:D:798:GLY:N	2.49	0.45
3:D:1738:LEU:HB2	3:D:2146:PRO:HD3	1.98	0.45
3:D:4638:TYR:O	3:D:4641:PRO:HD2	2.17	0.45
3:D:4744:ASP:O	3:D:4745:LEU:C	2.60	0.45
3:A:957:LYS:HA	3:A:960:MET:HE2	1.99	0.45
3:A:3780:LEU:HD22	3:A:3816:MET:HG2	1.99	0.45
3:A:4725:LEU:HD23	3:A:4725:LEU:C	2.42	0.45
3:A:4728:HIS:O	3:A:4729:GLY:C	2.60	0.45
3:B:957:LYS:HA	3:B:960:MET:HE2	1.99	0.45
3:B:1177:THR:OG1	3:B:1180:ARG:NH1	2.40	0.45
3:B:4725:LEU:HD23	3:B:4725:LEU:C	2.42	0.45
3:B:4953:ASP:OD1	3:B:4953:ASP:C	2.60	0.45
3:C:579:GLN:OE1	3:C:582:HIS:NE2	2.50	0.45
3:C:1653:LEU:HA	3:C:1656:ARG:HB2	1.98	0.45
3:D:597:HIS:HD2	3:D:1665:HIS:CE1	2.35	0.45
3:D:788:LYS:HG3	3:D:1629:GLN:HB3	1.98	0.45
3:D:4851:TYR:HD2	3:D:4920:PHE:CD2	2.35	0.45
3:A:699:GLY:HA3	3:A:705:ASN:HD21	1.81	0.45
3:A:1461:ASP:OD1	3:A:1461:ASP:N	2.49	0.45
3:B:3675:ASP:OD1	3:B:3675:ASP:N	2.49	0.45
3:B:4680:LYS:O	3:B:4680:LYS:HG2	2.15	0.45
3:B:4740:LEU:HG	3:B:4741:LEU:HD22	1.99	0.45
3:B:4932:ILE:O	3:B:4933:GLN:C	2.60	0.45
3:D:1443:GLN:OE1	3:D:1557:THR:N	2.47	0.45
3:D:2375:GLY:O	3:D:2379:ALA:N	2.45	0.45
3:D:3966:THR:O	3:D:3970:GLN:N	2.50	0.45
3:A:579:GLN:OE1	3:A:582:HIS:NE2	2.50	0.45
3:A:4638:TYR:O	3:A:4641:PRO:HD2	2.17	0.45
3:A:4851:TYR:HD2	3:A:4920:PHE:CD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1097:THR:OG1	3:B:1098:GLY:N	2.50	0.45
3:B:1738:LEU:HB2	3:B:2146:PRO:HD3	1.98	0.45
3:B:4638:TYR:CB	3:B:4641:PRO:HG2	2.47	0.45
3:C:221:ARG:NH2	3:C:254:THR:O	2.50	0.45
3:C:1008:SER:HB3	3:C:1017:ARG:HD2	1.99	0.45
3:C:3798:LEU:HD23	3:C:3798:LEU:HA	1.87	0.45
3:D:595:ARG:NH1	3:D:1643:GLU:OE2	2.45	0.45
3:D:1839:VAL:HG23	3:D:1935:VAL:HG22	1.98	0.45
3:D:3898:ASP:OD1	3:D:3898:ASP:N	2.46	0.45
3:D:4054:ASN:OD1	3:D:4054:ASN:N	2.44	0.45
3:D:4652:LEU:O	3:D:4654:ALA:N	2.50	0.45
3:A:1097:THR:OG1	3:A:1098:GLY:N	2.50	0.45
3:A:1810:LYS:HG2	3:A:1814:MET:HE2	1.97	0.45
3:A:4984:ASN:O	3:A:4987:ASN:HB2	2.17	0.45
3:B:1632:ASP:OD1	3:B:1632:ASP:N	2.38	0.45
3:B:4675:LYS:HA	3:B:4715:TYR:CD1	2.50	0.45
3:C:597:HIS:HD2	3:C:1665:HIS:CE1	2.35	0.45
2:I:45:THR:HG23	2:I:47:ALA:H	1.83	0.44
3:D:836:GLY:HA3	3:D:837:PRO:HD2	1.78	0.44
3:D:4779:LYS:HB3	3:D:4779:LYS:HE2	1.70	0.44
3:A:597:HIS:HD2	3:A:1665:HIS:CE1	2.35	0.44
3:A:2527:LEU:HD11	3:A:2582:MET:HB2	1.98	0.44
3:A:4744:ASP:O	3:A:4745:LEU:C	2.60	0.44
3:A:4780:PHE:HA	3:A:4783:ILE:CG1	2.46	0.44
3:A:4934:GLY:O	3:A:4935:LEU:C	2.60	0.44
3:B:3966:THR:O	3:B:3970:GLN:N	2.50	0.44
3:B:4863:TYR:OH	3:B:4886:HIS:NE2	2.46	0.44
3:C:4953:ASP:OD1	3:C:4953:ASP:C	2.60	0.44
3:C:4984:ASN:O	3:C:4987:ASN:HB2	2.17	0.44
3:D:221:ARG:NH2	3:D:254:THR:O	2.50	0.44
3:D:2434:GLY:O	3:D:2508:ARG:NE	2.37	0.44
3:D:3780:LEU:HD22	3:D:3816:MET:HG2	1.99	0.44
3:D:4243:PHE:O	3:D:4244:GLU:C	2.59	0.44
3:A:4674:GLU:OE2	3:A:4775:TYR:OH	2.29	0.44
3:B:123:THR:OG1	3:B:134:ASP:OD2	2.34	0.44
3:B:1008:SER:HB3	3:B:1017:ARG:HD2	1.99	0.44
3:B:2442:LEU:HD23	3:B:2442:LEU:HA	1.88	0.44
3:C:883:ALA:HB3	3:C:967:PRO:HG3	1.98	0.44
3:C:4728:HIS:O	3:C:4729:GLY:C	2.60	0.44
3:C:4798:MET:C	3:C:4812:HIS:CE1	2.93	0.44
2:L:45:THR:HG23	2:L:47:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:784:SER:OG	3:D:785:ALA:N	2.47	0.44
3:D:3361:THR:O	3:D:3365:LEU:N	2.51	0.44
3:D:4780:PHE:HA	3:D:4783:ILE:CG1	2.46	0.44
3:D:4995:LEU:HD23	3:D:4995:LEU:HA	1.84	0.44
3:A:123:THR:OG1	3:A:134:ASP:OD2	2.34	0.44
3:A:3361:THR:O	3:A:3365:LEU:N	2.51	0.44
3:A:4953:ASP:OD1	3:A:4953:ASP:C	2.60	0.44
3:B:167:ASP:OD1	3:B:167:ASP:N	2.50	0.44
3:B:4779:LYS:HE2	3:B:4779:LYS:HB3	1.70	0.44
3:B:4798:MET:C	3:B:4812:HIS:CE1	2.93	0.44
3:B:4936:ILE:HG13	3:C:4927:ILE:HD12	1.98	0.44
3:B:4984:ASN:O	3:B:4987:ASN:HB2	2.17	0.44
3:C:3966:THR:O	3:C:3970:GLN:N	2.50	0.44
3:C:4708:THR:CG2	3:C:4775:TYR:HB2	2.47	0.44
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.84	0.44
3:D:957:LYS:HA	3:D:960:MET:HE2	1.99	0.44
3:D:2532:ALA:O	3:D:2535:SER:OG	2.31	0.44
3:D:3900:GLN:NE2	3:D:3967:GLU:O	2.50	0.44
3:A:3675:ASP:N	3:A:3675:ASP:OD1	2.49	0.44
3:A:4172:GLU:OE2	3:A:4175:ARG:NH2	2.44	0.44
3:B:531:ARG:NH2	3:B:562:GLU:OE1	2.43	0.44
3:B:4638:TYR:O	3:B:4641:PRO:HD2	2.17	0.44
3:B:4744:ASP:O	3:B:4745:LEU:C	2.60	0.44
3:C:705:ASN:OD1	3:C:705:ASN:N	2.46	0.44
3:C:2442:LEU:HD23	3:C:2442:LEU:HA	1.88	0.44
3:C:4638:TYR:O	3:C:4641:PRO:HD2	2.17	0.44
3:C:4851:TYR:HD2	3:C:4920:PHE:CD2	2.35	0.44
3:C:4934:GLY:O	3:C:4935:LEU:C	2.60	0.44
3:D:579:GLN:OE1	3:D:582:HIS:NE2	2.50	0.44
3:D:1770:SER:N	3:D:1956:GLU:OE2	2.51	0.44
3:D:4725:LEU:HD23	3:D:4725:LEU:C	2.42	0.44
3:D:4740:LEU:HG	3:D:4741:LEU:HD22	1.99	0.44
3:A:4652:LEU:O	3:A:4654:ALA:N	2.50	0.44
3:A:4812:HIS:O	3:A:4814:LEU:N	2.51	0.44
3:B:266:ARG:NH1	3:B:269:TRP:O	2.44	0.44
3:B:3946:GLN:O	3:B:3950:ASN:ND2	2.43	0.44
3:B:4172:GLU:OE2	3:B:4175:ARG:NH2	2.44	0.44
3:C:957:LYS:HA	3:C:960:MET:HE2	1.99	0.44
3:C:4650:HIS:O	3:C:4650:HIS:ND1	2.51	0.44
3:C:4725:LEU:C	3:C:4725:LEU:HD23	2.42	0.44
3:C:4802:GLY:CA	3:C:4808:PHE:HB2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:106:LEU:HD22	2:K:126:ILE:HD11	2.00	0.44
3:D:131:LEU:HD22	3:C:2460:LEU:HA	2.00	0.44
3:D:1856:ASP:OD1	3:D:1856:ASP:N	2.46	0.44
3:D:4024:VAL:HA	3:D:4027:LEU:HD12	2.00	0.44
3:A:788:LYS:HG3	3:A:1629:GLN:HB3	1.98	0.44
3:A:3966:THR:O	3:A:3970:GLN:N	2.50	0.44
3:B:788:LYS:HG3	3:B:1629:GLN:HB3	1.98	0.44
3:B:1849:LEU:HD12	3:B:1849:LEU:HA	1.86	0.44
3:C:2186:MET:O	3:C:2192:TYR:OH	2.33	0.44
3:C:4674:GLU:OE2	3:C:4775:TYR:OH	2.29	0.44
3:C:4812:HIS:O	3:C:4814:LEU:N	2.51	0.44
3:C:4931:ILE:O	3:C:4932:ILE:C	2.60	0.44
3:D:1097:THR:OG1	3:D:1098:GLY:N	2.50	0.44
3:D:2596:THR:HG23	3:D:2599:GLN:H	1.83	0.44
3:D:4650:HIS:ND1	3:D:4650:HIS:O	2.51	0.44
3:D:4674:GLU:OE2	3:D:4775:TYR:OH	2.29	0.44
3:A:4971:THR:OG1	3:A:4972:PRO:HD2	2.18	0.44
3:B:350:HIS:HB3	3:B:353:SER:HB3	1.99	0.44
3:B:597:HIS:HD2	3:B:1665:HIS:CE1	2.35	0.44
3:B:1443:GLN:OE1	3:B:1557:THR:N	2.47	0.44
3:B:1839:VAL:HG23	3:B:1935:VAL:HG22	1.98	0.44
3:B:2367:ALA:O	3:B:2374:SER:N	2.51	0.44
3:C:1770:SER:N	3:C:1956:GLU:OE2	2.51	0.44
3:C:3675:ASP:N	3:C:3675:ASP:OD1	2.49	0.44
3:C:4235:VAL:HG11	3:C:5019:TRP:CZ3	2.53	0.44
3:C:4572:ALA:C	3:C:4574:ASN:N	2.76	0.44
1:F:47:LYS:HB3	1:F:47:LYS:HE2	1.80	0.44
3:D:4705:VAL:HG23	3:D:4708:THR:OG1	2.18	0.44
3:A:1552:VAL:HG11	3:A:1562:ILE:HD13	2.00	0.44
3:A:1838:PHE:HA	3:A:1841:VAL:HG12	1.99	0.44
3:B:221:ARG:NH2	3:B:254:THR:O	2.50	0.44
3:B:4235:VAL:HG21	3:B:5019:TRP:CZ2	2.53	0.44
3:B:4650:HIS:ND1	3:B:4650:HIS:O	2.51	0.44
3:B:4652:LEU:O	3:B:4654:ALA:N	2.50	0.44
3:B:4688:ILE:HG21	3:B:4737:ILE:HD12	1.99	0.44
3:C:4740:LEU:HG	3:C:4741:LEU:HD22	1.99	0.44
3:C:4744:ASP:O	3:C:4745:LEU:C	2.60	0.44
3:C:4951:LYS:HB2	3:C:4951:LYS:NZ	2.33	0.44
3:D:883:ALA:HB3	3:D:967:PRO:HG3	1.98	0.44
3:D:1177:THR:OG1	3:D:1180:ARG:NH1	2.40	0.44
3:D:4927:ILE:HD11	3:C:4936:ILE:HG13	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:618:GLN:OE1	3:A:1678:ASN:ND2	2.35	0.44
3:A:756:SER:OG	3:A:757:PHE:N	2.51	0.44
3:A:2186:MET:O	3:A:2192:TYR:OH	2.33	0.44
3:A:3900:GLN:NE2	3:A:3967:GLU:O	2.50	0.44
3:A:4706:LEU:H	3:A:4706:LEU:HD12	1.83	0.44
3:B:756:SER:OG	3:B:757:PHE:N	2.51	0.44
3:B:1552:VAL:HG11	3:B:1562:ILE:HD13	2.00	0.44
3:B:2460:LEU:HA	3:C:131:LEU:HD22	2.00	0.44
3:B:4812:HIS:O	3:B:4814:LEU:N	2.51	0.44
2:J:106:LEU:HD22	2:J:126:ILE:HD11	2.00	0.43
2:I:79:ASP:OD1	2:I:79:ASP:N	2.47	0.43
2:I:106:LEU:HD22	2:I:126:ILE:HD11	2.00	0.43
3:D:1868:PRO:O	3:D:1872:THR:OG1	2.29	0.43
3:D:4932:ILE:O	3:D:4933:GLN:C	2.60	0.43
3:D:4979:THR:HG23	7:D:5104:ATP:C6	2.53	0.43
3:A:221:ARG:NH2	3:A:254:THR:O	2.50	0.43
3:A:717:ASP:OD2	3:A:722:TRP:NE1	2.46	0.43
3:A:883:ALA:HB3	3:A:967:PRO:HG3	1.99	0.43
3:A:4863:TYR:OH	3:A:4886:HIS:NE2	2.46	0.43
3:B:4235:VAL:HG11	3:B:5019:TRP:CZ3	2.53	0.43
3:B:4706:LEU:H	3:B:4706:LEU:HD12	1.83	0.43
3:B:4971:THR:OG1	3:B:4972:PRO:HD2	2.18	0.43
3:B:4995:LEU:HD23	3:B:4995:LEU:HA	1.84	0.43
3:C:4235:VAL:HG21	3:C:5019:TRP:CZ2	2.53	0.43
3:D:63:ALA:HB2	3:D:261:ARG:HH22	1.83	0.43
3:D:1008:SER:HB3	3:D:1017:ARG:HD2	1.99	0.43
3:D:4953:ASP:OD1	3:D:4953:ASP:C	2.60	0.43
3:D:4984:ASN:O	3:D:4987:ASN:HB2	2.17	0.43
3:A:492:ASP:OD1	3:A:493:ARG:NH1	2.51	0.43
3:A:4936:ILE:HG13	3:B:4927:ILE:HD12	1.99	0.43
3:C:1028:ASP:OD1	3:C:1028:ASP:N	2.47	0.43
3:C:4979:THR:HG23	7:C:5104:ATP:C6	2.53	0.43
2:K:45:THR:HG23	2:K:47:ALA:H	1.83	0.43
2:K:70:LEU:HD12	2:K:70:LEU:HA	1.88	0.43
2:J:45:THR:HG23	2:J:47:ALA:H	1.83	0.43
3:D:1838:PHE:HA	3:D:1841:VAL:HG12	1.99	0.43
3:D:4728:HIS:O	3:D:4729:GLY:C	2.60	0.43
3:A:1008:SER:HB3	3:A:1017:ARG:HD2	1.99	0.43
3:A:4650:HIS:ND1	3:A:4650:HIS:O	2.51	0.43
3:A:4832:HIS:ND1	3:A:4943:LEU:HD11	2.33	0.43
3:B:717:ASP:OD1	3:B:720:HIS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4809:PHE:HA	3:B:4812:HIS:CD2	2.53	0.43
3:B:4851:TYR:HD2	3:B:4920:PHE:CD2	2.35	0.43
3:B:4933:GLN:HG3	3:C:4926:VAL:O	2.18	0.43
3:C:551:LEU:HD23	3:C:551:LEU:HA	1.86	0.43
3:C:756:SER:OG	3:C:757:PHE:N	2.51	0.43
3:C:1097:THR:OG1	3:C:1098:GLY:N	2.50	0.43
3:C:1431:THR:O	3:C:1431:THR:OG1	2.36	0.43
3:C:4715:TYR:HE2	3:C:4717:ASP:HB3	1.82	0.43
3:C:4938:ASP:C	3:C:4940:PHE:N	2.75	0.43
3:C:4971:THR:OG1	3:C:4972:PRO:HD2	2.18	0.43
3:D:194:SER:OG	3:D:195:PHE:N	2.44	0.43
3:D:4172:GLU:OE2	3:D:4175:ARG:NH2	2.44	0.43
3:D:4209:GLN:HE21	3:D:4665:LYS:HZ2	1.67	0.43
3:A:2458:ARG:O	3:A:2510:TYR:OH	2.32	0.43
3:A:3946:GLN:O	3:A:3950:ASN:ND2	2.43	0.43
3:B:2578:MET:HE2	3:B:2578:MET:HB3	1.81	0.43
3:B:4056:GLU:HA	3:B:4059:LEU:HB2	2.01	0.43
3:C:63:ALA:HB2	3:C:261:ARG:HH22	1.83	0.43
3:C:1838:PHE:HA	3:C:1841:VAL:HG12	1.99	0.43
3:C:2596:THR:HG23	3:C:2599:GLN:H	1.83	0.43
3:C:4705:VAL:HG23	3:C:4708:THR:OG1	2.18	0.43
3:C:4706:LEU:H	3:C:4706:LEU:HD12	1.83	0.43
3:C:4809:PHE:HA	3:C:4812:HIS:CD2	2.53	0.43
3:D:3675:ASP:OD1	3:D:3675:ASP:N	2.49	0.43
3:D:4235:VAL:HA	3:D:4238:CYS:HB2	2.00	0.43
3:D:4655:PHE:CB	3:D:4796:MET:HE1	2.39	0.43
3:D:4812:HIS:O	3:D:4814:LEU:N	2.51	0.43
3:D:4971:THR:OG1	3:D:4972:PRO:HD2	2.18	0.43
3:A:2367:ALA:O	3:A:2374:SER:N	2.51	0.43
3:A:2578:MET:HE2	3:A:2578:MET:HB3	1.81	0.43
3:A:4705:VAL:HG23	3:A:4708:THR:OG1	2.18	0.43
3:A:4806:ASN:O	3:A:4807:PHE:C	2.59	0.43
3:A:4979:THR:HG23	7:A:5104:ATP:C6	2.53	0.43
3:B:914:PRO:O	3:B:918:ARG:N	2.46	0.43
3:B:4544:LEU:HA	3:B:4547:GLN:HG2	2.01	0.43
3:B:4931:ILE:O	3:B:4932:ILE:C	2.60	0.43
3:C:3780:LEU:HD22	3:C:3816:MET:HG2	1.99	0.43
3:C:4060:LYS:HE2	3:C:4060:LYS:HB3	1.85	0.43
3:C:4235:VAL:HA	3:C:4238:CYS:HB2	2.00	0.43
3:C:4896:GLY:HA2	3:C:4925:ILE:CD1	2.49	0.43
3:C:4923:PHE:O	3:C:4927:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:350:HIS:HB3	3:D:353:SER:HB3	1.99	0.43
3:D:4235:VAL:HG11	3:D:5019:TRP:CZ3	2.53	0.43
3:D:4572:ALA:C	3:D:4574:ASN:N	2.76	0.43
3:D:4663:CYS:C	3:D:4664:LEU:HD23	2.44	0.43
3:D:4929:LEU:HD13	3:D:4929:LEU:HA	1.72	0.43
3:D:4951:LYS:HB2	3:D:4951:LYS:NZ	2.33	0.43
3:A:1044:ARG:O	3:A:1048:GLY:N	2.49	0.43
3:A:4235:VAL:HG11	3:A:5019:TRP:CZ3	2.53	0.43
3:A:4544:LEU:O	3:A:4547:GLN:HG2	2.18	0.43
3:A:4652:LEU:C	3:A:4654:ALA:N	2.77	0.43
3:B:1770:SER:N	3:B:1956:GLU:OE2	2.51	0.43
3:B:2548:LEU:HD23	3:B:2551:ASN:HD22	1.84	0.43
3:C:1452:TRP:HB3	3:C:1548:LEU:HD22	2.01	0.43
2:K:51:ASP:N	2:K:51:ASP:OD1	2.51	0.43
3:D:3903:LEU:HG	3:D:3915:ILE:HD12	2.01	0.43
3:D:4706:LEU:HD12	3:D:4706:LEU:H	1.83	0.43
3:D:4832:HIS:ND1	3:D:4943:LEU:HD11	2.33	0.43
3:A:1569:GLN:HB2	3:A:1572:ILE:HD11	2.00	0.43
3:A:2460:LEU:HA	3:B:131:LEU:HD22	2.00	0.43
3:A:4809:PHE:HA	3:A:4812:HIS:CD2	2.53	0.43
3:B:3798:LEU:HD23	3:B:3798:LEU:HA	1.87	0.43
3:B:3903:LEU:HG	3:B:3915:ILE:HD12	2.01	0.43
3:B:4979:THR:HG23	7:B:5104:ATP:C6	2.53	0.43
3:B:4983:HIS:CE1	3:B:5027:CYS:SG	3.12	0.43
3:C:350:HIS:HB3	3:C:353:SER:HB3	1.99	0.43
3:C:4056:GLU:HA	3:C:4059:LEU:HB2	2.01	0.43
3:C:4983:HIS:CE1	3:C:5027:CYS:SG	3.12	0.43
3:D:1548:LEU:HD23	3:D:1548:LEU:HA	1.89	0.43
3:D:1552:VAL:HG11	3:D:1562:ILE:HD13	2.00	0.43
3:D:4896:GLY:HA2	3:D:4925:ILE:CD1	2.49	0.43
3:A:38:ALA:HB1	3:A:64:ILE:HG13	2.00	0.43
3:A:914:PRO:O	3:A:918:ARG:N	2.46	0.43
3:A:2190:VAL:HA	3:A:2193:GLN:HE21	1.84	0.43
3:A:2532:ALA:O	3:A:2535:SER:OG	2.31	0.43
3:A:4923:PHE:O	3:A:4927:ILE:HB	2.19	0.43
3:B:1838:PHE:HA	3:B:1841:VAL:HG12	1.99	0.43
3:B:2128:TYR:HB3	3:B:3669:PHE:HD2	1.84	0.43
3:B:3780:LEU:HD22	3:B:3816:MET:HG2	1.99	0.43
3:B:4235:VAL:HA	3:B:4238:CYS:HB2	2.00	0.43
3:B:4780:PHE:HA	3:B:4783:ILE:CG1	2.46	0.43
3:C:1552:VAL:HG11	3:C:1562:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:VAL:HG21	3:D:1782:PHE:CE1	2.54	0.43
2:L:106:LEU:HD22	2:L:126:ILE:HD11	2.00	0.43
2:J:87:ARG:HA	2:J:87:ARG:HD2	1.90	0.43
3:D:1476:MET:HE2	3:D:1476:MET:HB3	1.87	0.43
3:D:4688:ILE:HG21	3:D:4737:ILE:HD12	1.99	0.43
3:D:4783:ILE:HG13	3:D:4784:PHE:CD1	2.45	0.43
3:A:63:ALA:HB2	3:A:261:ARG:HH22	1.83	0.43
3:A:1561:VAL:HG12	3:A:1562:ILE:HG23	2.01	0.43
3:A:4640:GLU:CB	3:A:4641:PRO:HD3	2.47	0.43
3:A:4688:ILE:HG21	3:A:4737:ILE:HD12	1.99	0.43
3:B:1561:VAL:HG12	3:B:1562:ILE:HG23	2.01	0.43
3:B:2596:THR:HG23	3:B:2599:GLN:H	1.83	0.43
3:B:3729:MET:HE2	3:B:3800:LEU:HD11	2.00	0.43
3:B:3915:ILE:O	3:B:3919:THR:N	2.52	0.43
3:B:4578:LEU:CD1	3:C:4849:TYR:CE2	2.98	0.43
3:C:320:LYS:HG3	3:C:356:TRP:CZ2	2.54	0.43
3:C:1561:VAL:HG12	3:C:1562:ILE:HG23	2.01	0.43
3:D:1569:GLN:HB2	3:D:1572:ILE:HD11	2.00	0.43
3:D:4544:LEU:O	3:D:4547:GLN:HG2	2.18	0.43
3:D:4661:TYR:CE2	3:D:4789:PHE:HD2	2.37	0.43
3:D:4809:PHE:HA	3:D:4812:HIS:CD2	2.53	0.43
3:D:4930:ALA:O	3:D:4931:ILE:C	2.61	0.43
3:A:350:HIS:HB3	3:A:353:SER:HB3	1.99	0.43
3:A:1770:SER:N	3:A:1956:GLU:OE2	2.51	0.43
3:A:3903:LEU:HG	3:A:3915:ILE:HD12	2.01	0.43
3:A:4544:LEU:HA	3:A:4547:GLN:HG2	2.01	0.43
3:A:4740:LEU:HG	3:A:4741:LEU:HD22	1.99	0.43
3:B:1452:TRP:HB3	3:B:1548:LEU:HD22	2.01	0.43
3:B:1812:LEU:HD23	3:B:1812:LEU:HA	1.86	0.43
3:B:2165:LEU:HD23	3:B:2170:MET:HE1	2.01	0.43
3:B:4024:VAL:HA	3:B:4027:LEU:HD12	2.00	0.43
3:B:4705:VAL:HG23	3:B:4708:THR:OG1	2.18	0.43
3:B:4923:PHE:O	3:B:4927:ILE:HB	2.19	0.43
3:B:4934:GLY:O	3:B:4935:LEU:C	2.60	0.43
3:C:38:ALA:HB1	3:C:64:ILE:HG13	2.01	0.43
3:C:2258:LEU:HD12	3:C:2258:LEU:HA	1.90	0.43
3:C:2434:GLY:O	3:C:2508:ARG:NE	2.37	0.43
3:C:4681:LEU:C	3:C:4681:LEU:HD23	2.44	0.43
1:F:90:VAL:HG21	3:B:1782:PHE:CE1	2.54	0.42
2:I:51:ASP:OD1	2:I:51:ASP:N	2.51	0.42
3:D:717:ASP:OD1	3:D:720:HIS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1044:ARG:O	3:D:1048:GLY:N	2.48	0.42
3:D:2367:ALA:O	3:D:2374:SER:N	2.51	0.42
3:A:2128:TYR:HB3	3:A:3669:PHE:HD2	1.84	0.42
3:A:4046:ASP:O	3:A:4050:GLU:N	2.43	0.42
3:A:4661:TYR:CE2	3:A:4789:PHE:HD2	2.37	0.42
3:A:4851:TYR:CD2	3:A:4920:PHE:HD2	2.36	0.42
3:A:4930:ALA:O	3:A:4931:ILE:C	2.61	0.42
3:B:1461:ASP:N	3:B:1461:ASP:OD1	2.49	0.42
3:B:1569:GLN:HB2	3:B:1572:ILE:HD11	2.00	0.42
3:B:4571:PHE:HD1	3:B:4571:PHE:HA	1.69	0.42
3:B:4681:LEU:HD23	3:B:4681:LEU:C	2.44	0.42
3:B:4832:HIS:ND1	3:B:4943:LEU:HD11	2.33	0.42
3:C:4024:VAL:HA	3:C:4027:LEU:HD12	2.00	0.42
3:C:4661:TYR:CE2	3:C:4789:PHE:HD2	2.37	0.42
1:E:90:VAL:HG21	3:C:1782:PHE:CE1	2.54	0.42
3:D:717:ASP:OD2	3:D:722:TRP:NE1	2.46	0.42
3:D:1561:VAL:HG12	3:D:1562:ILE:HG23	2.01	0.42
3:D:1763:PRO:HG3	3:D:2094:LEU:HD22	2.01	0.42
3:D:2165:LEU:HD23	3:D:2170:MET:HE1	2.01	0.42
3:D:4851:TYR:CD2	3:D:4920:PHE:HD2	2.36	0.42
3:A:167:ASP:OD1	3:A:167:ASP:N	2.50	0.42
3:A:1763:PRO:HG3	3:A:2094:LEU:HD22	2.01	0.42
3:A:1930:LYS:HE3	3:A:1930:LYS:HB3	1.79	0.42
3:A:2319:PRO:HD2	3:A:2394:GLY:HA2	2.01	0.42
3:A:4024:VAL:HA	3:A:4027:LEU:HD12	2.00	0.42
3:A:4235:VAL:HA	3:A:4238:CYS:HB2	2.00	0.42
3:A:4586:PRO:HB3	3:A:4628:VAL:CB	2.49	0.42
3:B:1231:GLN:HG2	3:B:1232:ARG:HG3	2.01	0.42
3:B:1455:PRO:HG3	3:B:1549:PHE:HE2	1.84	0.42
3:B:3820:LEU:O	3:B:3902:TYR:OH	2.37	0.42
3:B:4572:ALA:C	3:B:4574:ASN:N	2.76	0.42
3:B:4853:VAL:HG13	3:B:4854:VAL:N	2.34	0.42
3:B:4896:GLY:HA2	3:B:4925:ILE:CD1	2.49	0.42
3:C:492:ASP:OD1	3:C:493:ARG:NH1	2.51	0.42
3:C:1763:PRO:HG3	3:C:2094:LEU:HD22	2.01	0.42
3:C:2548:LEU:HD23	3:C:2551:ASN:HD22	1.84	0.42
3:C:4544:LEU:HA	3:C:4547:GLN:HG2	2.01	0.42
1:G:53:GLN:HE21	1:G:53:GLN:HB2	1.69	0.42
3:D:38:ALA:HB1	3:D:64:ILE:HG13	2.01	0.42
3:D:1452:TRP:HB3	3:D:1548:LEU:HD22	2.01	0.42
3:D:1599:MET:HE3	3:D:1599:MET:HB2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2190:VAL:HA	3:D:2193:GLN:HE21	1.84	0.42
3:D:4059:LEU:HD23	3:D:4059:LEU:HA	1.88	0.42
3:D:4586:PRO:HB3	3:D:4628:VAL:CB	2.49	0.42
3:D:4934:GLY:O	3:D:4935:LEU:C	2.60	0.42
3:D:4983:HIS:CE1	3:D:5027:CYS:SG	3.12	0.42
3:A:131:LEU:HD12	3:A:131:LEU:HA	1.86	0.42
3:A:1231:GLN:HG2	3:A:1232:ARG:HG3	2.01	0.42
3:A:1455:PRO:HG3	3:A:1549:PHE:HE2	1.84	0.42
3:A:4056:GLU:HA	3:A:4059:LEU:HB2	2.01	0.42
3:B:4209:GLN:HE21	3:B:4665:LYS:HZ1	1.66	0.42
3:B:4652:LEU:C	3:B:4654:ALA:N	2.77	0.42
3:B:4655:PHE:CB	3:B:4796:MET:HE1	2.39	0.42
3:C:4688:ILE:HG21	3:C:4737:ILE:HD12	1.99	0.42
3:C:4832:HIS:ND1	3:C:4943:LEU:HD11	2.33	0.42
1:G:90:VAL:HG21	3:A:1782:PHE:CE1	2.54	0.42
2:I:44:PRO:HB2	2:I:48:GLU:HB2	2.02	0.42
3:D:492:ASP:OD1	3:D:493:ARG:NH1	2.51	0.42
3:D:840:VAL:HG12	3:D:1199:VAL:HG22	2.02	0.42
3:D:3915:ILE:O	3:D:3919:THR:N	2.52	0.42
3:A:840:VAL:HG12	3:A:1199:VAL:HG22	2.02	0.42
3:A:2457:LEU:HB2	3:A:2509:VAL:HG21	2.01	0.42
3:A:2548:LEU:HD23	3:A:2551:ASN:HD22	1.84	0.42
3:A:4853:VAL:HG13	3:A:4854:VAL:N	2.34	0.42
3:A:4896:GLY:HA2	3:A:4925:ILE:HD12	2.01	0.42
3:A:4983:HIS:CE1	3:A:5027:CYS:SG	3.12	0.42
3:B:320:LYS:HG3	3:B:356:TRP:CZ2	2.54	0.42
3:B:492:ASP:OD1	3:B:493:ARG:NH1	2.51	0.42
3:B:1763:PRO:HG3	3:B:2094:LEU:HD22	2.01	0.42
3:B:4544:LEU:O	3:B:4547:GLN:HG2	2.18	0.42
3:B:4688:ILE:HD11	3:B:4728:HIS:CD2	2.54	0.42
3:C:1455:PRO:HG3	3:C:1549:PHE:HE2	1.84	0.42
3:C:4663:CYS:C	3:C:4664:LEU:HD23	2.44	0.42
3:C:4806:ASN:O	3:C:4807:PHE:C	2.59	0.42
3:C:4853:VAL:HG13	3:C:4854:VAL:N	2.34	0.42
3:C:4921:PHE:CD2	3:C:4922[B]:PHE:HD1	2.38	0.42
2:L:121:GLU:O	2:L:125:MET:N	2.48	0.42
3:D:1942:LEU:HD12	3:D:1942:LEU:HA	1.90	0.42
3:D:2610:LEU:HD12	3:D:2610:LEU:HA	1.88	0.42
3:D:3915:ILE:H	3:D:3915:ILE:HG13	1.58	0.42
3:D:4544:LEU:HA	3:D:4547:GLN:HG2	2.01	0.42
3:D:4853:VAL:HG13	3:D:4854:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4923:PHE:O	3:D:4927:ILE:HB	2.19	0.42
3:A:2596:THR:HG23	3:A:2599:GLN:H	1.83	0.42
3:A:4681:LEU:HD23	3:A:4681:LEU:C	2.44	0.42
3:A:4983:HIS:CE1	3:A:5027:CYS:HG	2.37	0.42
3:B:2319:PRO:HD2	3:B:2394:GLY:HA2	2.01	0.42
3:B:3832:ILE:HD13	3:B:3832:ILE:HA	1.92	0.42
3:B:4801:LEU:O	3:B:4808:PHE:HD2	2.03	0.42
3:B:4930:ALA:O	3:B:4931:ILE:C	2.61	0.42
3:C:3729:MET:HE2	3:C:3800:LEU:HD11	2.00	0.42
3:C:3903:LEU:HG	3:C:3915:ILE:HD12	2.01	0.42
3:C:4688:ILE:HD11	3:C:4728:HIS:CD2	2.54	0.42
3:C:4851:TYR:CD2	3:C:4920:PHE:HD2	2.36	0.42
1:H:47:LYS:HB3	1:H:47:LYS:HE2	1.80	0.42
2:L:44:PRO:HB2	2:L:48:GLU:HB2	2.02	0.42
2:J:70:LEU:HD12	2:J:70:LEU:HA	1.88	0.42
1:E:53:GLN:HE21	1:E:53:GLN:HB2	1.69	0.42
3:D:2319:PRO:HD2	3:D:2394:GLY:HA2	2.01	0.42
3:D:3694:LYS:HE3	3:D:3694:LYS:HB2	1.91	0.42
3:D:3860:ASN:OD1	3:D:3861:GLU:N	2.53	0.42
3:D:4056:GLU:HA	3:D:4059:LEU:HB2	2.01	0.42
3:D:4688:ILE:HD11	3:D:4728:HIS:CD2	2.54	0.42
3:A:3904:ARG:HA	3:A:3914:ASN:HA	2.02	0.42
3:A:4779:LYS:HE2	3:A:4779:LYS:HB3	1.70	0.42
3:A:4896:GLY:HA2	3:A:4925:ILE:CD1	2.49	0.42
3:B:1868:PRO:O	3:B:1872:THR:OG1	2.29	0.42
3:B:2190:VAL:HA	3:B:2193:GLN:HE21	1.84	0.42
3:B:2532:ALA:O	3:B:2535:SER:OG	2.31	0.42
3:B:4663:CYS:C	3:B:4664:LEU:HD23	2.44	0.42
3:B:4715:TYR:HE2	3:B:4717:ASP:HB3	1.82	0.42
3:C:2367:ALA:O	3:C:2374:SER:N	2.51	0.42
3:C:3626:LYS:HE2	3:C:3626:LYS:HB2	1.89	0.42
3:C:4672:LYS:HZ2	3:C:4672:LYS:HG3	1.48	0.42
2:L:51:ASP:OD1	2:L:51:ASP:N	2.51	0.42
3:D:320:LYS:HG3	3:D:356:TRP:CZ2	2.54	0.42
3:D:1291:LEU:HD23	3:D:1291:LEU:HA	1.90	0.42
3:D:4821:LYS:O	3:D:4825:THR:HG23	2.20	0.42
3:A:4978:HIS:O	3:A:4982:GLU:HB2	2.20	0.42
3:C:1569:GLN:HB2	3:C:1572:ILE:HD11	2.00	0.42
3:C:4586:PRO:HB3	3:C:4628:VAL:CB	2.49	0.42
3:C:4734:ARG:O	3:C:4735:GLU:C	2.63	0.42
3:C:4821:LYS:O	3:C:4825:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4930:ALA:O	3:C:4931:ILE:C	2.61	0.42
2:K:121:GLU:O	2:K:125:MET:N	2.48	0.42
1:E:47:LYS:HE2	1:E:47:LYS:HB3	1.80	0.42
3:D:552:ASP:OD1	3:D:552:ASP:N	2.47	0.42
3:D:1005:TRP:HH2	3:D:1013:ILE:HG23	1.84	0.42
3:D:3729:MET:HE2	3:D:3800:LEU:HD11	2.00	0.42
3:D:4681:LEU:HD23	3:D:4681:LEU:C	2.44	0.42
3:D:4806:ASN:O	3:D:4807:PHE:C	2.59	0.42
3:D:4807:PHE:O	3:D:4810:ALA:HB3	2.20	0.42
3:A:1005:TRP:HH2	3:A:1013:ILE:HG23	1.84	0.42
3:B:840:VAL:HG12	3:B:1199:VAL:HG22	2.02	0.42
3:B:4661:TYR:CE2	3:B:4789:PHE:HD2	2.37	0.42
3:C:205:ILE:HD12	3:C:205:ILE:HA	1.92	0.42
3:C:290:TYR:O	3:C:302:VAL:N	2.47	0.42
3:C:4978:HIS:O	3:C:4982:GLU:HB2	2.20	0.42
3:D:1455:PRO:HG3	3:D:1549:PHE:HE2	1.84	0.42
3:D:2128:TYR:HB3	3:D:3669:PHE:HD2	1.84	0.42
3:D:4235:VAL:HG21	3:D:5019:TRP:CZ2	2.53	0.42
3:D:4978:HIS:O	3:D:4982:GLU:HB2	2.20	0.42
3:A:453:GLU:HA	3:A:454:PRO:HD3	1.95	0.42
3:A:584:LYS:HE2	3:A:584:LYS:HB3	1.94	0.42
3:A:3729:MET:HE2	3:A:3800:LEU:HD11	2.00	0.42
3:A:4572:ALA:C	3:A:4574:ASN:N	2.76	0.42
3:A:4663:CYS:C	3:A:4664:LEU:HD23	2.44	0.42
3:B:38:ALA:HB1	3:B:64:ILE:HG13	2.01	0.42
3:B:63:ALA:HB2	3:B:261:ARG:HH22	1.83	0.42
3:B:1685:LEU:HD23	3:B:1685:LEU:HA	1.87	0.42
3:B:2186:MET:O	3:B:2192:TYR:OH	2.32	0.42
3:B:2358:ILE:HD12	3:C:195:PHE:HE1	1.84	0.42
3:B:4576:ILE:HG23	3:B:4639:MET:HB3	2.02	0.42
3:B:4672:LYS:HZ2	3:B:4672:LYS:HG3	1.48	0.42
3:B:4701:TRP:CZ2	3:B:4781:GLY:HA3	2.55	0.42
3:B:4722:ARG:HD3	3:B:4743:MET:CE	2.50	0.42
3:B:4896:GLY:HA2	3:B:4925:ILE:HD12	2.01	0.42
3:B:4921:PHE:CD2	3:B:4922[B]:PHE:HD1	2.38	0.42
3:C:840:VAL:HG12	3:C:1199:VAL:HG22	2.02	0.42
3:C:2128:TYR:HB3	3:C:3669:PHE:HD2	1.84	0.42
3:C:4046:ASP:O	3:C:4050:GLU:N	2.43	0.42
3:C:4544:LEU:O	3:C:4547:GLN:HG2	2.18	0.42
3:C:4649:LEU:O	3:C:4652:LEU:N	2.52	0.42
3:D:3703:LEU:HD23	3:D:3703:LEU:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4715:TYR:HE2	3:D:4717:ASP:HB3	1.83	0.42
3:A:3832:ILE:HD13	3:A:3832:ILE:HA	1.92	0.42
3:A:4235:VAL:HG21	3:A:5019:TRP:CZ2	2.53	0.42
3:A:4807:PHE:O	3:A:4810:ALA:HB3	2.20	0.42
3:A:4985:LEU:HD23	3:A:4985:LEU:H	1.85	0.42
3:B:1272:LEU:HD13	3:B:1289:LEU:HD11	2.02	0.42
3:B:1575:LEU:HD12	3:B:1575:LEU:HA	1.91	0.42
3:B:4044:MET:HE2	3:B:4044:MET:HB2	1.88	0.42
3:B:4821:LYS:O	3:B:4825:THR:HG23	2.20	0.42
3:C:418:LEU:HD23	3:C:493:ARG:HB3	2.02	0.42
3:C:1272:LEU:HD13	3:C:1289:LEU:HD11	2.02	0.42
3:C:4684:ASP:O	3:C:4684:ASP:OD1	2.38	0.42
3:C:4807:PHE:O	3:C:4810:ALA:HB3	2.20	0.42
2:J:94:ASP:OD2	2:J:99:GLY:N	2.53	0.41
3:D:2548:LEU:HD23	3:D:2551:ASN:HD22	1.84	0.41
3:D:4582:VAL:HG11	3:A:4860:ARG:NH1	2.34	0.41
3:D:4652:LEU:C	3:D:4654:ALA:N	2.77	0.41
3:A:769:GLU:N	3:A:1473:THR:O	2.50	0.41
3:A:1871:PHE:HZ	3:A:2094:LEU:HD13	1.85	0.41
3:A:2114:PRO:HB3	3:A:3707:ARG:HH12	1.85	0.41
3:A:4821:LYS:O	3:A:4825:THR:HG23	2.20	0.41
3:B:1599:MET:HB2	3:B:1599:MET:HE3	1.80	0.41
3:C:1005:TRP:HH2	3:C:1013:ILE:HG23	1.84	0.41
3:C:2457:LEU:HB2	3:C:2509:VAL:HG21	2.01	0.41
3:C:2750:LYS:O	3:C:2754:PHE:N	2.53	0.41
3:C:3361:THR:O	3:C:3365:LEU:N	2.51	0.41
3:C:4044:MET:HE2	3:C:4044:MET:HB2	1.88	0.41
3:C:4576:ILE:HG23	3:C:4639:MET:HB3	2.02	0.41
3:C:4896:GLY:HA2	3:C:4925:ILE:HD12	2.01	0.41
3:D:167:ASP:OD1	3:D:167:ASP:N	2.50	0.41
3:D:1231:GLN:HG2	3:D:1232:ARG:HG3	2.01	0.41
3:D:1272:LEU:HD13	3:D:1289:LEU:HD11	2.02	0.41
3:D:2516:ASP:O	3:D:2520:HIS:N	2.53	0.41
3:D:4921:PHE:CD2	3:D:4922[B]:PHE:HD1	2.38	0.41
3:A:320:LYS:HG3	3:A:356:TRP:CZ2	2.54	0.41
3:A:3768:SER:HA	3:A:3771:HIS:CE1	2.55	0.41
3:A:4801:LEU:O	3:A:4808:PHE:HD2	2.03	0.41
3:B:1029:GLU:HA	3:B:1032:LYS:HB2	2.02	0.41
3:B:1871:PHE:HZ	3:B:2094:LEU:HD13	1.85	0.41
3:B:2461:VAL:O	3:B:2510:TYR:OH	2.38	0.41
3:B:3361:THR:O	3:B:3365:LEU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3860:ASN:OD1	3:B:3861:GLU:N	2.53	0.41
3:B:4851:TYR:CD2	3:B:4920:PHE:HD2	2.36	0.41
3:C:1029:GLU:HA	3:C:1032:LYS:HB2	2.02	0.41
3:C:4655:PHE:CB	3:C:4796:MET:HE1	2.39	0.41
3:C:4722:ARG:HD3	3:C:4743:MET:CE	2.50	0.41
3:C:4985:LEU:HD23	3:C:4985:LEU:H	1.85	0.41
2:K:94:ASP:OD2	2:K:99:GLY:N	2.53	0.41
3:D:1667:LEU:HD23	3:D:1667:LEU:HA	1.89	0.41
3:D:2457:LEU:HB2	3:D:2509:VAL:HG21	2.01	0.41
3:A:1452:TRP:HB3	3:A:1548:LEU:HD22	2.01	0.41
3:A:2165:LEU:HD23	3:A:2170:MET:HE1	2.01	0.41
3:A:2358:ILE:HD12	3:B:195:PHE:HE1	1.85	0.41
3:B:2457:LEU:HB2	3:B:2509:VAL:HG21	2.01	0.41
3:B:2610:LEU:HD12	3:B:2610:LEU:HA	1.88	0.41
3:B:3768:SER:HA	3:B:3771:HIS:CE1	2.55	0.41
3:B:3904:ARG:HA	3:B:3914:ASN:HA	2.02	0.41
3:C:2319:PRO:HD2	3:C:2394:GLY:HA2	2.01	0.41
2:I:70:LEU:HD12	2:I:70:LEU:HA	1.88	0.41
3:D:205:ILE:HD12	3:D:205:ILE:HA	1.92	0.41
3:A:595:ARG:NH1	3:A:1643:GLU:OE2	2.45	0.41
3:A:717:ASP:OD1	3:A:720:HIS:N	2.51	0.41
3:A:1272:LEU:HD13	3:A:1289:LEU:HD11	2.02	0.41
3:A:4933:GLN:HG3	3:B:4926:VAL:O	2.19	0.41
3:B:76:ARG:HD3	3:B:76:ARG:HA	1.88	0.41
3:B:418:LEU:HD23	3:B:493:ARG:HB3	2.02	0.41
3:B:2458:ARG:O	3:B:2510:TYR:OH	2.32	0.41
3:B:4586:PRO:HB3	3:B:4628:VAL:CB	2.49	0.41
3:B:4978:HIS:O	3:B:4982:GLU:HB2	2.20	0.41
3:B:4985:LEU:HD23	3:B:4985:LEU:H	1.85	0.41
3:C:805:PRO:HA	3:C:806:PRO:HD3	1.93	0.41
3:C:1476:MET:HE2	3:C:1476:MET:HB3	1.87	0.41
3:C:2285:GLU:N	3:C:2285:GLU:OE1	2.54	0.41
2:L:94:ASP:OD2	2:L:99:GLY:N	2.53	0.41
2:K:44:PRO:HB2	2:K:48:GLU:HB2	2.02	0.41
1:F:56:ILE:H	1:F:56:ILE:HG12	1.66	0.41
3:D:2114:PRO:HB3	3:D:3707:ARG:HH12	1.85	0.41
3:D:3904:ARG:HA	3:D:3914:ASN:HA	2.02	0.41
3:D:4785:THR:O	3:D:4785:THR:HG22	2.20	0.41
3:D:4801:LEU:O	3:D:4808:PHE:HD2	2.03	0.41
3:A:1018:ASN:HB3	3:A:1021:LEU:HG	2.03	0.41
3:A:2285:GLU:OE1	3:A:2285:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2516:ASP:O	3:A:2520:HIS:N	2.53	0.41
3:A:4722:ARG:HD3	3:A:4743:MET:CE	2.50	0.41
3:B:205:ILE:HD12	3:B:205:ILE:HA	1.92	0.41
3:B:1667:LEU:HD23	3:B:1667:LEU:HA	1.89	0.41
3:B:2114:PRO:HB3	3:B:3707:ARG:HH12	1.86	0.41
3:B:3882:GLN:HE21	3:B:3882:GLN:HB3	1.67	0.41
3:B:4734:ARG:O	3:B:4735:GLU:C	2.63	0.41
3:C:221:ARG:HH21	3:C:259:LEU:HD21	1.85	0.41
3:C:717:ASP:OD1	3:C:720:HIS:N	2.52	0.41
3:C:721:LEU:HD23	3:C:721:LEU:HA	1.91	0.41
3:C:2165:LEU:HD23	3:C:2170:MET:HE1	2.01	0.41
3:C:3768:SER:HA	3:C:3771:HIS:CE1	2.55	0.41
3:C:3832:ILE:HD13	3:C:3832:ILE:HA	1.92	0.41
3:C:4640:GLU:CB	3:C:4641:PRO:HD3	2.47	0.41
3:C:4779:LYS:HE2	3:C:4779:LYS:HB3	1.70	0.41
3:D:756:SER:OG	3:D:757:PHE:N	2.51	0.41
3:D:2285:GLU:N	3:D:2285:GLU:OE1	2.54	0.41
3:D:2321:ILE:HD12	3:D:2418:LEU:HD12	2.03	0.41
3:D:2471:SER:HA	3:D:2525:GLY:HA2	2.02	0.41
3:D:4576:ILE:HG23	3:D:4639:MET:HB3	2.02	0.41
3:D:4733:GLY:O	3:D:4737:ILE:HG12	2.21	0.41
3:D:4896:GLY:HA2	3:D:4925:ILE:HD12	2.01	0.41
3:A:4701:TRP:CZ2	3:A:4781:GLY:HA3	2.55	0.41
3:A:4929:LEU:HD13	3:A:4929:LEU:HA	1.72	0.41
3:B:4574:ASN:OD1	3:B:4813:LEU:HB2	2.21	0.41
3:B:4807:PHE:O	3:B:4810:ALA:HB3	2.20	0.41
3:C:595:ARG:NH1	3:C:1643:GLU:OE2	2.45	0.41
3:C:728:ARG:HA	3:C:728:ARG:HD3	1.91	0.41
3:C:3860:ASN:OD1	3:C:3861:GLU:N	2.53	0.41
3:C:3940:LYS:HE2	3:C:3940:LYS:HB3	1.77	0.41
3:C:4701:TRP:CZ2	3:C:4781:GLY:HA3	2.55	0.41
3:C:4733:GLY:O	3:C:4737:ILE:HG12	2.21	0.41
3:C:4932:ILE:O	3:C:4933:GLN:C	2.60	0.41
3:C:4995:LEU:HD23	3:C:4995:LEU:HA	1.84	0.41
2:J:126:ILE:HD13	2:J:126:ILE:HA	1.90	0.41
3:D:1871:PHE:HZ	3:D:2094:LEU:HD13	1.85	0.41
3:D:2024:PRO:HG2	3:D:2027:ILE:HG12	2.02	0.41
3:D:2461:VAL:O	3:D:2510:TYR:OH	2.38	0.41
3:D:3768:SER:HA	3:D:3771:HIS:CE1	2.55	0.41
3:D:4039:MET:H	3:D:4039:MET:HG3	1.67	0.41
3:A:2442:LEU:HD23	3:A:2442:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2491:SER:O	3:A:2491:SER:OG	2.32	0.41
3:A:3860:ASN:OD1	3:A:3861:GLU:N	2.53	0.41
3:A:3915:ILE:O	3:A:3919:THR:N	2.52	0.41
3:A:4578:LEU:CD1	3:B:4849:TYR:CE2	2.97	0.41
3:A:4687:TYR:O	3:A:4691:GLN:NE2	2.54	0.41
3:A:4688:ILE:HD11	3:A:4728:HIS:CD2	2.54	0.41
3:A:4921:PHE:CD2	3:A:4922[B]:PHE:HD1	2.38	0.41
3:A:4951:LYS:HB2	3:A:4951:LYS:NZ	2.33	0.41
3:B:1005:TRP:HH2	3:B:1013:ILE:HG23	1.84	0.41
3:B:4180:ARG:HD3	3:B:4192:ARG:NH1	2.36	0.41
3:C:1231:GLN:HG2	3:C:1232:ARG:HG3	2.01	0.41
3:C:2190:VAL:HA	3:C:2193:GLN:HE21	1.84	0.41
3:C:4049:VAL:O	3:C:4052:SER:OG	2.39	0.41
3:C:4983:HIS:CE1	3:C:5027:CYS:HG	2.39	0.41
2:K:86:ILE:HG12	2:K:143:VAL:HG12	2.03	0.41
2:J:10:ILE:H	2:J:10:ILE:HG13	1.69	0.41
3:D:221:ARG:HH21	3:D:259:LEU:HD21	1.85	0.41
3:D:4025:VAL:HA	3:D:4028:LEU:HD12	2.03	0.41
3:D:4708:THR:CG2	3:D:4775:TYR:HB2	2.47	0.41
3:D:4985:LEU:HD23	3:D:4985:LEU:H	1.85	0.41
3:A:2461:VAL:O	3:A:2510:TYR:OH	2.38	0.41
3:A:4000:MET:HE1	3:A:4058:ILE:HG13	2.02	0.41
3:A:4932:ILE:O	3:A:4933:GLN:C	2.60	0.41
3:B:2516:ASP:O	3:B:2520:HIS:N	2.53	0.41
3:C:1599:MET:HE3	3:C:1599:MET:HB2	1.79	0.41
3:C:2003:GLN:O	3:C:2007:ASN:ND2	2.54	0.41
3:C:2471:SER:HA	3:C:2525:GLY:HA2	2.02	0.41
3:C:4000:MET:HE1	3:C:4058:ILE:HG13	2.02	0.41
2:L:86:ILE:HG12	2:L:143:VAL:HG12	2.03	0.41
2:J:44:PRO:HB2	2:J:48:GLU:HB2	2.02	0.41
1:E:66:MET:HE2	1:E:66:MET:HB3	1.95	0.41
3:D:4640:GLU:CB	3:D:4641:PRO:HD3	2.47	0.41
3:D:4684:ASP:OD1	3:D:4684:ASP:O	2.38	0.41
3:D:4722:ARG:HD3	3:D:4743:MET:CE	2.50	0.41
3:D:4727:LYS:NZ	3:D:4728:HIS:CE1	2.89	0.41
3:D:4968:PHE:O	3:D:4974:GLY:HA3	2.21	0.41
3:A:221:ARG:HH21	3:A:259:LEU:HD21	1.85	0.41
3:A:1029:GLU:HA	3:A:1032:LYS:HB2	2.02	0.41
3:A:2024:PRO:HG2	3:A:2027:ILE:HG12	2.02	0.41
3:A:4180:ARG:HD3	3:A:4192:ARG:NH1	2.36	0.41
3:A:4576:ILE:HG23	3:A:4639:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4684:ASP:OD1	3:A:4684:ASP:O	2.38	0.41
3:A:4727:LYS:NZ	3:A:4728:HIS:CE1	2.89	0.41
3:A:4733:GLY:O	3:A:4737:ILE:HG12	2.21	0.41
3:A:4938:ASP:C	3:A:4940:PHE:N	2.76	0.41
3:B:265:LEU:HD23	3:B:279:PRO:HB2	2.03	0.41
3:B:290:TYR:O	3:B:302:VAL:N	2.47	0.41
3:B:1018:ASN:HB3	3:B:1021:LEU:HG	2.03	0.41
3:B:1519:LEU:HD23	3:B:1519:LEU:HA	1.92	0.41
3:B:1930:LYS:HE3	3:B:1930:LYS:HB3	1.79	0.41
3:B:2285:GLU:OE1	3:B:2285:GLU:N	2.54	0.41
3:B:2434:GLY:O	3:B:2508:ARG:NE	2.37	0.41
3:B:2471:SER:HA	3:B:2525:GLY:HA2	2.02	0.41
3:B:4649:LEU:O	3:B:4652:LEU:N	2.52	0.41
3:B:4687:TYR:O	3:B:4691:GLN:NE2	2.54	0.41
3:B:4708:THR:CG2	3:B:4775:TYR:HB2	2.47	0.41
3:B:5027:CYS:C	3:B:5029:ARG:H	2.29	0.41
3:C:468:LEU:HD23	3:C:468:LEU:HA	1.84	0.41
3:C:1871:PHE:HZ	3:C:2094:LEU:HD13	1.85	0.41
3:C:2321:ILE:HD12	3:C:2418:LEU:HD12	2.03	0.41
3:C:2461:VAL:O	3:C:2510:TYR:OH	2.38	0.41
3:C:3769:ARG:HH11	3:C:3769:ARG:HD3	1.75	0.41
3:C:4574:ASN:OD1	3:C:4813:LEU:HB2	2.21	0.41
3:C:4727:LYS:NZ	3:C:4728:HIS:CE1	2.89	0.41
3:C:4785:THR:O	3:C:4785:THR:HG22	2.20	0.41
3:C:4968:PHE:O	3:C:4974:GLY:HA3	2.21	0.41
3:D:584:LYS:HE2	3:D:584:LYS:HB3	1.94	0.41
3:D:1018:ASN:HB3	3:D:1021:LEU:HG	2.03	0.41
3:D:2442:LEU:HD23	3:D:2442:LEU:HA	1.88	0.41
3:D:2750:LYS:O	3:D:2754:PHE:N	2.53	0.41
3:D:3626:LYS:HE2	3:D:3626:LYS:HB2	1.89	0.41
3:D:4574:ASN:OD1	3:D:4813:LEU:HB2	2.21	0.41
3:D:4919:THR:HG23	3:D:4920:PHE:N	2.36	0.41
3:A:2471:SER:HA	3:A:2525:GLY:HA2	2.02	0.41
3:A:4025:VAL:HA	3:A:4028:LEU:HD12	2.03	0.41
3:B:221:ARG:HH21	3:B:259:LEU:HD21	1.85	0.41
3:B:4727:LYS:NZ	3:B:4728:HIS:CE1	2.89	0.41
3:C:1849:LEU:HD12	3:C:1849:LEU:HA	1.86	0.41
3:C:1930:LYS:HB3	3:C:1930:LYS:HE3	1.79	0.41
3:C:3946:GLN:O	3:C:3950:ASN:ND2	2.43	0.41
3:C:4025:VAL:HA	3:C:4028:LEU:HD12	2.03	0.41
3:D:418:LEU:HD23	3:D:493:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:ALA:HB2	3:D:563:VAL:HG22	2.03	0.40
3:D:1519:LEU:HD23	3:D:1519:LEU:HA	1.92	0.40
3:D:1651:LEU:O	3:D:1654:SER:OG	2.34	0.40
3:D:2003:GLN:O	3:D:2007:ASN:ND2	2.54	0.40
3:D:4180:ARG:HD3	3:D:4192:ARG:NH1	2.36	0.40
3:D:4192:ARG:H	3:D:4192:ARG:HG2	1.64	0.40
3:A:2138:LEU:HD23	3:A:3658:LYS:HD3	2.03	0.40
3:A:4574:ASN:OD1	3:A:4813:LEU:HB2	2.21	0.40
3:A:4785:THR:O	3:A:4785:THR:HG22	2.20	0.40
3:A:5027:CYS:C	3:A:5029:ARG:H	2.30	0.40
3:B:618:GLN:OE1	3:B:1678:ASN:ND2	2.35	0.40
3:C:1667:LEU:HD23	3:C:1667:LEU:HA	1.89	0.40
3:C:2516:ASP:O	3:C:2520:HIS:N	2.53	0.40
3:C:3904:ARG:HA	3:C:3914:ASN:HA	2.02	0.40
3:C:4687:TYR:O	3:C:4691:GLN:NE2	2.54	0.40
3:C:4799:SER:CA	3:C:4812:HIS:CE1	3.04	0.40
3:C:4801:LEU:O	3:C:4808:PHE:HD2	2.03	0.40
3:C:4822:THR:O	3:C:4826:ILE:HD12	2.21	0.40
2:I:94:ASP:OD2	2:I:99:GLY:N	2.54	0.40
3:D:615:ARG:NH2	3:D:1676:LEU:O	2.51	0.40
3:D:2138:LEU:HD23	3:D:3658:LYS:HD3	2.03	0.40
3:D:3678:SER:OG	3:D:3773:ARG:NH2	2.54	0.40
3:D:3940:LYS:HB3	3:D:3940:LYS:HE2	1.77	0.40
3:D:4822:THR:O	3:D:4826:ILE:HD12	2.22	0.40
3:A:416:LYS:HA	3:A:419:ASP:HB2	2.03	0.40
3:A:4171:LEU:HD23	3:A:4171:LEU:HA	1.95	0.40
3:A:4637:GLY:O	3:A:4638:TYR:C	2.65	0.40
3:B:438:ILE:HD13	3:B:438:ILE:HA	1.97	0.40
3:B:1819:VAL:HG12	3:B:1926:LEU:HD13	2.03	0.40
3:B:2138:LEU:HD23	3:B:3658:LYS:HD3	2.03	0.40
3:B:3626:LYS:HE2	3:B:3626:LYS:HB2	1.89	0.40
3:B:4192:ARG:H	3:B:4192:ARG:HG2	1.64	0.40
3:B:4806:ASN:O	3:B:4807:PHE:C	2.59	0.40
3:C:1018:ASN:HB3	3:C:1021:LEU:HG	2.03	0.40
3:C:2138:LEU:HD23	3:C:3658:LYS:HD3	2.03	0.40
3:C:3915:ILE:O	3:C:3919:THR:N	2.52	0.40
3:C:4734:ARG:H	3:C:4734:ARG:HG2	1.62	0.40
1:E:23:VAL:HG23	1:E:105:ASN:H	1.86	0.40
2:I:28:ILE:HG13	2:I:64:ILE:HB	2.04	0.40
3:D:265:LEU:HD23	3:D:279:PRO:HB2	2.03	0.40
3:D:3703:LEU:O	3:D:3706:SER:OG	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4687:TYR:O	3:D:4691:GLN:NE2	2.54	0.40
3:D:4780:PHE:CA	3:D:4783:ILE:HG12	2.50	0.40
3:A:418:LEU:HD23	3:A:493:ARG:HB3	2.02	0.40
3:A:1519:LEU:HD23	3:A:1519:LEU:HA	1.92	0.40
3:A:1819:VAL:HG12	3:A:1926:LEU:HD13	2.03	0.40
3:A:2358:ILE:HB	3:B:195:PHE:CE1	2.56	0.40
3:B:416:LYS:HA	3:B:419:ASP:HB2	2.03	0.40
3:B:3678:SER:OG	3:B:3773:ARG:NH2	2.54	0.40
3:B:4000:MET:HE1	3:B:4058:ILE:HG13	2.02	0.40
3:B:4060:LYS:HE2	3:B:4060:LYS:HB3	1.85	0.40
3:B:4783:ILE:HG13	3:B:4784:PHE:CD1	2.45	0.40
3:B:4783:ILE:HG13	3:B:4784:PHE:N	2.37	0.40
3:B:4785:THR:O	3:B:4785:THR:HG22	2.20	0.40
3:C:2025:GLU:HA	3:C:2028:ARG:HE	1.86	0.40
3:C:3678:SER:OG	3:C:3773:ARG:NH2	2.54	0.40
3:C:4805:ASN:O	3:C:4807:PHE:N	2.54	0.40
3:C:5027:CYS:C	3:C:5029:ARG:H	2.30	0.40
3:D:416:LYS:HA	3:D:419:ASP:HB2	2.03	0.40
3:D:1029:GLU:HA	3:D:1032:LYS:HB2	2.02	0.40
3:D:2025:GLU:HA	3:D:2028:ARG:HE	1.87	0.40
3:D:3886:ARG:NH2	3:D:3889:GLN:OE1	2.50	0.40
3:D:4230:LYS:HD2	3:D:4959:PHE:CE1	2.57	0.40
3:D:4783:ILE:HG13	3:D:4784:PHE:N	2.37	0.40
3:A:1147:ASP:OD1	3:A:1147:ASP:N	2.40	0.40
3:A:3882:GLN:HE21	3:A:3882:GLN:HB3	1.67	0.40
3:A:3885:PHE:HA	3:A:3888:LEU:HB2	2.04	0.40
3:A:4968:PHE:O	3:A:4974:GLY:HA3	2.21	0.40
3:B:131:LEU:HD12	3:B:131:LEU:HA	1.86	0.40
3:B:4025:VAL:HA	3:B:4028:LEU:HD12	2.03	0.40
3:B:4241:THR:HA	3:B:4244:GLU:OE1	2.21	0.40
3:B:4573:ILE:O	3:B:4573:ILE:HG22	2.22	0.40
3:C:416:LYS:HA	3:C:419:ASP:HB2	2.03	0.40
3:C:1260:MET:N	3:C:1269:CYS:O	2.52	0.40
3:C:1456:ASP:N	3:C:1456:ASP:OD1	2.39	0.40
3:C:1575:LEU:HD12	3:C:1575:LEU:HA	1.91	0.40
3:C:2518:LEU:HD22	3:C:2568:LEU:HD23	2.04	0.40
3:C:4648:LEU:HD12	3:C:4648:LEU:HA	1.92	0.40
2:L:42:GLN:HE22	2:L:76:LYS:HD2	1.87	0.40
1:E:56:ILE:H	1:E:56:ILE:HG12	1.66	0.40
2:I:126:ILE:HD13	2:I:126:ILE:HA	1.90	0.40
3:D:2518:LEU:HD22	3:D:2568:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3885:PHE:HA	3:D:3888:LEU:HB2	2.04	0.40
3:D:4000:MET:HE1	3:D:4058:ILE:HG13	2.02	0.40
3:D:4637:GLY:O	3:D:4638:TYR:C	2.65	0.40
3:D:4672:LYS:HZ2	3:D:4672:LYS:HG3	1.48	0.40
3:D:4701:TRP:CZ2	3:D:4781:GLY:HA3	2.55	0.40
3:A:527:ALA:HB2	3:A:563:VAL:HG22	2.03	0.40
3:A:749:ASP:HB3	3:A:754:SER:HB3	2.04	0.40
3:A:1599:MET:HE3	3:A:1599:MET:HB2	1.80	0.40
3:A:2189:LYS:NZ	3:A:2193:GLN:HE22	2.20	0.40
3:A:3678:SER:OG	3:A:3773:ARG:NH2	2.54	0.40
3:A:4044:MET:HE2	3:A:4044:MET:HB2	1.88	0.40
3:B:2358:ILE:HB	3:C:195:PHE:CE1	2.55	0.40
3:B:4640:GLU:CB	3:B:4641:PRO:HD3	2.47	0.40
3:B:4733:GLY:O	3:B:4737:ILE:HG12	2.21	0.40
3:C:749:ASP:HB3	3:C:754:SER:HB3	2.04	0.40
3:C:2024:PRO:HG2	3:C:2027:ILE:HG12	2.02	0.40
3:C:2114:PRO:HB3	3:C:3707:ARG:HH12	1.86	0.40
3:C:3694:LYS:HA	3:C:3695:PRO:HD3	1.95	0.40
3:C:4180:ARG:HD3	3:C:4192:ARG:NH1	2.36	0.40
3:C:4230:LYS:HD2	3:C:4959:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	F	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	G	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
2	J	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
2	K	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
2	L	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
3	A	3813/5037 (76%)	3598 (94%)	205 (5%)	10 (0%)	36	70
3	B	3813/5037 (76%)	3597 (94%)	206 (5%)	10 (0%)	36	70
3	C	3813/5037 (76%)	3597 (94%)	206 (5%)	10 (0%)	36	70
3	D	3813/5037 (76%)	3597 (94%)	206 (5%)	10 (0%)	36	70
All	All	16204/21168 (76%)	15297 (94%)	867 (5%)	40 (0%)	44	75

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	837	PRO
3	D	4653	VAL
3	D	4745	LEU
3	A	837	PRO
3	A	4653	VAL
3	A	4745	LEU
3	B	837	PRO
3	B	4653	VAL
3	B	4745	LEU
3	C	837	PRO
3	C	4653	VAL
3	C	4745	LEU
3	D	4821	LYS
3	A	4821	LYS
3	B	4821	LYS
3	C	4821	LYS
3	D	4578	LEU
3	A	4578	LEU
3	B	4578	LEU
3	C	4578	LEU
3	A	834	PRO
3	B	834	PRO
3	D	834	PRO
3	D	3354	LEU
3	D	4568	PHE
3	D	4806	ASN

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Mol	Chain	Res	Type
3	D	4813	LEU
3	A	3354	LEU
3	A	4568	PHE
3	A	4806	ASN
3	A	4813	LEU
3	B	3354	LEU
3	B	4568	PHE
3	B	4806	ASN
3	B	4813	LEU
3	C	834	PRO
3	C	3354	LEU
3	C	4568	PHE
3	C	4806	ASN
3	C	4813	LEU

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	E	84/88 (96%)	84 (100%)	0	100	100
1	F	84/88 (96%)	84 (100%)	0	100	100
1	G	84/88 (96%)	84 (100%)	0	100	100
1	H	84/88 (96%)	84 (100%)	0	100	100
2	I	104/122 (85%)	103 (99%)	1 (1%)	68	76
2	J	104/122 (85%)	103 (99%)	1 (1%)	68	76
2	K	104/122 (85%)	103 (99%)	1 (1%)	68	76
2	L	104/122 (85%)	103 (99%)	1 (1%)	68	76
3	A	2475/4276 (58%)	2442 (99%)	33 (1%)	61	72
3	B	2475/4276 (58%)	2441 (99%)	34 (1%)	59	71
3	C	2475/4276 (58%)	2441 (99%)	34 (1%)	59	71
3	D	2475/4276 (58%)	2441 (99%)	34 (1%)	59	71
All	All	10652/17944 (59%)	10513 (99%)	139 (1%)	59	72

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	53	ILE
2	K	53	ILE
2	J	53	ILE
2	I	53	ILE
3	D	16	THR
3	D	135	VAL
3	D	355	LEU
3	D	587	ILE
3	D	781	VAL
3	D	1112	ASP
3	D	1597	VAL
3	D	3874	VAL
3	D	4036	VAL
3	D	4214	LYS
3	D	4230	LYS
3	D	4241	THR
3	D	4244	GLU
3	D	4571	PHE
3	D	4573	ILE
3	D	4577	LEU
3	D	4648	LEU
3	D	4649	LEU
3	D	4652	LEU
3	D	4657	ILE
3	D	4658	ILE
3	D	4672	LYS
3	D	4734	ARG
3	D	4812	HIS
3	D	4813	LEU
3	D	4814	LEU
3	D	4816	ILE
3	D	4822	THR
3	D	4825	THR
3	D	4852	THR
3	D	4928	LEU
3	D	4929	LEU
3	D	4932	ILE
3	D	4938	ASP
3	A	16	THR
3	A	135	VAL
3	A	355	LEU
3	A	587	ILE

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Mol	Chain	Res	Type
3	A	1112	ASP
3	A	1597	VAL
3	A	3874	VAL
3	A	4036	VAL
3	A	4214	LYS
3	A	4230	LYS
3	A	4241	THR
3	A	4244	GLU
3	A	4571	PHE
3	A	4573	ILE
3	A	4577	LEU
3	A	4648	LEU
3	A	4649	LEU
3	A	4652	LEU
3	A	4657	ILE
3	A	4658	ILE
3	A	4672	LYS
3	A	4734	ARG
3	A	4812	HIS
3	A	4813	LEU
3	A	4814	LEU
3	A	4816	ILE
3	A	4822	THR
3	A	4825	THR
3	A	4852	THR
3	A	4928	LEU
3	A	4929	LEU
3	A	4932	ILE
3	A	4938	ASP
3	B	16	THR
3	B	135	VAL
3	B	355	LEU
3	B	587	ILE
3	B	781	VAL
3	B	1112	ASP
3	B	1597	VAL
3	B	3874	VAL
3	B	4036	VAL
3	B	4214	LYS
3	B	4230	LYS
3	B	4241	THR
3	B	4244	GLU

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Mol	Chain	Res	Type
3	B	4571	PHE
3	B	4573	ILE
3	B	4577	LEU
3	B	4648	LEU
3	B	4649	LEU
3	B	4652	LEU
3	B	4657	ILE
3	B	4658	ILE
3	B	4672	LYS
3	B	4734	ARG
3	B	4812	HIS
3	B	4813	LEU
3	B	4814	LEU
3	B	4816	ILE
3	B	4822	THR
3	B	4825	THR
3	B	4852	THR
3	B	4928	LEU
3	B	4929	LEU
3	B	4932	ILE
3	B	4938	ASP
3	C	16	THR
3	C	135	VAL
3	C	355	LEU
3	C	587	ILE
3	C	781	VAL
3	C	1112	ASP
3	C	1597	VAL
3	C	3874	VAL
3	C	4036	VAL
3	C	4214	LYS
3	C	4230	LYS
3	C	4241	THR
3	C	4244	GLU
3	C	4571	PHE
3	C	4573	ILE
3	C	4577	LEU
3	C	4648	LEU
3	C	4649	LEU
3	C	4652	LEU
3	C	4657	ILE
3	C	4658	ILE

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Mol	Chain	Res	Type
3	C	4672	LYS
3	C	4734	ARG
3	C	4812	HIS
3	C	4813	LEU
3	C	4814	LEU
3	C	4816	ILE
3	C	4822	THR
3	C	4825	THR
3	C	4852	THR
3	C	4928	LEU
3	C	4929	LEU
3	C	4932	ILE
3	C	4938	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (257) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	25	HIS
1	H	32	ASN
1	H	53	GLN
1	H	94	ASN
2	L	42	GLN
2	L	54	ASN
1	G	20	GLN
1	G	25	HIS
1	G	53	GLN
1	G	94	ASN
2	K	42	GLN
2	K	54	ASN
2	K	108	HIS
2	K	112	ASN
1	F	25	HIS
1	F	53	GLN
1	F	94	ASN
2	J	42	GLN
1	E	20	GLN
1	E	25	HIS
1	E	53	GLN
1	E	94	ASN
2	I	42	GLN
2	I	54	ASN
2	I	98	ASN

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Mol	Chain	Res	Type
3	D	71	GLN
3	D	79	GLN
3	D	156	GLN
3	D	383	HIS
3	D	473	ASN
3	D	593	HIS
3	D	597	HIS
3	D	647	ASN
3	D	765	GLN
3	D	838	HIS
3	D	877	ASN
3	D	994	ASN
3	D	1041	GLN
3	D	1084	GLN
3	D	1130	GLN
3	D	1165	ASN
3	D	1229	ASN
3	D	1296	GLN
3	D	1299	GLN
3	D	1429	ASN
3	D	1459	GLN
3	D	1460	HIS
3	D	1491	ASN
3	D	1545	ASN
3	D	1563	GLN
3	D	1598	GLN
3	D	1660	GLN
3	D	1665	HIS
3	D	1691	GLN
3	D	1719	HIS
3	D	1776	HIS
3	D	1861	GLN
3	D	1938	GLN
3	D	2007	ASN
3	D	2169	GLN
3	D	2193	GLN
3	D	2213	ASN
3	D	2247	GLN
3	D	2284	ASN
3	D	2291	GLN
3	D	2551	ASN
3	D	3767	GLN

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Mol	Chain	Res	Type
3	D	3781	GLN
3	D	3837	GLN
3	D	3851	ASN
3	D	3882	GLN
3	D	3900	GLN
3	D	4020	GLN
3	D	4162	ASN
3	D	4204	GLN
3	D	4209	GLN
3	D	4216	GLN
3	D	4223	ASN
3	D	4250	GLN
3	D	4714	ASN
3	D	4812	HIS
3	D	5003	HIS
3	D	5006	GLN
3	A	71	GLN
3	A	79	GLN
3	A	156	GLN
3	A	383	HIS
3	A	473	ASN
3	A	475	GLN
3	A	593	HIS
3	A	597	HIS
3	A	647	ASN
3	A	765	GLN
3	A	838	HIS
3	A	877	ASN
3	A	994	ASN
3	A	1035	ASN
3	A	1041	GLN
3	A	1084	GLN
3	A	1130	GLN
3	A	1165	ASN
3	A	1229	ASN
3	A	1296	GLN
3	A	1299	GLN
3	A	1429	ASN
3	A	1459	GLN
3	A	1460	HIS
3	A	1491	ASN
3	A	1545	ASN

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Mol	Chain	Res	Type
3	A	1563	GLN
3	A	1598	GLN
3	A	1660	GLN
3	A	1665	HIS
3	A	1691	GLN
3	A	1719	HIS
3	A	1776	HIS
3	A	1861	GLN
3	A	1938	GLN
3	A	2007	ASN
3	A	2161	GLN
3	A	2169	GLN
3	A	2193	GLN
3	A	2213	ASN
3	A	2247	GLN
3	A	2284	ASN
3	A	2551	ASN
3	A	3767	GLN
3	A	3781	GLN
3	A	3837	GLN
3	A	3851	ASN
3	A	3882	GLN
3	A	3900	GLN
3	A	4020	GLN
3	A	4162	ASN
3	A	4204	GLN
3	A	4209	GLN
3	A	4216	GLN
3	A	4223	ASN
3	A	4250	GLN
3	A	4547	GLN
3	A	4714	ASN
3	A	4812	HIS
3	A	5003	HIS
3	B	156	GLN
3	B	383	HIS
3	B	473	ASN
3	B	475	GLN
3	B	593	HIS
3	B	597	HIS
3	B	647	ASN
3	B	765	GLN

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Mol	Chain	Res	Type
3	B	838	HIS
3	B	877	ASN
3	B	994	ASN
3	B	1035	ASN
3	B	1041	GLN
3	B	1084	GLN
3	B	1130	GLN
3	B	1165	ASN
3	B	1229	ASN
3	B	1296	GLN
3	B	1299	GLN
3	B	1429	ASN
3	B	1459	GLN
3	B	1460	HIS
3	B	1491	ASN
3	B	1545	ASN
3	B	1563	GLN
3	B	1598	GLN
3	B	1660	GLN
3	B	1691	GLN
3	B	1719	HIS
3	B	1776	HIS
3	B	1861	GLN
3	B	1938	GLN
3	B	2007	ASN
3	B	2169	GLN
3	B	2193	GLN
3	B	2213	ASN
3	B	2247	GLN
3	B	2284	ASN
3	B	2291	GLN
3	B	2551	ASN
3	B	3767	GLN
3	B	3781	GLN
3	B	3837	GLN
3	B	3851	ASN
3	B	3882	GLN
3	B	3900	GLN
3	B	3977	GLN
3	B	4020	GLN
3	B	4162	ASN
3	B	4204	GLN

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Mol	Chain	Res	Type
3	B	4209	GLN
3	B	4216	GLN
3	B	4223	ASN
3	B	4547	GLN
3	B	4714	ASN
3	B	4812	HIS
3	B	5003	HIS
3	B	5006	GLN
3	C	156	GLN
3	C	383	HIS
3	C	473	ASN
3	C	475	GLN
3	C	593	HIS
3	C	597	HIS
3	C	647	ASN
3	C	765	GLN
3	C	838	HIS
3	C	877	ASN
3	C	994	ASN
3	C	1035	ASN
3	C	1041	GLN
3	C	1084	GLN
3	C	1130	GLN
3	C	1165	ASN
3	C	1296	GLN
3	C	1299	GLN
3	C	1429	ASN
3	C	1459	GLN
3	C	1460	HIS
3	C	1491	ASN
3	C	1545	ASN
3	C	1598	GLN
3	C	1660	GLN
3	C	1665	HIS
3	C	1691	GLN
3	C	1719	HIS
3	C	1861	GLN
3	C	1938	GLN
3	C	2007	ASN
3	C	2169	GLN
3	C	2176	ASN
3	C	2193	GLN

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Mol	Chain	Res	Type
3	C	2213	ASN
3	C	2247	GLN
3	C	2284	ASN
3	C	2291	GLN
3	C	2551	ASN
3	C	3767	GLN
3	C	3781	GLN
3	C	3837	GLN
3	C	3851	ASN
3	C	3882	GLN
3	C	3900	GLN
3	C	4020	GLN
3	C	4162	ASN
3	C	4204	GLN
3	C	4209	GLN
3	C	4216	GLN
3	C	4223	ASN
3	C	4250	GLN
3	C	4714	ASN
3	C	4812	HIS
3	C	5003	HIS
3	C	5006	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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
4	A1LVX	A	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.94	3 (5%)
8	CFF	C	5105	-	15,15,15	1.68	4 (26%)	23,23,23	1.71	5 (21%)
7	ATP	A	5104	-	32,33,33	3.09	12 (37%)	48,52,52	1.74	9 (18%)
8	CFF	A	5105	-	15,15,15	1.67	3 (20%)	23,23,23	1.70	5 (21%)
4	A1LVX	C	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.93	3 (5%)
7	ATP	B	5104	-	32,33,33	3.10	12 (37%)	48,52,52	1.74	9 (18%)
7	ATP	C	5104	-	32,33,33	3.10	12 (37%)	48,52,52	1.75	9 (18%)
7	ATP	D	5104	-	32,33,33	3.10	12 (37%)	48,52,52	1.74	9 (18%)
8	CFF	B	5105	-	15,15,15	1.68	4 (26%)	23,23,23	1.70	6 (26%)
4	A1LVX	B	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.93	3 (5%)
4	A1LVX	D	5101	-	38,39,39	1.00	2 (5%)	57,63,63	0.93	3 (5%)
8	CFF	D	5105	-	15,15,15	1.68	4 (26%)	23,23,23	1.70	5 (21%)

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
4	A1LVX	A	5101	-	-	1/47/47/47	0/2/2/2
8	CFF	C	5105	-	-	-	0/2/2/2
7	ATP	A	5104	-	-	11/22/38/38	0/3/3/3
8	CFF	A	5105	-	-	-	0/2/2/2
4	A1LVX	C	5101	-	-	1/47/47/47	0/2/2/2
7	ATP	B	5104	-	-	12/22/38/38	0/3/3/3
7	ATP	C	5104	-	-	11/22/38/38	0/3/3/3
7	ATP	D	5104	-	-	12/22/38/38	0/3/3/3
8	CFF	B	5105	-	-	-	0/2/2/2
4	A1LVX	B	5101	-	-	1/47/47/47	0/2/2/2
4	A1LVX	D	5101	-	-	1/47/47/47	0/2/2/2
8	CFF	D	5105	-	-	-	0/2/2/2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5104	ATP	C2'-C3'	-8.66	1.29	1.53
7	C	5104	ATP	C2'-C3'	-8.66	1.29	1.53
7	B	5104	ATP	C2'-C3'	-8.64	1.29	1.53
7	D	5104	ATP	C2'-C3'	-8.64	1.29	1.53
7	B	5104	ATP	C6-N6	6.00	1.49	1.34
7	D	5104	ATP	C6-N6	6.00	1.49	1.34
7	A	5104	ATP	C6-N6	6.00	1.49	1.34
7	C	5104	ATP	C6-N6	6.00	1.49	1.34
7	D	5104	ATP	PB-O3A	5.74	1.65	1.59
7	C	5104	ATP	PB-O3A	5.71	1.65	1.59
7	A	5104	ATP	PB-O3A	5.69	1.65	1.59
7	B	5104	ATP	PB-O3A	5.69	1.65	1.59
7	B	5104	ATP	PB-O3B	5.58	1.65	1.59
7	A	5104	ATP	PB-O3B	5.51	1.65	1.59
7	B	5104	ATP	PA-O3A	5.51	1.65	1.59
7	C	5104	ATP	PA-O3A	5.51	1.65	1.59
7	D	5104	ATP	PB-O3B	5.51	1.65	1.59
7	C	5104	ATP	PB-O3B	5.50	1.65	1.59
7	A	5104	ATP	PA-O3A	5.48	1.65	1.59
7	D	5104	ATP	PA-O3A	5.47	1.65	1.59
7	C	5104	ATP	O4'-C1'	-5.39	1.29	1.42
7	D	5104	ATP	O4'-C1'	-5.37	1.29	1.42
7	A	5104	ATP	O4'-C1'	-5.34	1.29	1.42
7	B	5104	ATP	O4'-C1'	-5.34	1.29	1.42
7	A	5104	ATP	O4'-C4'	4.35	1.54	1.45
7	B	5104	ATP	O4'-C4'	4.34	1.54	1.45
7	D	5104	ATP	O4'-C4'	4.33	1.54	1.45
7	C	5104	ATP	O4'-C4'	4.33	1.54	1.45
7	C	5104	ATP	C5'-C4'	-3.46	1.41	1.51
7	A	5104	ATP	C5'-C4'	-3.46	1.41	1.51
7	D	5104	ATP	C5'-C4'	-3.45	1.41	1.51
7	B	5104	ATP	C5'-C4'	-3.43	1.41	1.51
8	B	5105	CFF	C4-N3	-3.20	1.32	1.38
8	C	5105	CFF	C4-N3	-3.19	1.32	1.38
8	D	5105	CFF	C4-N3	-3.16	1.33	1.38
8	A	5105	CFF	C4-N3	-3.13	1.33	1.38
4	C	5101	A1LVX	C17-I1	-3.11	2.03	2.10
8	B	5105	CFF	C5-N7	-3.10	1.32	1.38
8	D	5105	CFF	C5-N7	-3.10	1.32	1.38
8	A	5105	CFF	C5-N7	-3.09	1.33	1.38
8	C	5105	CFF	C5-N7	-3.09	1.33	1.38
4	D	5101	A1LVX	C17-I1	-3.09	2.03	2.10
4	A	5101	A1LVX	C17-I1	-3.09	2.03	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5101	A1LVX	C17-I1	-3.09	2.03	2.10
7	C	5104	ATP	C2'-C1'	2.84	1.62	1.53
7	A	5104	ATP	O3'-C3'	2.83	1.50	1.43
7	C	5104	ATP	O3'-C3'	2.83	1.50	1.43
7	D	5104	ATP	C2'-C1'	2.82	1.62	1.53
7	A	5104	ATP	C2'-C1'	2.81	1.62	1.53
7	D	5104	ATP	O3'-C3'	2.81	1.49	1.43
7	B	5104	ATP	C2'-C1'	2.81	1.62	1.53
7	B	5104	ATP	O3'-C3'	2.80	1.49	1.43
7	B	5104	ATP	C8-N9	-2.62	1.33	1.37
7	C	5104	ATP	C8-N9	-2.61	1.33	1.37
7	D	5104	ATP	C8-N9	-2.60	1.33	1.37
7	A	5104	ATP	C8-N9	-2.59	1.33	1.37
8	A	5105	CFF	C5-C4	2.56	1.45	1.37
8	C	5105	CFF	C5-C4	2.56	1.45	1.37
8	D	5105	CFF	C5-C4	2.53	1.45	1.37
8	B	5105	CFF	C5-C4	2.52	1.45	1.37
4	A	5101	A1LVX	C8-C9	2.34	1.54	1.52
4	B	5101	A1LVX	C8-C9	2.34	1.54	1.52
7	A	5104	ATP	C5-N7	-2.32	1.34	1.39
7	C	5104	ATP	C5-N7	-2.32	1.34	1.39
4	D	5101	A1LVX	C8-C9	2.31	1.54	1.52
7	D	5104	ATP	C5-N7	-2.28	1.34	1.39
7	B	5104	ATP	C5-N7	-2.26	1.35	1.39
4	C	5101	A1LVX	C8-C9	2.24	1.54	1.52
8	B	5105	CFF	C5-C6	2.04	1.48	1.43
8	C	5105	CFF	C5-C6	2.03	1.48	1.43
8	D	5105	CFF	C5-C6	2.02	1.48	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	5104	ATP	C5-C4-N3	-5.14	119.64	126.72
7	C	5104	ATP	C5-C4-N3	-5.13	119.65	126.72
7	D	5104	ATP	C5-C4-N3	-5.13	119.66	126.72
7	A	5104	ATP	C5-C4-N3	-5.11	119.69	126.72
7	B	5104	ATP	N3-C2-N1	-4.69	121.48	128.58
7	C	5104	ATP	N3-C2-N1	-4.69	121.48	128.58
7	A	5104	ATP	N3-C2-N1	-4.68	121.50	128.58
7	D	5104	ATP	N3-C2-N1	-4.67	121.51	128.58
8	C	5105	CFF	N3-C2-N1	4.06	122.22	117.14
8	B	5105	CFF	N3-C2-N1	4.05	122.20	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	5105	CFF	N3-C2-N1	4.04	122.19	117.14
8	A	5105	CFF	N3-C2-N1	4.04	122.18	117.14
7	C	5104	ATP	N3-C4-N9	3.80	133.63	127.17
7	D	5104	ATP	N3-C4-N9	3.77	133.57	127.17
7	A	5104	ATP	N3-C4-N9	3.77	133.57	127.17
7	B	5104	ATP	N3-C4-N9	3.76	133.56	127.17
7	C	5104	ATP	C2-N3-C4	3.48	120.34	111.83
7	B	5104	ATP	C2-N3-C4	3.47	120.32	111.83
7	D	5104	ATP	C2-N3-C4	3.47	120.31	111.83
7	A	5104	ATP	C2-N3-C4	3.46	120.28	111.83
7	C	5104	ATP	N9-C8-N7	-3.28	109.28	113.94
7	A	5104	ATP	N9-C8-N7	-3.26	109.31	113.94
7	D	5104	ATP	N9-C8-N7	-3.25	109.32	113.94
7	B	5104	ATP	N9-C8-N7	-3.22	109.36	113.94
4	A	5101	A1LVX	O2-S1-C5	-3.04	106.05	108.87
7	B	5104	ATP	C4-C5-N7	-3.03	107.12	110.58
7	A	5104	ATP	C5-N7-C8	3.03	108.21	103.45
7	C	5104	ATP	C5-N7-C8	3.03	108.21	103.45
7	D	5104	ATP	C5-N7-C8	3.02	108.19	103.45
4	B	5101	A1LVX	O2-S1-C5	-3.02	106.07	108.87
4	D	5101	A1LVX	O2-S1-C5	-3.01	106.07	108.87
7	D	5104	ATP	C4-C5-N7	-3.01	107.14	110.58
7	B	5104	ATP	C5-N7-C8	2.99	108.15	103.45
7	A	5104	ATP	C4-C5-N7	-2.99	107.16	110.58
7	C	5104	ATP	C4-C5-N7	-2.99	107.16	110.58
4	C	5101	A1LVX	O2-S1-C5	-2.95	106.12	108.87
8	A	5105	CFF	C6-N1-C2	-2.87	120.99	125.66
8	C	5105	CFF	C6-N1-C2	-2.87	120.99	125.66
8	B	5105	CFF	C6-N1-C2	-2.86	121.02	125.66
8	D	5105	CFF	C6-N1-C2	-2.85	121.02	125.66
7	C	5104	ATP	C4-N9-C8	2.75	108.63	105.74
8	C	5105	CFF	N3-C4-N9	2.74	130.58	126.27
8	A	5105	CFF	N3-C4-N9	2.72	130.54	126.27
7	D	5104	ATP	C4-N9-C8	2.71	108.58	105.74
8	D	5105	CFF	N3-C4-N9	2.70	130.51	126.27
7	A	5104	ATP	C4-N9-C8	2.70	108.57	105.74
7	B	5104	ATP	C4-N9-C8	2.69	108.56	105.74
8	B	5105	CFF	N3-C4-N9	2.68	130.49	126.27
4	B	5101	A1LVX	C7-C17-I1	-2.36	117.22	122.88
4	D	5101	A1LVX	C7-C17-I1	-2.35	117.24	122.88
8	C	5105	CFF	C5-C4-N9	-2.35	107.45	112.10
4	A	5101	A1LVX	C7-C17-I1	-2.34	117.25	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5101	A1LVX	O1-S1-C5	-2.34	106.69	108.87
8	B	5105	CFF	C5-C4-N9	-2.33	107.47	112.10
4	C	5101	A1LVX	O1-S1-C5	-2.33	106.70	108.87
8	D	5105	CFF	C5-C4-N9	-2.33	107.48	112.10
8	A	5105	CFF	C5-C4-N9	-2.33	107.48	112.10
4	C	5101	A1LVX	C7-C17-I1	-2.33	117.29	122.88
4	D	5101	A1LVX	O1-S1-C5	-2.32	106.71	108.87
4	B	5101	A1LVX	O1-S1-C5	-2.32	106.72	108.87
7	B	5104	ATP	C4'-O4'-C1'	-2.25	104.51	109.47
7	A	5104	ATP	C4'-O4'-C1'	-2.23	104.54	109.47
7	D	5104	ATP	C4'-O4'-C1'	-2.23	104.54	109.47
7	C	5104	ATP	C4'-O4'-C1'	-2.22	104.57	109.47
8	A	5105	CFF	C6-C5-C4	-2.13	120.23	122.92
8	B	5105	CFF	C6-C5-C4	-2.13	120.23	122.92
8	D	5105	CFF	C6-C5-C4	-2.13	120.24	122.92
8	C	5105	CFF	C6-C5-C4	-2.13	120.24	122.92
8	B	5105	CFF	O11-C2-N3	-2.00	118.56	121.33

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	5104	ATP	PB-O3B-PG-O3G
7	D	5104	ATP	C5'-O5'-PA-O3A
7	A	5104	ATP	PB-O3B-PG-O3G
7	A	5104	ATP	C5'-O5'-PA-O3A
7	B	5104	ATP	PB-O3B-PG-O3G
7	B	5104	ATP	C5'-O5'-PA-O3A
7	C	5104	ATP	PB-O3B-PG-O3G
7	C	5104	ATP	C5'-O5'-PA-O3A
7	D	5104	ATP	PB-O3B-PG-O2G
7	A	5104	ATP	PB-O3B-PG-O2G
7	B	5104	ATP	PB-O3B-PG-O2G
7	C	5104	ATP	PB-O3B-PG-O2G
7	D	5104	ATP	PB-O3A-PA-O2A
7	A	5104	ATP	PB-O3A-PA-O2A
7	B	5104	ATP	PB-O3A-PA-O2A
7	C	5104	ATP	PB-O3A-PA-O2A
7	D	5104	ATP	C5'-O5'-PA-O1A
7	D	5104	ATP	C5'-O5'-PA-O2A
7	A	5104	ATP	C5'-O5'-PA-O1A
7	B	5104	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
7	B	5104	ATP	C5'-O5'-PA-O2A
7	C	5104	ATP	C5'-O5'-PA-O1A
7	D	5104	ATP	C4'-C5'-O5'-PA
7	A	5104	ATP	C4'-C5'-O5'-PA
7	B	5104	ATP	C4'-C5'-O5'-PA
7	C	5104	ATP	C4'-C5'-O5'-PA
7	D	5104	ATP	PG-O3B-PB-O3A
7	A	5104	ATP	PG-O3B-PB-O3A
7	B	5104	ATP	PG-O3B-PB-O3A
7	C	5104	ATP	PG-O3B-PB-O3A
7	D	5104	ATP	PB-O3B-PG-O1G
7	A	5104	ATP	PB-O3B-PG-O1G
7	B	5104	ATP	PB-O3B-PG-O1G
7	C	5104	ATP	PB-O3B-PG-O1G
7	D	5104	ATP	O4'-C4'-C5'-O5'
7	A	5104	ATP	O4'-C4'-C5'-O5'
7	B	5104	ATP	O4'-C4'-C5'-O5'
7	C	5104	ATP	O4'-C4'-C5'-O5'
7	D	5104	ATP	PG-O3B-PB-O1B
7	A	5104	ATP	PG-O3B-PB-O1B
7	B	5104	ATP	PG-O3B-PB-O1B
7	C	5104	ATP	PG-O3B-PB-O1B
4	D	5101	A1LVX	C11-C12-N2-C19
4	B	5101	A1LVX	C11-C12-N2-C19
4	A	5101	A1LVX	C11-C12-N2-C19
4	C	5101	A1LVX	C11-C12-N2-C19
7	A	5104	ATP	C3'-C4'-C5'-O5'
7	C	5104	ATP	C3'-C4'-C5'-O5'
7	D	5104	ATP	C3'-C4'-C5'-O5'
7	B	5104	ATP	C3'-C4'-C5'-O5'

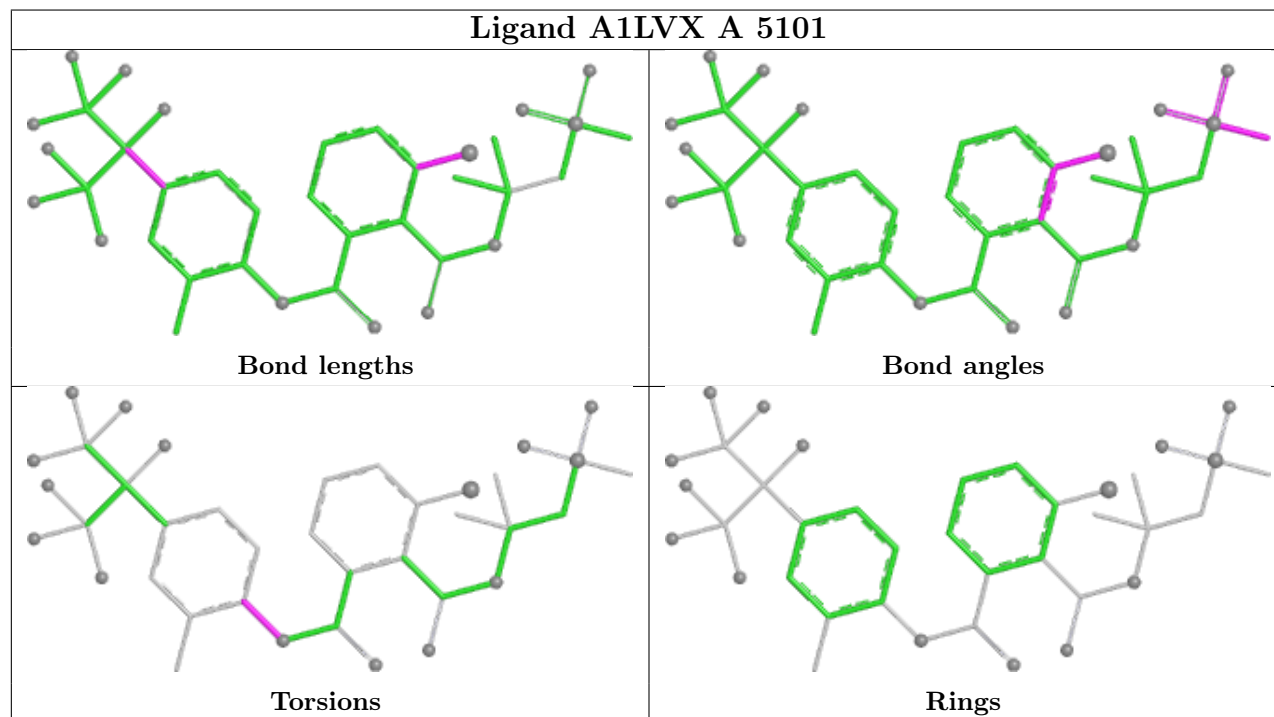
There are no ring outliers.

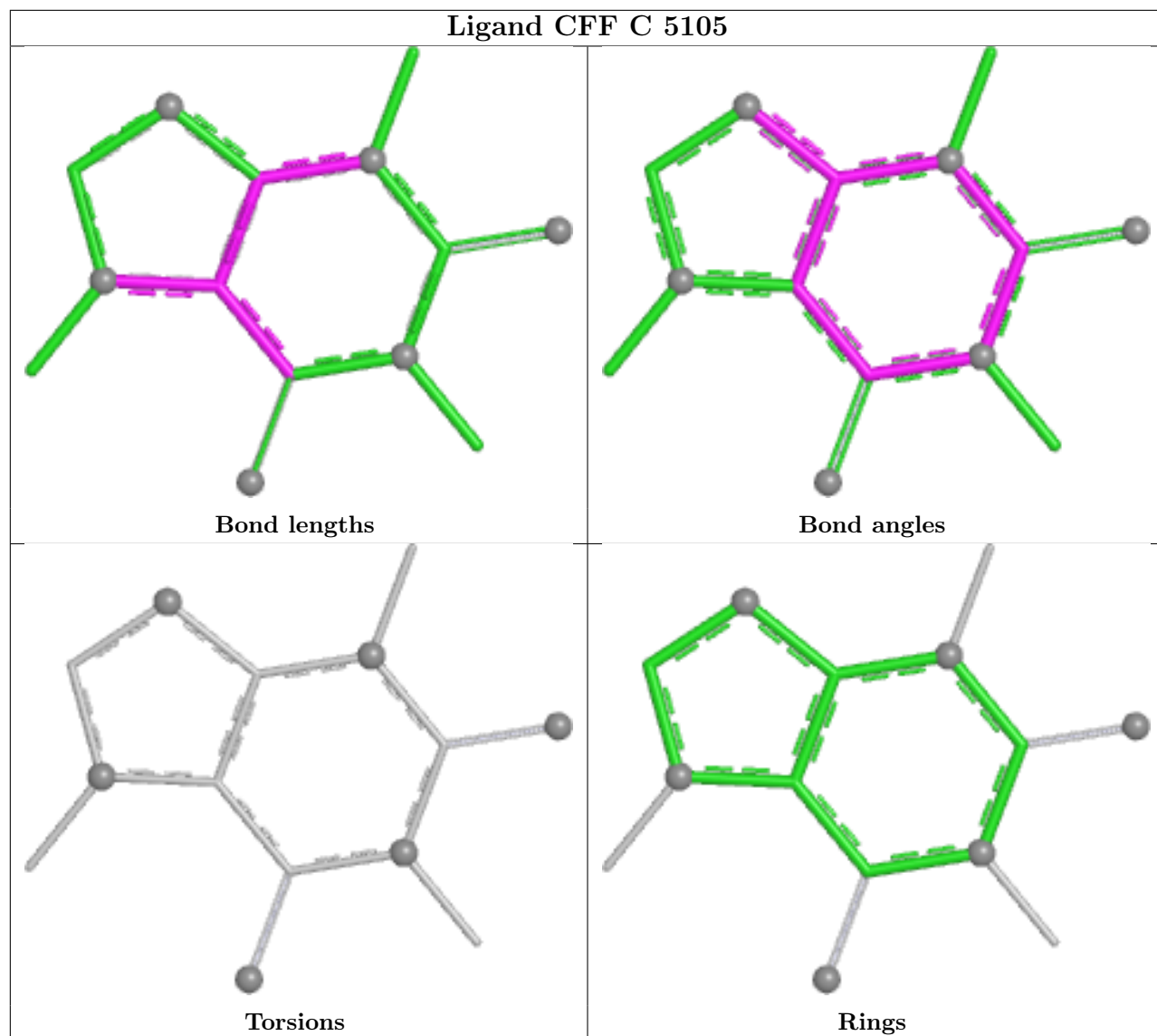
4 monomers are involved in 8 short contacts:

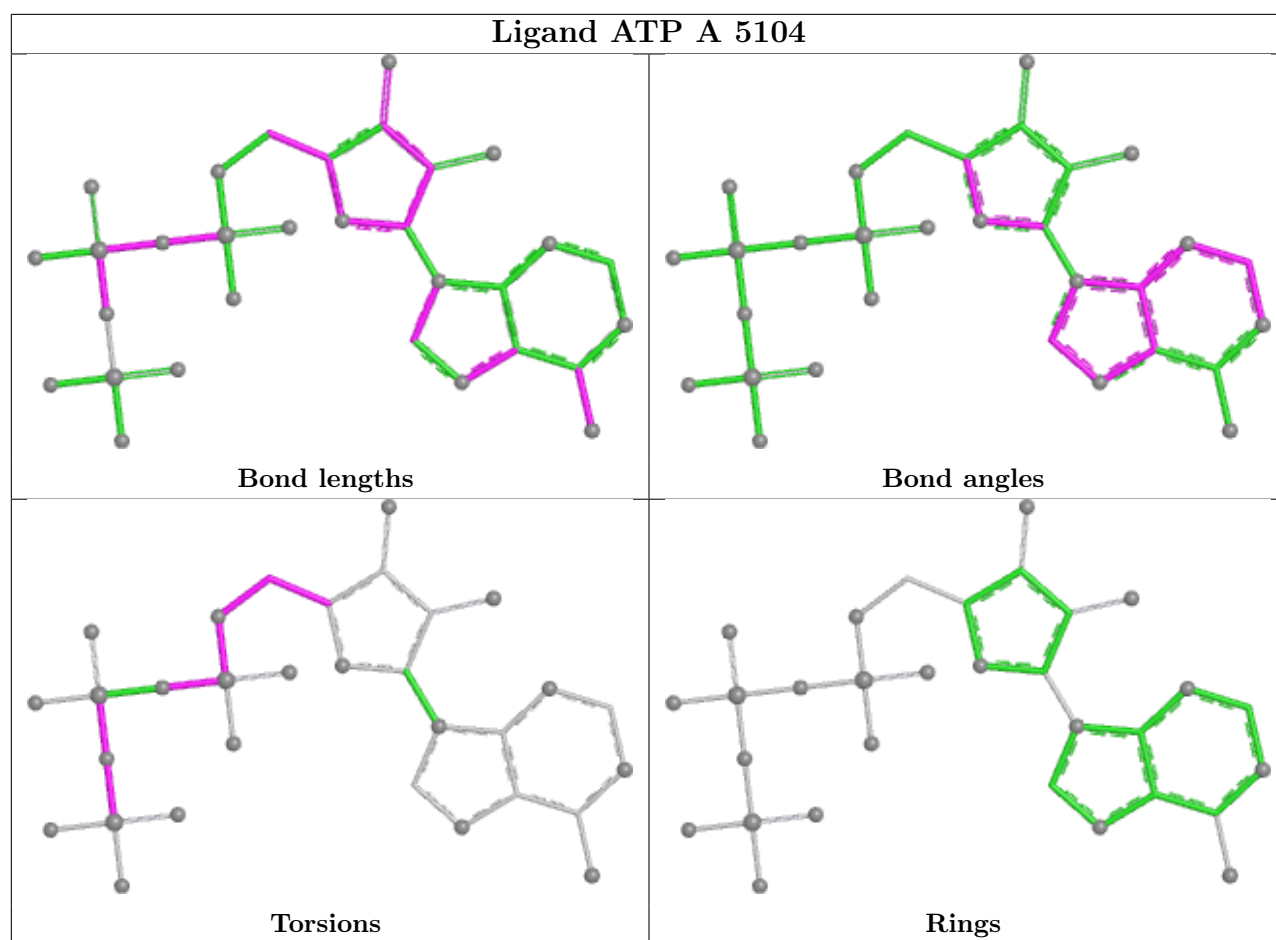
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	5104	ATP	2	0
7	B	5104	ATP	2	0
7	C	5104	ATP	2	0
7	D	5104	ATP	2	0

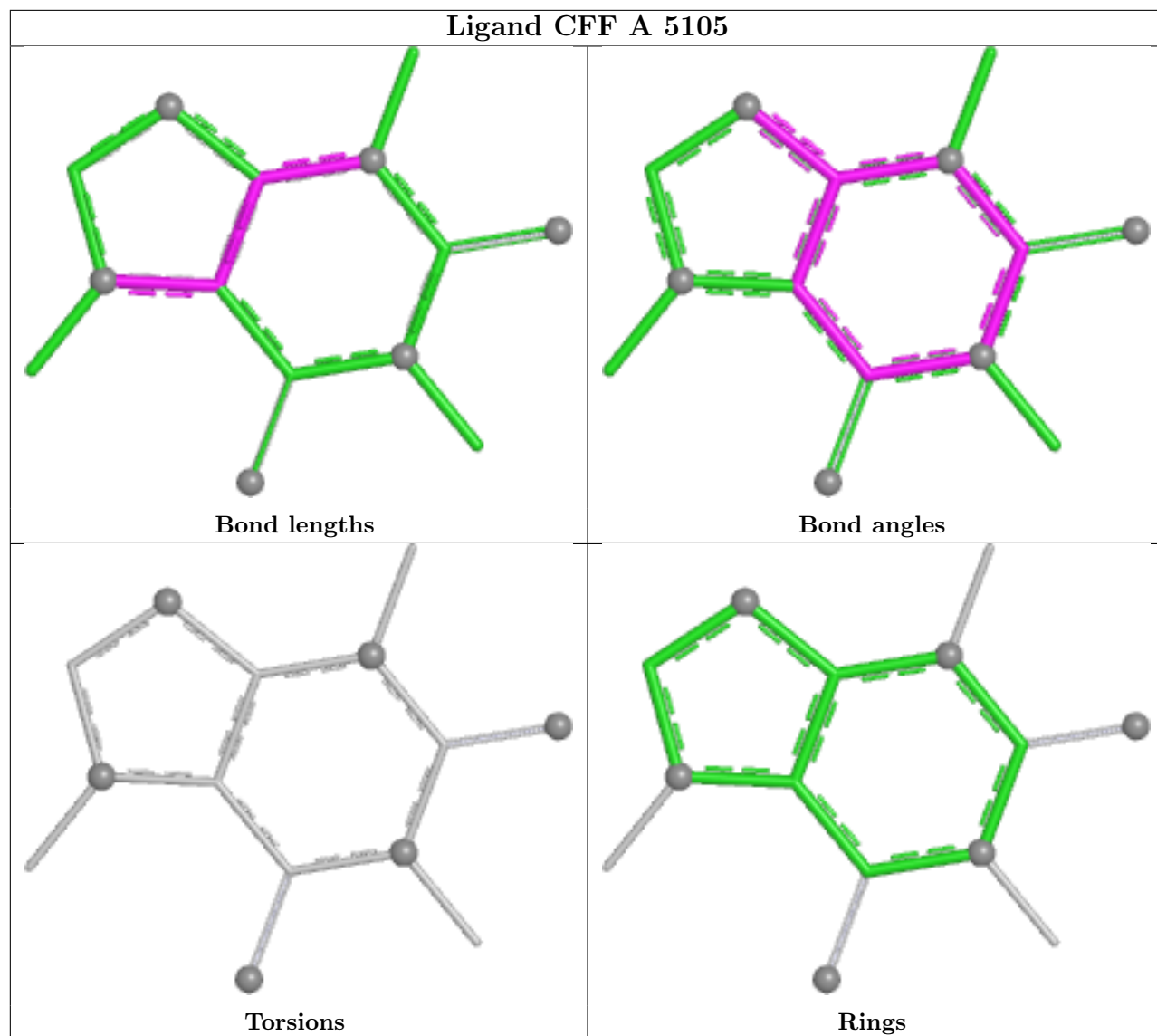
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

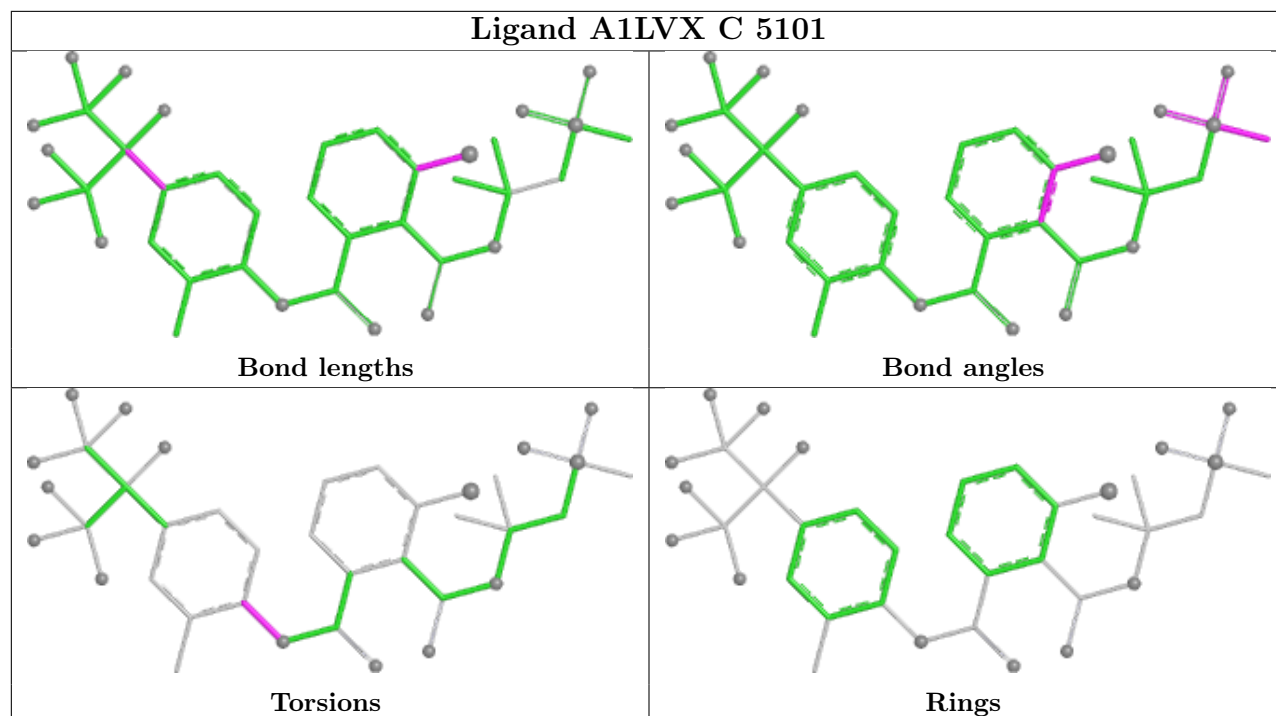




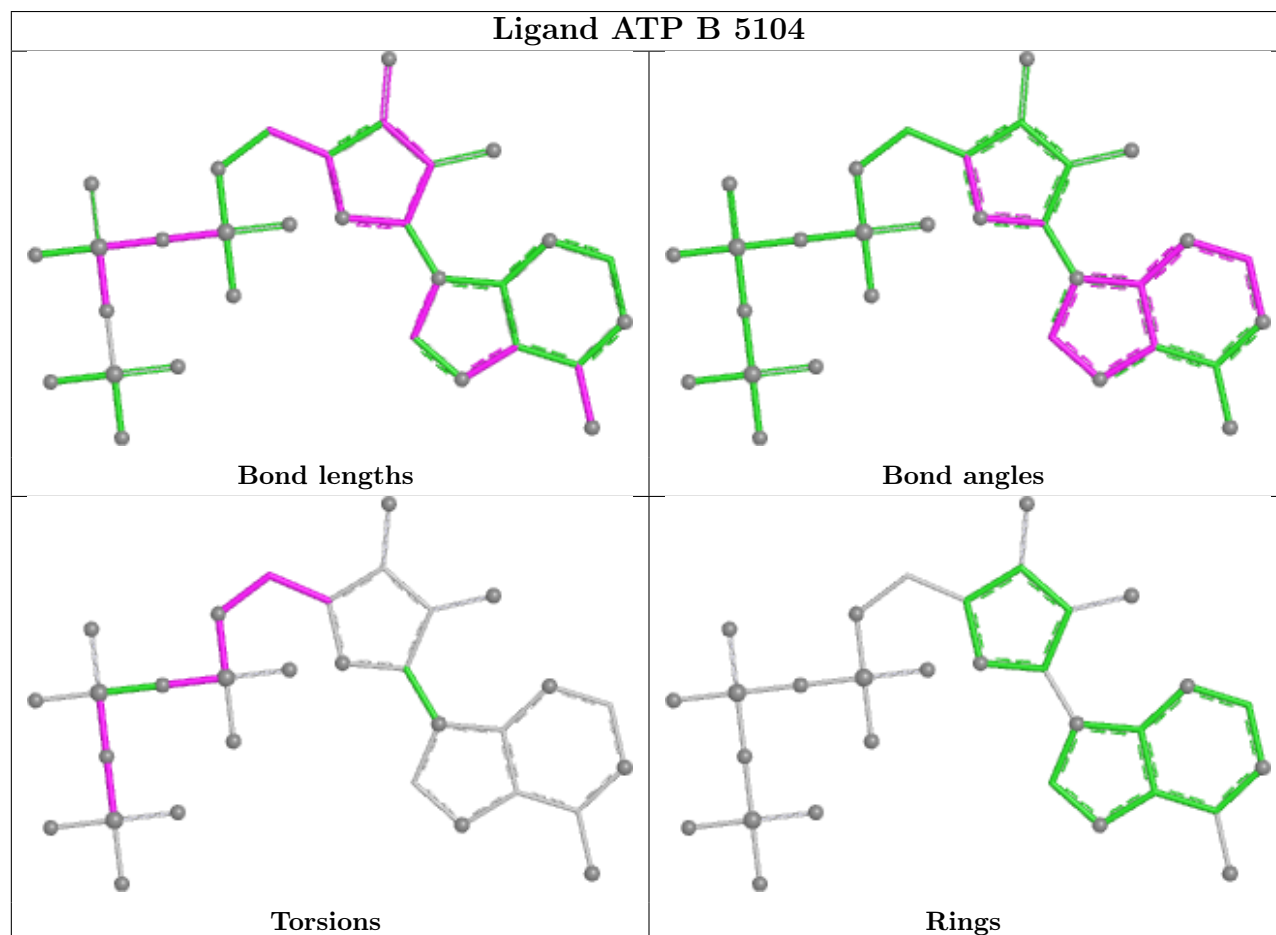


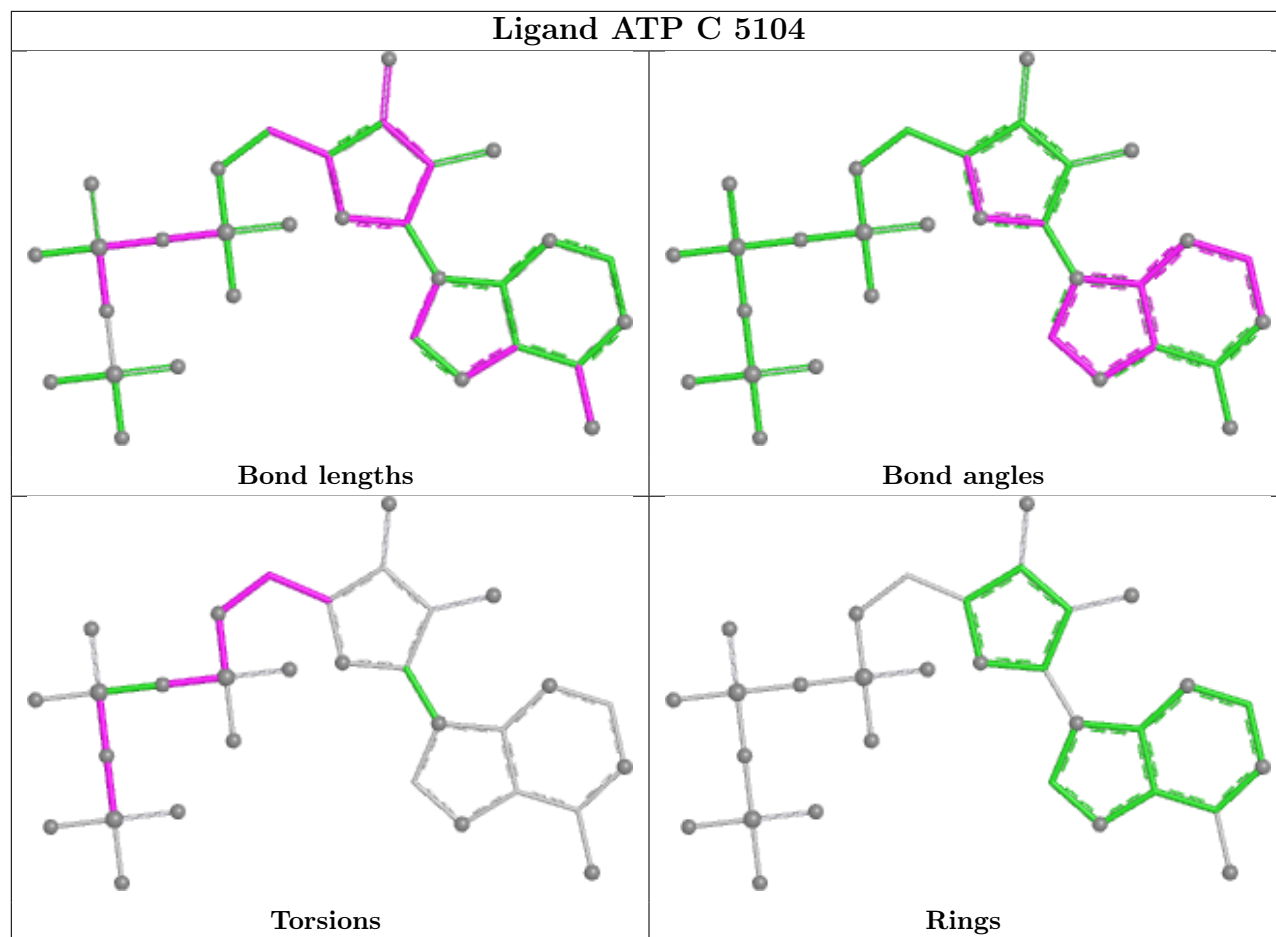


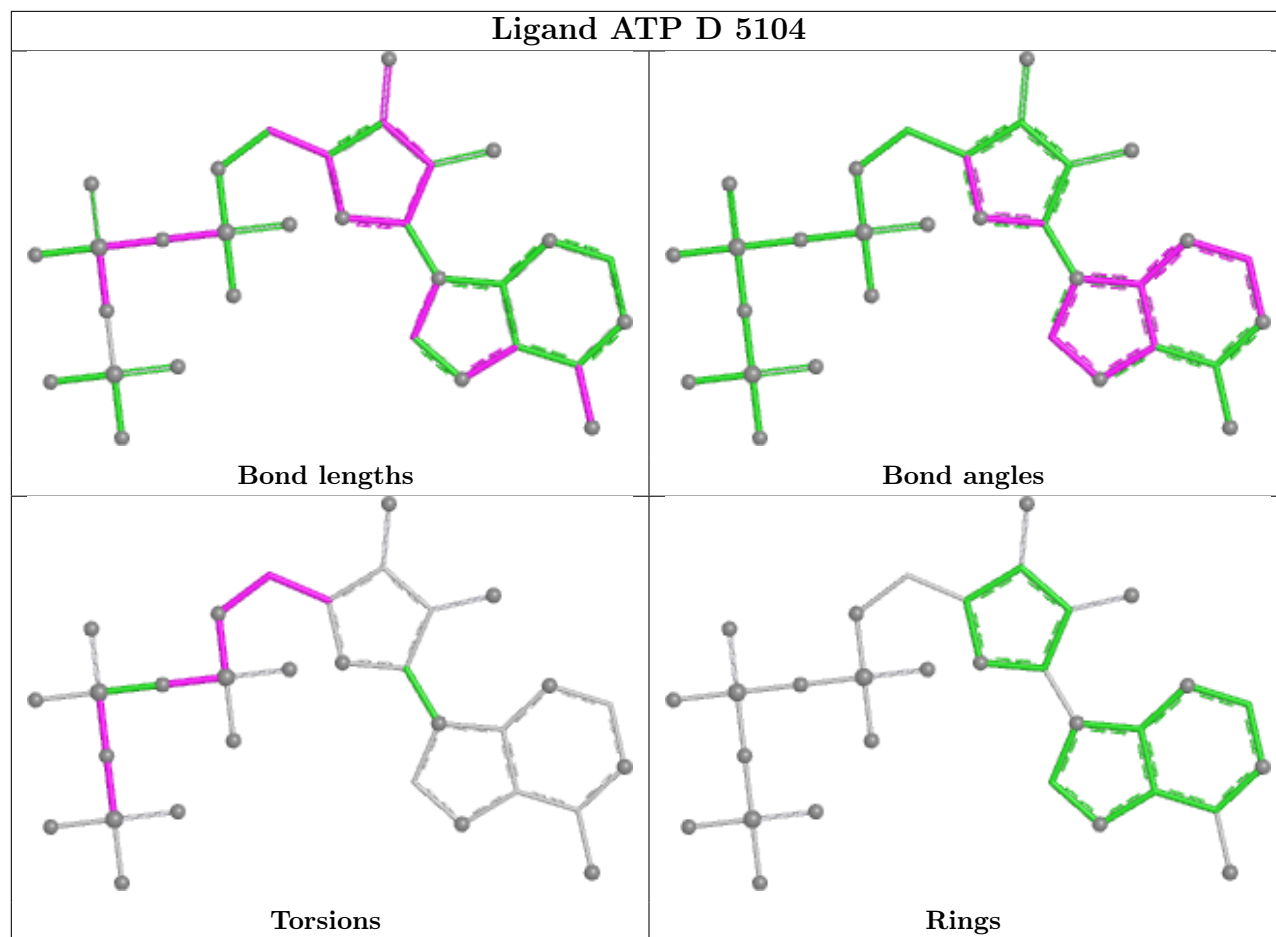
Ligand A1LVX C 5101

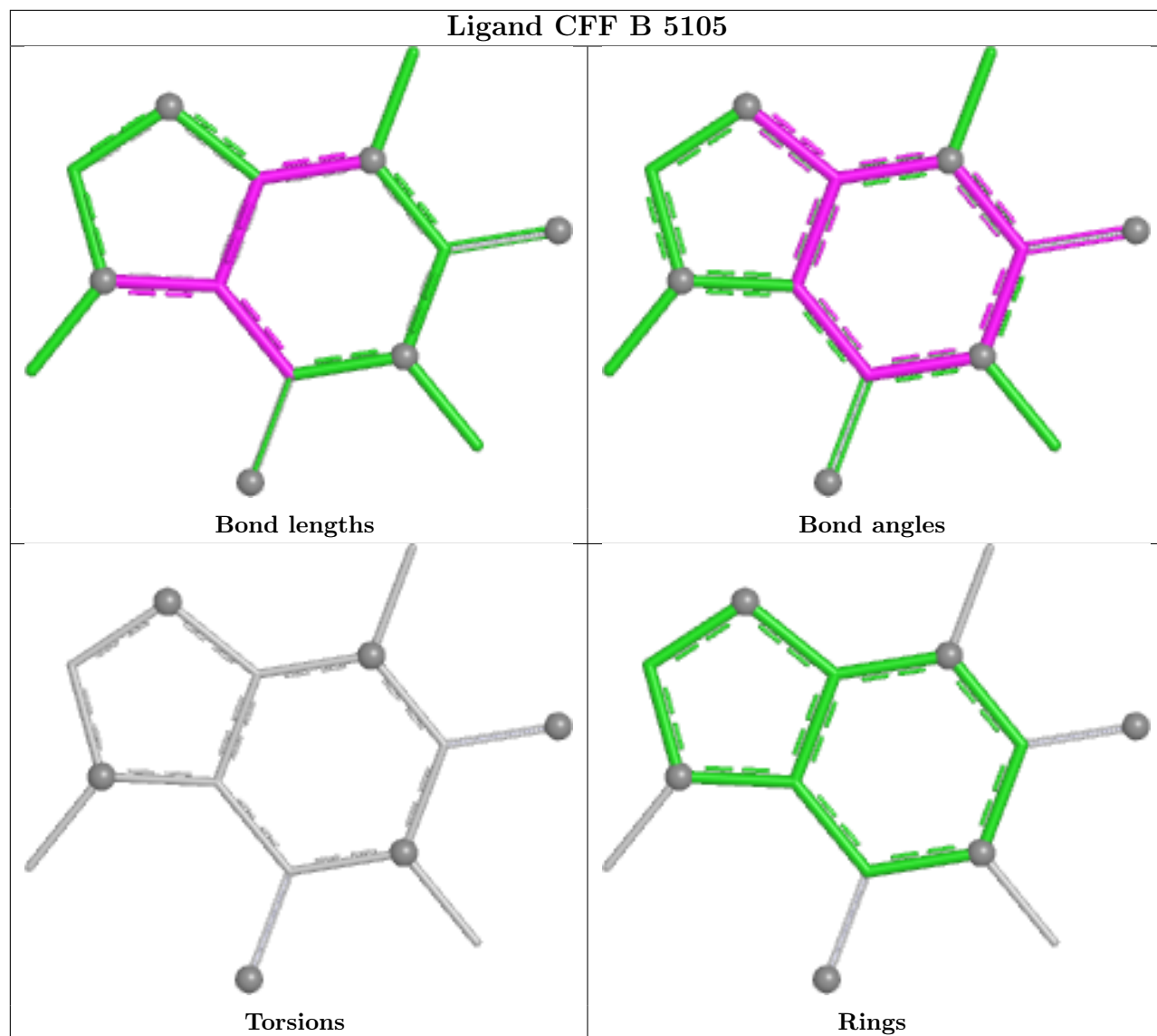


Ligand ATP B 5104

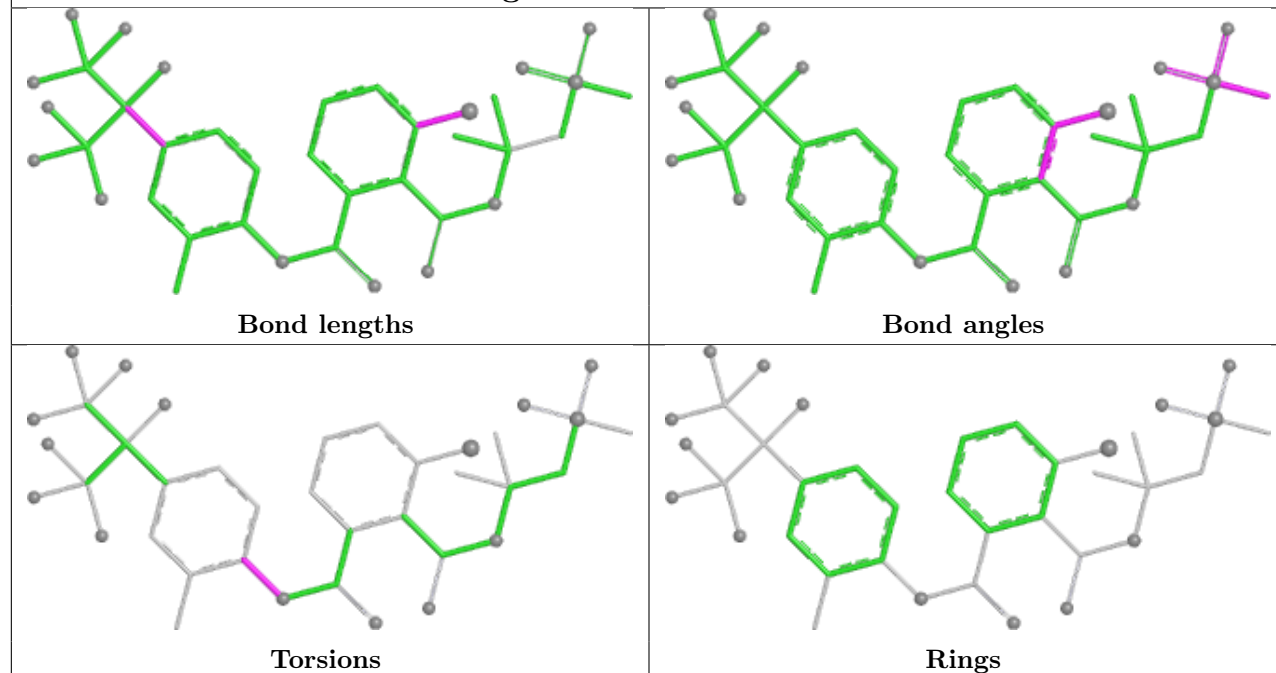




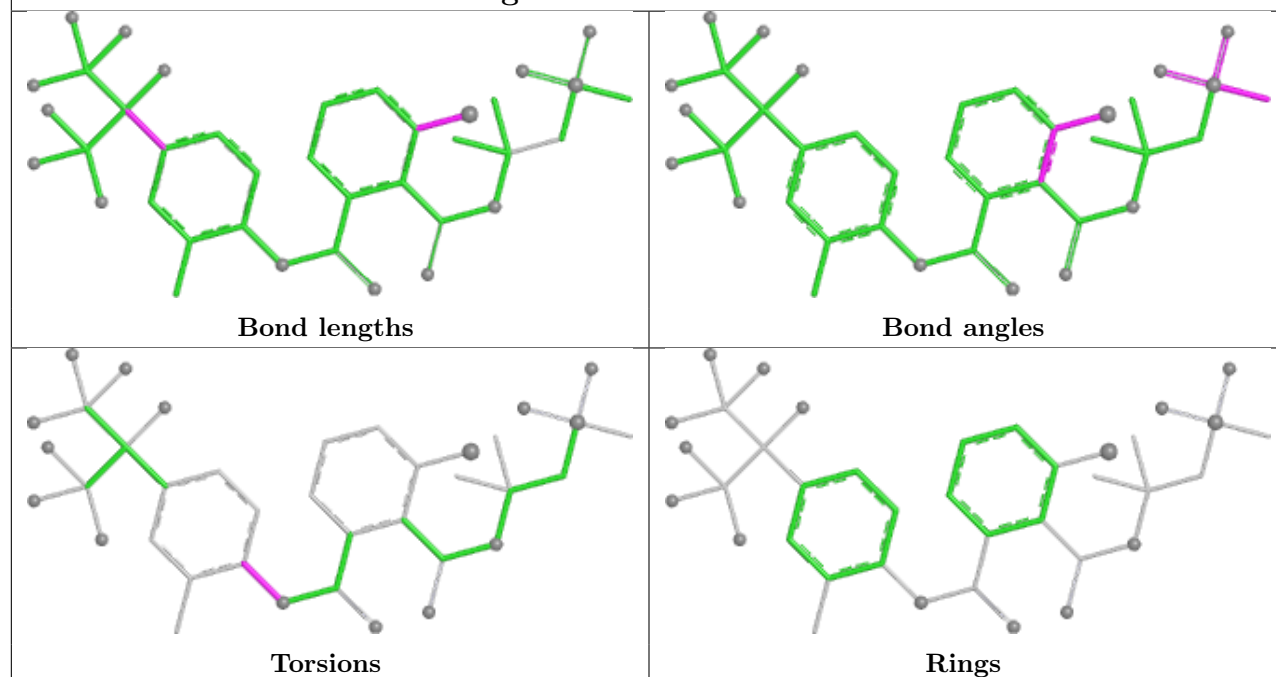


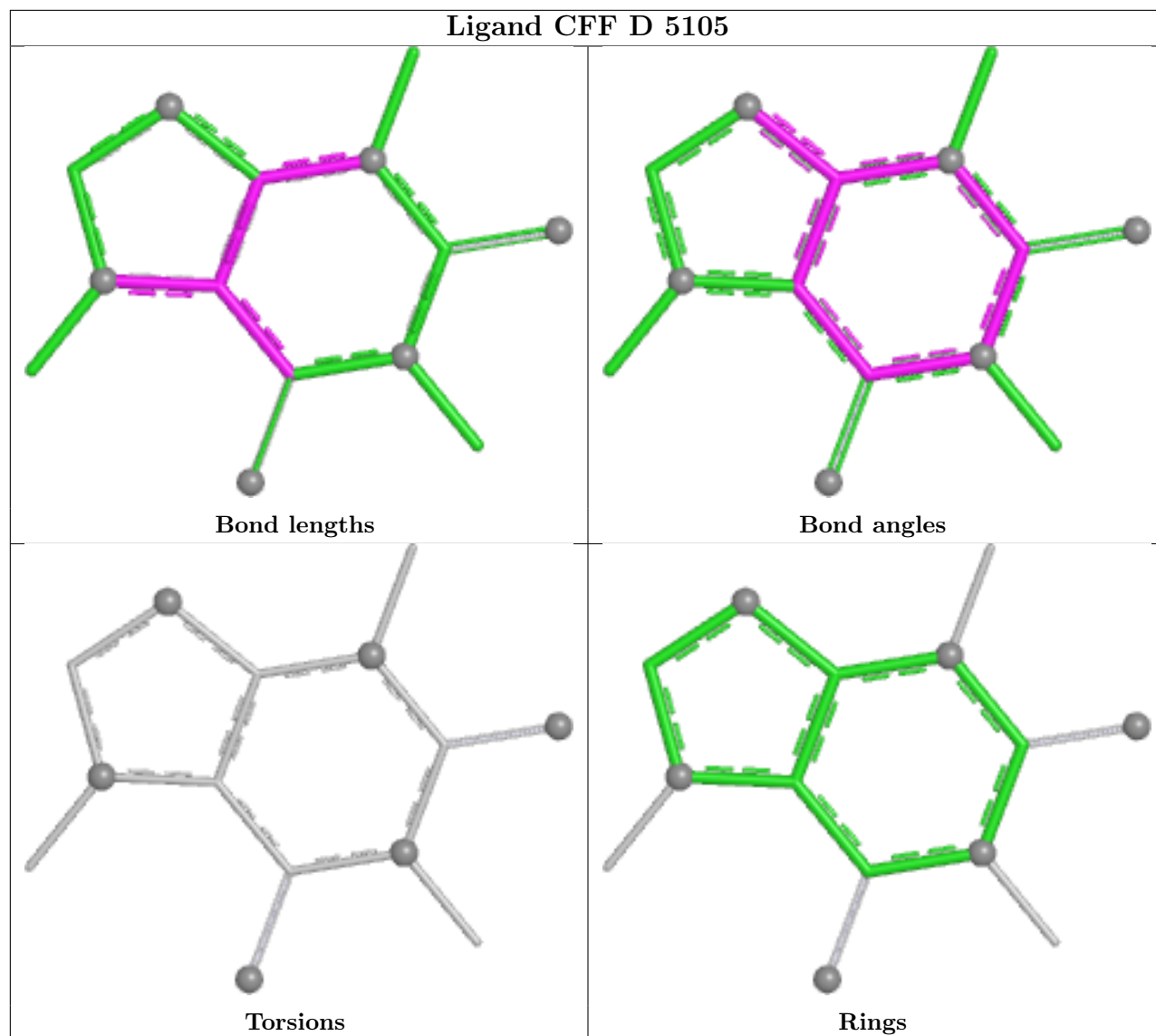


Ligand A1LVX B 5101



Ligand A1LVX D 5101





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

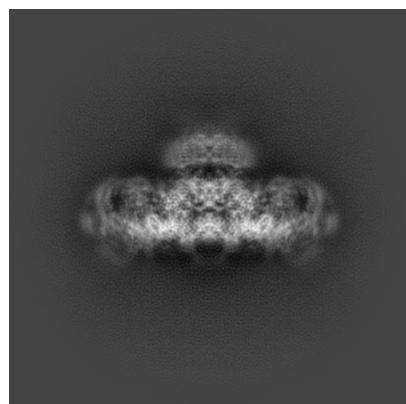
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38398. These allow visual inspection of the internal detail of the map and identification of artifacts.

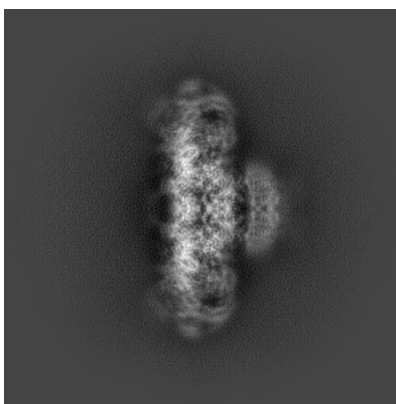
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

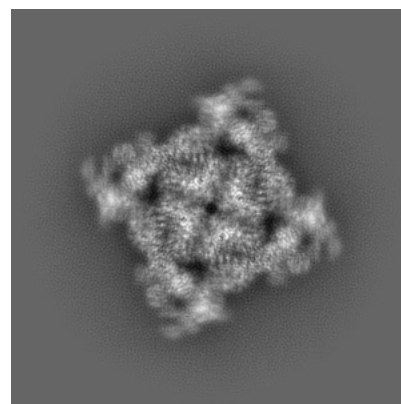
6.1.1 Primary map



X

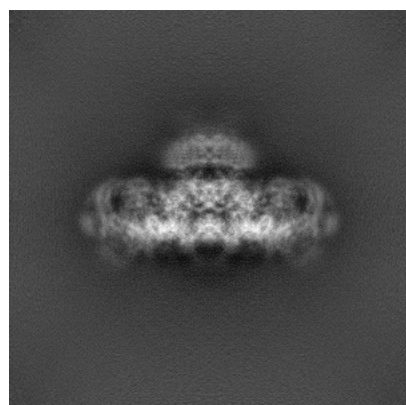


Y

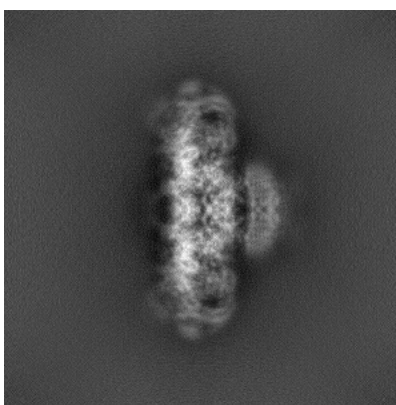


Z

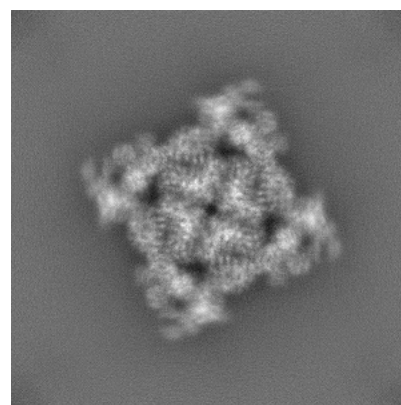
6.1.2 Raw map



X



Y

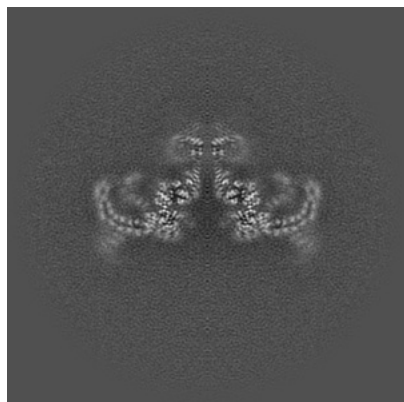


Z

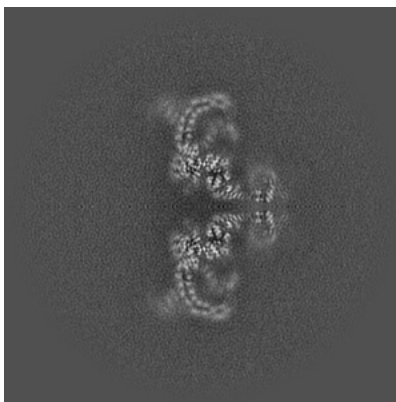
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

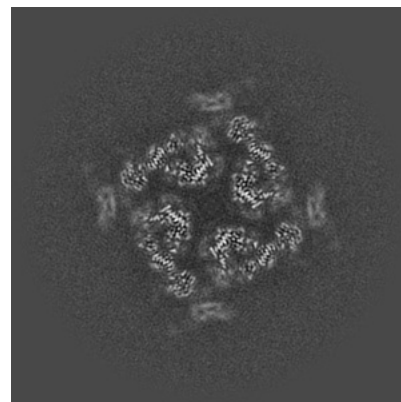
6.2.1 Primary map



X Index: 256

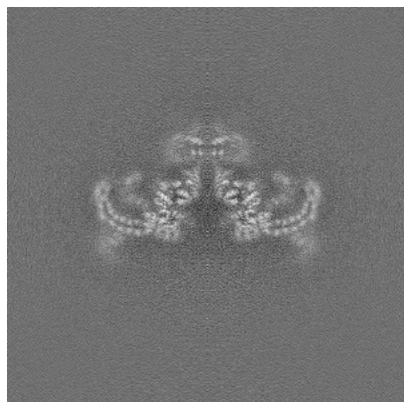


Y Index: 256

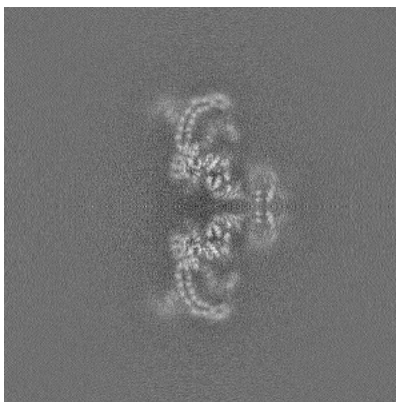


Z Index: 256

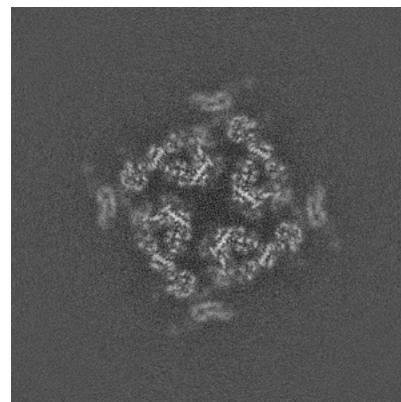
6.2.2 Raw map



X Index: 256



Y Index: 256

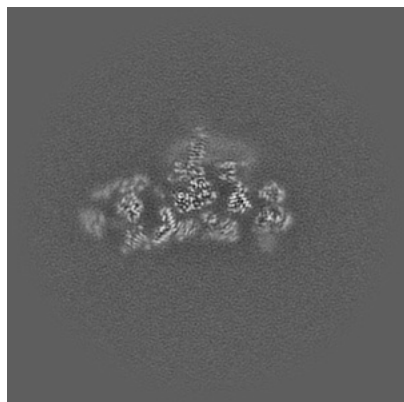


Z Index: 256

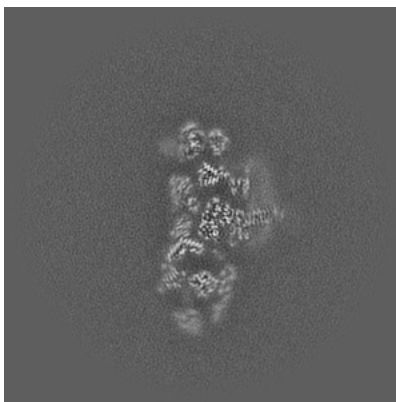
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

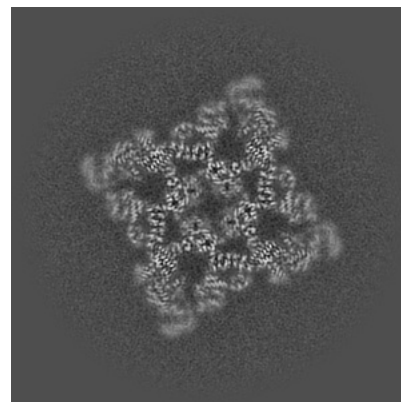
6.3.1 Primary map



X Index: 221

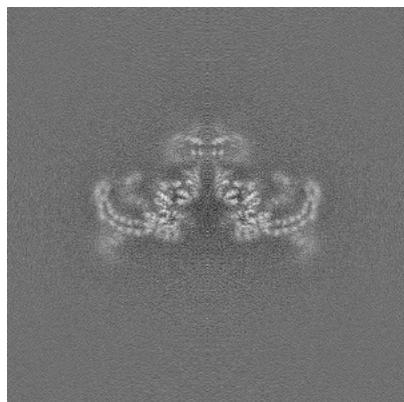


Y Index: 291

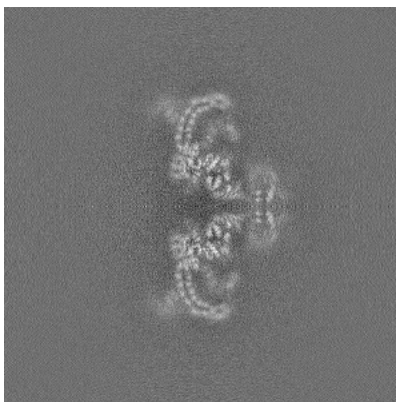


Z Index: 236

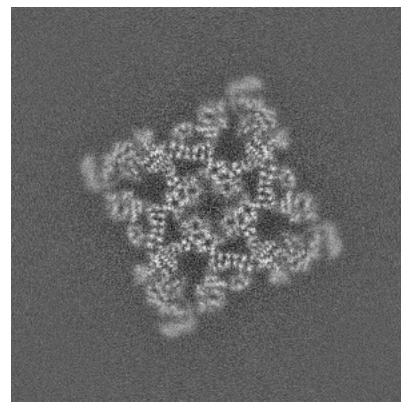
6.3.2 Raw map



X Index: 256



Y Index: 256

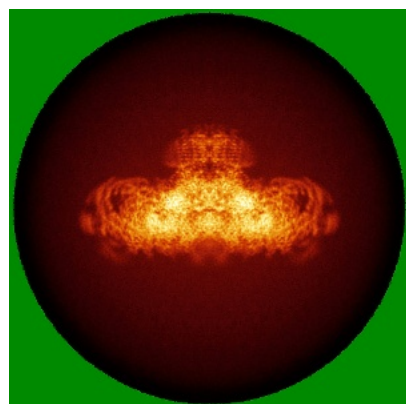


Z Index: 236

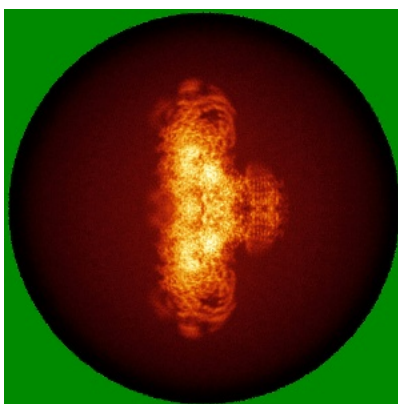
The images above show the largest variance slices of the map in three orthogonal directions.

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

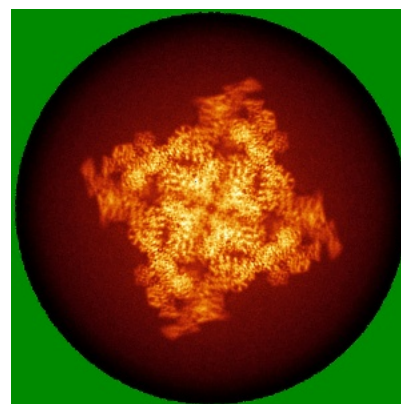
6.4.1 Primary map



X

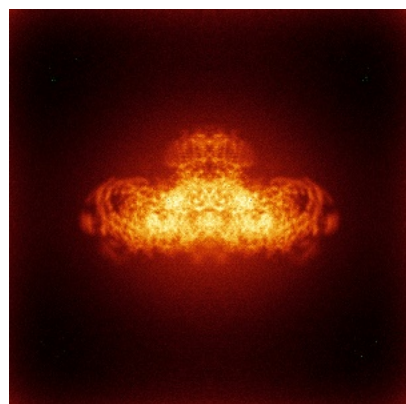


Y

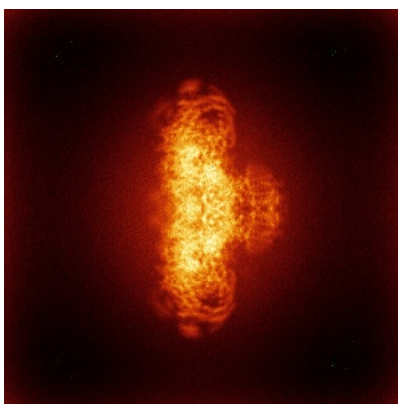


Z

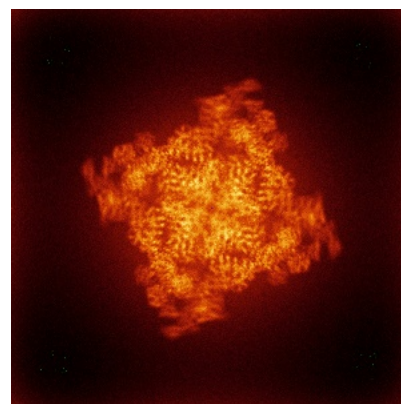
6.4.2 Raw map



X



Y

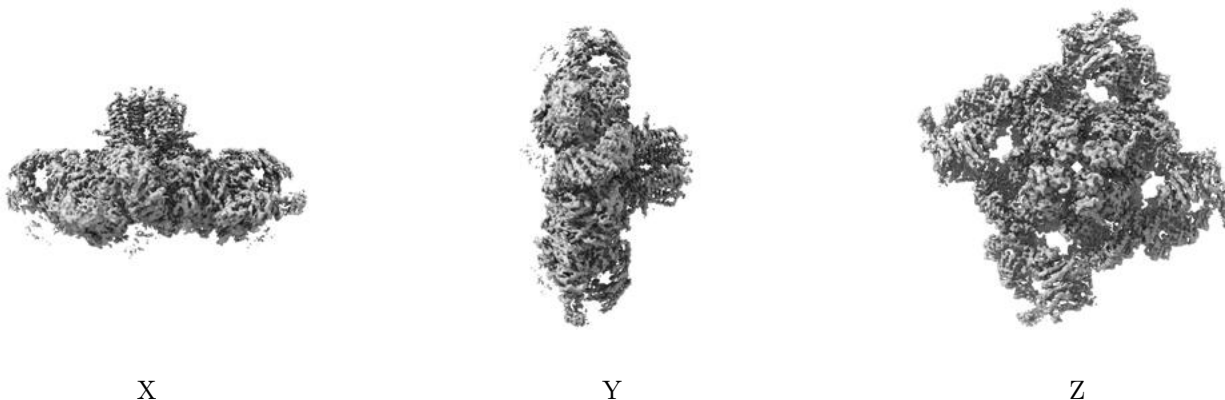


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

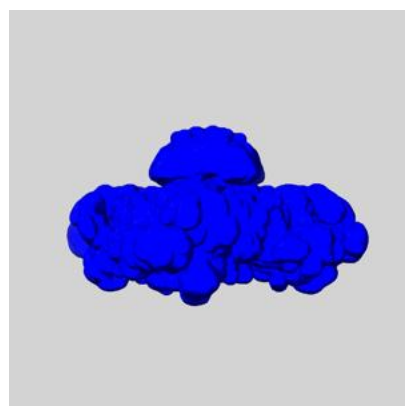
6.6 Mask visualisation [i](#)

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

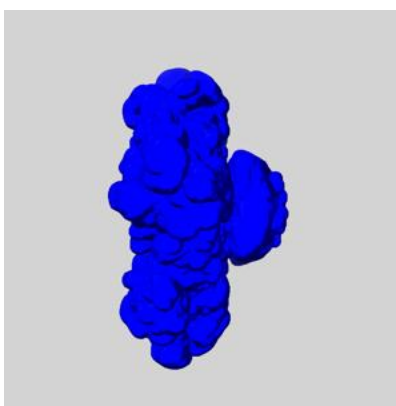
A mask typically either:

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

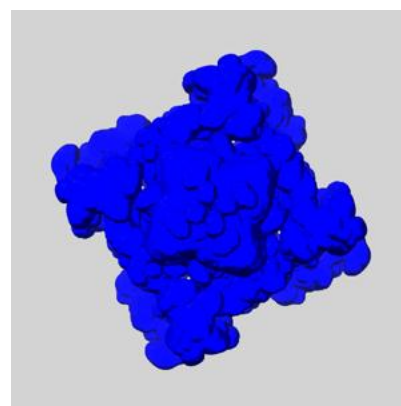
6.6.1 emd_38398_msk_1.map [i](#)



X



Y

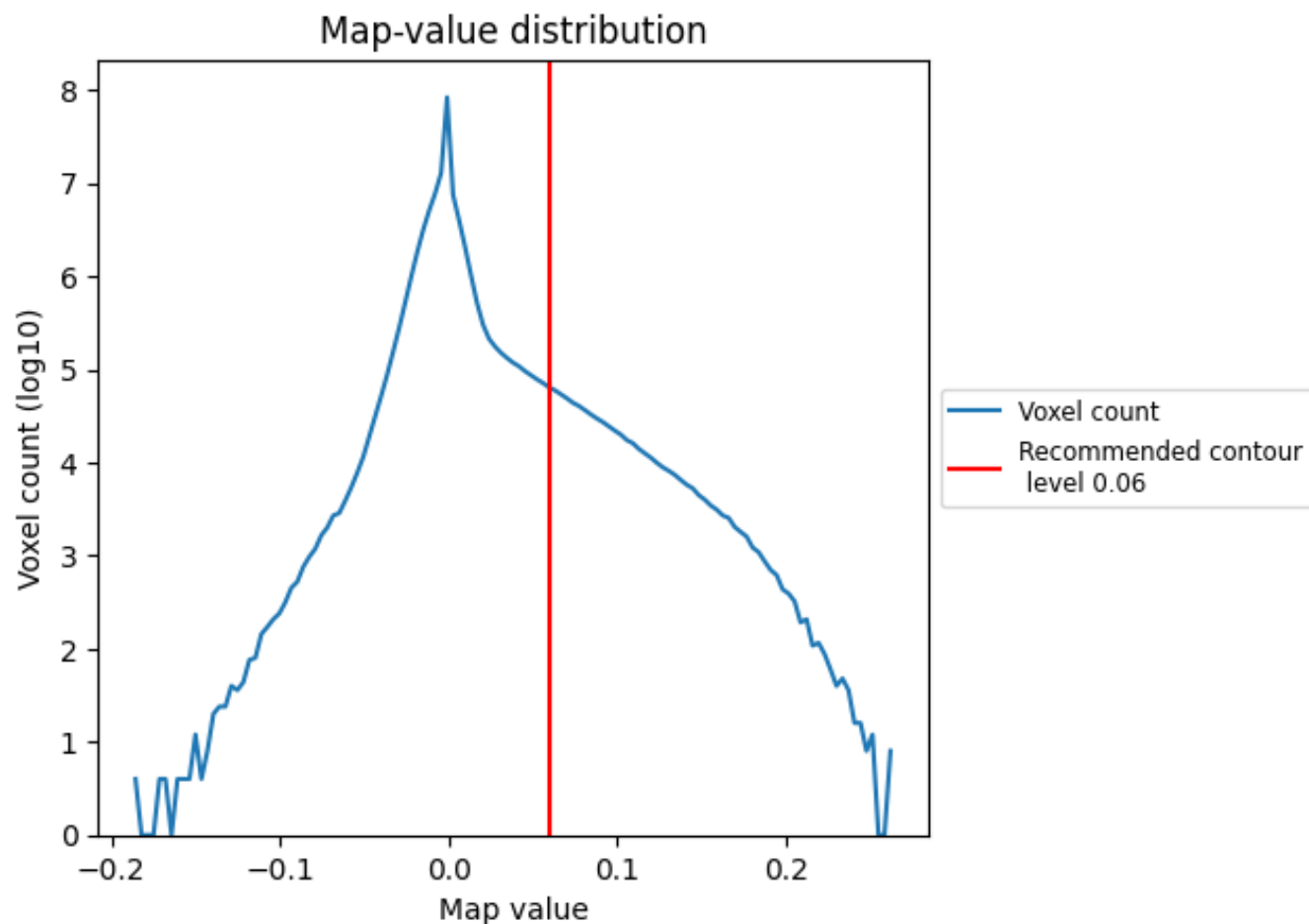


Z

7 Map analysis [i](#)

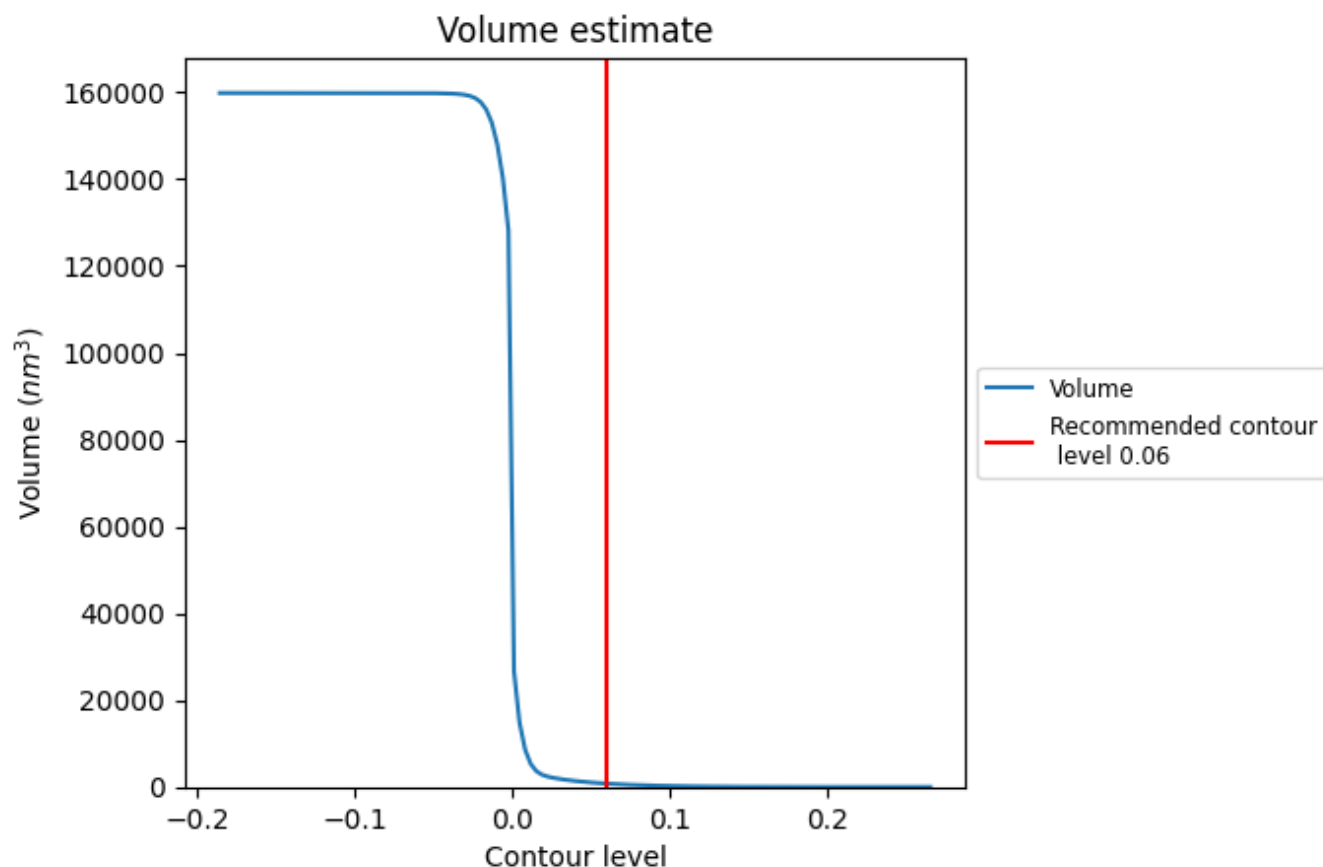
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

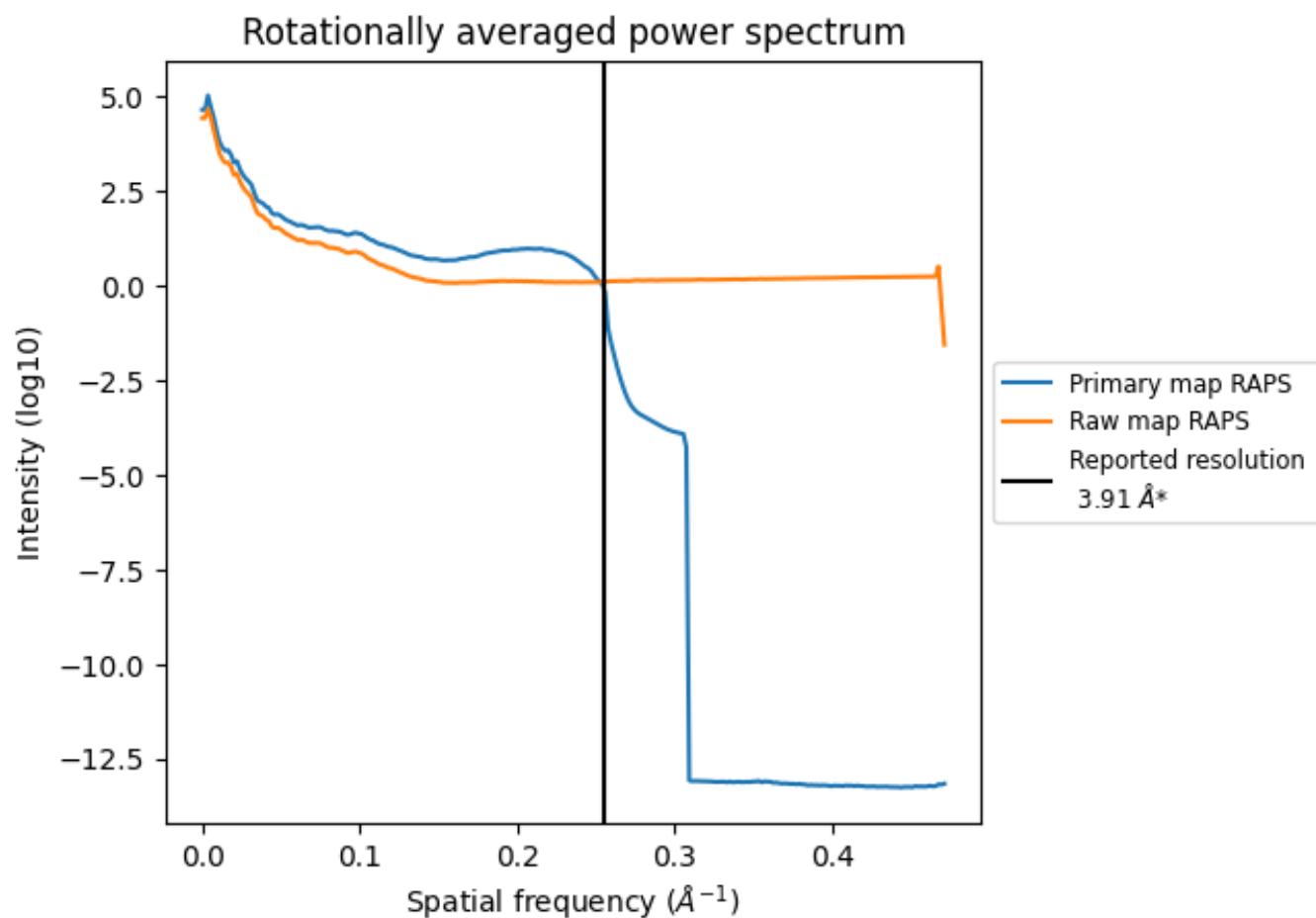
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 783 nm³; this corresponds to an approximate mass of 707 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 ⓘ

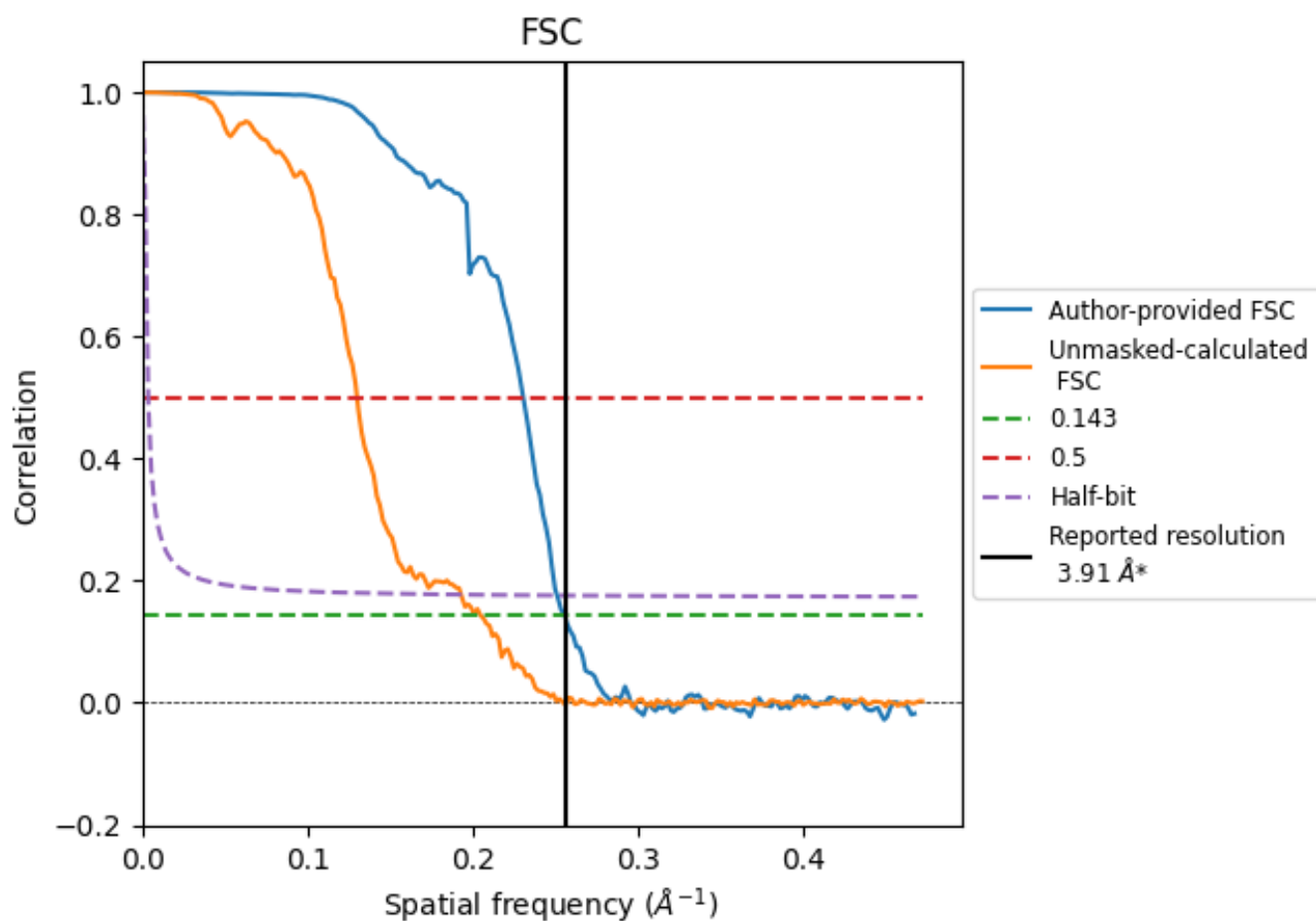


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

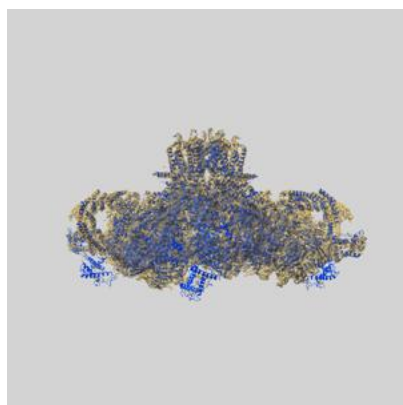
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.91	4.34	3.99
Unmasked-calculated*	4.89	7.70	5.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.89 differs from the reported value 3.91 by more than 10 %

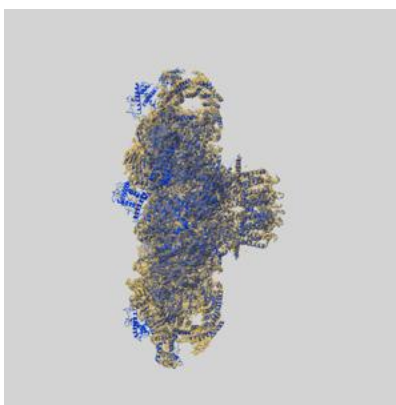
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38398 and PDB model 8XJI. Per-residue inclusion information can be found in section 3 on page 9.

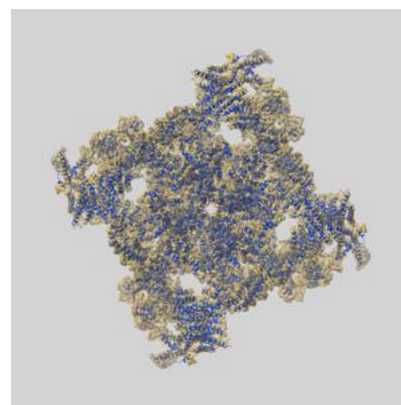
9.1 Map-model overlay [i](#)



X



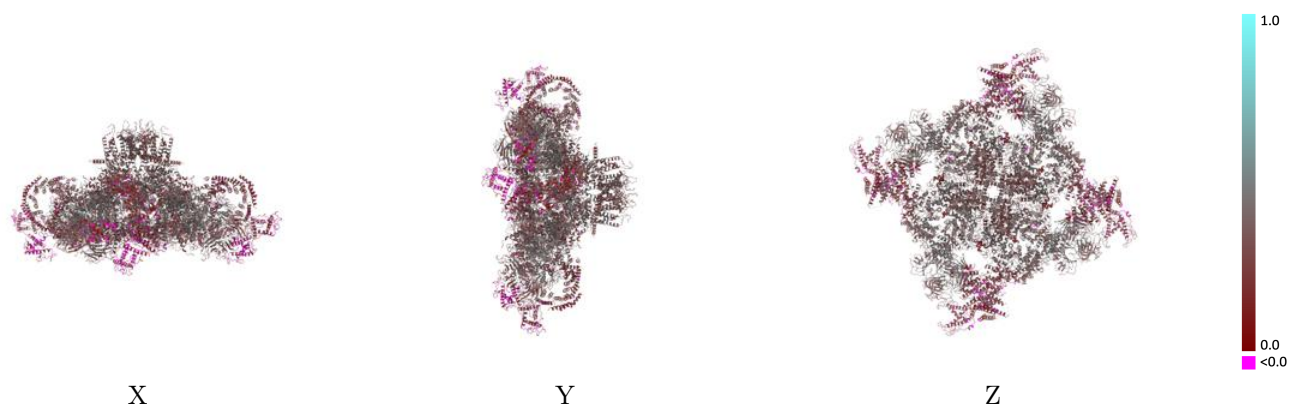
Y



Z

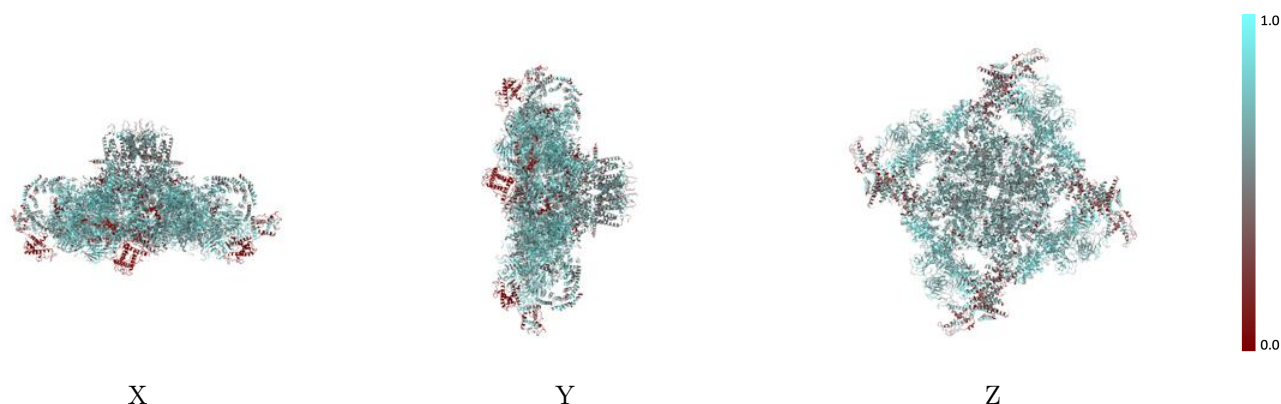
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



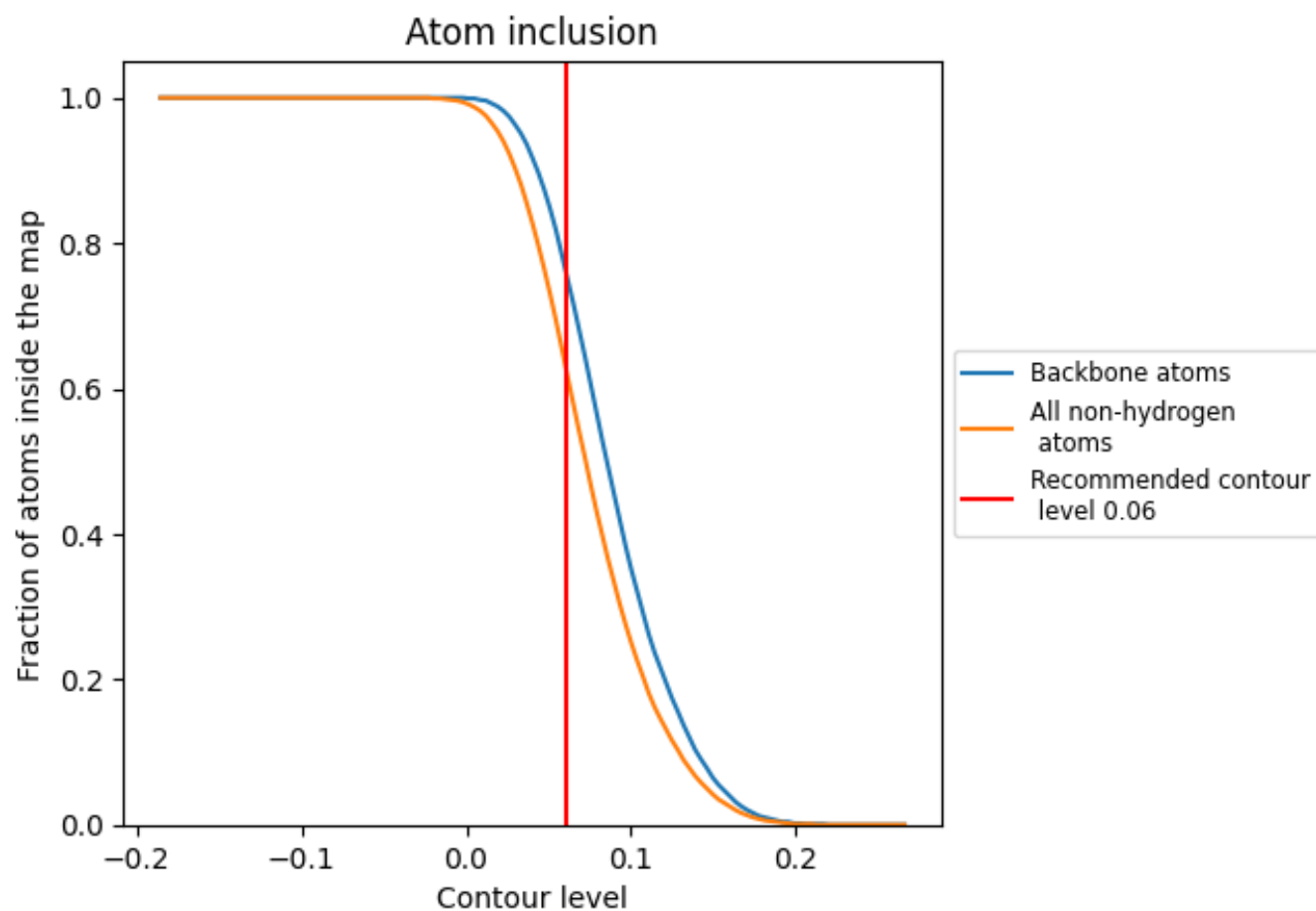
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 63% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6320	0.3400
A	0.6360	0.3410
B	0.6370	0.3410
C	0.6370	0.3410
D	0.6430	0.3490
E	0.6620	0.3580
F	0.6600	0.3580
G	0.6600	0.3630
H	0.6630	0.3690
I	0.4580	0.2340
J	0.4570	0.2330
K	0.4550	0.2350
L	0.4490	0.2300

1.0

0.0

<0.0