



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:21 AM UTC

PDB ID : 8VK4 / pdb_00008vk4
EMDB ID : EMD-43304
Title : Structure of mouse RyR1 in complex with S100A1 (high-Ca²⁺/CFF/ATP dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2024-01-08
Resolution : 3.56 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:

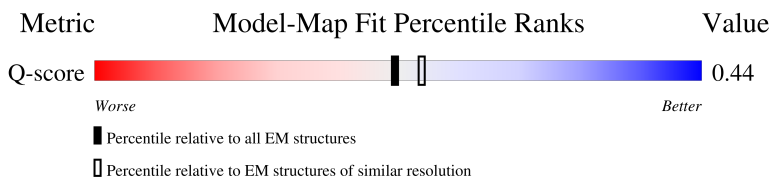
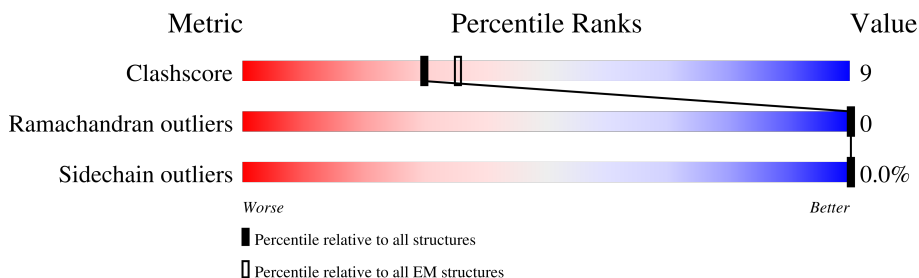
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.56 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	12750 (3.06 - 4.06)

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	108	
1	F	108	
1	G	108	
1	H	108	

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Mol	Chain	Length	Quality of chain
2	I	94	
2	J	94	
2	K	94	
2	L	94	
2	M	94	
2	N	94	
2	O	94	
2	P	94	
3	A	5035	
3	B	5035	
3	C	5035	
3	D	5035	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 149304 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 FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- Molecule 2 is a protein called Protein S100A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	J	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	K	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	L	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	N	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	M	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	O	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	P	93	Total	C	N	O	S	0	0
			729	460	114	152	3		

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		
3	B	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		
3	C	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	I	2	Total	Ca	0
			2	2	
4	J	2	Total	Ca	0
			2	2	
4	D	1	Total	Ca	0
			1	1	
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	K	2	Total	Ca	0
			2	2	
4	L	2	Total	Ca	0
			2	2	
4	N	2	Total	Ca	0
			2	2	
4	M	2	Total	Ca	0
			2	2	
4	O	2	Total	Ca	0
			2	2	
4	P	2	Total	Ca	0
			2	2	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

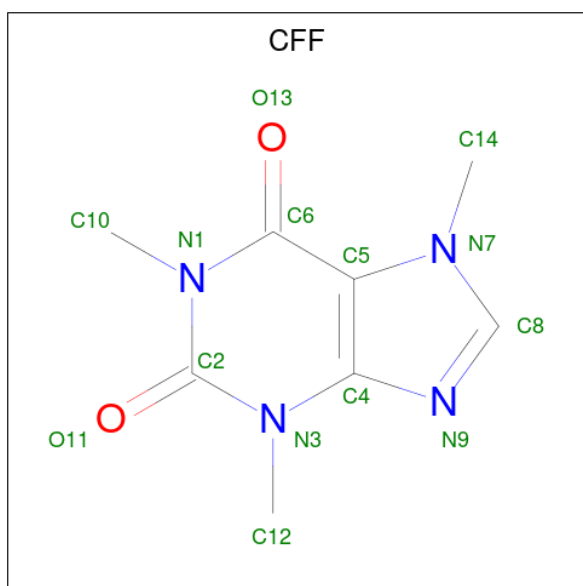
Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	

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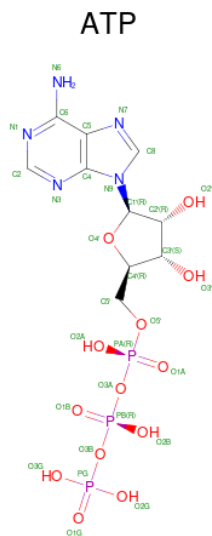
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



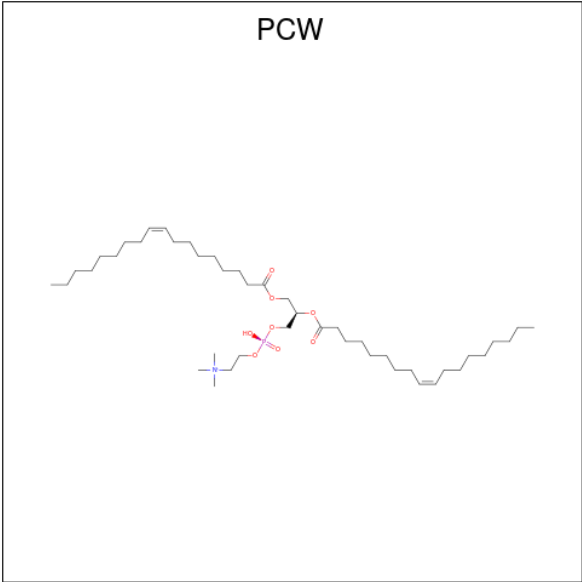
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	4	2	
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



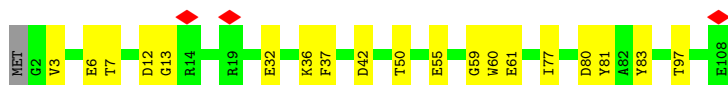
Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 



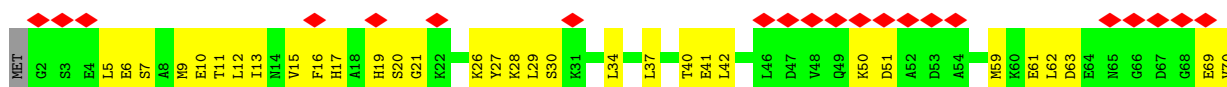
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

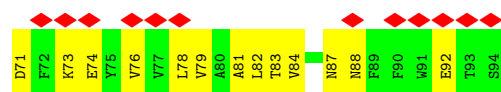
Chain H: 



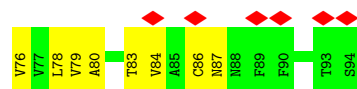
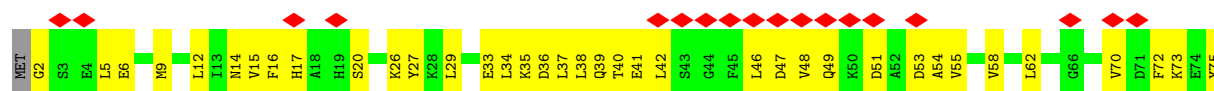
- Molecule 2: Protein S100A1

Chain I: 

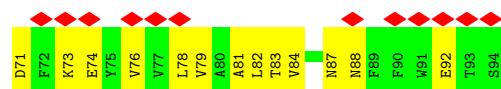
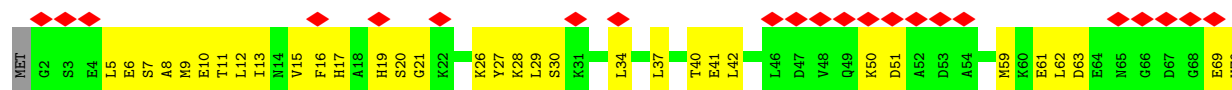




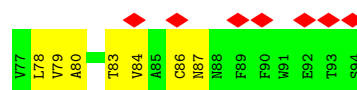
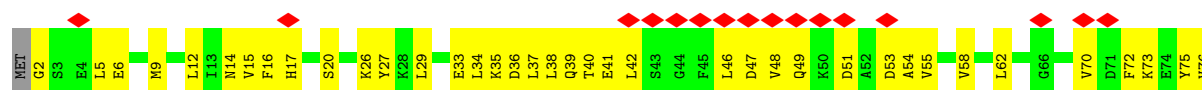
• Molecule 2: Protein S100A1



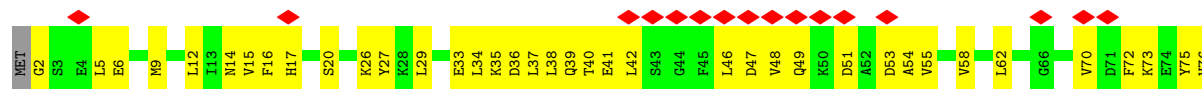
• Molecule 2: Protein S100A1



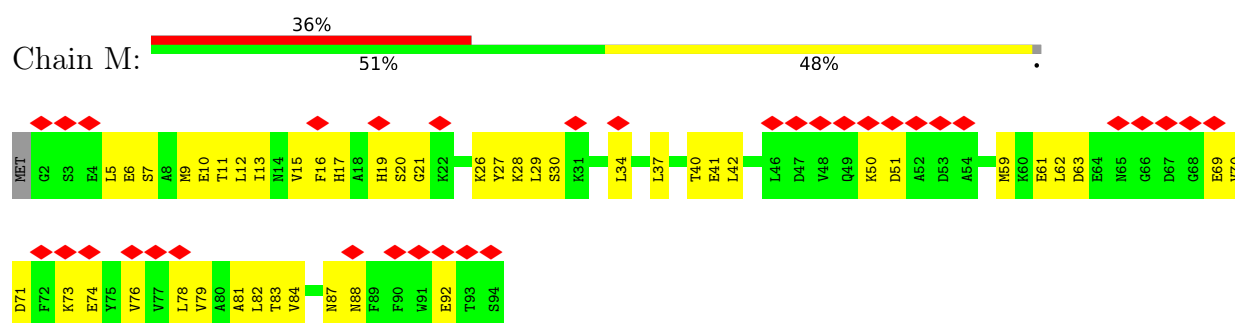
• Molecule 2: Protein S100A1



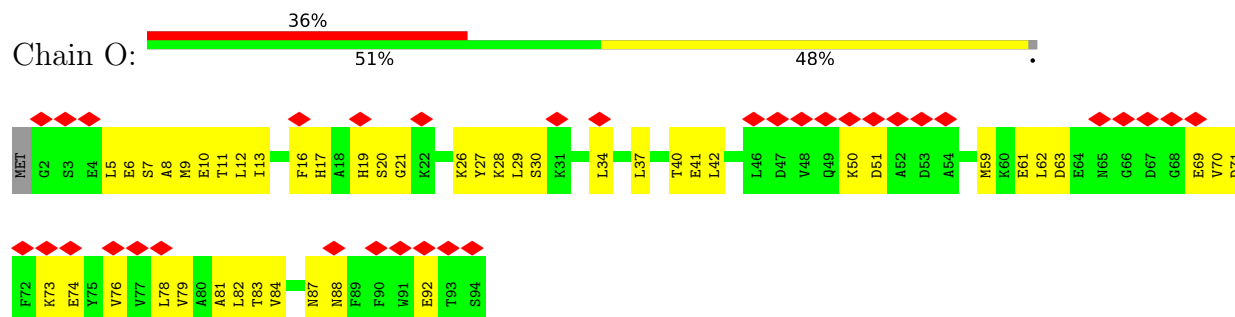
• Molecule 2: Protein S100A1



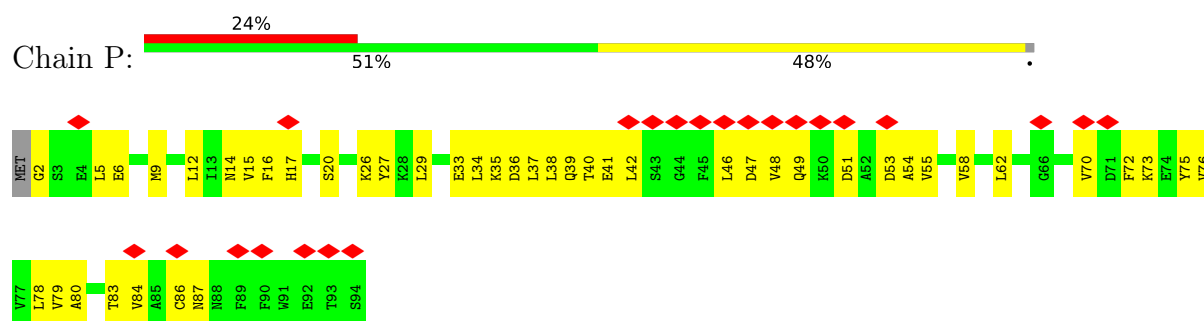
• Molecule 2: Protein S100A1



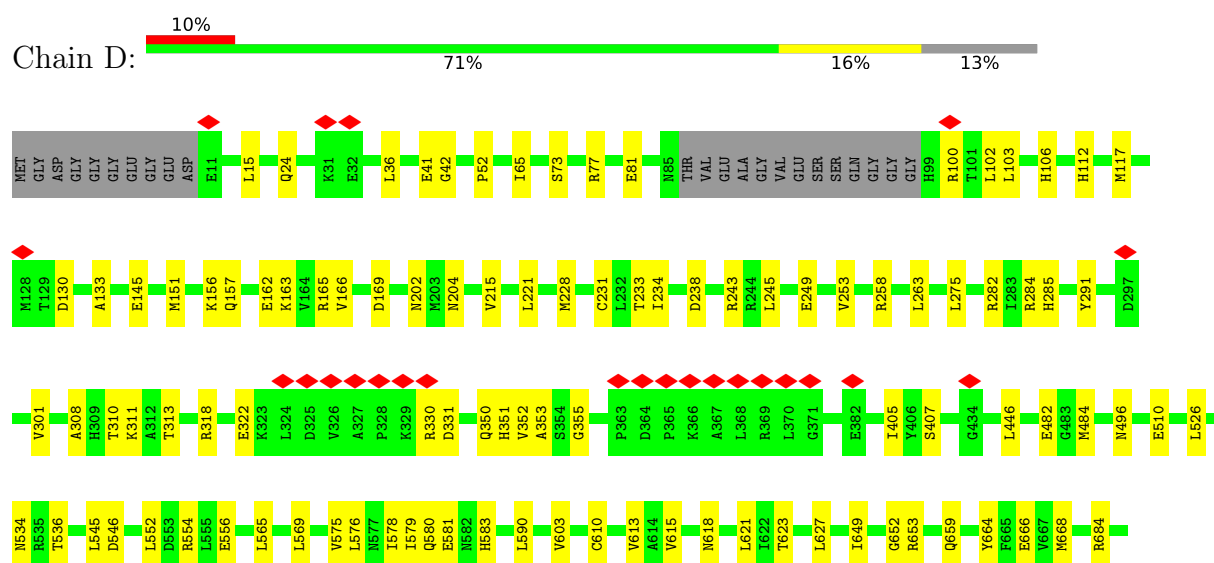
- Molecule 2: Protein S100A1



- Molecule 2: Protein S100A1



- Molecule 3: Ryanodine receptor 1

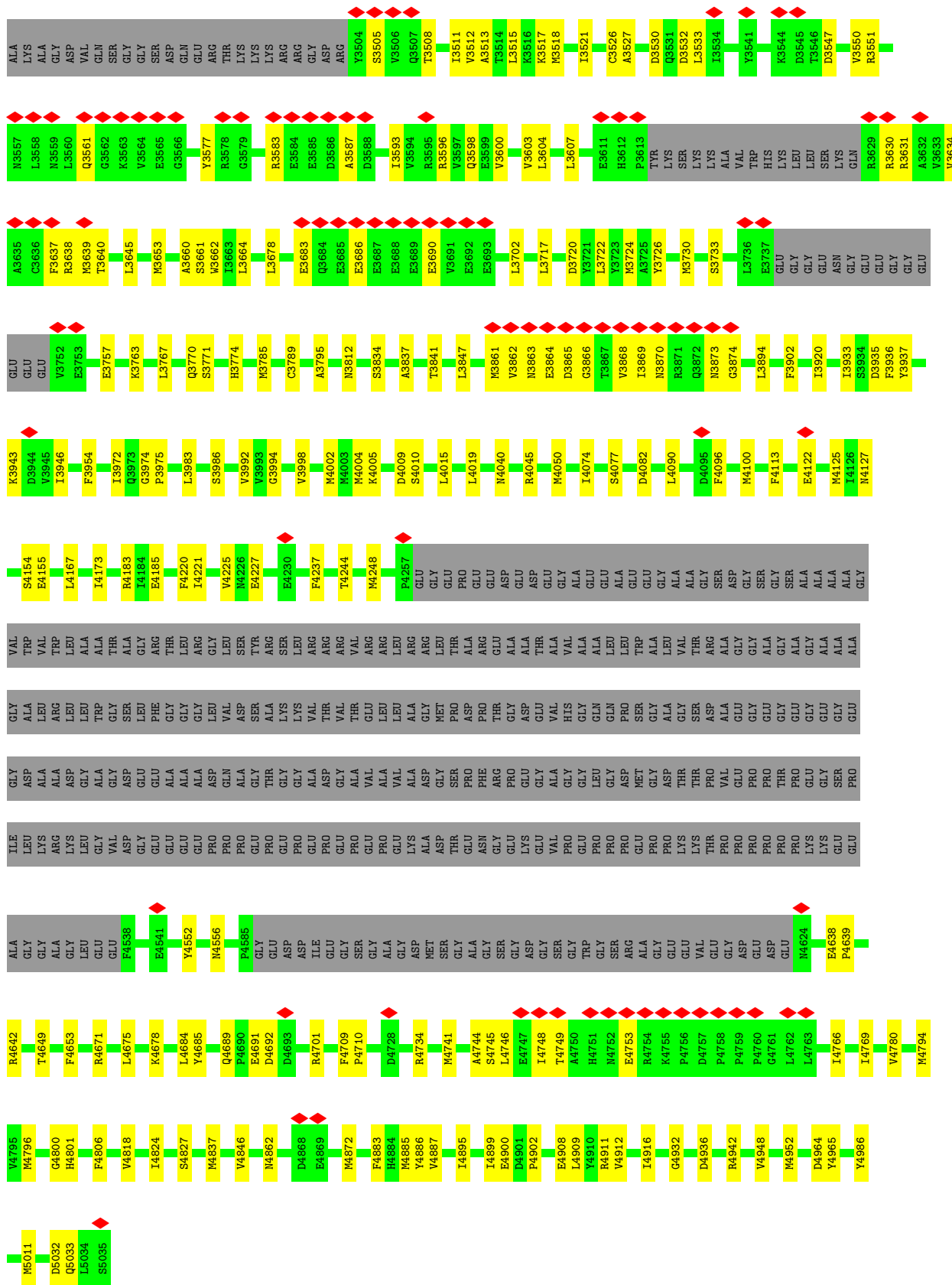








E3398	F3399	S3400	V3401	L3402	C3403	R3404	D3405	L3406	Y3407	A3408	L3409	Y3410	F3411	L3412	L3413	L3414	R3415	R3421		N3431	A3432		L3435		M3438	V3439	G3440	F3441	F3442	F3443	I3444		S3447		N3451	F3452	R3453	R3454	E3455	E3456																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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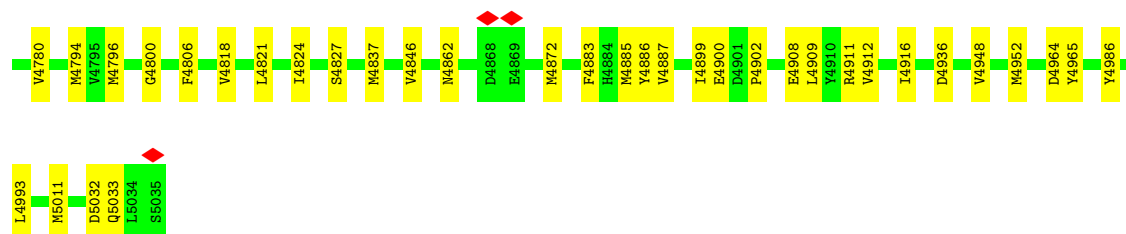


- Molecule 3: Ryanodine receptor 1

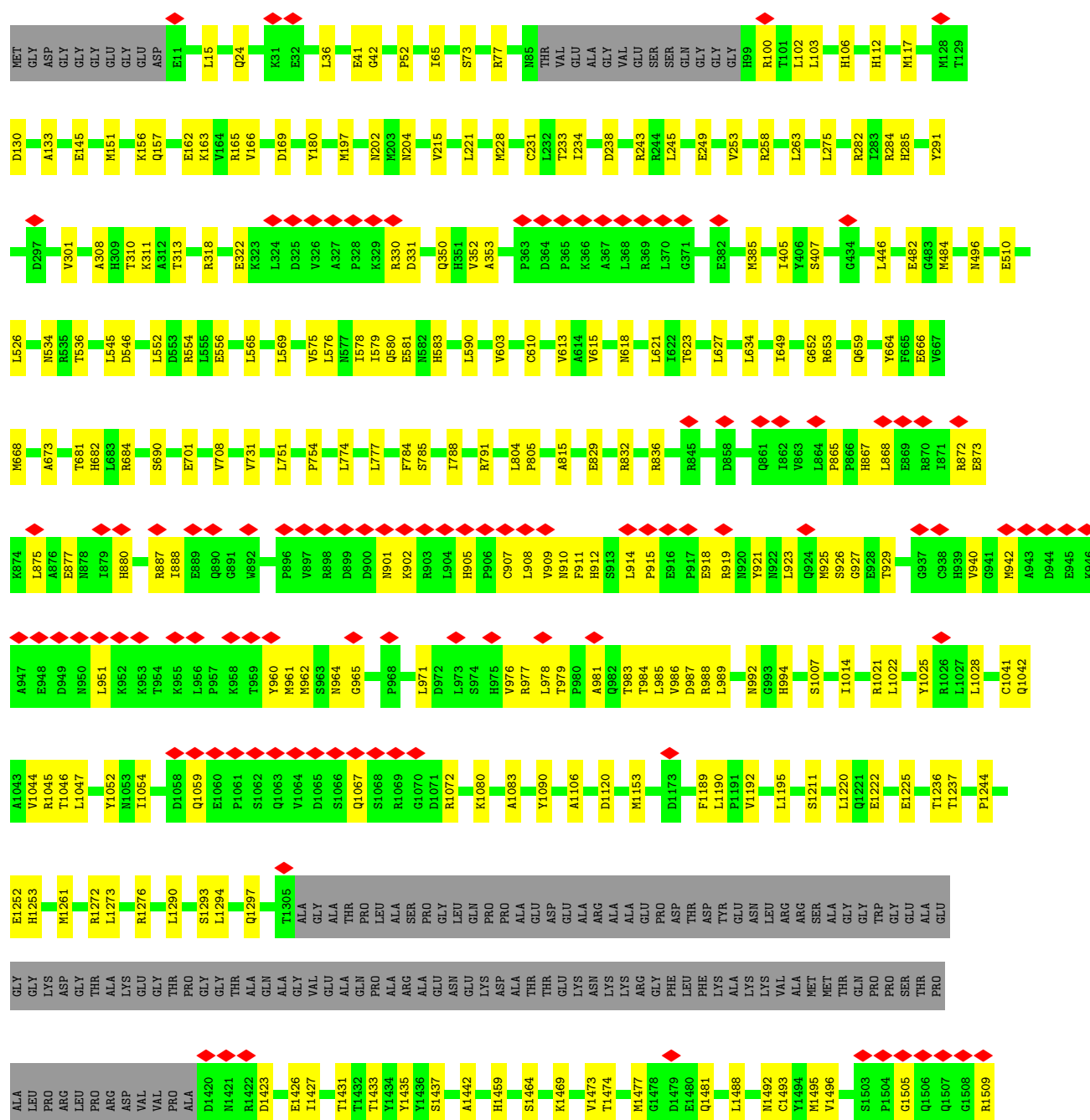




N3319	I3320	R3321	R3322	I3323	I3324	V3325	I3330	D3331	E3332	A3333	M3336	K3337	A3343	P3344	I3345	I3346	V3347	E3353	I3354	L3355	R3356	I3360	I3363	R3367	V3373	V3374	A3375	E3376	E3377	E3378	I3379	L3380	R3381	L3382	E3383	A3384	R3385	A3386	E3387	A3388	E3389	E3390	G3391	E3392	L3393	L3394	V3395	R3396	D3397	E3398	F3399																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
S3400	V3401	L3402	C3403	R3404	D3405	I3406	Y3407	A3408	L3409	Y3410	P3411	I3412	L3413	I3414	R3415	R3421	N3431	A3432	L3435	M3438	Y3439	G3440	E3441	I3442	F3443	I3444	S3447	N3451	F3452	K3453	R3454	E3455	E3456	Q3457	N3458	F3459	V3460	V3461	Q3462	N3463	E3464	I3465	N3466	N3467	M3468	S3469	F3470	L3471	T3472	ALA	ASN	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
SER	LYS	MET	ALA	LYS	ALA	GLY	ASP	VAL	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	GLY	GLY	ASP	ASP	ARG	Y3504	S3505	F3506	Q3507	T3508	I3511	V3512	A3513	T3514	L3515	K3516	K3517	M3518	I3521	C3526	A3527	D3530	Q3531	D3532	L3533	I3534	Y3541	R3544	D3545	T3546	D3547																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
V3550	R3551	N3557	L3558	N3559	L3560	Q3561	Q3562	K3563	V3564	E3565	G3566	L3576	Y3577	R3578	G3579	V3580	R3583	E3584	E3585	D3586	A3587	D3588	I3593	V3594	R3595	R3596	V3597	Q3598	E3599	V3600	V3603	L3604	L3607	E3611	H3612	P3613	TVR	LYS	SER	LYS	LYS	ALA	VAL	TRP	HIS	LYS	LEU	SER	GLY	GLN	R3629																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
R3630	R3631	V3634	A3635	C3636	F3637	R3638	M3639	T3640	L3645	C3651	N3652	M3653	A3660	L3664	L3678	E3683	Q3684	E3685	E3686	E3687	E3688	E3689	E3690	V3691	E3692	E3693	L3702	L3717	D3720	Y3721	L3722	T3723	M3724	A3725	Y3726	M3730	S3733	L3736	E3737	GLU	GLY	GLY	GLU	ASN	LYS	GLY	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
GLU	GLY	GLY	GLU	GLU	GLU	GLU	V3752	E3753	E3757	K3763	L3767	Q3770	S3771	H3774	M3785	C3789	A3795	N3812	S3834	A3837	T3841	L3847	M3861	V3862	N3863	E3864	D3865	G3866	T3867	V3868	L3869	N3870	K3871	Q3872	N3873	G3874	L3894	F3902	I3920	T3933	S3934																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
D3935	F3936	Y3937	D3944	V3945	I3946	F3954	I3972	Q3973	G3974	P3975	L3983	S3986	V3992	L3993	G3994	V3998	M4002	M4003	M4004	K4005	D4009	S4010	L4015	L4019	M4040	R4045	M4050	I4074	S4077	D4082	R4088	G4089	L4090	D4095	F4096	M4100	F4113																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
E4122	M4125	I4126	N4127	S4154	E4155	L4167	I4173	R4183	I4184	E4185	F4220	I4221	V4225	N4226	E4227	E4230	F4237	T4244	M4248	P4257	GLU	GLY	GLU	PRO	GLU	GLU	ASP	ALA	GLU	ASP	GLY	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA	VAL	ALA</

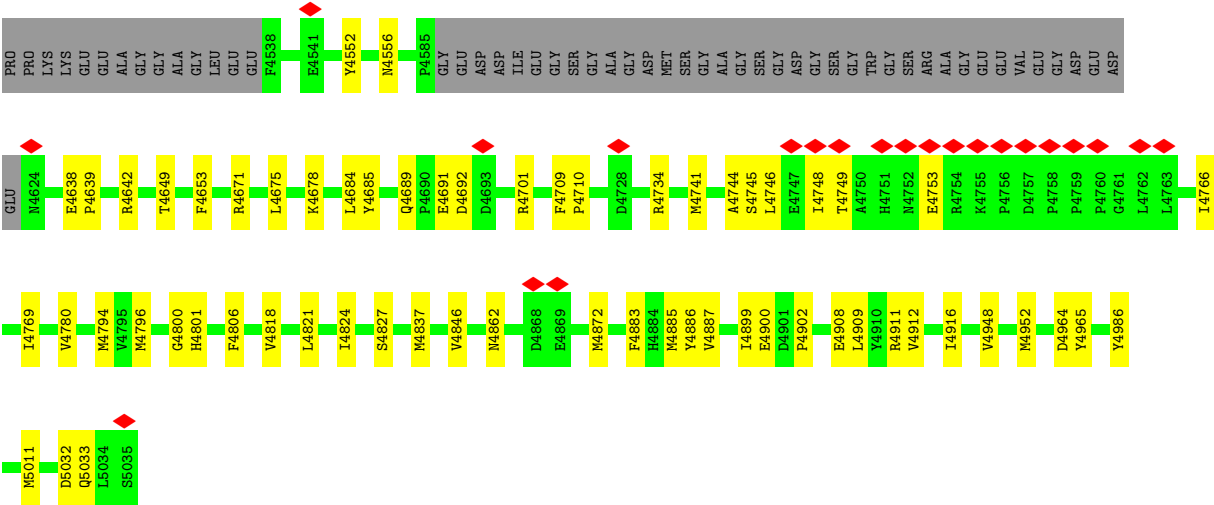


• Molecule 3: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31572	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.19	0/847	0.34	0/1142
1	F	0.19	0/847	0.34	0/1142
1	G	0.19	0/847	0.33	0/1142
1	H	0.19	0/847	0.33	0/1142
2	I	0.17	0/739	0.49	0/992
2	J	0.21	0/739	0.53	0/992
2	K	0.17	0/739	0.49	0/992
2	L	0.21	0/739	0.53	0/992
2	M	0.17	0/739	0.49	0/992
2	N	0.21	0/739	0.53	0/992
2	O	0.18	0/739	0.49	0/992
2	P	0.21	0/739	0.53	0/992
3	A	0.20	0/35638	0.36	0/48272
3	B	0.20	0/35638	0.36	0/48272
3	C	0.20	0/35638	0.36	0/48272
3	D	0.20	0/35638	0.36	0/48272
All	All	0.20	0/151852	0.37	0/205592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	829	0	826	13	0
1	F	829	0	826	11	0
1	G	829	0	826	11	0
1	H	829	0	826	11	0
2	I	729	0	705	53	0
2	J	729	0	705	56	0
2	K	729	0	705	53	0
2	L	729	0	705	55	0
2	M	729	0	705	53	0
2	N	729	0	705	57	0
2	O	729	0	705	52	0
2	P	729	0	705	55	0
3	A	34849	0	34448	596	0
3	B	34849	0	34448	590	0
3	C	34849	0	34448	594	0
3	D	34849	0	34448	586	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	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	14	0	10	0	0
6	B	14	0	10	0	0
6	C	14	0	10	0	0
6	D	14	0	10	0	0
7	A	62	0	24	3	0
7	B	62	0	24	4	0
7	C	62	0	24	4	0
7	D	62	0	24	4	0
8	A	108	0	167	6	0
8	B	108	0	167	5	0
8	C	108	0	167	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	108	0	167	5	0
All	All	149304	0	147540	2692	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 9.

All (2692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:GLU:OE2	3:A:2694:GLN:NE2	1.72	1.23
3:C:2694:GLN:NE2	2:M:10:GLU:OE2	1.72	1.23
3:D:2694:GLN:NE2	2:O:10:GLU:OE2	1.72	1.22
3:B:2694:GLN:NE2	2:K:10:GLU:OE2	1.72	1.21
3:A:875:LEU:HD11	3:A:1047:LEU:HD21	1.41	1.02
3:D:875:LEU:HD11	3:D:1047:LEU:HD21	1.41	1.01
3:C:875:LEU:HD11	3:C:1047:LEU:HD21	1.41	0.98
3:B:875:LEU:HD11	3:B:1047:LEU:HD21	1.41	0.98
2:I:6:GLU:OE2	2:J:42:LEU:HD13	1.65	0.95
2:N:42:LEU:HD13	2:M:6:GLU:OE2	1.65	0.95
2:O:6:GLU:OE2	2:P:42:LEU:HD13	1.65	0.94
2:K:6:GLU:OE2	2:L:42:LEU:HD13	1.65	0.94
3:A:4040:ASN:O	3:A:4045:ARG:NH1	2.12	0.83
3:B:4040:ASN:O	3:B:4045:ARG:NH1	2.12	0.83
3:C:4040:ASN:O	3:C:4045:ARG:NH1	2.12	0.82
2:I:41:GLU:OE1	2:J:2:GLY:N	2.13	0.82
2:N:2:GLY:N	2:M:41:GLU:OE1	2.13	0.82
2:K:41:GLU:OE1	2:L:2:GLY:N	2.13	0.81
3:D:4040:ASN:O	3:D:4045:ARG:NH1	2.12	0.81
2:K:84:VAL:HG13	2:L:72:PHE:HE2	1.44	0.81
2:O:41:GLU:OE1	2:P:2:GLY:N	2.13	0.81
3:C:3319:ASN:O	3:C:3323:ILE:HD12	1.80	0.81
3:D:3319:ASN:O	3:D:3323:ILE:HD12	1.80	0.81
2:I:84:VAL:HG13	2:J:72:PHE:HE2	1.44	0.81
3:D:145:GLU:OE1	3:C:2453:ARG:NH2	2.14	0.80
3:A:3309:THR:OG1	3:A:3311:ASP:OD1	1.99	0.80
3:D:3309:THR:OG1	3:D:3311:ASP:OD1	2.00	0.80
2:O:84:VAL:HG13	2:P:72:PHE:HE2	1.44	0.80
3:A:3319:ASN:O	3:A:3323:ILE:HD12	1.80	0.80
3:B:3319:ASN:O	3:B:3323:ILE:HD12	1.80	0.80
2:N:72:PHE:HE2	2:M:84:VAL:HG13	1.44	0.80
3:A:3236:SER:OG	3:A:3239:GLU:OE1	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3309:THR:OG1	3:B:3311:ASP:OD1	2.00	0.79
3:D:1713:TYR:OH	3:D:1816:MET:SD	2.41	0.79
3:D:156:LYS:CG	3:C:228:MET:SD	2.71	0.79
3:B:1435:TYR:OH	3:B:1570:GLN:N	2.16	0.79
3:B:2183:ILE:HG22	3:B:2187:MET:HE2	1.65	0.79
3:C:1713:TYR:OH	3:C:1816:MET:SD	2.41	0.79
3:C:3309:THR:OG1	3:C:3311:ASP:OD1	2.00	0.79
3:D:1435:TYR:OH	3:D:1570:GLN:N	2.16	0.79
3:B:2453:ARG:NH2	3:C:145:GLU:OE1	2.14	0.79
3:C:1435:TYR:OH	3:C:1570:GLN:N	2.16	0.79
3:C:2183:ILE:HG22	3:C:2187:MET:HE2	1.65	0.79
3:A:2183:ILE:HG22	3:A:2187:MET:HE2	1.65	0.78
3:A:4082:ASP:OD2	3:B:4734:ARG:NH1	2.16	0.78
3:B:3236:SER:OG	3:B:3239:GLU:OE1	2.01	0.78
3:A:1713:TYR:OH	3:A:1816:MET:SD	2.41	0.78
3:B:3367:ARG:NH1	3:B:3441:GLU:OE2	2.16	0.78
3:D:2183:ILE:HG22	3:D:2187:MET:HE2	1.65	0.78
3:A:2213:VAL:HG11	3:A:2257:TYR:HE2	1.48	0.78
3:B:1713:TYR:OH	3:B:1816:MET:SD	2.41	0.78
3:C:3236:SER:OG	3:C:3239:GLU:OE1	2.01	0.78
3:C:3367:ARG:NH1	3:C:3441:GLU:OE2	2.16	0.78
3:D:1653:GLU:OE1	3:D:1657:ARG:NH1	2.17	0.78
3:D:3236:SER:OG	3:D:3239:GLU:OE1	2.01	0.78
3:D:3367:ARG:NH1	3:D:3441:GLU:OE2	2.16	0.78
3:A:1653:GLU:OE1	3:A:1657:ARG:NH1	2.17	0.78
3:A:3367:ARG:NH1	3:A:3441:GLU:OE2	2.17	0.78
3:B:2269:GLN:NE2	3:B:2413:GLU:OE2	2.17	0.78
3:D:2213:VAL:HG11	3:D:2257:TYR:HE2	1.48	0.78
3:A:2453:ARG:NH2	3:B:145:GLU:OE1	2.16	0.78
3:D:1423:ASP:OD2	3:D:1569:LYS:NZ	2.17	0.78
3:C:1423:ASP:OD2	3:C:1569:LYS:NZ	2.17	0.78
3:C:2269:GLN:NE2	3:C:2413:GLU:OE2	2.17	0.78
3:A:2269:GLN:NE2	3:A:2413:GLU:OE2	2.17	0.77
3:B:3316:LEU:O	3:B:3320:ILE:HD12	1.85	0.77
3:A:3316:LEU:O	3:A:3320:ILE:HD12	1.85	0.77
3:B:228:MET:SD	3:C:156:LYS:CG	2.71	0.77
3:C:2156:LEU:HD21	3:C:2199:MET:HE1	1.66	0.77
3:D:2269:GLN:NE2	3:D:2413:GLU:OE2	2.17	0.77
3:D:2453:ARG:NH2	3:A:145:GLU:OE1	2.18	0.77
3:A:1435:TYR:OH	3:A:1570:GLN:N	2.16	0.77
3:B:1653:GLU:OE1	3:B:1657:ARG:NH1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2213:VAL:HG11	3:B:2257:TYR:HE2	1.48	0.77
3:B:2156:LEU:HD21	3:B:2199:MET:HE1	1.66	0.77
3:C:1653:GLU:OE1	3:C:1657:ARG:NH1	2.17	0.77
3:C:2213:VAL:HG11	3:C:2257:TYR:HE2	1.48	0.77
3:B:3435:LEU:HD22	3:B:3518:MET:HE2	1.67	0.76
3:B:1423:ASP:OD2	3:B:1569:LYS:NZ	2.17	0.76
3:D:3316:LEU:O	3:D:3320:ILE:HD12	1.85	0.76
2:J:53:ASP:OD2	2:J:54:ALA:N	2.19	0.76
3:D:2156:LEU:HD21	3:D:2199:MET:HE1	1.66	0.76
2:N:53:ASP:OD2	2:N:54:ALA:N	2.19	0.76
3:C:3316:LEU:O	3:C:3320:ILE:HD12	1.85	0.76
3:D:3400:SER:OG	3:D:3455:GLU:OE1	2.04	0.76
3:A:1042:GLN:O	3:A:1046:THR:HG23	1.86	0.76
3:B:3407:TYR:OH	3:B:3456:GLU:OE2	2.04	0.76
3:C:1042:GLN:O	3:C:1046:THR:HG23	1.86	0.76
3:D:3435:LEU:HD22	3:D:3518:MET:HE2	1.67	0.76
3:C:3435:LEU:HD22	3:C:3518:MET:HE2	1.67	0.76
2:L:53:ASP:OD2	2:L:54:ALA:N	2.19	0.76
3:A:836:ARG:NH2	3:A:1211:SER:O	2.20	0.75
3:D:156:LYS:HG2	3:C:228:MET:SD	2.27	0.75
3:D:2873:GLN:OE1	3:D:2921:ARG:NH2	2.19	0.75
3:A:2156:LEU:HD21	3:A:2199:MET:HE1	1.66	0.75
3:B:1042:GLN:O	3:B:1046:THR:HG23	1.86	0.75
3:B:4744:ALA:O	3:B:4748:ILE:HD12	1.87	0.75
3:C:2873:GLN:OE1	3:C:2921:ARG:NH2	2.19	0.75
3:D:24:GLN:OE1	3:D:204:ASN:ND2	2.20	0.75
3:C:836:ARG:NH2	3:C:1211:SER:O	2.20	0.75
3:C:2813:SER:OG	3:C:2883:TYR:OH	2.03	0.75
3:A:4744:ALA:O	3:A:4748:ILE:HD12	1.87	0.75
3:B:836:ARG:NH2	3:B:1211:SER:O	2.20	0.75
3:C:4744:ALA:O	3:C:4748:ILE:HD12	1.87	0.75
2:P:53:ASP:OD2	2:P:54:ALA:N	2.19	0.75
3:D:4744:ALA:O	3:D:4748:ILE:HD12	1.87	0.75
3:A:24:GLN:OE1	3:A:204:ASN:ND2	2.20	0.75
3:A:2873:GLN:OE1	3:A:2921:ARG:NH2	2.19	0.75
3:B:228:MET:SD	3:C:156:LYS:HG2	2.27	0.75
3:D:836:ARG:NH2	3:D:1211:SER:O	2.20	0.75
3:A:3400:SER:OG	3:A:3455:GLU:OE1	2.04	0.75
3:A:3407:TYR:OH	3:A:3456:GLU:OE2	2.04	0.75
3:C:24:GLN:OE1	3:C:204:ASN:ND2	2.20	0.75
3:D:3407:TYR:OH	3:D:3456:GLU:OE2	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4900:GLU:O	3:D:4911:ARG:NH2	2.21	0.74
3:A:228:MET:SD	3:B:156:LYS:CG	2.75	0.74
3:D:330:ARG:NH1	3:D:331:ASP:OD1	2.21	0.74
3:D:2813:SER:OG	3:D:2883:TYR:OH	2.03	0.74
3:A:330:ARG:NH1	3:A:331:ASP:OD1	2.21	0.74
3:B:2873:GLN:OE1	3:B:2921:ARG:NH2	2.19	0.74
3:C:4900:GLU:O	3:C:4911:ARG:NH2	2.21	0.74
2:J:80:ALA:O	2:J:84:VAL:HG22	1.88	0.74
3:B:24:GLN:OE1	3:B:204:ASN:ND2	2.20	0.74
2:P:80:ALA:O	2:P:84:VAL:HG22	1.88	0.74
3:C:3400:SER:OG	3:C:3455:GLU:OE1	2.04	0.74
3:C:3407:TYR:OH	3:C:3456:GLU:OE2	2.04	0.74
3:A:3435:LEU:HD22	3:A:3518:MET:HE2	1.67	0.74
2:N:80:ALA:O	2:N:84:VAL:HG22	1.88	0.74
3:B:330:ARG:NH1	3:B:331:ASP:OD1	2.21	0.74
3:D:1042:GLN:O	3:D:1046:THR:HG23	1.86	0.74
3:B:3400:SER:OG	3:B:3455:GLU:OE1	2.04	0.73
3:C:330:ARG:NH1	3:C:331:ASP:OD1	2.21	0.73
3:A:1423:ASP:OD2	3:A:1569:LYS:NZ	2.17	0.73
3:D:908:LEU:O	3:D:964:ASN:ND2	2.22	0.73
3:B:4900:GLU:O	3:B:4911:ARG:NH2	2.21	0.73
3:B:4638:GLU:OE2	3:B:4642:ARG:NH1	2.21	0.73
3:D:4638:GLU:OE2	3:D:4642:ARG:NH1	2.21	0.73
3:A:4900:GLU:O	3:A:4911:ARG:NH2	2.20	0.73
3:B:908:LEU:O	3:B:964:ASN:ND2	2.22	0.73
3:A:951:LEU:HB3	3:A:971:LEU:HD23	1.71	0.73
3:A:908:LEU:O	3:A:964:ASN:ND2	2.22	0.73
3:C:4638:GLU:OE2	3:C:4642:ARG:NH1	2.21	0.73
2:L:80:ALA:O	2:L:84:VAL:HG22	1.88	0.72
3:A:4638:GLU:OE2	3:A:4642:ARG:NH1	2.21	0.72
3:B:951:LEU:HB3	3:B:971:LEU:HD23	1.71	0.72
3:C:908:LEU:O	3:C:964:ASN:ND2	2.22	0.72
3:C:914:LEU:HD21	3:C:918:GLU:OE1	1.90	0.72
3:D:951:LEU:HB3	3:D:971:LEU:HD23	1.71	0.72
3:D:4074:ILE:O	3:D:4077:SER:OG	2.06	0.72
3:B:1505:GLY:O	3:B:1509:ARG:NH1	2.23	0.72
3:B:914:LEU:HD21	3:B:918:GLU:OE1	1.90	0.72
3:B:2889:ARG:O	3:B:2893:GLN:NE2	2.23	0.72
2:P:5:LEU:HD23	2:P:9:MET:HE1	1.72	0.72
3:D:3111:LEU:O	3:D:3183:TYR:OH	2.07	0.72
3:A:4883:PHE:O	3:A:4887:VAL:HG22	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:951:LEU:HB3	3:C:971:LEU:HD23	1.71	0.72
3:D:2889:ARG:O	3:D:2893:GLN:NE2	2.23	0.72
3:A:914:LEU:HD21	3:A:918:GLU:OE1	1.90	0.71
3:B:4883:PHE:O	3:B:4887:VAL:HG22	1.90	0.71
3:C:1505:GLY:O	3:C:1509:ARG:NH1	2.23	0.71
3:D:228:MET:SD	3:A:156:LYS:CG	2.78	0.71
2:L:5:LEU:HD23	2:L:9:MET:HE1	1.72	0.71
3:A:2889:ARG:O	3:A:2893:GLN:NE2	2.23	0.71
1:E:37:PHE:O	3:A:1688:SER:OG	2.07	0.71
3:D:914:LEU:HD21	3:D:918:GLU:OE1	1.90	0.71
3:D:1505:GLY:O	3:D:1509:ARG:NH1	2.23	0.71
3:D:4883:PHE:O	3:D:4887:VAL:HG22	1.90	0.71
3:C:2698:ARG:NH2	2:M:17:HIS:ND1	2.38	0.71
3:C:4883:PHE:O	3:C:4887:VAL:HG22	1.90	0.71
3:B:2698:ARG:NH2	2:K:17:HIS:ND1	2.38	0.71
3:A:1505:GLY:O	3:A:1509:ARG:NH1	2.23	0.71
3:A:3111:LEU:O	3:A:3183:TYR:OH	2.07	0.71
3:C:2889:ARG:O	3:C:2893:GLN:NE2	2.23	0.71
2:N:5:LEU:HD23	2:N:9:MET:HE1	1.72	0.71
2:I:17:HIS:ND1	3:A:2698:ARG:NH2	2.38	0.70
1:G:37:PHE:O	3:C:1688:SER:OG	2.07	0.70
3:D:2564:THR:HG22	3:D:2607:CYS:HA	1.74	0.70
2:J:5:LEU:HD23	2:J:9:MET:HE1	1.72	0.70
3:D:2698:ARG:NH2	2:O:17:HIS:ND1	2.38	0.70
3:D:4082:ASP:OD2	3:A:4734:ARG:NH1	2.24	0.70
3:A:2564:THR:HG22	3:A:2607:CYS:HA	1.74	0.70
3:C:3111:LEU:O	3:C:3183:TYR:OH	2.07	0.70
3:A:228:MET:SD	3:B:156:LYS:HG2	2.31	0.70
2:I:61:GLU:O	3:A:3638:ARG:NH1	2.25	0.70
3:C:3638:ARG:NH1	2:M:61:GLU:O	2.25	0.70
3:C:2564:THR:HG22	3:C:2607:CYS:HA	1.74	0.70
3:D:3638:ARG:NH1	2:O:61:GLU:O	2.25	0.69
3:B:829:GLU:OE2	3:B:832:ARG:NH1	2.26	0.69
3:B:2564:THR:HG22	3:B:2607:CYS:HA	1.74	0.69
3:C:829:GLU:OE2	3:C:832:ARG:NH1	2.26	0.69
3:C:2539:THR:O	3:C:2543:SER:OG	2.10	0.69
3:D:829:GLU:OE2	3:D:832:ARG:NH1	2.26	0.69
3:D:3108:VAL:HG21	3:D:3172:SER:HB2	1.73	0.69
1:H:37:PHE:O	3:D:1688:SER:OG	2.06	0.69
3:D:4734:ARG:NH1	3:C:4082:ASP:OD2	2.26	0.69
3:B:1431:THR:HG22	3:B:1433:THR:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3111:LEU:O	3:B:3183:TYR:OH	2.07	0.69
3:B:3638:ARG:NH1	2:K:61:GLU:O	2.25	0.69
3:C:3108:VAL:HG21	3:C:3172:SER:HB2	1.74	0.69
3:C:3467:ASN:ND2	3:C:3508:THR:O	2.26	0.69
2:M:37:LEU:O	2:M:40:THR:OG1	2.10	0.69
3:D:3467:ASN:ND2	3:D:3508:THR:O	2.26	0.69
3:A:3108:VAL:HG21	3:A:3172:SER:HB2	1.74	0.69
3:B:3108:VAL:HG21	3:B:3172:SER:HB2	1.74	0.69
3:C:3530:ASP:OD1	3:C:3561:GLN:NE2	2.26	0.69
3:D:3208:GLU:OE1	3:D:3281:TYR:OH	2.11	0.68
3:A:1431:THR:HG22	3:A:1433:THR:H	1.58	0.68
3:B:3530:ASP:OD1	3:B:3561:GLN:NE2	2.26	0.68
3:C:1431:THR:HG22	3:C:1433:THR:H	1.58	0.68
3:D:3530:ASP:OD1	3:D:3561:GLN:NE2	2.26	0.68
3:B:41:GLU:OE2	3:B:407:SER:OG	2.11	0.68
3:C:1273:LEU:HD22	3:C:1290:LEU:HD11	1.76	0.68
3:D:3053:HIS:NE2	3:D:3103:ASP:OD1	2.27	0.68
3:B:3053:HIS:NE2	3:B:3103:ASP:OD1	2.27	0.68
3:A:3053:HIS:NE2	3:A:3103:ASP:OD1	2.27	0.68
3:A:3530:ASP:OD1	3:A:3561:GLN:NE2	2.26	0.68
3:B:2560:LEU:O	3:B:2564:THR:HG23	1.94	0.68
1:E:32:GLU:OE1	1:E:97:THR:OG1	2.10	0.68
3:B:4074:ILE:O	3:B:4077:SER:OG	2.06	0.68
3:C:2560:LEU:O	3:C:2564:THR:HG23	1.94	0.68
3:A:1273:LEU:HD22	3:A:1290:LEU:HD11	1.76	0.68
3:B:1273:LEU:HD22	3:B:1290:LEU:HD11	1.76	0.68
3:D:1297:GLN:NE2	3:D:1546:ASN:OD1	2.27	0.68
3:D:2560:LEU:O	3:D:2564:THR:HG23	1.94	0.68
3:A:2523:LEU:HD11	3:A:2583:MET:SD	2.33	0.68
3:B:4082:ASP:OD2	3:C:4734:ARG:NH1	2.26	0.68
3:C:3053:HIS:NE2	3:C:3103:ASP:OD1	2.27	0.68
3:D:1273:LEU:HD22	3:D:1290:LEU:HD11	1.76	0.68
3:A:829:GLU:OE2	3:A:832:ARG:NH1	2.26	0.68
3:C:1297:GLN:NE2	3:C:1546:ASN:OD1	2.27	0.68
3:A:2560:LEU:O	3:A:2564:THR:HG23	1.94	0.67
3:B:3467:ASN:ND2	3:B:3508:THR:O	2.26	0.67
3:C:2588:TYR:OH	3:C:2592:ARG:NH2	2.28	0.67
3:D:2523:LEU:HD11	3:D:2583:MET:SD	2.34	0.67
3:A:3467:ASN:ND2	3:A:3508:THR:O	2.26	0.67
3:B:2523:LEU:HD11	3:B:2583:MET:SD	2.34	0.67
3:B:2588:TYR:OH	3:B:2592:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:910:ASN:O	3:D:914:LEU:N	2.28	0.67
3:D:2588:TYR:OH	3:D:2592:ARG:NH2	2.28	0.67
3:A:2588:TYR:OH	3:A:2592:ARG:NH2	2.28	0.67
3:C:3530:ASP:OD2	3:C:3596:ARG:NH2	2.28	0.67
1:F:37:PHE:O	3:B:1688:SER:OG	2.07	0.67
3:A:910:ASN:O	3:A:914:LEU:N	2.28	0.67
3:B:3530:ASP:OD2	3:B:3596:ARG:NH2	2.28	0.67
3:C:2523:LEU:HD11	3:C:2583:MET:SD	2.34	0.67
3:B:1297:GLN:NE2	3:B:1546:ASN:OD1	2.27	0.67
3:D:1431:THR:HG22	3:D:1433:THR:H	1.58	0.67
3:A:1297:GLN:NE2	3:A:1546:ASN:OD1	2.26	0.67
3:B:910:ASN:O	3:B:914:LEU:N	2.28	0.67
3:D:552:LEU:HD11	3:D:565:LEU:HD22	1.77	0.67
3:A:552:LEU:HD11	3:A:565:LEU:HD22	1.77	0.67
3:B:3208:GLU:OE1	3:B:3281:TYR:OH	2.11	0.67
2:I:37:LEU:O	2:I:40:THR:OG1	2.11	0.67
3:B:552:LEU:HD11	3:B:565:LEU:HD22	1.77	0.67
3:D:41:GLU:OE2	3:D:407:SER:OG	2.11	0.66
3:A:3530:ASP:OD2	3:A:3596:ARG:NH2	2.28	0.66
3:C:3505:SER:O	3:C:3508:THR:OG1	2.12	0.66
2:I:84:VAL:HG22	2:J:72:PHE:CD2	2.31	0.66
3:C:3344:GLN:O	3:C:3347:VAL:HG22	1.95	0.66
2:N:72:PHE:CD2	2:M:84:VAL:HG22	2.30	0.66
3:D:3344:GLN:O	3:D:3347:VAL:HG22	1.95	0.66
3:D:3530:ASP:OD2	3:D:3596:ARG:NH2	2.28	0.66
3:C:910:ASN:O	3:C:914:LEU:N	2.28	0.66
3:B:3076:LEU:HD23	3:B:3077:ASP:N	2.11	0.66
2:K:37:LEU:O	2:K:40:THR:OG1	2.11	0.66
3:D:3082:MET:O	3:D:3090:LYS:NZ	2.29	0.66
3:A:2539:THR:O	3:A:2543:SER:OG	2.10	0.66
3:C:41:GLU:OE2	3:C:407:SER:OG	2.11	0.66
3:C:552:LEU:HD11	3:C:565:LEU:HD22	1.77	0.66
3:D:228:MET:SD	3:A:156:LYS:HG2	2.34	0.66
3:B:3320:ILE:O	3:B:3324:ILE:HD12	1.96	0.66
3:B:3344:GLN:O	3:B:3347:VAL:HG22	1.95	0.66
2:K:84:VAL:HG22	2:L:72:PHE:CD2	2.31	0.66
3:B:1021:ARG:HE	7:B:8005:ATP:HN62	1.43	0.66
3:B:2752:LEU:HB3	3:B:2814:LEU:HD13	1.77	0.66
3:A:3344:GLN:O	3:A:3347:VAL:HG22	1.95	0.66
3:C:2703:CYS:O	3:C:2707:ILE:HD12	1.96	0.66
2:O:84:VAL:HG22	2:P:72:PHE:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3320:ILE:O	3:A:3324:ILE:HD12	1.96	0.66
3:B:3082:MET:O	3:B:3090:LYS:NZ	2.29	0.66
3:C:2752:LEU:HB3	3:C:2814:LEU:HD13	1.77	0.66
3:B:2260:GLU:OE2	3:B:2298:LYS:NZ	2.22	0.65
3:B:3505:SER:O	3:B:3508:THR:OG1	2.12	0.65
3:D:3076:LEU:HD23	3:D:3077:ASP:N	2.11	0.65
3:D:3532:ASP:OD1	3:D:3533:LEU:N	2.29	0.65
3:A:41:GLU:OE2	3:A:407:SER:OG	2.11	0.65
3:A:4074:ILE:O	3:A:4077:SER:OG	2.06	0.65
3:B:3532:ASP:OD1	3:B:3533:LEU:N	2.29	0.65
3:C:1021:ARG:HE	7:C:5106:ATP:HN62	1.43	0.65
3:C:3532:ASP:OD1	3:C:3533:LEU:N	2.29	0.65
3:D:701:GLU:OE2	3:D:1459:HIS:NE2	2.29	0.65
3:A:3082:MET:O	3:A:3090:LYS:NZ	2.29	0.65
2:K:6:GLU:OE2	2:L:42:LEU:CD1	2.44	0.65
3:A:701:GLU:OE2	3:A:1459:HIS:NE2	2.29	0.65
3:A:3208:GLU:OE1	3:A:3281:TYR:OH	2.11	0.65
3:A:3410:TYR:O	3:A:3413:LEU:N	2.30	0.65
3:A:3505:SER:O	3:A:3508:THR:OG1	2.12	0.65
2:N:37:LEU:O	2:N:40:THR:OG1	2.11	0.65
3:D:2703:CYS:O	3:D:2707:ILE:HD12	1.96	0.65
3:C:3076:LEU:HD23	3:C:3077:ASP:N	2.11	0.65
1:E:3:VAL:HG23	1:E:77:ILE:HD13	1.78	0.65
3:C:3082:MET:O	3:C:3090:LYS:NZ	2.29	0.65
3:D:3410:TYR:O	3:D:3413:LEU:N	2.30	0.65
3:D:3505:SER:O	3:D:3508:THR:OG1	2.12	0.65
3:A:1021:ARG:HE	7:A:8005:ATP:HN62	1.43	0.65
3:C:4824:ILE:O	3:C:4827:SER:OG	2.14	0.65
3:D:2752:LEU:HB3	3:D:2814:LEU:HD13	1.77	0.65
3:A:3532:ASP:OD1	3:A:3533:LEU:N	2.29	0.65
3:C:3320:ILE:O	3:C:3324:ILE:HD12	1.96	0.65
3:C:3410:TYR:O	3:C:3413:LEU:N	2.30	0.64
2:O:37:LEU:O	2:O:40:THR:OG1	2.11	0.64
3:A:2752:LEU:HB3	3:A:2814:LEU:HD13	1.77	0.64
3:A:3076:LEU:HD23	3:A:3077:ASP:N	2.11	0.64
2:N:72:PHE:CE2	2:M:84:VAL:HG13	2.31	0.64
1:F:3:VAL:HG23	1:F:77:ILE:HD13	1.80	0.64
1:H:32:GLU:OE1	1:H:97:THR:OG1	2.15	0.64
3:D:484:MET:HE2	3:D:484:MET:HA	1.80	0.64
3:A:2755:PHE:HD2	3:A:2814:LEU:HD11	1.63	0.64
3:C:484:MET:HA	3:C:484:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:84:VAL:HG13	2:L:72:PHE:CE2	2.31	0.64
2:N:42:LEU:CD1	2:M:6:GLU:OE2	2.44	0.64
2:J:72:PHE:HA	2:J:75:TYR:CE1	2.33	0.64
1:G:3:VAL:HG23	1:G:77:ILE:HD13	1.79	0.64
1:H:3:VAL:HG23	1:H:77:ILE:HD13	1.79	0.64
3:D:3235:ASN:OD1	3:D:3236:SER:N	2.31	0.64
3:B:2703:CYS:O	3:B:2707:ILE:HD12	1.96	0.64
3:C:701:GLU:OE2	3:C:1459:HIS:NE2	2.29	0.64
3:D:1021:ARG:HE	7:D:8005:ATP:HN62	1.43	0.64
3:D:3320:ILE:O	3:D:3324:ILE:HD12	1.96	0.64
2:P:72:PHE:HA	2:P:75:TYR:CE1	2.33	0.64
3:A:2703:CYS:O	3:A:2707:ILE:HD12	1.96	0.64
3:B:3410:TYR:O	3:B:3413:LEU:N	2.30	0.64
1:F:32:GLU:OE2	1:F:97:THR:OG1	2.15	0.64
3:D:4796:MET:CE	8:D:8007:PCW:H222	2.27	0.64
3:B:484:MET:HE2	3:B:484:MET:HA	1.80	0.64
3:B:2755:PHE:HD2	3:B:2814:LEU:HD11	1.63	0.64
2:L:72:PHE:HA	2:L:75:TYR:CE1	2.33	0.64
1:G:32:GLU:OE1	1:G:97:THR:OG1	2.15	0.64
3:B:3235:ASN:OD1	3:B:3236:SER:N	2.31	0.64
3:B:3443:PHE:CG	3:B:3515:LEU:HD22	2.33	0.64
3:C:3235:ASN:OD1	3:C:3236:SER:N	2.31	0.64
3:D:554:ARG:NE	3:D:556:GLU:OE2	2.31	0.64
2:N:72:PHE:HA	2:N:75:TYR:CE1	2.33	0.64
2:I:6:GLU:OE2	2:J:42:LEU:CD1	2.44	0.64
3:A:484:MET:HE2	3:A:484:MET:HA	1.79	0.63
3:A:3235:ASN:OD1	3:A:3236:SER:N	2.31	0.63
3:B:3212:ASN:OD1	3:B:3213:GLU:N	2.31	0.63
3:C:3208:GLU:OE1	3:C:3281:TYR:OH	2.11	0.63
3:A:2209:MET:O	3:A:2213:VAL:HG13	1.99	0.63
3:C:2599:ALA:O	3:C:2603:VAL:HG23	1.99	0.63
3:C:3212:ASN:OD1	3:C:3213:GLU:N	2.31	0.63
3:D:2539:THR:O	3:D:2543:SER:OG	2.10	0.63
3:D:3431:ASN:OD1	3:D:3432:ALA:N	2.32	0.63
3:D:4818:VAL:HG11	3:A:4837:MET:HE2	1.81	0.63
3:A:2260:GLU:OE2	3:A:2298:LYS:NZ	2.22	0.63
3:A:3443:PHE:CG	3:A:3515:LEU:HD22	2.33	0.63
3:B:554:ARG:NE	3:B:556:GLU:OE2	2.31	0.63
3:B:2209:MET:O	3:B:2213:VAL:HG13	1.99	0.63
3:B:3431:ASN:OD1	3:B:3432:ALA:N	2.32	0.63
3:C:3443:PHE:CG	3:C:3515:LEU:HD22	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:LEU:HD23	3:D:805:PRO:O	1.99	0.63
3:D:3770:GLN:OE1	3:D:3812:ASN:ND2	2.32	0.63
3:D:4796:MET:HE1	8:D:8007:PCW:H222	1.80	0.63
3:A:3212:ASN:OD1	3:A:3213:GLU:N	2.31	0.63
3:C:2755:PHE:HD2	3:C:2814:LEU:HD11	1.63	0.63
3:D:2209:MET:O	3:D:2213:VAL:HG13	1.99	0.63
3:D:2933:MET:SD	3:D:2934:ASN:N	2.72	0.63
3:D:2599:ALA:O	3:D:2603:VAL:HG23	1.99	0.63
3:B:1442:ALA:N	3:B:1514:ASP:OD1	2.32	0.63
3:D:2755:PHE:HD2	3:D:2814:LEU:HD11	1.63	0.62
3:D:3443:PHE:CG	3:D:3515:LEU:HD22	2.33	0.62
3:A:901:ASN:OD1	3:A:902:LYS:N	2.32	0.62
3:B:2933:MET:SD	3:B:2934:ASN:N	2.72	0.62
3:B:3864:GLU:O	3:B:3868:VAL:HG22	1.99	0.62
3:C:901:ASN:OD1	3:C:902:LYS:N	2.32	0.62
3:C:2933:MET:SD	3:C:2934:ASN:N	2.72	0.62
3:C:3770:GLN:OE1	3:C:3812:ASN:ND2	2.32	0.62
3:D:901:ASN:OD1	3:D:902:LYS:N	2.32	0.62
3:A:804:LEU:HD23	3:A:805:PRO:O	1.99	0.62
3:A:2297:GLU:OE1	3:A:2357:LEU:HD22	2.00	0.62
3:A:2599:ALA:O	3:A:2603:VAL:HG23	1.99	0.62
3:A:2933:MET:SD	3:A:2934:ASN:N	2.72	0.62
3:B:2297:GLU:OE1	3:B:2357:LEU:HD22	2.00	0.62
3:D:3212:ASN:OD1	3:D:3213:GLU:N	2.31	0.62
3:D:3864:GLU:O	3:D:3868:VAL:HG22	1.99	0.62
3:A:554:ARG:NE	3:A:556:GLU:OE2	2.31	0.62
3:B:4862:ASN:HB2	3:B:4872:MET:HE1	1.82	0.62
3:C:3864:GLU:O	3:C:3868:VAL:HG22	1.99	0.62
2:P:37:LEU:O	2:P:40:THR:OG1	2.11	0.62
2:I:84:VAL:HG13	2:J:72:PHE:CE2	2.31	0.62
3:A:3770:GLN:OE1	3:A:3812:ASN:ND2	2.32	0.62
3:B:2599:ALA:O	3:B:2603:VAL:HG23	1.99	0.62
2:I:82:LEU:HD12	3:A:3630:ARG:HD3	1.82	0.62
2:J:6:GLU:HA	2:J:9:MET:HE2	1.82	0.62
3:D:865:PRO:HD2	3:D:868:LEU:HD12	1.82	0.62
3:B:249:GLU:HB2	3:B:253:VAL:HG11	1.82	0.62
3:B:701:GLU:OE2	3:B:1459:HIS:NE2	2.29	0.62
2:O:84:VAL:HG13	2:P:72:PHE:CE2	2.31	0.62
3:D:4009:ASP:OD1	3:D:4010:SER:N	2.33	0.62
3:A:921:TYR:CE2	3:A:925:MET:HE3	2.35	0.62
3:A:3864:GLU:O	3:A:3868:VAL:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:901:ASN:OD1	3:B:902:LYS:N	2.32	0.62
3:C:554:ARG:NE	3:C:556:GLU:OE2	2.31	0.62
3:C:3954:PHE:CD2	3:C:4015:LEU:HD21	2.34	0.62
3:D:921:TYR:CE2	3:D:925:MET:HE3	2.35	0.62
3:D:1442:ALA:N	3:D:1514:ASP:OD1	2.32	0.62
3:A:4009:ASP:OD1	3:A:4010:SER:N	2.33	0.62
3:B:914:LEU:HD12	3:B:915:PRO:HD2	1.82	0.62
2:L:6:GLU:HA	2:L:9:MET:HE2	1.82	0.62
3:A:914:LEU:HD12	3:A:915:PRO:HD2	1.82	0.62
3:A:1442:ALA:N	3:A:1514:ASP:OD1	2.32	0.62
3:A:3954:PHE:CD2	3:A:4015:LEU:HD21	2.34	0.62
3:A:4796:MET:CE	8:A:8007:PCW:H222	2.29	0.62
3:A:4862:ASN:HB2	3:A:4872:MET:HE1	1.82	0.62
3:B:2749:PRO:HD2	3:B:2752:LEU:HD12	1.82	0.62
3:C:3431:ASN:OD1	3:C:3432:ALA:N	2.32	0.62
3:D:4824:ILE:O	3:D:4827:SER:OG	2.14	0.62
3:A:925:MET:HE1	7:A:8005:ATP:O4'	2.00	0.62
3:B:865:PRO:HD2	3:B:868:LEU:HD12	1.82	0.62
3:B:3630:ARG:HD3	2:K:82:LEU:HD12	1.82	0.62
3:B:4009:ASP:OD1	3:B:4010:SER:N	2.33	0.62
3:C:308:ALA:HB1	3:C:313:THR:HG21	1.81	0.62
3:C:914:LEU:HD12	3:C:915:PRO:HD2	1.82	0.62
2:N:6:GLU:HA	2:N:9:MET:HE2	1.82	0.62
2:J:42:LEU:HD23	2:J:46:LEU:HB2	1.82	0.62
3:D:2627:LEU:HD12	3:D:2641:PRO:HB3	1.81	0.62
3:A:249:GLU:HB2	3:A:253:VAL:HG11	1.82	0.62
3:A:2627:LEU:HD12	3:A:2641:PRO:HB3	1.81	0.62
3:B:1427:ILE:O	3:B:1431:THR:OG1	2.17	0.62
3:C:1442:ALA:N	3:C:1514:ASP:OD1	2.32	0.62
3:C:2209:MET:O	3:C:2213:VAL:HG13	1.99	0.62
3:C:4009:ASP:OD1	3:C:4010:SER:N	2.33	0.62
3:D:308:ALA:HB1	3:D:313:THR:HG21	1.81	0.61
3:D:914:LEU:HD12	3:D:915:PRO:HD2	1.82	0.61
3:A:865:PRO:HD2	3:A:868:LEU:HD12	1.82	0.61
3:B:925:MET:HE1	7:B:8005:ATP:O4'	2.00	0.61
3:C:804:LEU:HD23	3:C:805:PRO:O	1.99	0.61
3:C:925:MET:HE1	7:C:5106:ATP:O4'	2.00	0.61
2:J:37:LEU:O	2:J:40:THR:OG1	2.11	0.61
3:D:4862:ASN:HB2	3:D:4872:MET:HE1	1.82	0.61
3:C:2297:GLU:OE1	3:C:2357:LEU:HD22	2.00	0.61
3:C:2627:LEU:HD12	3:C:2641:PRO:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:GLU:HA	2:P:9:MET:HE2	1.82	0.61
3:D:2749:PRO:HD2	3:D:2752:LEU:HD12	1.82	0.61
3:D:3630:ARG:HD3	2:O:82:LEU:HD12	1.82	0.61
3:D:3954:PHE:CD2	3:D:4015:LEU:HD21	2.34	0.61
3:A:4818:VAL:HG11	3:B:4837:MET:HE2	1.81	0.61
3:B:2627:LEU:HD12	3:B:2641:PRO:HB3	1.81	0.61
3:B:3954:PHE:CD2	3:B:4015:LEU:HD21	2.34	0.61
3:C:2749:PRO:HD2	3:C:2752:LEU:HD12	1.82	0.61
3:A:2749:PRO:HD2	3:A:2752:LEU:HD12	1.82	0.61
2:P:42:LEU:HD23	2:P:46:LEU:HB2	1.82	0.61
3:B:2539:THR:O	3:B:2543:SER:OG	2.10	0.61
3:D:4900:GLU:O	3:D:4911:ARG:NH1	2.32	0.61
3:A:3311:ASP:OD1	3:A:3312:HIS:N	2.34	0.61
2:L:42:LEU:HD23	2:L:46:LEU:HB2	1.82	0.61
3:D:249:GLU:HB2	3:D:253:VAL:HG11	1.82	0.61
3:D:258:ARG:O	3:D:285:HIS:NE2	2.33	0.61
3:A:258:ARG:O	3:A:285:HIS:NE2	2.33	0.61
3:A:405:ILE:HG21	3:A:482:GLU:HG2	1.83	0.61
3:A:3431:ASN:OD1	3:A:3432:ALA:N	2.32	0.61
3:A:4221:ILE:HD13	3:A:4952:MET:HE2	1.82	0.61
3:B:3770:GLN:OE1	3:B:3812:ASN:ND2	2.32	0.61
3:C:921:TYR:CE2	3:C:925:MET:HE3	2.35	0.61
2:M:88:ASN:O	2:M:92:GLU:HG2	2.01	0.61
3:C:865:PRO:HD2	3:C:868:LEU:HD12	1.82	0.61
3:C:3630:ARG:HD3	2:M:82:LEU:HD12	1.82	0.61
3:A:914:LEU:O	3:A:919:ARG:NE	2.34	0.61
2:I:88:ASN:O	2:I:92:GLU:HG2	2.01	0.61
3:D:2179:MET:HE3	3:D:2183:ILE:HG13	1.83	0.61
3:B:282:ARG:NH1	3:B:313:THR:OG1	2.34	0.61
3:B:405:ILE:HG21	3:B:482:GLU:HG2	1.83	0.61
3:B:921:TYR:CE2	3:B:925:MET:HE3	2.35	0.61
3:C:282:ARG:NH1	3:C:313:THR:OG1	2.34	0.61
3:C:405:ILE:HG21	3:C:482:GLU:HG2	1.83	0.61
3:C:3311:ASP:OD1	3:C:3312:HIS:N	2.34	0.61
2:L:37:LEU:O	2:L:40:THR:OG1	2.11	0.61
3:D:925:MET:HE1	7:D:8005:ATP:O4'	2.00	0.60
3:D:2005:GLU:N	3:D:2005:GLU:OE1	2.34	0.60
3:A:282:ARG:NH1	3:A:313:THR:OG1	2.34	0.60
3:A:318:ARG:NH1	3:A:350:GLN:OE1	2.34	0.60
3:A:926:SER:O	3:A:929:THR:OG1	2.19	0.60
3:A:4900:GLU:O	3:A:4911:ARG:NH1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3311:ASP:OD1	3:B:3312:HIS:N	2.34	0.60
3:B:4900:GLU:O	3:B:4911:ARG:NH1	2.32	0.60
3:C:4900:GLU:O	3:C:4911:ARG:NH1	2.32	0.60
3:D:3311:ASP:OD1	3:D:3312:HIS:N	2.34	0.60
3:B:804:LEU:HD23	3:B:805:PRO:O	1.99	0.60
3:B:4221:ILE:HD13	3:B:4952:MET:HE2	1.82	0.60
3:C:4862:ASN:HB2	3:C:4872:MET:HE1	1.82	0.60
3:A:308:ALA:HB1	3:A:313:THR:HG21	1.81	0.60
3:B:258:ARG:O	3:B:285:HIS:NE2	2.33	0.60
3:B:914:LEU:O	3:B:919:ARG:NE	2.34	0.60
3:C:318:ARG:NH1	3:C:350:GLN:OE1	2.34	0.60
3:C:914:LEU:O	3:C:919:ARG:NE	2.34	0.60
3:C:2005:GLU:OE1	3:C:2005:GLU:N	2.34	0.60
3:A:2005:GLU:N	3:A:2005:GLU:OE1	2.34	0.60
3:A:2179:MET:HE3	3:A:2183:ILE:HG13	1.83	0.60
3:A:2394:ASP:OD1	3:A:2395:GLY:N	2.35	0.60
3:B:2394:ASP:OD1	3:B:2395:GLY:N	2.35	0.60
3:B:3660:ALA:HA	3:B:3664:LEU:HD12	1.84	0.60
3:D:282:ARG:NH1	3:D:313:THR:OG1	2.34	0.60
3:D:2297:GLU:OE1	3:D:2357:LEU:HD22	2.00	0.60
3:D:2623:LEU:O	3:D:2627:LEU:HD23	2.02	0.60
3:D:3660:ALA:HA	3:D:3664:LEU:HD12	1.84	0.60
3:B:308:ALA:HB1	3:B:313:THR:HG21	1.81	0.60
3:C:2179:MET:HE3	3:C:2183:ILE:HG13	1.83	0.60
3:C:4221:ILE:HD13	3:C:4952:MET:HE2	1.82	0.60
3:D:914:LEU:O	3:D:919:ARG:NE	2.34	0.60
3:A:2623:LEU:O	3:A:2627:LEU:HD23	2.02	0.60
3:C:249:GLU:HB2	3:C:253:VAL:HG11	1.82	0.60
3:C:1427:ILE:O	3:C:1431:THR:OG1	2.17	0.60
3:C:2623:LEU:O	3:C:2627:LEU:HD23	2.02	0.60
3:C:2879:LEU:HD21	3:C:2927:LEU:HD23	1.83	0.60
3:D:405:ILE:HG21	3:D:482:GLU:HG2	1.83	0.60
3:B:2005:GLU:OE1	3:B:2005:GLU:N	2.34	0.60
3:C:258:ARG:O	3:C:285:HIS:NE2	2.33	0.60
3:D:4221:ILE:HD13	3:D:4952:MET:HE2	1.82	0.60
3:A:3660:ALA:HA	3:A:3664:LEU:HD12	1.84	0.60
3:B:318:ARG:NH1	3:B:350:GLN:OE1	2.34	0.60
3:B:2179:MET:HE3	3:B:2183:ILE:HG13	1.83	0.60
3:C:3660:ALA:HA	3:C:3664:LEU:HD12	1.84	0.60
2:K:88:ASN:O	2:K:92:GLU:HG2	2.01	0.60
3:A:4796:MET:HE1	8:A:8007:PCW:H222	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2623:LEU:O	3:B:2627:LEU:HD23	2.02	0.60
3:B:4824:ILE:O	3:B:4827:SER:OG	2.14	0.60
3:C:2394:ASP:OD1	3:C:2395:GLY:N	2.35	0.60
2:N:42:LEU:HD23	2:N:46:LEU:HB2	1.82	0.60
3:D:926:SER:O	3:D:929:THR:OG1	2.19	0.59
3:D:2879:LEU:HD21	3:D:2927:LEU:HD23	1.83	0.59
3:D:3661:SER:HG	3:D:3662:TRP:CD1	2.20	0.59
2:O:88:ASN:O	2:O:92:GLU:HG2	2.01	0.59
3:D:318:ARG:NH1	3:D:350:GLN:OE1	2.34	0.59
3:B:4796:MET:CE	8:B:8007:PCW:H222	2.32	0.59
3:C:3220:TYR:CD1	3:C:3237:VAL:HG22	2.38	0.59
1:E:12:ASP:OD1	1:E:13:GLY:N	2.36	0.59
3:D:2394:ASP:OD1	3:D:2395:GLY:N	2.35	0.59
3:A:2570:PHE:CZ	3:A:2583:MET:HE1	2.37	0.59
3:D:3220:TYR:CD1	3:D:3237:VAL:HG22	2.38	0.59
3:B:2570:PHE:CZ	3:B:2583:MET:HE1	2.37	0.59
3:B:3347:VAL:HG21	3:B:3415:ARG:HB2	1.84	0.59
3:C:4796:MET:CE	8:C:5101:PCW:H222	2.33	0.59
3:D:3347:VAL:HG21	3:D:3415:ARG:HB2	1.84	0.59
3:C:3105:GLU:O	3:C:3109:GLU:OE1	2.21	0.59
3:C:3347:VAL:HG21	3:C:3415:ARG:HB2	1.84	0.59
3:D:4689:GLN:OE1	3:D:4701:ARG:NH2	2.36	0.59
3:B:926:SER:O	3:B:929:THR:OG1	2.19	0.59
3:C:1253:HIS:O	3:C:1276:ARG:NH1	2.36	0.59
3:D:1427:ILE:O	3:D:1431:THR:OG1	2.17	0.59
3:C:926:SER:O	3:C:929:THR:OG1	2.19	0.59
3:C:2570:PHE:CZ	3:C:2583:MET:HE1	2.37	0.59
3:C:3661:SER:HG	3:C:3662:TRP:CD1	2.20	0.59
3:A:1253:HIS:O	3:A:1276:ARG:NH1	2.36	0.59
3:B:3220:TYR:CD1	3:B:3237:VAL:HG22	2.38	0.59
3:B:4689:GLN:OE1	3:B:4701:ARG:NH2	2.36	0.59
3:C:1699:LEU:C	3:C:1816:MET:HE1	2.28	0.59
3:D:2570:PHE:CZ	3:D:2583:MET:HE1	2.37	0.59
3:B:2879:LEU:HD21	3:B:2927:LEU:HD23	1.83	0.59
3:B:3105:GLU:O	3:B:3109:GLU:OE1	2.21	0.59
2:N:84:VAL:HG21	2:M:76:VAL:HG11	1.85	0.59
3:D:1699:LEU:C	3:D:1816:MET:HE1	2.28	0.59
3:A:3220:TYR:CD1	3:A:3237:VAL:HG22	2.38	0.59
3:A:4689:GLN:OE1	3:A:4701:ARG:NH2	2.36	0.59
3:C:1618:THR:HG22	3:C:1629:VAL:HG12	1.85	0.59
3:A:1699:LEU:C	3:A:1816:MET:HE1	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3347:VAL:HG21	3:A:3415:ARG:HB2	1.84	0.58
3:B:615:VAL:HG23	3:B:618:ASN:HB2	1.85	0.58
3:A:615:VAL:HG23	3:A:618:ASN:HB2	1.85	0.58
3:C:2886:THR:HG22	3:C:2889:ARG:HH21	1.68	0.58
2:O:6:GLU:OE2	2:P:42:LEU:CD1	2.44	0.58
1:F:50:THR:N	1:F:55:GLU:OE1	2.34	0.58
3:D:2886:THR:HG22	3:D:2889:ARG:HH21	1.68	0.58
3:A:3661:SER:HG	3:A:3662:TRP:CD1	2.21	0.58
3:C:162:GLU:OE1	3:C:162:GLU:N	2.36	0.58
2:N:16:PHE:CE1	2:N:29:LEU:HD23	2.38	0.58
2:P:16:PHE:CE1	2:P:29:LEU:HD23	2.38	0.58
1:F:59:GLY:HA3	1:F:77:ILE:HD12	1.85	0.58
3:B:1253:HIS:O	3:B:1276:ARG:NH1	2.36	0.58
3:B:3406:LEU:HD11	3:B:3410:TYR:CZ	2.39	0.58
3:C:3954:PHE:HD2	3:C:4015:LEU:HD21	1.69	0.58
1:G:59:GLY:HA3	1:G:77:ILE:HD12	1.86	0.58
3:B:162:GLU:N	3:B:162:GLU:OE1	2.36	0.58
2:I:5:LEU:HD23	2:J:41:GLU:HB2	1.86	0.58
3:A:2879:LEU:HD21	3:A:2927:LEU:HD23	1.83	0.58
3:A:3406:LEU:HD11	3:A:3410:TYR:CZ	2.39	0.58
3:B:3954:PHE:HD2	3:B:4015:LEU:HD21	1.69	0.58
3:B:4185:GLU:O	3:B:4986:TYR:OH	2.20	0.58
3:B:4818:VAL:HG11	3:C:4837:MET:HE2	1.86	0.58
3:A:103:LEU:HD21	3:A:106:HIS:CE1	2.39	0.58
3:A:1618:THR:HG22	3:A:1629:VAL:HG12	1.85	0.58
3:B:1699:LEU:C	3:B:1816:MET:HE1	2.28	0.58
3:C:615:VAL:HG23	3:C:618:ASN:HB2	1.85	0.58
3:D:3105:GLU:O	3:D:3109:GLU:OE1	2.21	0.58
2:K:5:LEU:HD23	2:L:41:GLU:HB2	1.86	0.58
2:L:16:PHE:CE1	2:L:29:LEU:HD23	2.38	0.58
3:B:103:LEU:HD21	3:B:106:HIS:CE1	2.39	0.58
3:B:2886:THR:HG22	3:B:2889:ARG:HH21	1.68	0.58
3:C:2213:VAL:HG11	3:C:2257:TYR:CE2	2.35	0.58
3:C:3406:LEU:HD11	3:C:3410:TYR:CZ	2.39	0.58
3:D:103:LEU:HD23	3:D:103:LEU:H	1.69	0.58
2:O:5:LEU:HD23	2:P:41:GLU:HB2	1.86	0.58
3:D:2769:PHE:O	3:D:2772:ILE:HG22	2.04	0.57
3:D:4837:MET:HE2	3:C:4818:VAL:HG11	1.86	0.57
3:A:162:GLU:OE1	3:A:162:GLU:N	2.36	0.57
3:A:3105:GLU:O	3:A:3109:GLU:OE1	2.21	0.57
3:C:4689:GLN:OE1	3:C:4701:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:76:VAL:HG11	2:J:84:VAL:HG21	1.85	0.57
1:H:59:GLY:HA3	1:H:77:ILE:HD12	1.86	0.57
3:D:3406:LEU:HD11	3:D:3410:TYR:CZ	2.39	0.57
3:A:2886:THR:HG22	3:A:2889:ARG:HH21	1.68	0.57
3:C:3353:GLU:OE1	3:C:3353:GLU:N	2.37	0.57
2:K:76:VAL:HG11	2:L:84:VAL:HG21	1.85	0.57
2:O:76:VAL:HG11	2:P:84:VAL:HG21	1.85	0.57
2:J:29:LEU:HD13	2:J:33:GLU:HB3	1.87	0.57
3:D:162:GLU:OE1	3:D:162:GLU:N	2.36	0.57
3:D:3262:ALA:HB3	3:D:3267:MET:HE3	1.86	0.57
3:D:4675:LEU:HD23	3:D:4709:PHE:CE1	2.40	0.57
3:A:3353:GLU:OE1	3:A:3353:GLU:N	2.37	0.57
3:B:2769:PHE:O	3:B:2772:ILE:HG22	2.04	0.57
3:B:4675:LEU:HD23	3:B:4709:PHE:CE1	2.40	0.57
3:D:1253:HIS:O	3:D:1276:ARG:NH1	2.36	0.57
3:D:1618:THR:HG22	3:D:1629:VAL:HG12	1.85	0.57
3:A:1427:ILE:O	3:A:1431:THR:OG1	2.17	0.57
3:A:2769:PHE:O	3:A:2772:ILE:HG22	2.04	0.57
3:A:3262:ALA:HB3	3:A:3267:MET:HE3	1.87	0.57
3:B:2213:VAL:HG11	3:B:2257:TYR:CE2	2.35	0.57
3:B:3239:GLU:OE1	3:B:3239:GLU:N	2.38	0.57
3:B:3600:VAL:HG22	3:B:3604:LEU:HD13	1.87	0.57
3:C:3515:LEU:HD21	3:C:3603:VAL:HG13	1.87	0.57
3:D:615:VAL:HG23	3:D:618:ASN:HB2	1.85	0.57
3:A:873:GLU:O	3:A:877:GLU:OE1	2.23	0.57
3:C:4675:LEU:HD23	3:C:4709:PHE:CE1	2.40	0.57
3:C:4796:MET:HE1	8:C:5101:PCW:H222	1.87	0.57
2:J:16:PHE:CE1	2:J:29:LEU:HD23	2.38	0.57
3:D:3972:ILE:HG21	3:D:3983:LEU:HD12	1.86	0.57
3:B:1857:SER:OG	3:B:1860:ASP:OD1	2.22	0.57
3:A:4675:LEU:HD23	3:A:4709:PHE:CE1	2.40	0.57
3:C:103:LEU:HD23	3:C:103:LEU:H	1.69	0.57
3:C:103:LEU:HD21	3:C:106:HIS:CE1	2.39	0.57
3:C:3972:ILE:HG21	3:C:3983:LEU:HD12	1.86	0.57
2:N:41:GLU:HB2	2:M:5:LEU:HD23	1.86	0.57
2:P:29:LEU:HD13	2:P:33:GLU:HB3	1.87	0.57
3:A:3954:PHE:HD2	3:A:4015:LEU:HD21	1.69	0.57
3:B:4796:MET:HE1	8:B:8007:PCW:H222	1.86	0.57
3:C:3239:GLU:OE1	3:C:3239:GLU:N	2.38	0.57
1:E:59:GLY:HA3	1:E:77:ILE:HD12	1.87	0.57
3:D:103:LEU:HD21	3:D:106:HIS:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3954:PHE:HD2	3:D:4015:LEU:HD21	1.69	0.57
3:B:1618:THR:HG22	3:B:1629:VAL:HG12	1.85	0.57
3:D:3515:LEU:HD21	3:D:3603:VAL:HG13	1.87	0.57
3:A:2110:ASP:OD1	3:A:2111:PHE:N	2.38	0.57
3:A:3600:VAL:HG22	3:A:3604:LEU:HD13	1.87	0.57
3:A:3972:ILE:HG21	3:A:3983:LEU:HD12	1.86	0.57
3:C:873:GLU:O	3:C:877:GLU:OE1	2.23	0.57
2:N:29:LEU:HD13	2:N:33:GLU:HB3	1.87	0.57
3:A:103:LEU:HD23	3:A:103:LEU:H	1.69	0.56
3:A:2156:LEU:CD2	3:A:2199:MET:HE1	2.33	0.56
3:D:1857:SER:OG	3:D:1860:ASP:OD1	2.22	0.56
3:D:3239:GLU:OE1	3:D:3239:GLU:N	2.38	0.56
3:A:4741:MET:CE	3:A:4746:LEU:HD11	2.35	0.56
3:B:42:GLY:O	3:B:117:MET:HE1	2.05	0.56
3:B:3515:LEU:HD21	3:B:3603:VAL:HG13	1.87	0.56
3:C:2156:LEU:CD2	3:C:2199:MET:HE1	2.33	0.56
3:C:2769:PHE:O	3:C:2772:ILE:HG22	2.04	0.56
3:D:42:GLY:O	3:D:117:MET:HE1	2.05	0.56
3:D:3353:GLU:OE1	3:D:3353:GLU:N	2.37	0.56
3:D:4741:MET:CE	3:D:4746:LEU:HD11	2.35	0.56
3:A:42:GLY:O	3:A:117:MET:HE1	2.05	0.56
3:A:3239:GLU:OE1	3:A:3239:GLU:N	2.38	0.56
3:B:552:LEU:HD22	3:B:590:LEU:HD11	1.87	0.56
3:B:2516:GLN:OE1	3:B:2573:THR:HG22	2.06	0.56
3:B:3262:ALA:HB3	3:B:3267:MET:HE3	1.86	0.56
3:B:3353:GLU:N	3:B:3353:GLU:OE1	2.37	0.56
3:B:4709:PHE:HB3	3:B:4710:PRO:HD3	1.87	0.56
3:C:552:LEU:HD22	3:C:590:LEU:HD11	1.87	0.56
3:C:2260:GLU:OE2	3:C:2298:LYS:NZ	2.22	0.56
3:C:2482:LYS:O	3:C:2482:LYS:HD2	2.06	0.56
2:L:29:LEU:HD13	2:L:33:GLU:HB3	1.87	0.56
3:A:2756:ILE:HD13	3:A:2811:LYS:HG2	1.88	0.56
3:A:2921:ARG:O	3:A:2925:GLN:HG3	2.06	0.56
3:A:4824:ILE:O	3:A:4827:SER:OG	2.14	0.56
3:B:2110:ASP:OD1	3:B:2111:PHE:N	2.38	0.56
3:B:2156:LEU:CD2	3:B:2199:MET:HE1	2.33	0.56
3:B:2921:ARG:O	3:B:2925:GLN:HG3	2.06	0.56
3:C:42:GLY:O	3:C:117:MET:HE1	2.05	0.56
3:C:3262:ALA:HB3	3:C:3267:MET:HE3	1.87	0.56
3:C:3600:VAL:HG22	3:C:3604:LEU:HD13	1.87	0.56
3:D:3600:VAL:HG22	3:D:3604:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2469:GLY:O	3:A:2472:SER:OG	2.22	0.56
3:A:2482:LYS:HD2	3:A:2482:LYS:O	2.05	0.56
3:B:2756:ILE:HD13	3:B:2811:LYS:HG2	1.88	0.56
3:D:2119:ARG:NH2	3:D:3720:ASP:OD1	2.38	0.56
2:I:62:LEU:HD13	2:I:78:LEU:HD22	1.87	0.56
3:D:552:LEU:HD22	3:D:590:LEU:HD11	1.87	0.56
3:D:873:GLU:O	3:D:877:GLU:OE1	2.23	0.56
3:D:2753:ASP:HA	3:D:2756:ILE:HD12	1.88	0.56
3:D:4709:PHE:HB3	3:D:4710:PRO:HD3	1.87	0.56
3:A:2119:ARG:NH2	3:A:3720:ASP:OD1	2.38	0.56
3:B:103:LEU:HD23	3:B:103:LEU:H	1.69	0.56
3:B:2482:LYS:HD2	3:B:2482:LYS:O	2.06	0.56
2:K:62:LEU:HD13	2:K:78:LEU:HD22	1.87	0.56
3:B:1252:GLU:OE1	3:B:1252:GLU:N	2.39	0.56
3:B:4899:ILE:HG13	3:B:4911:ARG:NH2	2.20	0.56
2:L:26:LYS:HD2	2:L:27:TYR:N	2.21	0.56
2:O:13:ILE:HA	2:O:16:PHE:CE1	2.41	0.56
3:D:2213:VAL:HG11	3:D:2257:TYR:CE2	2.35	0.56
3:D:2516:GLN:OE1	3:D:2573:THR:HG22	2.06	0.56
3:A:2516:GLN:OE1	3:A:2573:THR:HG22	2.06	0.56
3:A:4185:GLU:O	3:A:4986:TYR:OH	2.20	0.56
3:C:2756:ILE:HD13	3:C:2811:LYS:HG2	1.88	0.56
3:D:1252:GLU:N	3:D:1252:GLU:OE1	2.39	0.56
3:D:2482:LYS:HD2	3:D:2482:LYS:O	2.06	0.56
3:D:4899:ILE:HG13	3:D:4911:ARG:NH2	2.20	0.56
3:C:2119:ARG:NH2	3:C:3720:ASP:OD1	2.38	0.56
3:D:2110:ASP:OD1	3:D:2111:PHE:N	2.38	0.55
3:D:2698:ARG:NH2	2:O:17:HIS:CE1	2.74	0.55
3:B:228:MET:SD	3:C:156:LYS:HG3	2.46	0.55
3:B:873:GLU:O	3:B:877:GLU:OE1	2.23	0.55
3:B:4753:GLU:N	3:B:4753:GLU:OE1	2.39	0.55
3:C:2516:GLN:OE1	3:C:2573:THR:HG22	2.06	0.55
3:C:3050:LEU:O	3:C:3054:ARG:NH1	2.40	0.55
2:L:35:LYS:O	2:L:39:GLN:OE1	2.24	0.55
2:N:35:LYS:O	2:N:39:GLN:OE1	2.24	0.55
2:P:26:LYS:HD2	2:P:27:TYR:N	2.21	0.55
3:A:964:ASN:OD1	3:A:965:GLY:N	2.39	0.55
3:A:4899:ILE:HG13	3:A:4911:ARG:NH2	2.20	0.55
3:B:653:ARG:NH1	3:B:751:LEU:O	2.40	0.55
3:B:2119:ARG:NH2	3:B:3720:ASP:OD1	2.38	0.55
3:B:2643:LYS:HD2	3:B:2699:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3690:GLU:OE1	3:B:3690:GLU:N	2.39	0.55
3:C:653:ARG:NH1	3:C:751:LEU:O	2.40	0.55
3:C:2469:GLY:O	3:C:2472:SER:OG	2.22	0.55
3:C:2643:LYS:HD2	3:C:2699:ILE:HD12	1.88	0.55
3:C:4741:MET:CE	3:C:4746:LEU:HD11	2.35	0.55
2:I:17:HIS:CE1	3:A:2698:ARG:NH2	2.74	0.55
3:D:2156:LEU:CD2	3:D:2199:MET:HE1	2.33	0.55
3:A:2368:ALA:CB	3:A:2380:ALA:HB2	2.36	0.55
3:A:2753:ASP:HA	3:A:2756:ILE:HD12	1.88	0.55
3:B:4741:MET:CE	3:B:4746:LEU:HD11	2.35	0.55
2:K:13:ILE:HA	2:K:16:PHE:CE1	2.41	0.55
2:K:84:VAL:HG22	2:L:72:PHE:CE2	2.42	0.55
2:J:26:LYS:HD2	2:J:27:TYR:N	2.21	0.55
3:D:653:ARG:NH1	3:D:751:LEU:O	2.40	0.55
3:A:3515:LEU:HD21	3:A:3603:VAL:HG13	1.87	0.55
3:A:4709:PHE:HB3	3:A:4710:PRO:HD3	1.87	0.55
3:A:4753:GLU:OE1	3:A:4753:GLU:N	2.39	0.55
3:B:3972:ILE:HG21	3:B:3983:LEU:HD12	1.86	0.55
3:C:964:ASN:OD1	3:C:965:GLY:N	2.39	0.55
3:C:1237:THR:OG1	3:C:1609:MET:SD	2.61	0.55
2:N:26:LYS:HD2	2:N:27:TYR:N	2.21	0.55
2:M:62:LEU:HD13	2:M:78:LEU:HD22	1.87	0.55
3:D:2368:ALA:CB	3:D:2380:ALA:HB2	2.37	0.55
3:A:1252:GLU:N	3:A:1252:GLU:OE1	2.39	0.55
3:A:3050:LEU:O	3:A:3054:ARG:NH1	2.40	0.55
3:B:2701:MET:HE3	3:B:2702:PRO:CD	2.37	0.55
3:C:1488:LEU:HD22	3:C:1544:GLU:OE2	2.07	0.55
3:C:2110:ASP:OD1	3:C:2111:PHE:N	2.38	0.55
3:C:2753:ASP:HA	3:C:2756:ILE:HD12	1.88	0.55
3:C:2921:ARG:O	3:C:2925:GLN:HG3	2.06	0.55
3:C:4899:ILE:HG13	3:C:4911:ARG:NH2	2.20	0.55
2:P:35:LYS:O	2:P:39:GLN:OE1	2.24	0.55
3:D:2921:ARG:O	3:D:2925:GLN:HG3	2.06	0.55
3:A:65:ILE:O	3:A:112:HIS:NE2	2.39	0.55
3:B:3167:TYR:OH	3:B:3204:VAL:HG11	2.07	0.55
3:C:163:LYS:O	3:C:165:ARG:NH1	2.38	0.55
3:C:1189:PHE:C	3:C:1190:LEU:HD12	2.32	0.55
3:C:4753:GLU:OE1	3:C:4753:GLU:N	2.39	0.55
2:K:78:LEU:O	2:K:82:LEU:HD23	2.07	0.55
2:N:12:LEU:HD21	2:N:76:VAL:HG12	1.89	0.55
3:D:2701:MET:HE3	3:D:2702:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2756:ILE:HD13	3:D:2811:LYS:HG2	1.88	0.55
3:B:1237:THR:OG1	3:B:1609:MET:SD	2.61	0.55
3:B:2469:GLY:O	3:B:2472:SER:OG	2.22	0.55
3:C:2378:LEU:O	3:C:2382:GLU:OE1	2.25	0.55
2:L:34:LEU:O	2:L:38:LEU:HD13	2.07	0.55
2:N:72:PHE:CE2	2:M:84:VAL:HG22	2.42	0.55
2:O:62:LEU:HD13	2:O:78:LEU:HD22	1.87	0.55
2:P:34:LEU:O	2:P:38:LEU:HD13	2.07	0.55
2:I:84:VAL:HG22	2:J:72:PHE:CE2	2.42	0.55
3:D:1488:LEU:HD22	3:D:1544:GLU:OE2	2.07	0.55
3:D:4753:GLU:OE1	3:D:4753:GLU:N	2.39	0.55
3:A:552:LEU:HD22	3:A:590:LEU:HD11	1.87	0.55
3:A:652:GLY:N	3:A:659:GLN:OE1	2.39	0.55
3:A:653:ARG:NH1	3:A:751:LEU:O	2.40	0.55
3:A:1189:PHE:C	3:A:1190:LEU:HD12	2.32	0.55
3:B:964:ASN:OD1	3:B:965:GLY:N	2.39	0.55
3:B:1488:LEU:HD22	3:B:1544:GLU:OE2	2.07	0.55
3:C:4709:PHE:HB3	3:C:4710:PRO:HD3	1.87	0.55
2:O:78:LEU:O	2:O:82:LEU:HD23	2.07	0.55
2:P:12:LEU:HD21	2:P:76:VAL:HG12	1.89	0.55
2:I:10:GLU:CD	3:A:2694:GLN:NE2	2.63	0.55
2:I:13:ILE:HA	2:I:16:PHE:CE1	2.41	0.55
2:J:12:LEU:HD21	2:J:76:VAL:HG12	1.89	0.55
2:J:35:LYS:O	2:J:39:GLN:OE1	2.24	0.55
3:D:2378:LEU:O	3:D:2382:GLU:OE1	2.25	0.55
3:D:2643:LYS:HD2	3:D:2699:ILE:HD12	1.88	0.55
2:M:78:LEU:O	2:M:82:LEU:HD23	2.07	0.55
2:I:12:LEU:O	2:I:16:PHE:CD1	2.60	0.55
3:D:981:ALA:O	3:D:984:THR:OG1	2.25	0.55
3:D:1237:THR:OG1	3:D:1609:MET:SD	2.61	0.55
3:D:2971:SER:HA	3:D:2974:PHE:CE1	2.42	0.55
3:B:2368:ALA:CB	3:B:2380:ALA:HB2	2.37	0.55
3:B:2753:ASP:HA	3:B:2756:ILE:HD12	1.88	0.55
3:D:3167:TYR:OH	3:D:3204:VAL:HG11	2.07	0.54
3:A:3690:GLU:OE1	3:A:3690:GLU:N	2.39	0.54
3:B:1189:PHE:C	3:B:1190:LEU:HD12	2.32	0.54
3:B:2378:LEU:O	3:B:2382:GLU:OE1	2.25	0.54
3:C:2698:ARG:NH2	2:M:17:HIS:CE1	2.74	0.54
3:C:3167:TYR:OH	3:C:3204:VAL:HG11	2.07	0.54
2:M:12:LEU:O	2:M:16:PHE:CD1	2.61	0.54
2:O:84:VAL:HG22	2:P:72:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1189:PHE:C	3:D:1190:LEU:HD12	2.32	0.54
3:A:2213:VAL:HG11	3:A:2257:TYR:CE2	2.35	0.54
3:C:1252:GLU:OE1	3:C:1252:GLU:N	2.39	0.54
3:C:1857:SER:OG	3:C:1860:ASP:OD1	2.22	0.54
2:N:34:LEU:O	2:N:38:LEU:HD13	2.07	0.54
2:O:19:HIS:HB2	2:O:37:LEU:HD12	1.89	0.54
3:D:964:ASN:OD1	3:D:965:GLY:N	2.39	0.54
3:D:3447:SER:O	3:D:3453:LYS:NZ	2.38	0.54
3:A:2643:LYS:HD2	3:A:2699:ILE:HD12	1.88	0.54
3:B:981:ALA:O	3:B:984:THR:OG1	2.25	0.54
3:B:3050:LEU:O	3:B:3054:ARG:NH1	2.40	0.54
3:C:2701:MET:HE3	3:C:2702:PRO:CD	2.37	0.54
2:K:12:LEU:O	2:K:16:PHE:CD1	2.61	0.54
2:L:12:LEU:HD21	2:L:76:VAL:HG12	1.89	0.54
2:M:13:ILE:HA	2:M:16:PHE:CE1	2.41	0.54
1:H:7:THR:HG23	1:H:7:THR:O	2.07	0.54
3:D:2999:PHE:HA	3:D:3003:LEU:HD12	1.89	0.54
3:D:3690:GLU:OE1	3:D:3690:GLU:N	2.39	0.54
3:D:4185:GLU:O	3:D:4986:TYR:OH	2.20	0.54
3:A:1435:TYR:HB2	3:A:1519:CYS:O	2.08	0.54
3:A:1488:LEU:HD22	3:A:1544:GLU:OE2	2.07	0.54
3:C:652:GLY:N	3:C:659:GLN:OE1	2.39	0.54
3:C:682:HIS:H	3:C:785:SER:HG	1.56	0.54
3:C:2368:ALA:CB	3:C:2380:ALA:HB2	2.37	0.54
2:I:78:LEU:O	2:I:82:LEU:HD23	2.07	0.54
2:J:34:LEU:O	2:J:38:LEU:HD13	2.07	0.54
3:D:3771:SER:HA	3:D:3774:HIS:CE1	2.43	0.54
3:A:2907:VAL:HG22	3:A:2908:PRO:HD2	1.89	0.54
3:A:3771:SER:HA	3:A:3774:HIS:CE1	2.43	0.54
3:B:3868:VAL:HG23	3:B:3870:ASN:H	1.73	0.54
3:C:3690:GLU:OE1	3:C:3690:GLU:N	2.39	0.54
2:M:19:HIS:HB2	2:M:37:LEU:HD12	1.90	0.54
3:A:2999:PHE:HA	3:A:3003:LEU:HD12	1.89	0.54
3:A:3253:GLU:O	3:A:3257:LEU:HD12	2.08	0.54
3:B:2698:ARG:NH2	2:K:17:HIS:CE1	2.74	0.54
3:B:2999:PHE:HA	3:B:3003:LEU:HD12	1.89	0.54
3:B:3771:SER:HA	3:B:3774:HIS:CE1	2.43	0.54
3:B:5032:ASP:OD2	3:B:5033:GLN:N	2.41	0.54
3:C:3262:ALA:HB3	3:C:3267:MET:CE	2.38	0.54
3:D:5032:ASP:OD2	3:D:5033:GLN:N	2.41	0.54
3:A:2701:MET:HE3	3:A:2702:PRO:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:65:ILE:O	3:B:112:HIS:NE2	2.39	0.54
3:C:623:THR:HG23	3:C:627:LEU:HD12	1.90	0.54
3:C:2907:VAL:HG22	3:C:2908:PRO:HD2	1.89	0.54
3:C:2971:SER:HA	3:C:2974:PHE:CE1	2.42	0.54
3:C:2999:PHE:HA	3:C:3003:LEU:HD12	1.89	0.54
3:D:623:THR:HG23	3:D:627:LEU:HD12	1.90	0.54
3:A:2378:LEU:O	3:A:2382:GLU:OE1	2.25	0.54
3:A:3167:TYR:OH	3:A:3204:VAL:HG11	2.07	0.54
2:O:12:LEU:O	2:O:16:PHE:CD1	2.60	0.54
3:D:3050:LEU:O	3:D:3054:ARG:NH1	2.40	0.54
3:B:1435:TYR:HB2	3:B:1519:CYS:O	2.08	0.54
3:C:1435:TYR:HB2	3:C:1519:CYS:O	2.08	0.54
3:C:5032:ASP:OD2	3:C:5033:GLN:N	2.41	0.54
2:I:19:HIS:HB2	2:I:37:LEU:HD12	1.89	0.54
3:A:2971:SER:HA	3:A:2974:PHE:CE1	2.42	0.54
3:B:446:LEU:HD23	3:B:526:LEU:HD22	1.90	0.54
3:B:1025:TYR:CD1	3:B:1028:LEU:HD12	2.43	0.54
3:B:2348:GLU:OE2	3:B:2352:ASN:ND2	2.41	0.54
3:C:976:VAL:O	3:C:977:ARG:NE	2.41	0.54
3:D:1435:TYR:HB2	3:D:1519:CYS:O	2.08	0.53
3:D:2907:VAL:HG22	3:D:2908:PRO:HD2	1.89	0.53
3:D:3065:VAL:O	3:D:3069:LEU:HD23	2.08	0.53
3:A:976:VAL:O	3:A:977:ARG:NE	2.41	0.53
3:A:994:HIS:CD2	3:A:1028:LEU:HD11	2.43	0.53
3:B:2907:VAL:HG22	3:B:2908:PRO:HD2	1.89	0.53
3:C:3868:VAL:HG23	3:C:3870:ASN:H	1.73	0.53
2:I:28:LYS:NZ	2:I:71:ASP:OD1	2.42	0.53
3:D:156:LYS:HG3	3:C:228:MET:SD	2.46	0.53
3:D:923:LEU:O	3:D:926:SER:OG	2.23	0.53
3:A:5032:ASP:OD2	3:A:5033:GLN:N	2.41	0.53
3:B:976:VAL:O	3:B:977:ARG:NE	2.41	0.53
3:B:3262:ALA:HB3	3:B:3267:MET:CE	2.38	0.53
3:B:3785:MET:HA	3:B:3785:MET:HE3	1.90	0.53
3:C:3065:VAL:O	3:C:3069:LEU:HD23	2.08	0.53
3:D:994:HIS:CD2	3:D:1028:LEU:HD11	2.43	0.53
3:A:2925:GLN:OE1	3:A:2929:LYS:HE2	2.08	0.53
3:B:2971:SER:HA	3:B:2974:PHE:CE1	2.42	0.53
3:B:3253:GLU:O	3:B:3257:LEU:HD12	2.08	0.53
3:D:3262:ALA:HB3	3:D:3267:MET:CE	2.38	0.53
3:A:1025:TYR:CD1	3:A:1028:LEU:HD12	2.43	0.53
3:B:994:HIS:CD2	3:B:1028:LEU:HD11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2925:GLN:OE1	3:B:2929:LYS:HE2	2.08	0.53
3:C:994:HIS:CD2	3:C:1028:LEU:HD11	2.43	0.53
3:C:3055:VAL:HG21	3:C:3135:VAL:HG11	1.90	0.53
2:J:16:PHE:HE1	2:J:29:LEU:HD23	1.74	0.53
3:D:2925:GLN:OE1	3:D:2929:LYS:HE2	2.08	0.53
3:C:1025:TYR:CD1	3:C:1028:LEU:HD12	2.43	0.53
2:L:16:PHE:HE1	2:L:29:LEU:HD23	1.74	0.53
3:D:3868:VAL:HG23	3:D:3870:ASN:H	1.73	0.53
3:A:3065:VAL:O	3:A:3069:LEU:HD23	2.08	0.53
3:B:163:LYS:O	3:B:165:ARG:NH1	2.38	0.53
3:C:3785:MET:HA	3:C:3785:MET:HE3	1.90	0.53
3:D:1558:THR:HG22	3:D:1558:THR:O	2.09	0.53
3:D:3055:VAL:HG21	3:D:3135:VAL:HG11	1.90	0.53
3:D:4883:PHE:CE1	3:D:4887:VAL:HG21	2.44	0.53
3:A:4225:VAL:HG11	3:A:4948:VAL:HA	1.91	0.53
3:B:2594:ARG:O	3:B:2595:SER:OG	2.25	0.53
2:P:16:PHE:HE1	2:P:29:LEU:HD23	1.74	0.53
3:D:976:VAL:O	3:D:977:ARG:NE	2.41	0.53
3:D:1025:TYR:CD1	3:D:1028:LEU:HD12	2.43	0.53
3:D:4741:MET:HE2	3:D:4746:LEU:HD11	1.91	0.53
3:A:3868:VAL:HG23	3:A:3870:ASN:H	1.73	0.53
3:B:3065:VAL:O	3:B:3069:LEU:HD23	2.08	0.53
3:B:4741:MET:HE2	3:B:4746:LEU:HD11	1.91	0.53
3:C:496:ASN:OD1	3:C:554:ARG:NE	2.42	0.53
3:C:3253:GLU:O	3:C:3257:LEU:HD12	2.08	0.53
3:C:4883:PHE:CE1	3:C:4887:VAL:HG21	2.44	0.53
3:A:4741:MET:HE2	3:A:4746:LEU:HD11	1.91	0.53
3:A:4883:PHE:CE1	3:A:4887:VAL:HG21	2.44	0.53
3:C:1558:THR:O	3:C:1558:THR:HG22	2.09	0.53
3:C:3771:SER:HA	3:C:3774:HIS:CE1	2.43	0.53
3:C:4741:MET:HE2	3:C:4746:LEU:HD11	1.91	0.53
2:N:16:PHE:HE1	2:N:29:LEU:HD23	1.74	0.53
3:B:3763:LYS:O	3:B:3767:LEU:HD13	2.09	0.53
3:C:1083:ALA:HB2	3:C:1190:LEU:HD11	1.91	0.53
3:D:3943:LYS:O	3:D:4005:LYS:NZ	2.34	0.52
3:A:623:THR:HG23	3:A:627:LEU:HD12	1.90	0.52
3:A:1758:GLY:N	3:A:1759:PRO:CD	2.72	0.52
3:A:3079:ARG:NE	3:A:3156:ASP:OD2	2.36	0.52
3:A:3142:THR:HG23	3:A:3197:ARG:HG3	1.92	0.52
3:A:3262:ALA:HB3	3:A:3267:MET:CE	2.38	0.52
3:B:623:THR:HG23	3:B:627:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4090:LEU:HB3	3:B:4125:MET:HE3	1.92	0.52
3:B:4883:PHE:CE1	3:B:4887:VAL:HG21	2.44	0.52
3:C:2925:GLN:OE1	3:C:2929:LYS:HE2	2.08	0.52
3:C:3763:LYS:O	3:C:3767:LEU:HD13	2.09	0.52
2:K:19:HIS:HB2	2:K:37:LEU:HD12	1.90	0.52
2:P:36:ASP:O	2:P:40:THR:HG23	2.09	0.52
3:D:65:ILE:O	3:D:112:HIS:NE2	2.39	0.52
3:A:446:LEU:HD23	3:A:526:LEU:HD22	1.90	0.52
3:A:3055:VAL:HG21	3:A:3135:VAL:HG11	1.90	0.52
3:B:1758:GLY:N	3:B:1759:PRO:CD	2.72	0.52
3:B:2910:ASP:OD1	3:B:2911:THR:N	2.43	0.52
3:B:3055:VAL:HG21	3:B:3135:VAL:HG11	1.90	0.52
3:C:65:ILE:O	3:C:112:HIS:NE2	2.39	0.52
3:C:546:ASP:OD1	3:C:583:HIS:NE2	2.39	0.52
2:O:28:LYS:NZ	2:O:71:ASP:OD1	2.42	0.52
3:D:1083:ALA:HB2	3:D:1190:LEU:HD11	1.91	0.52
3:D:3142:THR:HG23	3:D:3197:ARG:HG3	1.91	0.52
3:D:3785:MET:HA	3:D:3785:MET:HE3	1.90	0.52
3:A:3763:LYS:O	3:A:3767:LEU:HD13	2.09	0.52
3:A:4090:LEU:HB3	3:A:4125:MET:HE3	1.92	0.52
3:A:4745:SER:O	3:A:4749:THR:HG23	2.10	0.52
3:B:3142:THR:HG23	3:B:3197:ARG:HG3	1.91	0.52
1:E:80:ASP:OD2	1:E:81:TYR:N	2.43	0.52
3:D:2348:GLU:OE2	3:D:2352:ASN:ND2	2.41	0.52
3:D:3253:GLU:O	3:D:3257:LEU:HD12	2.08	0.52
3:C:3142:THR:HG23	3:C:3197:ARG:HG3	1.91	0.52
2:L:36:ASP:O	2:L:40:THR:HG23	2.09	0.52
1:G:7:THR:O	1:G:7:THR:HG23	2.09	0.52
3:D:1758:GLY:N	3:D:1759:PRO:CD	2.72	0.52
3:D:3763:LYS:O	3:D:3767:LEU:HD13	2.09	0.52
3:D:4090:LEU:HB3	3:D:4125:MET:HE3	1.92	0.52
3:B:1558:THR:HG22	3:B:1558:THR:O	2.09	0.52
3:C:545:LEU:HD21	3:C:579:ILE:HD13	1.91	0.52
3:C:1758:GLY:N	3:C:1759:PRO:CD	2.72	0.52
3:C:2910:ASP:OD1	3:C:2911:THR:N	2.43	0.52
3:C:3661:SER:HG	3:C:3662:TRP:HD1	1.56	0.52
3:D:446:LEU:HD23	3:D:526:LEU:HD22	1.90	0.52
3:D:2910:ASP:OD1	3:D:2911:THR:N	2.43	0.52
3:D:3717:LEU:HD11	3:D:3785:MET:HE1	1.92	0.52
3:A:2577:ALA:CB	3:A:2619:MET:HE1	2.40	0.52
3:B:4225:VAL:HG11	3:B:4948:VAL:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4745:SER:O	3:B:4749:THR:HG23	2.10	0.52
3:D:1793:ALA:O	3:D:1794:THR:OG1	2.23	0.52
3:D:3972:ILE:CG2	3:D:3983:LEU:HD12	2.40	0.52
2:K:28:LYS:NZ	2:K:71:ASP:OD1	2.42	0.52
3:D:2179:MET:HE3	3:D:2183:ILE:CG1	2.40	0.52
3:A:875:LEU:HD11	3:A:1047:LEU:CD2	2.29	0.52
3:A:3785:MET:HA	3:A:3785:MET:HE3	1.90	0.52
3:C:2694:GLN:NE2	2:M:10:GLU:CD	2.63	0.52
3:D:3576:LEU:HD21	3:A:1220:LEU:HD22	1.92	0.52
3:A:545:LEU:HD21	3:A:579:ILE:HD13	1.91	0.52
3:A:3717:LEU:HD11	3:A:3785:MET:HE1	1.92	0.52
3:C:4090:LEU:HB3	3:C:4125:MET:HE3	1.92	0.52
3:D:496:ASN:OD1	3:D:554:ARG:NE	2.42	0.52
3:D:985:LEU:O	3:D:989:LEU:HG	2.10	0.52
3:A:2179:MET:HE3	3:A:2183:ILE:CG1	2.40	0.52
3:A:3661:SER:HG	3:A:3662:TRP:HD1	1.58	0.52
3:C:1927:LEU:HD13	3:C:1940:MET:HE1	1.92	0.52
3:C:1985:PHE:CZ	2:M:92:GLU:OE2	2.63	0.52
2:M:28:LYS:NZ	2:M:71:ASP:OD1	2.42	0.52
2:P:16:PHE:CG	2:P:75:TYR:OH	2.60	0.52
3:D:228:MET:SD	3:A:156:LYS:HG3	2.50	0.51
3:D:979:THR:O	3:D:983:THR:HG23	2.11	0.51
3:D:2469:GLY:O	3:D:2472:SER:OG	2.22	0.51
3:B:496:ASN:OD1	3:B:554:ARG:NE	2.42	0.51
3:B:1083:ALA:HB2	3:B:1190:LEU:HD11	1.91	0.51
3:B:2577:ALA:CB	3:B:2619:MET:HE1	2.40	0.51
3:C:3447:SER:O	3:C:3453:LYS:NZ	2.38	0.51
3:C:3972:ILE:CG2	3:C:3983:LEU:HD12	2.40	0.51
3:D:2577:ALA:CB	3:D:2619:MET:HE1	2.40	0.51
2:N:36:ASP:O	2:N:40:THR:HG23	2.09	0.51
3:A:496:ASN:OD1	3:A:554:ARG:NE	2.42	0.51
3:B:1562:VAL:HG12	3:B:1563:VAL:HG13	1.93	0.51
3:C:981:ALA:O	3:C:984:THR:OG1	2.25	0.51
3:C:985:LEU:O	3:C:989:LEU:HG	2.10	0.51
3:C:1562:VAL:HG12	3:C:1563:VAL:HG13	1.93	0.51
3:D:545:LEU:HD21	3:D:579:ILE:HD13	1.91	0.51
3:D:1737:VAL:HG11	3:D:1960:ALA:CB	2.40	0.51
3:D:2824:VAL:HG12	3:D:2938:VAL:HB	1.92	0.51
3:D:4745:SER:O	3:D:4749:THR:HG23	2.10	0.51
3:A:979:THR:O	3:A:983:THR:HG23	2.11	0.51
3:A:985:LEU:O	3:A:989:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2910:ASP:OD1	3:A:2911:THR:N	2.43	0.51
3:A:3220:TYR:CE1	3:A:3237:VAL:HG22	2.46	0.51
3:A:3837:ALA:O	3:A:3841:THR:HG23	2.11	0.51
3:B:545:LEU:HD21	3:B:579:ILE:HD13	1.91	0.51
3:B:2156:LEU:HD21	3:B:2199:MET:CE	2.40	0.51
3:C:4225:VAL:HG11	3:C:4948:VAL:HA	1.91	0.51
3:D:3079:ARG:NE	3:D:3156:ASP:OD2	2.36	0.51
3:D:3661:SER:HG	3:D:3662:TRP:HD1	1.56	0.51
3:A:1737:VAL:HG11	3:A:1960:ALA:CB	2.40	0.51
3:A:3374:VAL:O	3:A:3378:GLU:OE1	2.29	0.51
3:A:4675:LEU:HD23	3:A:4709:PHE:HE1	1.76	0.51
3:B:546:ASP:OD1	3:B:583:HIS:NE2	2.39	0.51
3:B:3861:MET:HB2	3:B:3868:VAL:HG21	1.93	0.51
3:C:446:LEU:HD23	3:C:526:LEU:HD22	1.90	0.51
3:C:979:THR:O	3:C:983:THR:HG23	2.11	0.51
2:I:92:GLU:OE2	3:A:1985:PHE:CZ	2.63	0.51
3:D:1927:LEU:HD13	3:D:1940:MET:HE1	1.92	0.51
3:D:4225:VAL:HG11	3:D:4948:VAL:HA	1.91	0.51
3:D:4675:LEU:HD23	3:D:4709:PHE:HE1	1.76	0.51
3:A:2177:ASN:O	3:A:2181:GLN:OE1	2.29	0.51
3:C:2177:ASN:O	3:C:2181:GLN:OE1	2.29	0.51
3:C:2179:MET:HE3	3:C:2183:ILE:CG1	2.40	0.51
3:C:2577:ALA:CB	3:C:2619:MET:HE1	2.40	0.51
3:D:3374:VAL:O	3:D:3378:GLU:OE1	2.29	0.51
3:D:3837:ALA:O	3:D:3841:THR:HG23	2.11	0.51
3:A:1083:ALA:HB2	3:A:1190:LEU:HD11	1.91	0.51
3:B:1737:VAL:HG11	3:B:1960:ALA:CB	2.40	0.51
3:B:1927:LEU:HD13	3:B:1940:MET:HE1	1.92	0.51
3:B:2103:VAL:HG13	3:B:2121:MET:HB2	1.93	0.51
3:B:3227:GLU:O	3:B:3228:ARG:HG2	2.11	0.51
3:A:1562:VAL:HG12	3:A:1563:VAL:HG13	1.93	0.51
3:B:3276:PRO:HA	3:B:3279:CYS:SG	2.51	0.51
3:C:2348:GLU:OE2	3:C:2352:ASN:ND2	2.41	0.51
3:C:4745:SER:O	3:C:4749:THR:HG23	2.10	0.51
2:L:16:PHE:CG	2:L:75:TYR:OH	2.60	0.51
2:M:62:LEU:HD13	2:M:78:LEU:CD2	2.41	0.51
2:O:76:VAL:HG21	2:P:84:VAL:HG21	1.93	0.51
2:J:36:ASP:O	2:J:40:THR:HG23	2.09	0.51
3:A:3227:GLU:O	3:A:3228:ARG:HG2	2.11	0.51
3:A:3276:PRO:HA	3:A:3279:CYS:SG	2.51	0.51
3:A:3861:MET:HB2	3:A:3868:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:872:ARG:HE	3:B:927:GLY:HA3	1.76	0.51
3:B:985:LEU:O	3:B:989:LEU:HG	2.10	0.51
3:B:1985:PHE:CZ	2:K:92:GLU:OE2	2.63	0.51
3:D:3227:GLU:O	3:D:3228:ARG:HG2	2.11	0.51
3:B:2179:MET:HE3	3:B:2183:ILE:CG1	2.40	0.51
3:B:3972:ILE:CG2	3:B:3983:LEU:HD12	2.40	0.51
3:C:2103:VAL:HG13	3:C:2121:MET:HB2	1.93	0.51
3:C:2824:VAL:HG12	3:C:2938:VAL:HB	1.92	0.51
3:C:3717:LEU:HD11	3:C:3785:MET:HE1	1.92	0.51
2:I:76:VAL:HG21	2:J:84:VAL:HG21	1.93	0.50
1:G:80:ASP:OD2	1:G:81:TYR:N	2.44	0.50
3:A:228:MET:SD	3:B:156:LYS:HG3	2.49	0.50
3:A:981:ALA:O	3:A:984:THR:OG1	2.25	0.50
3:A:1558:THR:O	3:A:1558:THR:HG22	2.09	0.50
3:A:2677:ARG:NH2	3:A:2715:TYR:O	2.45	0.50
3:B:652:GLY:N	3:B:659:GLN:OE1	2.39	0.50
3:B:2677:ARG:NH2	3:B:2715:TYR:O	2.45	0.50
3:B:3220:TYR:CE1	3:B:3237:VAL:HG22	2.46	0.50
3:B:3837:ALA:O	3:B:3841:THR:HG23	2.11	0.50
3:C:872:ARG:HE	3:C:927:GLY:HA3	1.76	0.50
3:C:1737:VAL:HG13	3:C:1737:VAL:O	2.12	0.50
3:C:2677:ARG:NH2	3:C:2715:TYR:O	2.45	0.50
2:K:62:LEU:HD13	2:K:78:LEU:CD2	2.41	0.50
2:O:62:LEU:HD13	2:O:78:LEU:CD2	2.41	0.50
1:G:50:THR:N	1:G:55:GLU:OE2	2.39	0.50
3:D:872:ARG:HE	3:D:927:GLY:HA3	1.76	0.50
3:D:1562:VAL:HG12	3:D:1563:VAL:HG13	1.93	0.50
3:D:2177:ASN:O	3:D:2181:GLN:OE1	2.29	0.50
3:D:3278:LEU:O	3:D:3282:LEU:HD23	2.11	0.50
3:A:2348:GLU:OE2	3:A:2352:ASN:ND2	2.41	0.50
3:A:3278:LEU:O	3:A:3282:LEU:HD23	2.11	0.50
3:B:3374:VAL:O	3:B:3378:GLU:OE1	2.29	0.50
3:B:3717:LEU:HD11	3:B:3785:MET:HE1	1.92	0.50
3:C:923:LEU:O	3:C:926:SER:OG	2.23	0.50
3:C:3220:TYR:CE1	3:C:3237:VAL:HG22	2.46	0.50
1:E:7:THR:HG23	1:E:7:THR:O	2.12	0.50
3:D:652:GLY:N	3:D:659:GLN:OE1	2.39	0.50
3:A:872:ARG:HE	3:A:927:GLY:HA3	1.76	0.50
3:A:1737:VAL:O	3:A:1737:VAL:HG13	2.12	0.50
3:B:2177:ASN:O	3:B:2181:GLN:OE1	2.29	0.50
3:C:3276:PRO:HA	3:C:3279:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ASP:OD2	1:H:81:TYR:N	2.44	0.50
3:A:1572:ASN:O	3:A:1573:ILE:HD13	2.12	0.50
3:A:1927:LEU:HD13	3:A:1940:MET:HE1	1.92	0.50
3:C:3227:GLU:O	3:C:3228:ARG:HG2	2.11	0.50
3:C:3278:LEU:O	3:C:3282:LEU:HD23	2.11	0.50
3:A:1857:SER:OG	3:A:1860:ASP:OD1	2.22	0.50
3:A:3972:ILE:CG2	3:A:3983:LEU:HD12	2.40	0.50
3:C:2156:LEU:HD21	3:C:2199:MET:CE	2.40	0.50
3:C:3374:VAL:O	3:C:3378:GLU:OE1	2.29	0.50
3:C:3837:ALA:O	3:C:3841:THR:HG23	2.10	0.50
3:D:1985:PHE:CZ	2:O:92:GLU:OE2	2.63	0.50
3:D:3220:TYR:CE1	3:D:3237:VAL:HG22	2.46	0.50
3:B:1572:ASN:O	3:B:1573:ILE:HD13	2.12	0.50
3:B:2824:VAL:HG12	3:B:2938:VAL:HB	1.92	0.50
3:B:3104:ILE:O	3:B:3108:VAL:HG23	2.12	0.50
3:C:1737:VAL:HG11	3:C:1960:ALA:CB	2.40	0.50
3:C:3861:MET:HB2	3:C:3868:VAL:HG21	1.93	0.50
2:I:62:LEU:HD13	2:I:78:LEU:CD2	2.41	0.50
3:D:546:ASP:OD1	3:D:583:HIS:NE2	2.39	0.50
3:D:3276:PRO:HA	3:D:3279:CYS:SG	2.51	0.50
3:D:3717:LEU:HD21	3:D:3785:MET:CE	2.42	0.50
3:B:784:PHE:CB	3:B:788:ILE:HD13	2.42	0.50
3:B:979:THR:O	3:B:983:THR:HG23	2.11	0.50
3:B:2694:GLN:NE2	2:K:10:GLU:CD	2.63	0.50
3:B:3278:LEU:O	3:B:3282:LEU:HD23	2.11	0.50
3:D:1572:ASN:O	3:D:1573:ILE:HD13	2.12	0.50
3:D:2103:VAL:HG13	3:D:2121:MET:HB2	1.93	0.50
3:D:2677:ARG:NH2	3:D:2715:TYR:O	2.45	0.50
3:D:3861:MET:HB2	3:D:3868:VAL:HG21	1.93	0.50
3:B:1007:SER:C	3:B:1022:LEU:HD23	2.37	0.50
3:B:1793:ALA:O	3:B:1794:THR:OG1	2.23	0.50
3:B:3894:LEU:HB3	3:B:3902:PHE:CE2	2.47	0.50
3:C:1007:SER:C	3:C:1022:LEU:HD23	2.37	0.50
3:C:2249:ARG:CD	3:C:2287:LEU:HD21	2.42	0.50
3:C:3104:ILE:O	3:C:3108:VAL:HG23	2.12	0.50
2:K:76:VAL:HA	2:K:79:VAL:HG22	1.94	0.50
1:F:80:ASP:OD2	1:F:81:TYR:N	2.44	0.50
3:D:3894:LEU:HB3	3:D:3902:PHE:CE2	2.47	0.50
3:A:546:ASP:OD1	3:A:583:HIS:NE2	2.39	0.50
3:C:2898:LYS:HZ1	3:C:2900:GLY:C	2.20	0.50
2:M:76:VAL:HA	2:M:79:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:84:VAL:HG22	2:P:72:PHE:HD2	1.77	0.50
3:A:784:PHE:CB	3:A:788:ILE:HD13	2.42	0.49
3:A:2117:LEU:O	3:A:2121:MET:HG2	2.12	0.49
3:A:2668:THR:HG21	3:A:2673:LEU:HD21	1.94	0.49
3:B:3717:LEU:HD21	3:B:3785:MET:CE	2.42	0.49
3:C:784:PHE:CB	3:C:788:ILE:HD13	2.42	0.49
3:C:2918:ALA:O	3:C:2922:GLU:OE1	2.30	0.49
3:C:4675:LEU:HD23	3:C:4709:PHE:HE1	1.76	0.49
2:K:76:VAL:HG21	2:L:84:VAL:HG21	1.93	0.49
2:O:76:VAL:HA	2:O:79:VAL:HG22	1.94	0.49
2:J:51:ASP:O	2:J:55:VAL:HG23	2.12	0.49
3:D:2117:LEU:O	3:D:2121:MET:HG2	2.12	0.49
3:A:1007:SER:C	3:A:1022:LEU:HD23	2.37	0.49
3:A:2249:ARG:CD	3:A:2287:LEU:HD21	2.42	0.49
3:A:2824:VAL:HG12	3:A:2938:VAL:HB	1.92	0.49
3:B:2249:ARG:CD	3:B:2287:LEU:HD21	2.42	0.49
3:C:2594:ARG:O	3:C:2595:SER:OG	2.25	0.49
3:C:3183:TYR:O	3:C:3187:LEU:HD23	2.12	0.49
2:N:51:ASP:O	2:N:55:VAL:HG23	2.12	0.49
1:F:7:THR:HG23	1:F:7:THR:O	2.12	0.49
3:A:1793:ALA:O	3:A:1794:THR:OG1	2.23	0.49
3:A:3894:LEU:HB3	3:A:3902:PHE:CE2	2.47	0.49
3:A:510:GLU:N	3:A:510:GLU:OE2	2.44	0.49
3:A:2103:VAL:HG13	3:A:2121:MET:HB2	1.93	0.49
3:B:3447:SER:O	3:B:3453:LYS:NZ	2.38	0.49
2:N:84:VAL:HG21	2:M:76:VAL:HG21	1.93	0.49
3:D:784:PHE:CB	3:D:788:ILE:HD13	2.42	0.49
3:D:1007:SER:C	3:D:1022:LEU:HD23	2.37	0.49
3:D:3847:LEU:CD2	3:D:3936:PHE:HD1	2.26	0.49
3:B:2918:ALA:O	3:B:2922:GLU:OE1	2.30	0.49
3:B:4244:THR:HG22	3:B:4248:MET:HE3	1.94	0.49
3:B:4675:LEU:HD23	3:B:4709:PHE:HE1	1.76	0.49
3:C:1572:ASN:O	3:C:1573:ILE:HD13	2.12	0.49
3:C:3847:LEU:CD2	3:C:3936:PHE:HD1	2.26	0.49
2:I:76:VAL:HA	2:I:79:VAL:HG22	1.94	0.49
2:I:84:VAL:HG22	2:J:72:PHE:HD2	1.77	0.49
3:D:3183:TYR:O	3:D:3187:LEU:HD23	2.13	0.49
3:A:664:TYR:OH	3:A:666:GLU:OE2	2.27	0.49
3:A:2577:ALA:HB2	3:A:2619:MET:HE1	1.95	0.49
3:A:3183:TYR:O	3:A:3187:LEU:HD23	2.13	0.49
3:B:2166:LEU:HD21	3:B:2178:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4684:LEU:HD23	3:B:4685:TYR:CE1	2.48	0.49
3:C:3394:LEU:O	3:C:3398:GLU:OE1	2.30	0.49
3:C:3410:TYR:O	3:C:3411:PRO:C	2.56	0.49
3:D:2577:ALA:HB2	3:D:2619:MET:HE1	1.95	0.49
3:D:3141:LEU:HD11	3:D:3145:PHE:CZ	2.48	0.49
3:D:4244:THR:HG22	3:D:4248:MET:HE3	1.94	0.49
3:A:163:LYS:O	3:A:165:ARG:NH1	2.37	0.49
3:A:2156:LEU:HD21	3:A:2199:MET:CE	2.40	0.49
3:A:3394:LEU:O	3:A:3398:GLU:OE1	2.30	0.49
3:B:318:ARG:NH2	3:B:322:GLU:O	2.46	0.49
1:E:50:THR:N	1:E:55:GLU:OE2	2.39	0.49
1:H:50:THR:N	1:H:55:GLU:OE2	2.38	0.49
3:D:1737:VAL:O	3:D:1737:VAL:HG13	2.12	0.49
3:D:2249:ARG:CD	3:D:2287:LEU:HD21	2.42	0.49
3:D:2393:ARG:O	3:D:2419:LEU:HD12	2.13	0.49
3:D:3394:LEU:O	3:D:3398:GLU:OE1	2.30	0.49
3:A:1481:GLN:OE1	3:A:1481:GLN:N	2.46	0.49
3:A:2393:ARG:O	3:A:2419:LEU:HD12	2.13	0.49
3:A:4684:LEU:HD23	3:A:4685:TYR:CE1	2.48	0.49
3:B:2577:ALA:HB2	3:B:2619:MET:HE1	1.95	0.49
3:B:3394:LEU:O	3:B:3398:GLU:OE1	2.30	0.49
3:B:4886:TYR:HA	3:C:4916:ILE:HD11	1.95	0.49
3:C:2577:ALA:HB2	3:C:2619:MET:HE1	1.95	0.49
3:C:3717:LEU:HD21	3:C:3785:MET:CE	2.42	0.49
3:C:3894:LEU:HB3	3:C:3902:PHE:CE2	2.47	0.49
2:P:51:ASP:O	2:P:55:VAL:HG23	2.12	0.49
3:D:102:LEU:HD23	3:D:102:LEU:H	1.78	0.49
3:A:3104:ILE:O	3:A:3108:VAL:HG23	2.12	0.49
3:A:3410:TYR:O	3:A:3411:PRO:C	2.56	0.49
3:B:942:MET:HG2	3:B:942:MET:O	2.13	0.49
3:B:1481:GLN:N	3:B:1481:GLN:OE1	2.46	0.49
3:B:1737:VAL:HG13	3:B:1737:VAL:O	2.12	0.49
3:C:684:ARG:NH1	3:C:708:VAL:O	2.43	0.49
3:C:1481:GLN:OE1	3:C:1481:GLN:N	2.46	0.49
3:C:3079:ARG:NE	3:C:3156:ASP:OD2	2.36	0.49
2:I:37:LEU:O	2:I:41:GLU:HG2	2.13	0.49
2:J:72:PHE:O	2:J:76:VAL:HG13	2.13	0.49
1:F:6:GLU:N	1:F:6:GLU:OE2	2.46	0.49
3:D:510:GLU:OE2	3:D:510:GLU:N	2.44	0.49
3:D:2668:THR:HG21	3:D:2673:LEU:HD21	1.95	0.49
3:D:2898:LYS:HZ1	3:D:2900:GLY:C	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3104:ILE:O	3:D:3108:VAL:HG23	2.12	0.49
3:A:3717:LEU:HD21	3:A:3785:MET:CE	2.42	0.49
3:A:3847:LEU:CD2	3:A:3936:PHE:HD1	2.26	0.49
3:A:4122:GLU:OE1	3:A:4122:GLU:N	2.44	0.49
3:B:3183:TYR:O	3:B:3187:LEU:HD23	2.12	0.49
3:B:3847:LEU:CD2	3:B:3936:PHE:HD1	2.26	0.49
3:B:3873:ASN:OD1	3:B:3874:GLY:N	2.46	0.49
3:C:2166:LEU:HD21	3:C:2178:LEU:HD23	1.95	0.49
2:M:37:LEU:O	2:M:41:GLU:HG2	2.13	0.49
3:D:3344:GLN:OE1	3:D:3415:ARG:NH2	2.46	0.48
3:D:3410:TYR:O	3:D:3411:PRO:C	2.56	0.48
3:D:3873:ASN:OD1	3:D:3874:GLY:N	2.46	0.48
3:A:1237:THR:OG1	3:A:1609:MET:SD	2.61	0.48
3:A:3344:GLN:OE1	3:A:3415:ARG:NH2	2.46	0.48
3:B:2668:THR:HG21	3:B:2673:LEU:HD21	1.95	0.48
3:C:102:LEU:HD23	3:C:102:LEU:H	1.78	0.48
3:C:664:TYR:OH	3:C:666:GLU:OE2	2.27	0.48
3:C:3141:LEU:HD11	3:C:3145:PHE:CZ	2.48	0.48
3:C:3344:GLN:OE1	3:C:3415:ARG:NH2	2.46	0.48
3:C:3873:ASN:OD1	3:C:3874:GLY:N	2.46	0.48
2:L:51:ASP:O	2:L:55:VAL:HG23	2.12	0.48
2:N:72:PHE:HD2	2:M:84:VAL:HG22	1.77	0.48
3:A:942:MET:O	3:A:942:MET:HG2	2.13	0.48
3:A:2166:LEU:HD21	3:A:2178:LEU:HD23	1.94	0.48
3:B:510:GLU:N	3:B:510:GLU:OE2	2.44	0.48
3:C:4244:THR:HG22	3:C:4248:MET:HE3	1.94	0.48
3:D:3865:ASP:OD1	3:D:3866:GLY:N	2.46	0.48
3:A:318:ARG:NH2	3:A:322:GLU:O	2.46	0.48
3:A:3141:LEU:HD11	3:A:3145:PHE:CZ	2.48	0.48
3:B:2523:LEU:HD22	3:B:2579:MET:SD	2.54	0.48
3:B:3344:GLN:OE1	3:B:3415:ARG:NH2	2.46	0.48
3:D:1481:GLN:OE1	3:D:1481:GLN:N	2.46	0.48
3:D:2166:LEU:HD21	3:D:2178:LEU:HD23	1.95	0.48
3:A:578:ILE:O	3:A:580:GLN:NE2	2.47	0.48
3:A:4902:PRO:HB3	3:A:4911:ARG:HD3	1.96	0.48
3:B:102:LEU:HD23	3:B:102:LEU:H	1.78	0.48
3:B:3141:LEU:HD11	3:B:3145:PHE:CZ	2.48	0.48
3:C:2739:ARG:O	3:C:2885:ASN:ND2	2.47	0.48
3:C:4684:LEU:HD23	3:C:4685:TYR:CE1	2.48	0.48
2:P:72:PHE:O	2:P:76:VAL:HG13	2.13	0.48
3:A:2523:LEU:HD22	3:A:2579:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4244:THR:HG22	3:A:4248:MET:HE3	1.94	0.48
3:A:4691:GLU:O	3:A:4692:ASP:CG	2.57	0.48
3:B:3253:GLU:O	3:B:3256:GLY:N	2.47	0.48
3:B:4691:GLU:O	3:B:4692:ASP:CG	2.57	0.48
3:C:2117:LEU:O	3:C:2121:MET:HG2	2.12	0.48
2:N:72:PHE:O	2:N:76:VAL:HG13	2.13	0.48
2:M:30:SER:N	2:M:69:GLU:OE2	2.47	0.48
2:P:86:CYS:SG	2:P:87:ASN:N	2.87	0.48
3:D:2739:ARG:O	3:D:2885:ASN:ND2	2.47	0.48
3:D:2918:ALA:O	3:D:2922:GLU:OE1	2.30	0.48
3:A:1067:GLN:OE1	3:A:1072:ARG:NH2	2.47	0.48
3:A:2206:GLU:OE1	3:A:2206:GLU:N	2.46	0.48
3:C:4900:GLU:O	3:C:4911:ARG:CZ	2.62	0.48
2:M:7:SER:O	2:M:11:THR:HG23	2.14	0.48
2:O:37:LEU:O	2:O:41:GLU:HG2	2.13	0.48
3:D:942:MET:HG2	3:D:942:MET:O	2.13	0.48
3:D:2908:PRO:O	3:D:2911:THR:OG1	2.30	0.48
3:A:2918:ALA:O	3:A:2922:GLU:OE1	2.30	0.48
3:B:1067:GLN:OE1	3:B:1072:ARG:NH2	2.47	0.48
3:B:2362:PRO:O	3:B:2370:ARG:NH1	2.47	0.48
2:I:30:SER:N	2:I:69:GLU:OE2	2.47	0.48
3:A:569:LEU:HD12	3:A:603:VAL:HG13	1.96	0.48
3:A:2362:PRO:O	3:A:2370:ARG:NH1	2.47	0.48
3:A:3865:ASP:OD1	3:A:3866:GLY:N	2.46	0.48
3:B:578:ILE:O	3:B:580:GLN:NE2	2.47	0.48
3:B:2117:LEU:O	3:B:2121:MET:HG2	2.12	0.48
3:B:2739:ARG:O	3:B:2885:ASN:ND2	2.47	0.48
3:B:3079:ARG:NE	3:B:3156:ASP:OD2	2.36	0.48
3:B:3182:PRO:O	3:B:3185:GLU:HG3	2.14	0.48
3:C:2523:LEU:HD22	3:C:2579:MET:SD	2.54	0.48
3:C:2668:THR:HG21	3:C:2673:LEU:HD21	1.95	0.48
3:C:3253:GLU:O	3:C:3256:GLY:N	2.47	0.48
2:K:7:SER:O	2:K:11:THR:HG23	2.14	0.48
2:K:37:LEU:O	2:K:41:GLU:HG2	2.13	0.48
2:J:42:LEU:CD2	2:J:46:LEU:HB2	2.44	0.48
3:D:875:LEU:HD11	3:D:1047:LEU:CD2	2.29	0.48
3:D:2362:PRO:O	3:D:2370:ARG:NH1	2.47	0.48
3:D:4684:LEU:HD23	3:D:4685:TYR:CE1	2.48	0.48
3:D:4691:GLU:O	3:D:4692:ASP:CG	2.57	0.48
3:D:4916:ILE:HD11	3:C:4886:TYR:HA	1.95	0.48
3:A:3253:GLU:O	3:A:3256:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1758:GLY:N	3:B:1759:PRO:HD2	2.29	0.48
3:B:3865:ASP:OD1	3:B:3866:GLY:N	2.46	0.48
3:B:4902:PRO:HB3	3:B:4911:ARG:HD3	1.96	0.48
3:C:4122:GLU:OE1	3:C:4122:GLU:N	2.44	0.48
3:C:4691:GLU:O	3:C:4692:ASP:CG	2.57	0.48
2:K:30:SER:N	2:K:69:GLU:OE2	2.47	0.48
2:O:7:SER:O	2:O:11:THR:HG23	2.14	0.48
2:P:58:VAL:HG13	2:P:62:LEU:HD23	1.96	0.48
3:D:318:ARG:NH2	3:D:322:GLU:O	2.46	0.48
3:D:2875:MET:HE1	3:D:2938:VAL:HG11	1.96	0.48
3:D:4900:GLU:O	3:D:4911:ARG:CZ	2.62	0.48
3:A:2473:LEU:O	3:A:2500:LYS:NZ	2.45	0.48
3:B:2197:ASN:OD1	3:B:2200:ARG:NH2	2.46	0.48
3:B:2206:GLU:OE1	3:B:2206:GLU:N	2.46	0.48
3:C:1793:ALA:O	3:C:1794:THR:OG1	2.23	0.48
3:C:2393:ARG:O	3:C:2419:LEU:HD12	2.13	0.48
3:C:2875:MET:HE1	3:C:2938:VAL:HG11	1.96	0.48
2:N:42:LEU:CD2	2:N:46:LEU:HB2	2.44	0.48
3:D:578:ILE:O	3:D:580:GLN:NE2	2.47	0.47
3:A:1758:GLY:N	3:A:1759:PRO:HD2	2.29	0.47
3:A:4908:GLU:O	3:A:4912:VAL:HG13	2.14	0.47
3:B:1659:ASP:OD1	3:B:1659:ASP:N	2.47	0.47
3:B:2393:ARG:O	3:B:2419:LEU:HD12	2.13	0.47
3:C:510:GLU:OE2	3:C:510:GLU:N	2.44	0.47
3:C:3865:ASP:OD1	3:C:3866:GLY:N	2.46	0.47
2:K:84:VAL:HG22	2:L:72:PHE:HD2	1.77	0.47
2:J:86:CYS:SG	2:J:87:ASN:N	2.87	0.47
3:D:2197:ASN:OD1	3:D:2200:ARG:NH2	2.46	0.47
3:D:3107:MET:O	3:D:3108:VAL:C	2.57	0.47
3:D:3253:GLU:O	3:D:3256:GLY:N	2.47	0.47
3:D:4902:PRO:HB3	3:D:4911:ARG:HD3	1.96	0.47
3:A:4900:GLU:O	3:A:4911:ARG:CZ	2.62	0.47
3:B:4908:GLU:O	3:B:4912:VAL:HG13	2.14	0.47
2:O:30:SER:N	2:O:69:GLU:OE2	2.47	0.47
3:A:3182:PRO:O	3:A:3185:GLU:HG3	2.14	0.47
3:B:2368:ALA:HB2	3:B:2380:ALA:HB2	1.96	0.47
3:B:3410:TYR:O	3:B:3411:PRO:C	2.56	0.47
3:C:318:ARG:NH2	3:C:322:GLU:O	2.46	0.47
3:C:888:ILE:HG12	3:C:960:TYR:HA	1.97	0.47
2:L:72:PHE:O	2:L:76:VAL:HG13	2.13	0.47
2:L:86:CYS:SG	2:L:87:ASN:N	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:888:ILE:HG12	3:D:960:TYR:HA	1.97	0.47
3:D:2368:ALA:HB2	3:D:2380:ALA:HB2	1.96	0.47
3:D:2523:LEU:HD22	3:D:2579:MET:SD	2.54	0.47
3:A:910:ASN:OD1	3:A:911:PHE:N	2.48	0.47
3:A:3873:ASN:OD1	3:A:3874:GLY:N	2.46	0.47
3:B:569:LEU:HD12	3:B:603:VAL:HG13	1.96	0.47
3:B:3164:VAL:HG22	3:B:3233:LEU:HD11	1.96	0.47
3:C:754:PRO:HG3	3:C:774:LEU:HD11	1.96	0.47
3:C:875:LEU:HD11	3:C:1047:LEU:CD2	2.29	0.47
3:C:942:MET:O	3:C:942:MET:HG2	2.13	0.47
3:C:1435:TYR:OH	3:C:1569:LYS:C	2.58	0.47
3:C:1659:ASP:OD1	3:C:1659:ASP:N	2.47	0.47
3:C:2473:LEU:O	3:C:2500:LYS:NZ	2.45	0.47
3:C:3182:PRO:O	3:C:3185:GLU:HG3	2.14	0.47
2:N:54:ALA:O	2:N:58:VAL:HG23	2.15	0.47
2:N:86:CYS:SG	2:N:87:ASN:N	2.87	0.47
1:F:83:TYR:OH	3:B:1784:PHE:O	2.28	0.47
3:D:2472:SER:HB3	3:D:2525:VAL:HG12	1.97	0.47
2:I:7:SER:O	2:I:11:THR:HG23	2.14	0.47
1:H:6:GLU:N	1:H:6:GLU:OE1	2.47	0.47
3:D:2156:LEU:HD21	3:D:2199:MET:CE	2.40	0.47
3:D:3176:LEU:HD23	3:D:3176:LEU:C	2.40	0.47
3:D:3182:PRO:O	3:D:3185:GLU:HG3	2.14	0.47
3:D:4653:PHE:N	3:D:4794:MET:HE1	2.30	0.47
8:D:8006:PCW:H62	8:C:5101:PCW:O31	2.15	0.47
3:B:754:PRO:HG3	3:B:774:LEU:HD11	1.96	0.47
3:B:4900:GLU:O	3:B:4911:ARG:CZ	2.62	0.47
3:C:578:ILE:O	3:C:580:GLN:NE2	2.47	0.47
3:D:569:LEU:HD12	3:D:603:VAL:HG13	1.96	0.47
3:D:910:ASN:OD1	3:D:911:PHE:N	2.48	0.47
3:D:1067:GLN:OE1	3:D:1072:ARG:NH2	2.47	0.47
3:D:2694:GLN:NE2	2:O:10:GLU:CD	2.63	0.47
3:D:3600:VAL:O	3:D:3604:LEU:HD13	2.15	0.47
3:A:534:ASN:OD1	3:A:536:THR:OG1	2.31	0.47
3:A:888:ILE:HG12	3:A:960:TYR:HA	1.97	0.47
3:A:2368:ALA:HB2	3:A:2380:ALA:HB2	1.95	0.47
3:A:2739:ARG:O	3:A:2885:ASN:ND2	2.47	0.47
3:A:2875:MET:HE1	3:A:2938:VAL:HG11	1.96	0.47
3:A:3107:MET:O	3:A:3108:VAL:C	2.57	0.47
3:A:3176:LEU:HD23	3:A:3176:LEU:C	2.40	0.47
3:A:3992:VAL:HG11	3:A:4050:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:8007:PCW:O31	8:B:8006:PCW:H62	2.15	0.47
3:B:2875:MET:HE1	3:B:2938:VAL:HG11	1.96	0.47
3:B:2898:LYS:HZ1	3:B:2900:GLY:C	2.22	0.47
3:B:4122:GLU:OE1	3:B:4122:GLU:N	2.44	0.47
3:C:233:THR:HG21	3:C:253:VAL:HG21	1.97	0.47
3:C:1067:GLN:OE1	3:C:1072:ARG:NH2	2.47	0.47
3:C:1758:GLY:N	3:C:1759:PRO:HD2	2.29	0.47
3:C:2362:PRO:O	3:C:2370:ARG:NH1	2.47	0.47
3:C:3600:VAL:O	3:C:3604:LEU:HD13	2.15	0.47
3:C:4653:PHE:N	3:C:4794:MET:HE1	2.30	0.47
2:N:5:LEU:HD23	2:N:9:MET:CE	2.44	0.47
2:P:42:LEU:CD2	2:P:46:LEU:HB2	2.44	0.47
3:D:233:THR:HG21	3:D:253:VAL:HG21	1.97	0.47
3:D:1435:TYR:OH	3:D:1569:LYS:C	2.58	0.47
3:D:2370:ARG:NE	3:D:2370:ARG:HA	2.30	0.47
3:A:2370:ARG:NE	3:A:2370:ARG:HA	2.30	0.47
3:A:3547:ASP:O	3:A:3550:VAL:HG22	2.15	0.47
3:B:910:ASN:OD1	3:B:911:PHE:N	2.48	0.47
3:B:3107:MET:O	3:B:3108:VAL:C	2.57	0.47
3:B:3730:MET:O	3:B:3733:SER:OG	2.31	0.47
3:C:2206:GLU:OE1	3:C:2206:GLU:N	2.46	0.47
3:C:3176:LEU:HD23	3:C:3176:LEU:C	2.40	0.47
3:C:3547:ASP:O	3:C:3550:VAL:HG22	2.15	0.47
3:C:4902:PRO:HB3	3:C:4911:ARG:HD3	1.96	0.47
2:L:42:LEU:CD2	2:L:46:LEU:HB2	2.44	0.47
2:L:54:ALA:O	2:L:58:VAL:HG23	2.15	0.47
2:L:58:VAL:HG13	2:L:62:LEU:HD23	1.96	0.47
1:E:6:GLU:N	1:E:6:GLU:OE1	2.48	0.47
3:D:664:TYR:OH	3:D:666:GLU:OE2	2.27	0.47
3:D:1758:GLY:N	3:D:1759:PRO:HD2	2.29	0.47
3:D:2625:ARG:HD2	3:D:2907:VAL:HG21	1.97	0.47
3:A:102:LEU:HD23	3:A:102:LEU:H	1.78	0.47
3:B:233:THR:HG21	3:B:253:VAL:HG21	1.97	0.47
3:C:2370:ARG:NE	3:C:2370:ARG:HA	2.30	0.47
2:N:58:VAL:HG13	2:N:62:LEU:HD23	1.96	0.47
2:P:54:ALA:O	2:P:58:VAL:HG23	2.15	0.47
3:D:1659:ASP:OD1	3:D:1659:ASP:N	2.47	0.47
3:A:4964:ASP:OD1	3:A:4965:TYR:N	2.47	0.47
3:C:569:LEU:HD12	3:C:603:VAL:HG13	1.96	0.47
3:C:2625:ARG:HD2	3:C:2907:VAL:HG21	1.97	0.47
2:K:83:THR:O	2:K:87:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:TYR:OH	3:C:1784:PHE:O	2.27	0.46
3:D:163:LYS:O	3:D:165:ARG:NH1	2.38	0.46
3:A:754:PRO:HG3	3:A:774:LEU:HD11	1.96	0.46
3:A:2874:ALA:O	3:A:2878:GLN:OE1	2.33	0.46
3:A:2898:LYS:HZ1	3:A:2900:GLY:C	2.22	0.46
3:A:4691:GLU:O	3:A:4692:ASP:OD1	2.33	0.46
3:B:1435:TYR:OH	3:B:1569:LYS:C	2.58	0.46
3:B:2625:ARG:HD2	3:B:2907:VAL:HG21	1.97	0.46
3:B:3212:ASN:ND2	3:B:3237:VAL:HG21	2.31	0.46
3:B:3600:VAL:O	3:B:3604:LEU:HD13	2.15	0.46
3:C:2472:SER:HB3	3:C:2525:VAL:HG12	1.97	0.46
3:C:3164:VAL:HG22	3:C:3233:LEU:HD11	1.96	0.46
2:J:58:VAL:HG13	2:J:62:LEU:HD23	1.96	0.46
3:D:3164:VAL:HG22	3:D:3233:LEU:HD11	1.96	0.46
3:A:3600:VAL:O	3:A:3604:LEU:HD13	2.15	0.46
3:B:888:ILE:HG12	3:B:960:TYR:HA	1.97	0.46
3:B:3176:LEU:C	3:B:3176:LEU:HD23	2.40	0.46
3:B:4964:ASP:OD1	3:B:4965:TYR:N	2.47	0.46
3:C:3943:LYS:O	3:C:4005:LYS:NZ	2.34	0.46
3:C:4185:GLU:O	3:C:4986:TYR:OH	2.20	0.46
2:I:81:ALA:O	2:I:84:VAL:HB	2.16	0.46
3:D:2972:GLN:O	3:D:2975:ILE:HG22	2.16	0.46
3:D:4649:THR:HG1	3:D:4801:HIS:CD2	2.31	0.46
3:D:4692:ASP:OD1	3:D:4692:ASP:C	2.59	0.46
3:A:2972:GLN:O	3:A:2975:ILE:HG22	2.16	0.46
3:B:923:LEU:O	3:B:926:SER:OG	2.23	0.46
3:B:2370:ARG:NE	3:B:2370:ARG:HA	2.30	0.46
3:B:2972:GLN:O	3:B:2975:ILE:HG22	2.16	0.46
3:B:3547:ASP:O	3:B:3550:VAL:HG22	2.15	0.46
3:B:4653:PHE:N	3:B:4794:MET:HE1	2.30	0.46
8:B:8007:PCW:O31	8:C:5107:PCW:H62	2.15	0.46
3:D:754:PRO:HG3	3:D:774:LEU:HD11	1.96	0.46
3:D:3992:VAL:HG11	3:D:4050:MET:HE2	1.97	0.46
3:D:4908:GLU:O	3:D:4912:VAL:HG13	2.14	0.46
3:A:233:THR:HG21	3:A:253:VAL:HG21	1.97	0.46
3:A:2564:THR:HG22	3:A:2607:CYS:CA	2.45	0.46
3:B:231:CYS:SG	3:B:253:VAL:HG13	2.56	0.46
3:B:2472:SER:HB3	3:B:2525:VAL:HG12	1.97	0.46
3:C:910:ASN:OD1	3:C:911:PHE:N	2.48	0.46
3:C:2197:ASN:OD1	3:C:2200:ARG:NH2	2.46	0.46
3:C:2368:ALA:HB2	3:C:2380:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3107:MET:O	3:C:3108:VAL:C	2.57	0.46
3:C:3402:LEU:C	3:C:3402:LEU:HD23	2.40	0.46
3:C:3992:VAL:HG11	3:C:4050:MET:HE2	1.97	0.46
3:C:4908:GLU:O	3:C:4912:VAL:HG13	2.14	0.46
2:M:83:THR:O	2:M:87:ASN:ND2	2.48	0.46
1:G:6:GLU:OE1	1:G:6:GLU:N	2.48	0.46
3:D:2206:GLU:N	3:D:2206:GLU:OE1	2.46	0.46
3:A:1659:ASP:N	3:A:1659:ASP:OD1	2.47	0.46
3:A:3330:ILE:O	3:A:3404:ARG:NH2	2.49	0.46
3:A:3355:LEU:HD12	3:A:3356:ARG:N	2.30	0.46
3:C:2311:CYS:O	3:C:2315:LEU:HD23	2.16	0.46
3:C:2889:ARG:HG2	3:C:2893:GLN:HE22	1.81	0.46
3:C:3212:ASN:ND2	3:C:3237:VAL:HG21	2.31	0.46
2:J:16:PHE:CG	2:J:75:TYR:OH	2.60	0.46
2:J:38:LEU:HB3	2:J:46:LEU:HD21	1.98	0.46
3:D:3212:ASN:ND2	3:D:3237:VAL:HG21	2.31	0.46
3:D:3293:PRO:O	3:D:3295:PRO:HD3	2.16	0.46
3:A:3004:LEU:HB2	3:A:3005:PRO:HD3	1.98	0.46
3:B:984:THR:HA	3:B:987:ASP:OD2	2.16	0.46
3:B:2889:ARG:HG2	3:B:2893:GLN:HE22	1.80	0.46
3:B:3686:GLU:OE1	3:B:3686:GLU:N	2.49	0.46
3:C:231:CYS:SG	3:C:253:VAL:HG13	2.56	0.46
3:C:243:ARG:NH1	3:C:482:GLU:OE2	2.48	0.46
3:C:2564:THR:HG22	3:C:2607:CYS:CA	2.45	0.46
3:C:3355:LEU:HD12	3:C:3356:ARG:N	2.30	0.46
3:C:3920:ILE:HD12	3:C:3986:SER:HB3	1.98	0.46
2:L:38:LEU:HB3	2:L:46:LEU:HD21	1.98	0.46
3:D:231:CYS:SG	3:D:253:VAL:HG13	2.56	0.46
3:D:1435:TYR:OH	3:D:1570:GLN:HG2	2.15	0.46
3:D:1700:GLU:OE1	3:D:1812:LYS:NZ	2.49	0.46
3:D:2311:CYS:O	3:D:2315:LEU:HD23	2.16	0.46
3:D:3547:ASP:O	3:D:3550:VAL:HG22	2.15	0.46
3:A:2625:ARG:HD2	3:A:2907:VAL:HG21	1.97	0.46
3:A:3686:GLU:OE1	3:A:3686:GLU:N	2.49	0.46
3:B:3004:LEU:HB2	3:B:3005:PRO:HD3	1.98	0.46
3:C:2820:TRP:O	3:C:2821:GLU:HB2	2.16	0.46
3:C:4691:GLU:O	3:C:4692:ASP:OD1	2.33	0.46
2:K:81:ALA:O	2:K:84:VAL:HB	2.16	0.46
2:O:81:ALA:O	2:O:84:VAL:HB	2.16	0.46
2:I:83:THR:O	2:I:87:ASN:ND2	2.48	0.46
2:J:54:ALA:O	2:J:58:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:234:ILE:HD12	3:D:243:ARG:HB3	1.98	0.46
3:D:1699:LEU:HD11	3:D:1716:LEU:HD13	1.98	0.46
3:D:3330:ILE:O	3:D:3404:ARG:NH2	2.49	0.46
8:D:8007:PCW:O31	8:A:8006:PCW:H62	2.15	0.46
3:A:231:CYS:SG	3:A:253:VAL:HG13	2.56	0.46
3:A:2472:SER:HB3	3:A:2525:VAL:HG12	1.97	0.46
3:A:2942:LEU:O	3:A:2945:MET:HG2	2.16	0.46
3:A:3212:ASN:ND2	3:A:3237:VAL:HG21	2.30	0.46
3:B:951:LEU:CB	3:B:971:LEU:HD23	2.45	0.46
3:B:1495:MET:HE1	3:B:1554:PHE:CZ	2.51	0.46
3:B:4691:GLU:O	3:B:4692:ASP:OD1	2.33	0.46
3:C:1293:SER:C	3:C:1294:LEU:HD22	2.41	0.46
3:C:3004:LEU:HB2	3:C:3005:PRO:HD3	1.98	0.46
2:N:72:PHE:O	2:N:76:VAL:HG22	2.16	0.46
2:J:72:PHE:O	2:J:76:VAL:HG22	2.16	0.46
3:D:1220:LEU:HD22	3:C:3576:LEU:HD21	1.98	0.46
3:D:1293:SER:C	3:D:1294:LEU:HD22	2.41	0.46
3:D:2874:ALA:O	3:D:2878:GLN:OE1	2.33	0.46
3:D:2942:LEU:O	3:D:2945:MET:HG2	2.16	0.46
3:D:4091:ILE:O	3:D:4126:ILE:N	2.39	0.46
3:A:2311:CYS:O	3:A:2315:LEU:HD23	2.16	0.46
3:A:3402:LEU:HD23	3:A:3402:LEU:C	2.40	0.46
3:A:3920:ILE:HD12	3:A:3986:SER:HB3	1.97	0.46
3:B:668:MET:SD	3:B:791:ARG:NH2	2.87	0.46
3:B:1772:SER:OG	3:B:1957:GLU:OE2	2.23	0.46
3:B:3355:LEU:HD12	3:B:3356:ARG:N	2.30	0.46
3:B:3402:LEU:HD23	3:B:3402:LEU:C	2.40	0.46
3:B:3992:VAL:HG11	3:B:4050:MET:HE2	1.97	0.46
3:C:234:ILE:HD12	3:C:243:ARG:HB3	1.98	0.46
3:C:1699:LEU:HD11	3:C:1716:LEU:HD13	1.98	0.46
3:C:2874:ALA:O	3:C:2878:GLN:OE1	2.33	0.46
3:C:2942:LEU:O	3:C:2945:MET:HG2	2.16	0.46
2:L:72:PHE:O	2:L:76:VAL:HG22	2.16	0.46
2:N:14:ASN:HA	2:N:17:HIS:HD1	1.81	0.46
3:D:3355:LEU:HD12	3:D:3356:ARG:N	2.30	0.46
3:A:1700:GLU:OE1	3:A:1812:LYS:NZ	2.49	0.46
3:A:3047:LEU:CD2	3:A:3069:LEU:HD22	2.46	0.46
3:A:3164:VAL:HG22	3:A:3233:LEU:HD11	1.97	0.46
3:B:2311:CYS:O	3:B:2315:LEU:HD23	2.16	0.46
3:B:2564:THR:HG22	3:B:2607:CYS:CA	2.45	0.46
3:B:2570:PHE:CE1	3:B:2583:MET:HE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1495:MET:HE1	3:C:1554:PHE:CZ	2.51	0.46
3:C:2570:PHE:CE1	3:C:2583:MET:HE1	2.51	0.46
3:C:3267:MET:HG3	3:C:3267:MET:O	2.16	0.46
2:N:16:PHE:CG	2:N:75:TYR:OH	2.60	0.46
3:D:2570:PHE:CE1	3:D:2583:MET:HE1	2.51	0.45
3:D:2594:ARG:O	3:D:2595:SER:OG	2.25	0.45
3:D:3004:LEU:HB2	3:D:3005:PRO:HD3	1.98	0.45
3:D:3267:MET:HG3	3:D:3267:MET:O	2.16	0.45
3:D:3600:VAL:HG22	3:D:3604:LEU:CD1	2.46	0.45
3:D:3937:TYR:CD1	3:D:4002:MET:HE3	2.52	0.45
3:D:4886:TYR:HA	3:A:4916:ILE:HD11	1.97	0.45
3:A:234:ILE:HD12	3:A:243:ARG:HB3	1.98	0.45
3:A:668:MET:SD	3:A:791:ARG:NH2	2.87	0.45
3:A:3333:ALA:HB3	3:A:3336:MET:HE2	1.98	0.45
3:B:1435:TYR:OH	3:B:1570:GLN:HG2	2.15	0.45
3:B:1700:GLU:OE1	3:B:1812:LYS:NZ	2.49	0.45
3:B:2874:ALA:O	3:B:2878:GLN:OE1	2.33	0.45
3:B:3600:VAL:HG22	3:B:3604:LEU:CD1	2.46	0.45
3:C:3293:PRO:O	3:C:3295:PRO:HD3	2.16	0.45
3:C:4649:THR:HG1	3:C:4801:HIS:CD2	2.33	0.45
3:D:2505:LEU:HD23	3:D:2505:LEU:C	2.42	0.45
3:A:243:ARG:NH1	3:A:482:GLU:OE2	2.48	0.45
3:A:1435:TYR:OH	3:A:1569:LYS:C	2.58	0.45
3:A:2594:ARG:O	3:A:2595:SER:OG	2.25	0.45
3:A:2889:ARG:HG2	3:A:2893:GLN:HE22	1.81	0.45
3:B:3267:MET:O	3:B:3267:MET:HG3	2.16	0.45
3:B:3333:ALA:HB3	3:B:3336:MET:HE2	1.98	0.45
3:C:887:ARG:NH2	7:C:5106:ATP:O3G	2.49	0.45
3:C:4692:ASP:OD1	3:C:4692:ASP:C	2.59	0.45
2:O:20:SER:OG	2:O:29:LEU:HD23	2.17	0.45
2:O:83:THR:O	2:O:87:ASN:ND2	2.48	0.45
2:P:14:ASN:HA	2:P:17:HIS:HD1	1.81	0.45
2:P:38:LEU:HB3	2:P:46:LEU:HD21	1.98	0.45
3:D:36:LEU:HD23	3:D:52:PRO:HA	1.99	0.45
3:D:668:MET:SD	3:D:791:ARG:NH2	2.87	0.45
3:D:3271:ILE:H	3:D:3271:ILE:HD12	1.81	0.45
3:D:4122:GLU:OE1	3:D:4122:GLU:N	2.44	0.45
3:A:4653:PHE:N	3:A:4794:MET:HE1	2.30	0.45
3:A:4692:ASP:OD1	3:A:4692:ASP:C	2.59	0.45
3:B:887:ARG:NH2	7:B:8005:ATP:O3G	2.49	0.45
3:B:3330:ILE:O	3:B:3404:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1435:TYR:OH	3:C:1570:GLN:HG2	2.15	0.45
3:C:1700:GLU:OE1	3:C:1812:LYS:NZ	2.49	0.45
3:C:3686:GLU:OE1	3:C:3686:GLU:N	2.49	0.45
2:N:38:LEU:HB3	2:N:46:LEU:HD21	1.98	0.45
2:P:72:PHE:O	2:P:76:VAL:HG22	2.16	0.45
3:D:2249:ARG:HD2	3:D:2287:LEU:HD21	1.98	0.45
3:D:2382:GLU:O	3:D:2385:ILE:HG22	2.17	0.45
3:D:2889:ARG:HG2	3:D:2893:GLN:HE22	1.80	0.45
3:D:3730:MET:O	3:D:3733:SER:OG	2.31	0.45
3:A:984:THR:HA	3:A:987:ASP:OD2	2.16	0.45
3:A:1435:TYR:OH	3:A:1570:GLN:HG2	2.16	0.45
3:A:1699:LEU:HD11	3:A:1716:LEU:HD13	1.98	0.45
3:B:1699:LEU:HD11	3:B:1716:LEU:HD13	1.98	0.45
3:B:2249:ARG:HD2	3:B:2287:LEU:HD21	1.98	0.45
3:B:2382:GLU:O	3:B:2385:ILE:HG22	2.17	0.45
3:B:3937:TYR:CD1	3:B:4002:MET:HE3	2.52	0.45
3:C:668:MET:SD	3:C:791:ARG:NH2	2.87	0.45
3:C:951:LEU:CB	3:C:971:LEU:HD23	2.45	0.45
2:L:78:LEU:HD12	2:L:79:VAL:N	2.32	0.45
1:H:54:GLN:OE1	1:H:54:GLN:N	2.50	0.45
3:D:984:THR:HA	3:D:987:ASP:OD2	2.16	0.45
3:D:3333:ALA:HB3	3:D:3336:MET:HE2	1.98	0.45
3:D:3402:LEU:HD23	3:D:3402:LEU:C	2.40	0.45
3:D:3443:PHE:CD2	3:D:3515:LEU:HD22	2.52	0.45
3:D:3686:GLU:N	3:D:3686:GLU:OE1	2.49	0.45
3:D:4691:GLU:O	3:D:4692:ASP:OD1	2.33	0.45
3:D:4964:ASP:OD1	3:D:4965:TYR:N	2.47	0.45
3:A:2528:LEU:HA	3:A:2531:MET:CE	2.47	0.45
3:A:3447:SER:O	3:A:3453:LYS:NZ	2.38	0.45
8:A:8007:PCW:H232	8:A:8007:PCW:H20	1.76	0.45
3:B:234:ILE:HD12	3:B:243:ARG:HB3	1.98	0.45
3:B:2746:VAL:HG22	3:B:2747:ILE:N	2.32	0.45
3:B:3047:LEU:CD2	3:B:3069:LEU:HD22	2.46	0.45
3:B:3724:MET:CE	3:B:3795:ALA:HB1	2.47	0.45
3:B:4692:ASP:OD1	3:B:4692:ASP:C	2.59	0.45
3:C:534:ASN:OD1	3:C:536:THR:OG1	2.31	0.45
3:C:984:THR:HA	3:C:987:ASP:OD2	2.16	0.45
3:C:2125:LEU:CD2	3:C:3678:LEU:HD21	2.47	0.45
3:C:2972:GLN:O	3:C:2975:ILE:HG22	2.16	0.45
3:C:3600:VAL:HG22	3:C:3604:LEU:CD1	2.46	0.45
3:C:3702:LEU:HD21	3:C:3726:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3724:MET:CE	3:C:3795:ALA:HB1	2.47	0.45
2:P:73:LYS:O	2:P:76:VAL:HG22	2.16	0.45
2:P:79:VAL:O	2:P:83:THR:HG22	2.17	0.45
2:J:78:LEU:HD12	2:J:79:VAL:N	2.32	0.45
3:D:992:ASN:C	3:D:992:ASN:HD22	2.25	0.45
3:D:1464:SER:O	3:D:1469:LYS:NZ	2.46	0.45
3:D:2528:LEU:HA	3:D:2531:MET:CE	2.47	0.45
3:D:3036:GLU:HA	3:D:3039:MET:HE3	1.98	0.45
3:D:3047:LEU:CD2	3:D:3069:LEU:HD22	2.46	0.45
3:D:3724:MET:CE	3:D:3795:ALA:HB1	2.47	0.45
3:D:3920:ILE:HD12	3:D:3986:SER:HB3	1.98	0.45
3:A:330:ARG:NH1	3:A:331:ASP:O	2.50	0.45
3:A:1222:GLU:OE1	3:A:1222:GLU:N	2.49	0.45
3:A:3036:GLU:HA	3:A:3039:MET:HE3	1.98	0.45
3:A:3293:PRO:O	3:A:3295:PRO:HD3	2.16	0.45
3:A:3443:PHE:CD2	3:A:3515:LEU:HD22	2.52	0.45
3:B:731:VAL:HA	3:B:1477:MET:HE3	1.99	0.45
3:B:2125:LEU:CD2	3:B:3678:LEU:HD21	2.47	0.45
3:B:2473:LEU:O	3:B:2500:LYS:NZ	2.45	0.45
3:B:2645:LEU:HD13	3:B:2679:LEU:HD11	1.98	0.45
3:B:2820:TRP:O	3:B:2821:GLU:HB2	2.16	0.45
3:B:2942:LEU:O	3:B:2945:MET:HG2	2.16	0.45
3:B:3920:ILE:HD12	3:B:3986:SER:HB3	1.97	0.45
3:B:4800:GLY:HA2	3:B:4806:PHE:HB2	1.99	0.45
3:C:3047:LEU:CD2	3:C:3069:LEU:HD22	2.46	0.45
3:C:3330:ILE:O	3:C:3404:ARG:NH2	2.49	0.45
2:L:73:LYS:O	2:L:76:VAL:HG22	2.16	0.45
3:D:534:ASN:OD1	3:D:536:THR:OG1	2.31	0.45
3:D:2125:LEU:CD2	3:D:3678:LEU:HD21	2.47	0.45
3:D:3136:ALA:O	3:D:3140:VAL:HG12	2.17	0.45
3:D:3421:ARG:NH2	3:D:3517:LYS:O	2.50	0.45
3:D:3521:ILE:H	3:D:3521:ILE:HD12	1.82	0.45
3:D:3702:LEU:HD21	3:D:3726:TYR:CD1	2.52	0.45
3:A:36:LEU:HD23	3:A:52:PRO:HA	1.98	0.45
3:A:887:ARG:NH2	7:A:8005:ATP:O3G	2.49	0.45
3:A:1293:SER:C	3:A:1294:LEU:HD22	2.41	0.45
3:A:2249:ARG:HD2	3:A:2287:LEU:HD21	1.98	0.45
3:A:3320:ILE:HD12	3:A:3320:ILE:H	1.82	0.45
3:A:3933:ILE:HG22	3:A:3998:VAL:HG11	1.99	0.45
3:B:330:ARG:NH1	3:B:331:ASP:O	2.50	0.45
3:B:1261:MET:HE1	3:B:1272:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2505:LEU:C	3:C:2505:LEU:HD23	2.42	0.45
3:C:3443:PHE:CD2	3:C:3515:LEU:HD22	2.52	0.45
2:K:20:SER:OG	2:K:29:LEU:HD23	2.17	0.45
2:N:73:LYS:O	2:N:76:VAL:HG22	2.16	0.45
1:H:83:TYR:OH	3:D:1784:PHE:O	2.28	0.45
3:D:887:ARG:NH2	7:D:8005:ATP:O3G	2.49	0.45
3:D:1222:GLU:OE1	3:D:1222:GLU:N	2.49	0.45
3:D:1495:MET:HE1	3:D:1554:PHE:CZ	2.51	0.45
3:D:3320:ILE:HD12	3:D:3320:ILE:H	1.82	0.45
3:D:4909:LEU:HA	3:D:4912:VAL:HG22	1.99	0.45
3:A:2952:ILE:H	3:A:2952:ILE:HD12	1.82	0.45
3:B:684:ARG:NH1	3:B:708:VAL:O	2.43	0.45
3:B:1973:ASN:ND2	3:B:2025:PRO:HD3	2.32	0.45
3:B:3322:ARG:HA	3:B:3325:VAL:HG12	1.99	0.45
3:B:3394:LEU:HD23	3:B:3398:GLU:OE1	2.17	0.45
3:B:4090:LEU:C	3:B:4125:MET:HE3	2.42	0.45
3:C:36:LEU:HD23	3:C:52:PRO:HA	1.99	0.45
3:C:330:ARG:NH1	3:C:331:ASP:O	2.50	0.45
3:C:731:VAL:HA	3:C:1477:MET:HE3	1.99	0.45
3:C:1261:MET:HE1	3:C:1272:ARG:CZ	2.47	0.45
3:C:2249:ARG:HD2	3:C:2287:LEU:HD21	1.98	0.45
3:C:3421:ARG:NH2	3:C:3517:LYS:O	2.50	0.45
2:K:84:VAL:CG1	2:L:72:PHE:HE2	2.23	0.45
2:M:50:LYS:NZ	2:M:51:ASP:OD2	2.50	0.45
1:E:83:TYR:OH	3:A:1784:PHE:O	2.28	0.45
2:I:9:MET:HG2	2:J:84:VAL:HG12	1.99	0.45
1:G:54:GLN:OE1	1:G:54:GLN:N	2.50	0.45
3:D:912:HIS:O	3:D:919:ARG:NH1	2.50	0.45
3:D:2645:LEU:HD13	3:D:2679:LEU:HD11	1.98	0.45
3:D:3227:GLU:O	3:D:3228:ARG:CG	2.65	0.45
3:D:3789:CYS:SG	3:D:3834:SER:OG	2.75	0.45
3:A:1261:MET:HE1	3:A:1272:ARG:CZ	2.47	0.45
3:A:1973:ASN:ND2	3:A:2025:PRO:HD3	2.32	0.45
3:A:3322:ARG:HA	3:A:3325:VAL:HG12	1.99	0.45
3:A:3521:ILE:H	3:A:3521:ILE:HD12	1.82	0.45
3:A:3937:TYR:CD1	3:A:4002:MET:HE3	2.51	0.45
3:A:4090:LEU:C	3:A:4125:MET:HE3	2.42	0.45
3:B:581:GLU:HG3	3:B:621:LEU:HD22	1.99	0.45
3:B:1293:SER:C	3:B:1294:LEU:HD22	2.41	0.45
3:B:3136:ALA:O	3:B:3140:VAL:HG12	2.17	0.45
3:B:3257:LEU:HB3	3:B:3267:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3421:ARG:NH2	3:B:3517:LYS:O	2.50	0.45
3:C:1090:TYR:N	3:C:1225:GLU:O	2.50	0.45
3:C:3521:ILE:H	3:C:3521:ILE:HD12	1.82	0.45
3:C:4800:GLY:HA2	3:C:4806:PHE:HB2	1.99	0.45
2:M:34:LEU:CD1	2:M:70:VAL:HG21	2.47	0.45
2:O:9:MET:HG2	2:P:84:VAL:HG12	1.99	0.45
2:I:20:SER:OG	2:I:29:LEU:HD23	2.17	0.45
3:D:2746:VAL:HG22	3:D:2747:ILE:N	2.32	0.45
3:D:3394:LEU:HD23	3:D:3398:GLU:OE1	2.17	0.45
3:A:731:VAL:HA	3:A:1477:MET:HE3	1.99	0.45
3:A:1090:TYR:N	3:A:1225:GLU:O	2.50	0.45
3:A:2125:LEU:CD2	3:A:3678:LEU:HD21	2.47	0.45
3:A:3208:GLU:OE1	3:A:3208:GLU:N	2.50	0.45
3:A:3257:LEU:HB3	3:A:3267:MET:HE1	1.99	0.45
3:A:3267:MET:HG3	3:A:3267:MET:O	2.16	0.45
3:A:3724:MET:CE	3:A:3795:ALA:HB1	2.47	0.45
3:B:484:MET:HE2	3:B:484:MET:CA	2.46	0.45
3:B:2528:LEU:HA	3:B:2531:MET:CE	2.47	0.45
3:B:2952:ILE:H	3:B:2952:ILE:HD12	1.82	0.45
3:B:3208:GLU:OE1	3:B:3208:GLU:N	2.50	0.45
3:B:3293:PRO:O	3:B:3295:PRO:HD3	2.16	0.45
3:B:3576:LEU:HD21	3:C:1220:LEU:HD22	1.97	0.45
3:C:1529:THR:OG1	3:C:1536:GLU:OE2	2.35	0.45
3:C:3257:LEU:HB3	3:C:3267:MET:HE1	1.99	0.45
3:C:3271:ILE:H	3:C:3271:ILE:HD12	1.81	0.45
3:C:4090:LEU:C	3:C:4125:MET:HE3	2.42	0.45
2:K:50:LYS:NZ	2:K:51:ASP:OD2	2.50	0.45
2:L:79:VAL:O	2:L:83:THR:HG22	2.17	0.45
2:N:78:LEU:HD12	2:N:79:VAL:N	2.32	0.45
2:I:41:GLU:C	2:I:42:LEU:HD22	2.42	0.44
2:J:79:VAL:O	2:J:83:THR:HG22	2.17	0.44
3:D:3869:ILE:HG22	3:D:3869:ILE:O	2.17	0.44
3:A:130:ASP:OD1	3:A:133:ALA:N	2.50	0.44
3:A:215:VAL:CG1	3:A:275:LEU:HD12	2.47	0.44
3:A:923:LEU:O	3:A:926:SER:OG	2.23	0.44
3:A:1495:MET:HE1	3:A:1554:PHE:CZ	2.51	0.44
3:A:2382:GLU:O	3:A:2385:ILE:HG22	2.17	0.44
3:A:2570:PHE:CE1	3:A:2583:MET:HE1	2.51	0.44
3:A:2782:ILE:HG23	3:A:2790:PRO:CD	2.47	0.44
3:A:3402:LEU:HD23	3:A:3402:LEU:O	2.18	0.44
3:A:3702:LEU:HD21	3:A:3726:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3227:GLU:O	3:B:3228:ARG:CG	2.65	0.44
3:C:4155:GLU:OE2	3:C:4183:ARG:NH1	2.50	0.44
2:K:9:MET:HG2	2:L:84:VAL:HG12	1.99	0.44
2:K:41:GLU:C	2:K:42:LEU:HD22	2.42	0.44
2:M:41:GLU:C	2:M:42:LEU:HD22	2.42	0.44
2:P:78:LEU:HD12	2:P:79:VAL:N	2.32	0.44
3:D:731:VAL:HA	3:D:1477:MET:HE3	1.99	0.44
3:D:1090:TYR:N	3:D:1225:GLU:O	2.50	0.44
3:D:1261:MET:HE1	3:D:1272:ARG:CZ	2.47	0.44
3:D:2820:TRP:O	3:D:2821:GLU:HB2	2.16	0.44
3:D:3270:VAL:HG12	3:D:3275:LEU:HD23	1.99	0.44
3:D:3402:LEU:HD23	3:D:3402:LEU:O	2.17	0.44
3:D:3577:TYR:CZ	3:D:3583:ARG:HD3	2.53	0.44
3:D:4821:LEU:HG	3:A:4837:MET:HE3	2.00	0.44
3:A:2645:LEU:HD13	3:A:2679:LEU:HD11	1.98	0.44
3:A:2746:VAL:HG22	3:A:2747:ILE:N	2.32	0.44
3:A:2820:TRP:O	3:A:2821:GLU:HB2	2.16	0.44
3:A:3227:GLU:O	3:A:3228:ARG:CG	2.65	0.44
3:A:3270:VAL:HG12	3:A:3275:LEU:HD23	2.00	0.44
3:B:3104:ILE:O	3:B:3107:MET:HB3	2.17	0.44
3:B:3521:ILE:HD12	3:B:3521:ILE:H	1.82	0.44
3:B:4155:GLU:OE2	3:B:4183:ARG:NH1	2.50	0.44
7:B:8005:ATP:O1A	7:B:8005:ATP:O3'	2.28	0.44
3:C:169:ASP:OD1	3:C:202:ASN:ND2	2.51	0.44
3:C:2782:ILE:HG23	3:C:2790:PRO:CD	2.47	0.44
3:C:3869:ILE:O	3:C:3869:ILE:HG22	2.17	0.44
2:K:34:LEU:CD1	2:K:70:VAL:HG21	2.47	0.44
2:N:42:LEU:HD13	2:M:6:GLU:CD	2.40	0.44
2:N:62:LEU:HD13	2:N:78:LEU:HD21	2.00	0.44
2:M:81:ALA:O	2:M:84:VAL:HB	2.16	0.44
2:P:62:LEU:HD13	2:P:78:LEU:HD21	2.00	0.44
3:D:2782:ILE:HG23	3:D:2790:PRO:CD	2.47	0.44
3:D:3104:ILE:O	3:D:3107:MET:HB3	2.17	0.44
3:D:3511:ILE:HG23	3:D:3512:VAL:N	2.33	0.44
3:A:245:LEU:HD23	3:A:301:VAL:HG12	1.99	0.44
3:A:912:HIS:O	3:A:919:ARG:NH1	2.50	0.44
3:A:3600:VAL:HG22	3:A:3604:LEU:CD1	2.46	0.44
3:A:4886:TYR:HA	3:B:4916:ILE:HD11	1.99	0.44
3:B:2782:ILE:HG23	3:B:2790:PRO:CD	2.47	0.44
3:B:3271:ILE:H	3:B:3271:ILE:HD12	1.81	0.44
3:C:581:GLU:HG3	3:C:621:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2247:ASN:O	3:C:2250:SER:OG	2.28	0.44
3:C:2382:GLU:O	3:C:2385:ILE:HG22	2.17	0.44
3:C:3104:ILE:O	3:C:3107:MET:HB3	2.17	0.44
3:C:3136:ALA:O	3:C:3140:VAL:HG12	2.17	0.44
3:C:3208:GLU:OE1	3:C:3208:GLU:N	2.50	0.44
3:C:3937:TYR:CD1	3:C:4002:MET:HE3	2.52	0.44
2:L:14:ASN:HA	2:L:17:HIS:HD1	1.81	0.44
2:O:34:LEU:CD1	2:O:70:VAL:HG21	2.47	0.44
3:D:130:ASP:OD1	3:D:133:ALA:N	2.50	0.44
3:D:215:VAL:CG1	3:D:275:LEU:HD12	2.47	0.44
3:D:330:ARG:NH1	3:D:331:ASP:O	2.50	0.44
3:D:3257:LEU:HB3	3:D:3267:MET:HE1	1.99	0.44
3:D:4090:LEU:C	3:D:4125:MET:HE3	2.42	0.44
3:A:169:ASP:OD1	3:A:202:ASN:ND2	2.51	0.44
3:A:951:LEU:CB	3:A:971:LEU:HD23	2.45	0.44
3:A:2505:LEU:HD23	3:A:2505:LEU:C	2.42	0.44
3:A:3136:ALA:O	3:A:3140:VAL:HG12	2.17	0.44
3:A:3271:ILE:H	3:A:3271:ILE:HD12	1.82	0.44
3:A:3577:TYR:CZ	3:A:3583:ARG:HD3	2.53	0.44
3:A:3869:ILE:HG22	3:A:3869:ILE:O	2.17	0.44
3:B:576:LEU:HD22	3:B:610:CYS:HB2	1.99	0.44
3:B:921:TYR:CZ	3:B:925:MET:HE3	2.53	0.44
3:B:1222:GLU:OE1	3:B:1222:GLU:N	2.49	0.44
3:B:3270:VAL:HG12	3:B:3275:LEU:HD23	1.99	0.44
3:C:484:MET:HE2	3:C:484:MET:CA	2.46	0.44
3:C:912:HIS:O	3:C:919:ARG:NH1	2.50	0.44
3:C:921:TYR:CZ	3:C:925:MET:HE3	2.53	0.44
3:C:3322:ARG:HA	3:C:3325:VAL:HG12	1.99	0.44
3:C:3511:ILE:HG23	3:C:3512:VAL:N	2.33	0.44
2:L:62:LEU:HD13	2:L:78:LEU:HD21	1.99	0.44
2:N:72:PHE:HE2	2:M:84:VAL:CG1	2.23	0.44
2:N:79:VAL:O	2:N:83:THR:HG22	2.17	0.44
2:N:84:VAL:HG12	2:M:9:MET:HG2	1.99	0.44
2:I:34:LEU:CD1	2:I:70:VAL:HG21	2.47	0.44
2:J:14:ASN:HA	2:J:17:HIS:HD1	1.81	0.44
2:J:62:LEU:HD13	2:J:78:LEU:HD21	2.00	0.44
3:D:3208:GLU:OE1	3:D:3208:GLU:N	2.50	0.44
3:A:3394:LEU:HD23	3:A:3398:GLU:OE1	2.17	0.44
3:A:3421:ARG:NH2	3:A:3517:LYS:O	2.50	0.44
3:B:2239:TYR:O	3:B:2243:ILE:HG12	2.18	0.44
3:B:3036:GLU:HA	3:B:3039:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3320:ILE:HD12	3:B:3320:ILE:H	1.82	0.44
3:B:3363:ILE:HG23	3:B:3438:MET:HE2	2.00	0.44
3:B:3577:TYR:CZ	3:B:3583:ARG:HD3	2.53	0.44
3:B:3702:LEU:HD21	3:B:3726:TYR:CD1	2.52	0.44
3:C:1973:ASN:ND2	3:C:2025:PRO:HD3	2.32	0.44
3:C:2171:MET:SD	3:C:2229:MET:HE1	2.58	0.44
3:C:3227:GLU:O	3:C:3228:ARG:CG	2.65	0.44
3:C:3363:ILE:HG23	3:C:3438:MET:HE2	2.00	0.44
3:C:4173:ILE:H	3:C:4173:ILE:HD12	1.83	0.44
2:M:20:SER:OG	2:M:29:LEU:HD23	2.17	0.44
3:D:1473:VAL:HG22	3:D:1474:THR:N	2.33	0.44
3:D:1529:THR:OG1	3:D:1536:GLU:OE2	2.35	0.44
3:D:1973:ASN:ND2	3:D:2025:PRO:HD3	2.32	0.44
3:D:3322:ARG:HA	3:D:3325:VAL:HG12	1.99	0.44
3:A:2171:MET:SD	3:A:2229:MET:HE1	2.58	0.44
3:B:130:ASP:OD1	3:B:133:ALA:N	2.50	0.44
3:B:2624:LEU:O	3:B:2628:VAL:HG23	2.18	0.44
3:B:3402:LEU:HD23	3:B:3402:LEU:O	2.17	0.44
3:B:3443:PHE:CD2	3:B:3515:LEU:HD22	2.52	0.44
3:B:3639:MET:O	3:B:3640:THR:C	2.61	0.44
3:C:130:ASP:OD1	3:C:133:ALA:N	2.50	0.44
3:C:576:LEU:HD22	3:C:610:CYS:HB2	1.99	0.44
3:C:3036:GLU:HA	3:C:3039:MET:HE3	1.98	0.44
3:C:3320:ILE:HD12	3:C:3320:ILE:H	1.82	0.44
3:C:3333:ALA:HB3	3:C:3336:MET:HE2	1.98	0.44
3:C:3402:LEU:HD23	3:C:3402:LEU:O	2.17	0.44
2:L:20:SER:HB3	2:L:27:TYR:HA	1.99	0.44
2:O:41:GLU:C	2:O:42:LEU:HD22	2.42	0.44
3:D:684:ARG:NH1	3:D:708:VAL:O	2.43	0.44
3:D:2268:MET:O	3:D:2269:GLN:HB3	2.18	0.44
3:D:2830:GLY:N	3:D:2934:ASN:OD1	2.51	0.44
3:D:3373:VAL:HG22	3:D:3399:PHE:CE1	2.53	0.44
3:D:3380:LEU:HD21	3:D:3392:GLU:HA	2.00	0.44
3:D:4227:GLU:N	3:D:4227:GLU:OE2	2.51	0.44
3:A:484:MET:HE2	3:A:484:MET:CA	2.46	0.44
3:A:1492:ASN:OD1	3:A:1493:CYS:N	2.51	0.44
3:A:3373:VAL:HG22	3:A:3399:PHE:CE1	2.53	0.44
3:A:4909:LEU:HA	3:A:4912:VAL:HG22	1.99	0.44
3:B:912:HIS:O	3:B:919:ARG:NH1	2.50	0.44
3:B:3406:LEU:HD11	3:B:3410:TYR:OH	2.18	0.44
3:B:3451:ASN:O	3:B:3454:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:VAL:CG1	3:C:275:LEU:HD12	2.47	0.44
3:C:2528:LEU:HA	3:C:2531:MET:CE	2.47	0.44
3:C:2624:LEU:O	3:C:2628:VAL:HG23	2.18	0.44
3:C:4227:GLU:N	3:C:4227:GLU:OE2	2.51	0.44
2:N:20:SER:HB3	2:N:27:TYR:HA	1.99	0.44
2:I:50:LYS:NZ	2:I:51:ASP:OD2	2.50	0.44
2:J:73:LYS:O	2:J:76:VAL:HG22	2.16	0.44
3:D:245:LEU:HD23	3:D:301:VAL:HG12	1.99	0.44
3:D:1426:GLU:HG2	3:D:1427:ILE:N	2.33	0.44
3:D:3933:ILE:HG22	3:D:3998:VAL:HG11	1.99	0.44
3:D:4155:GLU:OE2	3:D:4183:ARG:NH1	2.50	0.44
3:D:4766:ILE:HA	3:D:4769:ILE:HD12	1.99	0.44
3:A:978:LEU:HD21	3:A:1045:ARG:HG2	2.00	0.44
3:A:1529:THR:OG1	3:A:1536:GLU:OE2	2.36	0.44
3:A:3943:LYS:O	3:A:4005:LYS:NZ	2.34	0.44
3:B:36:LEU:HD23	3:B:52:PRO:HA	1.99	0.44
3:B:169:ASP:OD1	3:B:202:ASN:ND2	2.51	0.44
3:B:1473:VAL:HG22	3:B:1474:THR:N	2.33	0.44
3:B:2505:LEU:HD23	3:B:2505:LEU:C	2.42	0.44
3:B:2528:LEU:HA	3:B:2531:MET:HE3	2.00	0.44
3:B:2830:GLY:N	3:B:2934:ASN:OD1	2.51	0.44
3:B:4909:LEU:HA	3:B:4912:VAL:HG22	1.99	0.44
3:C:673:ALA:O	3:C:681:THR:OG1	2.35	0.44
3:C:2239:TYR:O	3:C:2243:ILE:HG12	2.18	0.44
3:C:2528:LEU:HA	3:C:2531:MET:HE3	2.00	0.44
3:C:2645:LEU:HD13	3:C:2679:LEU:HD11	1.98	0.44
3:C:2746:VAL:HG22	3:C:2747:ILE:N	2.32	0.44
3:C:3270:VAL:HG12	3:C:3275:LEU:HD23	1.99	0.44
3:C:3394:LEU:HD23	3:C:3398:GLU:OE1	2.17	0.44
3:C:3407:TYR:O	3:C:3411:PRO:CD	2.66	0.44
3:C:3789:CYS:SG	3:C:3834:SER:OG	2.75	0.44
2:N:12:LEU:O	2:N:15:VAL:HG12	2.18	0.44
2:M:21:GLY:HA2	2:M:26:LYS:HA	2.00	0.44
2:O:50:LYS:NZ	2:O:51:ASP:OD2	2.50	0.44
2:J:12:LEU:O	2:J:15:VAL:HG12	2.18	0.44
3:D:2171:MET:SD	3:D:2229:MET:HE1	2.58	0.44
3:D:3406:LEU:HD11	3:D:3410:TYR:OH	2.18	0.44
3:D:3407:TYR:O	3:D:3411:PRO:CD	2.66	0.44
3:A:581:GLU:HG3	3:A:621:LEU:HD22	1.99	0.44
3:A:619:GLN:OE1	3:A:1679:ASN:ND2	2.49	0.44
3:A:921:TYR:CZ	3:A:925:MET:HE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3104:ILE:O	3:A:3107:MET:HB3	2.17	0.44
3:A:3380:LEU:HD21	3:A:3392:GLU:HA	2.00	0.44
3:A:3451:ASN:O	3:A:3454:ARG:HG2	2.18	0.44
3:A:3639:MET:O	3:A:3640:THR:C	2.61	0.44
3:B:875:LEU:HD11	3:B:1047:LEU:CD2	2.29	0.44
3:B:992:ASN:HD22	3:B:992:ASN:C	2.25	0.44
3:B:3380:LEU:HD21	3:B:3392:GLU:HA	2.00	0.44
3:C:1426:GLU:HG2	3:C:1427:ILE:N	2.33	0.44
3:C:2830:GLY:N	3:C:2934:ASN:OD1	2.51	0.44
3:C:3577:TYR:CZ	3:C:3583:ARG:HD3	2.53	0.44
3:D:2239:TYR:O	3:D:2243:ILE:HG12	2.18	0.43
3:D:2952:ILE:H	3:D:2952:ILE:HD12	1.82	0.43
3:A:3406:LEU:HD11	3:A:3410:TYR:OH	2.18	0.43
3:A:3511:ILE:HG23	3:A:3512:VAL:N	2.33	0.43
3:A:4766:ILE:HA	3:A:4769:ILE:HD12	1.99	0.43
3:A:4800:GLY:HA2	3:A:4806:PHE:HB2	1.99	0.43
3:B:73:SER:O	3:B:100:ARG:NH1	2.51	0.43
3:B:1120:ASP:OD1	3:B:1120:ASP:N	2.50	0.43
3:B:2171:MET:SD	3:B:2229:MET:HE1	2.58	0.43
3:B:2758:LYS:O	3:B:2761:GLU:HG3	2.18	0.43
3:B:3407:TYR:O	3:B:3411:PRO:CD	2.66	0.43
3:B:3789:CYS:SG	3:B:3834:SER:OG	2.75	0.43
3:C:575:VAL:O	3:C:579:ILE:HG12	2.18	0.43
3:C:690:SER:N	3:C:777:LEU:O	2.52	0.43
3:C:3451:ASN:O	3:C:3454:ARG:HG2	2.18	0.43
2:L:12:LEU:O	2:L:15:VAL:HG12	2.18	0.43
2:P:20:SER:HB3	2:P:27:TYR:HA	1.99	0.43
3:D:73:SER:O	3:D:100:ARG:NH1	2.51	0.43
3:D:2199:MET:HE2	3:D:2199:MET:HA	2.01	0.43
3:D:2528:LEU:HA	3:D:2531:MET:HE3	2.00	0.43
3:D:2758:LYS:O	3:D:2761:GLU:HG3	2.18	0.43
3:D:4173:ILE:HD12	3:D:4173:ILE:H	1.83	0.43
3:D:4800:GLY:HA2	3:D:4806:PHE:HB2	1.99	0.43
3:A:992:ASN:C	3:A:992:ASN:HD22	2.25	0.43
3:A:2239:TYR:O	3:A:2243:ILE:HG12	2.18	0.43
3:A:2268:MET:O	3:A:2269:GLN:HB3	2.18	0.43
3:B:1090:TYR:N	3:B:1225:GLU:O	2.50	0.43
3:B:2930:PHE:HA	3:B:2933:MET:HG3	1.99	0.43
3:B:3869:ILE:O	3:B:3869:ILE:HG22	2.17	0.43
3:C:1014:ILE:H	3:C:1014:ILE:HD12	1.84	0.43
3:C:2764:HIS:NE2	3:C:2791:MET:SD	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3639:MET:O	3:C:3640:THR:C	2.61	0.43
2:K:74:GLU:O	2:K:78:LEU:HD13	2.19	0.43
2:L:48:VAL:HG23	2:L:49:GLN:N	2.34	0.43
2:P:48:VAL:HG23	2:P:49:GLN:N	2.33	0.43
3:D:921:TYR:CZ	3:D:925:MET:HE3	2.53	0.43
3:A:1120:ASP:N	3:A:1120:ASP:OD1	2.50	0.43
3:A:1426:GLU:HG2	3:A:1427:ILE:N	2.33	0.43
3:A:1473:VAL:HG22	3:A:1474:THR:N	2.33	0.43
3:A:2624:LEU:O	3:A:2628:VAL:HG23	2.18	0.43
3:A:4155:GLU:OE2	3:A:4183:ARG:NH1	2.50	0.43
3:A:4227:GLU:N	3:A:4227:GLU:OE2	2.51	0.43
3:B:1492:ASN:OD1	3:B:1493:CYS:N	2.51	0.43
3:B:4227:GLU:N	3:B:4227:GLU:OE2	2.51	0.43
3:C:245:LEU:HD23	3:C:301:VAL:HG12	1.99	0.43
3:C:1473:VAL:HG22	3:C:1474:THR:N	2.33	0.43
3:C:2268:MET:O	3:C:2269:GLN:HB3	2.18	0.43
3:C:3380:LEU:HD21	3:C:3392:GLU:HA	2.00	0.43
3:C:3406:LEU:HD11	3:C:3410:TYR:OH	2.18	0.43
3:C:3937:TYR:HD1	3:C:4002:MET:HE3	1.84	0.43
2:M:74:GLU:O	2:M:78:LEU:HD13	2.19	0.43
2:O:21:GLY:HA2	2:O:26:LYS:HA	2.00	0.43
2:J:20:SER:HB3	2:J:27:TYR:HA	1.99	0.43
3:D:228:MET:HE1	3:A:157:GLN:H	1.84	0.43
3:D:978:LEU:HD21	3:D:1045:ARG:HG2	2.00	0.43
3:D:3337:LYS:HD2	3:D:3465:ILE:HD11	2.01	0.43
3:D:4004:MET:HE3	3:D:4113:PHE:CZ	2.54	0.43
3:D:4846:VAL:HG11	3:D:4885:MET:HG2	2.01	0.43
3:A:351:HIS:O	3:A:355:GLY:N	2.44	0.43
3:A:784:PHE:CG	3:A:788:ILE:HD11	2.53	0.43
3:A:2764:HIS:NE2	3:A:2791:MET:SD	2.92	0.43
3:A:3324:ILE:HG23	3:A:3336:MET:SD	2.59	0.43
3:A:3526:CYS:SG	3:A:3527:ALA:N	2.92	0.43
3:A:3937:TYR:HD1	3:A:4002:MET:HE3	1.83	0.43
3:A:4846:VAL:HG11	3:A:4885:MET:HG2	2.01	0.43
3:B:784:PHE:CG	3:B:788:ILE:HD11	2.54	0.43
3:B:1462:ASP:OD2	3:B:1469:LYS:NZ	2.47	0.43
3:B:1529:THR:OG1	3:B:1536:GLU:OE2	2.35	0.43
3:B:2199:MET:HE2	3:B:2199:MET:HA	2.01	0.43
3:B:3320:ILE:O	3:B:3324:ILE:CD1	2.65	0.43
3:B:3337:LYS:HD2	3:B:3465:ILE:HD11	2.01	0.43
3:C:2758:LYS:O	3:C:2761:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2952:ILE:HD12	3:C:2952:ILE:H	1.82	0.43
3:C:3324:ILE:HG23	3:C:3336:MET:SD	2.59	0.43
3:C:3933:ILE:HG22	3:C:3998:VAL:HG11	1.99	0.43
3:C:4004:MET:HE3	3:C:4113:PHE:CZ	2.54	0.43
2:P:14:ASN:O	2:P:17:HIS:ND1	2.52	0.43
2:P:51:ASP:HB3	2:P:54:ALA:HB3	2.01	0.43
3:D:575:VAL:O	3:D:579:ILE:HG12	2.18	0.43
3:D:690:SER:N	3:D:777:LEU:O	2.52	0.43
3:D:951:LEU:CB	3:D:971:LEU:HD23	2.45	0.43
3:D:1195:LEU:N	3:D:1195:LEU:HD12	2.34	0.43
3:D:1492:ASN:OD1	3:D:1493:CYS:N	2.51	0.43
3:D:2764:HIS:NE2	3:D:2791:MET:SD	2.92	0.43
3:D:3227:GLU:C	3:D:3229:ALA:H	2.27	0.43
3:D:3607:LEU:O	3:D:3607:LEU:HD23	2.19	0.43
3:A:73:SER:O	3:A:100:ARG:NH1	2.51	0.43
3:A:1195:LEU:HD12	3:A:1195:LEU:N	2.34	0.43
3:A:2199:MET:HA	3:A:2199:MET:HE2	2.01	0.43
3:B:1014:ILE:H	3:B:1014:ILE:HD12	1.84	0.43
3:B:2239:TYR:CE2	3:B:2243:ILE:HD11	2.54	0.43
3:B:3086:PRO:O	3:B:3089:VAL:HG22	2.19	0.43
3:B:3511:ILE:HG23	3:B:3512:VAL:N	2.33	0.43
3:B:4173:ILE:H	3:B:4173:ILE:HD12	1.83	0.43
3:B:4638:GLU:HB3	3:B:4639:PRO:HD3	2.01	0.43
3:B:4846:VAL:HG11	3:B:4885:MET:HG2	2.01	0.43
3:C:1222:GLU:OE1	3:C:1222:GLU:N	2.49	0.43
3:C:1492:ASN:OD1	3:C:1493:CYS:N	2.51	0.43
3:C:2239:TYR:CE2	3:C:2243:ILE:HD11	2.54	0.43
3:C:3320:ILE:O	3:C:3324:ILE:CD1	2.65	0.43
3:C:3337:LYS:HD2	3:C:3465:ILE:HD11	2.01	0.43
3:C:3526:CYS:SG	3:C:3527:ALA:N	2.92	0.43
3:C:4909:LEU:HA	3:C:4912:VAL:HG22	1.99	0.43
2:P:12:LEU:O	2:P:15:VAL:HG12	2.18	0.43
2:J:48:VAL:HG23	2:J:49:GLN:N	2.33	0.43
3:D:169:ASP:OD1	3:D:202:ASN:ND2	2.51	0.43
3:D:576:LEU:HD22	3:D:610:CYS:HB2	1.99	0.43
3:D:581:GLU:HG3	3:D:621:LEU:HD22	1.99	0.43
3:D:784:PHE:CG	3:D:788:ILE:HD11	2.54	0.43
3:D:1014:ILE:H	3:D:1014:ILE:HD12	1.84	0.43
3:D:3320:ILE:O	3:D:3324:ILE:CD1	2.65	0.43
3:D:3722:LEU:HD11	3:D:3726:TYR:HE2	1.84	0.43
3:A:576:LEU:HD22	3:A:610:CYS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1014:ILE:H	3:A:1014:ILE:HD12	1.84	0.43
3:A:1080:LYS:HA	3:A:1190:LEU:HD21	2.01	0.43
3:A:1496:VAL:HG12	3:A:1539:THR:HG21	2.00	0.43
3:A:3407:TYR:O	3:A:3411:PRO:CD	2.66	0.43
3:A:4173:ILE:H	3:A:4173:ILE:HD12	1.83	0.43
3:B:1195:LEU:N	3:B:1195:LEU:HD12	2.34	0.43
3:B:2268:MET:O	3:B:2269:GLN:HB3	2.18	0.43
3:B:2755:PHE:CZ	3:B:2931:LEU:HD23	2.54	0.43
3:C:73:SER:O	3:C:100:ARG:NH1	2.51	0.43
3:C:3157:VAL:HG13	3:C:3158:ILE:N	2.34	0.43
3:C:3607:LEU:O	3:C:3607:LEU:HD23	2.19	0.43
3:C:4638:GLU:HB3	3:C:4639:PRO:HD3	2.01	0.43
2:I:5:LEU:HD21	2:J:15:VAL:HG11	2.01	0.43
2:I:74:GLU:O	2:I:78:LEU:HD13	2.19	0.43
2:J:51:ASP:HB3	2:J:54:ALA:HB3	2.01	0.43
3:D:575:VAL:HA	3:D:578:ILE:HG22	2.01	0.43
3:D:2384:ALA:HB1	3:D:2423:ILE:CG2	2.49	0.43
3:D:2695:GLU:OE2	2:O:27:TYR:OH	2.37	0.43
3:D:2930:PHE:HA	3:D:2933:MET:HG3	1.99	0.43
3:D:3324:ILE:HG23	3:D:3336:MET:SD	2.59	0.43
3:D:3937:TYR:HD1	3:D:4002:MET:HE3	1.84	0.43
3:D:4935:ILE:HG12	3:A:4932:GLY:HA2	2.00	0.43
3:A:2830:GLY:N	3:A:2934:ASN:OD1	2.51	0.43
3:B:215:VAL:CG1	3:B:275:LEU:HD12	2.47	0.43
3:B:1080:LYS:HA	3:B:1190:LEU:HD21	2.00	0.43
3:B:3157:VAL:HG13	3:B:3158:ILE:N	2.34	0.43
3:C:784:PHE:CG	3:C:788:ILE:HD11	2.54	0.43
3:C:914:LEU:HD23	3:C:919:ARG:HA	2.01	0.43
3:C:2755:PHE:CZ	3:C:2931:LEU:HD23	2.54	0.43
3:C:2883:TYR:HB2	3:C:2920:ASP:OD2	2.19	0.43
3:C:3373:VAL:HG22	3:C:3399:PHE:CE1	2.53	0.43
3:C:4846:VAL:HG11	3:C:4885:MET:HG2	2.01	0.43
2:L:46:LEU:HD23	2:L:47:ASP:N	2.34	0.43
2:P:62:LEU:HD12	2:P:70:VAL:HG11	2.01	0.43
3:A:2758:LYS:O	3:A:2761:GLU:HG3	2.18	0.43
3:A:3157:VAL:HG13	3:A:3158:ILE:N	2.34	0.43
3:A:3337:LYS:HD2	3:A:3465:ILE:HD11	2.01	0.43
3:B:2764:HIS:NE2	3:B:2791:MET:SD	2.92	0.43
3:B:3933:ILE:HG22	3:B:3998:VAL:HG11	1.99	0.43
3:C:575:VAL:HA	3:C:578:ILE:HG22	2.01	0.43
3:C:992:ASN:C	3:C:992:ASN:HD22	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2199:MET:HE2	3:C:2199:MET:HA	2.01	0.43
3:C:3086:PRO:O	3:C:3089:VAL:HG22	2.19	0.43
2:N:48:VAL:HG23	2:N:49:GLN:N	2.34	0.43
2:O:5:LEU:HD21	2:P:15:VAL:HG11	2.01	0.43
1:E:36:LYS:NZ	1:E:42:ASP:OD2	2.39	0.43
2:J:46:LEU:HD23	2:J:47:ASP:N	2.34	0.43
3:D:484:MET:HE2	3:D:484:MET:CA	2.46	0.43
3:D:2247:ASN:O	3:D:2250:SER:OG	2.28	0.43
3:D:3451:ASN:O	3:D:3454:ARG:HG2	2.18	0.43
3:D:3526:CYS:SG	3:D:3527:ALA:N	2.92	0.43
3:D:3639:MET:O	3:D:3640:THR:C	2.61	0.43
3:D:4671:ARG:NH1	3:D:4780:VAL:HG22	2.34	0.43
3:A:2528:LEU:HA	3:A:2531:MET:HE3	2.00	0.43
3:A:2755:PHE:CZ	3:A:2931:LEU:HD23	2.54	0.43
3:A:2930:PHE:HA	3:A:2933:MET:HG3	1.99	0.43
3:A:4004:MET:HE3	3:A:4113:PHE:CZ	2.54	0.43
3:B:234:ILE:O	3:B:258:ARG:NH2	2.47	0.43
3:B:961:MET:SD	3:B:962:MET:O	2.77	0.43
3:B:3324:ILE:HG23	3:B:3336:MET:SD	2.59	0.43
3:B:3722:LEU:HD11	3:B:3726:TYR:HE2	1.84	0.43
3:B:3847:LEU:CD1	3:C:77:ARG:HE	2.32	0.43
3:B:4004:MET:HE3	3:B:4113:PHE:CZ	2.54	0.43
3:C:880:HIS:CE1	3:C:909:VAL:O	2.72	0.43
3:C:2384:ALA:HB1	3:C:2423:ILE:CG2	2.49	0.43
2:N:46:LEU:HD23	2:N:47:ASP:N	2.34	0.43
3:D:961:MET:SD	3:D:962:MET:O	2.77	0.43
3:D:1106:ALA:HB2	3:D:1192:VAL:HG11	2.01	0.43
3:A:880:HIS:CE1	3:A:909:VAL:O	2.72	0.43
3:A:2523:LEU:HD23	3:A:2523:LEU:C	2.44	0.43
3:A:3227:GLU:C	3:A:3229:ALA:H	2.27	0.43
3:A:4638:GLU:HB3	3:A:4639:PRO:HD3	2.01	0.43
3:B:238:ASP:OD1	3:B:238:ASP:O	2.37	0.43
3:B:245:LEU:HD23	3:B:301:VAL:HG12	1.99	0.43
3:B:385:MET:HE1	3:C:169:ASP:OD2	2.18	0.43
3:B:575:VAL:HA	3:B:578:ILE:HG22	2.01	0.43
3:B:2949:THR:O	3:B:2950:SER:C	2.62	0.43
3:B:3373:VAL:HG22	3:B:3399:PHE:CE1	2.53	0.43
3:C:1106:ALA:HB2	3:C:1192:VAL:HG11	2.01	0.43
3:C:1437:SER:OG	3:C:1566:GLU:HB2	2.19	0.43
3:C:2523:LEU:HD23	3:C:2523:LEU:C	2.44	0.43
3:C:3227:GLU:C	3:C:3229:ALA:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4964:ASP:OD1	3:C:4965:TYR:N	2.47	0.43
2:N:14:ASN:O	2:N:17:HIS:ND1	2.52	0.43
2:O:29:LEU:HB2	2:O:70:VAL:HB	2.01	0.43
3:D:77:ARG:HE	3:C:3847:LEU:CD1	2.32	0.42
3:D:238:ASP:OD1	3:D:238:ASP:O	2.37	0.42
3:D:2239:TYR:CE2	3:D:2243:ILE:HD11	2.54	0.42
3:A:690:SER:N	3:A:777:LEU:O	2.52	0.42
3:A:2384:ALA:HB1	3:A:2423:ILE:CG2	2.49	0.42
3:A:3320:ILE:O	3:A:3324:ILE:CD1	2.65	0.42
3:B:880:HIS:CE1	3:B:909:VAL:O	2.72	0.42
3:B:1426:GLU:HG2	3:B:1427:ILE:N	2.33	0.42
3:B:2883:TYR:HB2	3:B:2920:ASP:OD2	2.19	0.42
3:C:4671:ARG:NH1	3:C:4780:VAL:HG22	2.34	0.42
3:C:4766:ILE:HA	3:C:4769:ILE:HD12	1.99	0.42
2:K:29:LEU:HB2	2:K:70:VAL:HB	2.01	0.42
2:N:15:VAL:HG11	2:M:5:LEU:HD21	2.01	0.42
2:P:16:PHE:HE2	2:P:27:TYR:CE2	2.37	0.42
2:P:46:LEU:HD23	2:P:47:ASP:N	2.34	0.42
2:J:14:ASN:O	2:J:17:HIS:ND1	2.52	0.42
3:D:880:HIS:CE1	3:D:909:VAL:O	2.72	0.42
3:D:1496:VAL:HG12	3:D:1539:THR:HG21	2.00	0.42
3:D:2523:LEU:HD23	3:D:2523:LEU:C	2.44	0.42
3:D:3363:ILE:HG23	3:D:3438:MET:HE2	2.00	0.42
8:D:8007:PCW:H232	8:D:8007:PCW:H20	1.76	0.42
3:A:575:VAL:HA	3:A:578:ILE:HG22	2.00	0.42
3:A:961:MET:SD	3:A:962:MET:O	2.77	0.42
3:A:1462:ASP:OD2	3:A:1469:LYS:NZ	2.47	0.42
3:A:2239:TYR:CE2	3:A:2243:ILE:HD11	2.54	0.42
3:A:2883:TYR:HB2	3:A:2920:ASP:OD2	2.19	0.42
3:A:2918:ALA:O	3:A:2922:GLU:CD	2.62	0.42
3:A:3356:ARG:HA	3:A:3360:ILE:HD12	2.01	0.42
3:A:3363:ILE:HG23	3:A:3438:MET:HE2	2.00	0.42
3:B:1106:ALA:HB2	3:B:1192:VAL:HG11	2.01	0.42
3:B:2384:ALA:HB1	3:B:2423:ILE:CG2	2.49	0.42
3:B:3405:ASP:O	3:B:3409:LEU:HD23	2.19	0.42
3:B:3645:LEU:CD2	3:B:3653:MET:HE1	2.49	0.42
3:C:961:MET:SD	3:C:962:MET:O	2.77	0.42
3:C:2695:GLU:OE2	2:M:27:TYR:OH	2.37	0.42
3:C:3440:GLY:O	3:C:3444:ILE:HG12	2.19	0.42
3:C:3722:LEU:HD11	3:C:3726:TYR:HE2	1.84	0.42
2:N:16:PHE:HE2	2:N:27:TYR:CE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:62:LEU:HD21	2:O:70:VAL:HG11	2.01	0.42
2:O:74:GLU:O	2:O:78:LEU:HD13	2.18	0.42
2:J:16:PHE:HE2	2:J:27:TYR:CE2	2.37	0.42
3:D:234:ILE:O	3:D:258:ARG:NH2	2.47	0.42
3:D:1090:TYR:HD1	3:D:1153:MET:HG2	1.84	0.42
3:D:3356:ARG:HA	3:D:3360:ILE:HD12	2.01	0.42
3:D:3440:GLY:O	3:D:3444:ILE:HG12	2.19	0.42
3:A:684:ARG:NH1	3:A:708:VAL:O	2.43	0.42
3:A:2197:ASN:OD1	3:A:2200:ARG:NH2	2.46	0.42
3:A:3645:LEU:CD2	3:A:3653:MET:HE1	2.49	0.42
3:A:4671:ARG:NH1	3:A:4780:VAL:HG22	2.34	0.42
3:B:575:VAL:O	3:B:579:ILE:HG12	2.18	0.42
3:B:914:LEU:HD23	3:B:919:ARG:HA	2.01	0.42
3:B:3607:LEU:HD23	3:B:3607:LEU:O	2.19	0.42
3:B:4671:ARG:NH1	3:B:4780:VAL:HG22	2.34	0.42
3:B:4766:ILE:HA	3:B:4769:ILE:HD12	1.99	0.42
3:C:914:LEU:O	3:C:919:ARG:NH2	2.53	0.42
3:C:978:LEU:HD21	3:C:1045:ARG:HG2	2.00	0.42
3:C:1120:ASP:OD1	3:C:1120:ASP:N	2.50	0.42
3:C:2438:ALA:HB2	3:C:2510:VAL:HG22	2.01	0.42
3:C:2930:PHE:HA	3:C:2933:MET:HG3	1.99	0.42
2:K:5:LEU:HD21	2:L:15:VAL:HG11	2.01	0.42
2:K:21:GLY:HA2	2:K:26:LYS:HA	2.00	0.42
2:I:27:TYR:OH	3:A:2695:GLU:OE2	2.37	0.42
3:D:2755:PHE:CZ	3:D:2931:LEU:HD23	2.54	0.42
3:D:3645:LEU:CD2	3:D:3653:MET:HE1	2.49	0.42
3:A:352:VAL:HG23	3:A:353:ALA:N	2.35	0.42
3:A:1106:ALA:HB2	3:A:1192:VAL:HG11	2.01	0.42
3:A:4649:THR:HG1	3:A:4801:HIS:CD2	2.35	0.42
3:B:978:LEU:HD21	3:B:1045:ARG:HG2	2.00	0.42
3:B:4220:PHE:CZ	3:B:4237:PHE:HA	2.55	0.42
3:C:1195:LEU:HD12	3:C:1195:LEU:N	2.34	0.42
2:I:29:LEU:HB2	2:I:70:VAL:HB	2.01	0.42
2:J:5:LEU:HD23	2:J:9:MET:CE	2.44	0.42
3:D:102:LEU:HD12	3:D:151:MET:SD	2.60	0.42
3:D:351:HIS:O	3:D:355:GLY:N	2.44	0.42
3:D:1120:ASP:N	3:D:1120:ASP:OD1	2.50	0.42
3:D:2438:ALA:HB2	3:D:2510:VAL:HG22	2.01	0.42
3:D:2624:LEU:O	3:D:2628:VAL:HG23	2.18	0.42
3:D:3157:VAL:HG13	3:D:3158:ILE:N	2.34	0.42
3:D:4638:GLU:HB3	3:D:4639:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:234:ILE:O	3:A:258:ARG:NH2	2.46	0.42
3:A:238:ASP:OD1	3:A:238:ASP:O	2.37	0.42
3:A:310:THR:HG23	3:A:311:LYS:N	2.34	0.42
3:A:575:VAL:O	3:A:579:ILE:HG12	2.18	0.42
3:A:1437:SER:OG	3:A:1566:GLU:HB2	2.19	0.42
3:A:3086:PRO:O	3:A:3089:VAL:HG22	2.19	0.42
3:A:3789:CYS:SG	3:A:3834:SER:OG	2.75	0.42
3:B:690:SER:N	3:B:777:LEU:O	2.51	0.42
3:B:3135:VAL:HG13	3:B:3136:ALA:N	2.35	0.42
3:C:984:THR:C	3:C:988:ARG:HE	2.27	0.42
3:C:1080:LYS:HA	3:C:1190:LEU:HD21	2.00	0.42
3:C:3771:SER:OG	3:C:3775:ASN:OD1	2.33	0.42
2:L:16:PHE:HE2	2:L:27:TYR:CE2	2.37	0.42
2:I:21:GLY:HA2	2:I:26:LYS:HA	2.00	0.42
2:I:84:VAL:CG1	2:J:72:PHE:HE2	2.23	0.42
3:D:352:VAL:HG23	3:D:353:ALA:N	2.35	0.42
3:D:1080:LYS:HA	3:D:1190:LEU:HD21	2.00	0.42
3:D:2160:LEU:HD13	3:D:2204:MET:HG2	2.02	0.42
3:D:3937:TYR:HD1	3:D:4002:MET:CE	2.33	0.42
3:A:102:LEU:HD12	3:A:151:MET:SD	2.60	0.42
3:A:1090:TYR:HD1	3:A:1153:MET:HG2	1.84	0.42
3:A:2679:LEU:HD23	3:A:2679:LEU:C	2.45	0.42
3:A:3937:TYR:HD1	3:A:4002:MET:CE	2.33	0.42
3:B:1437:SER:OG	3:B:1566:GLU:HB2	2.19	0.42
3:B:2523:LEU:C	3:B:2523:LEU:HD23	2.44	0.42
3:B:3227:GLU:C	3:B:3229:ALA:H	2.27	0.42
3:B:3638:ARG:CZ	2:K:61:GLU:O	2.67	0.42
3:C:238:ASP:O	3:C:238:ASP:OD1	2.37	0.42
3:C:2679:LEU:HD23	3:C:2679:LEU:C	2.45	0.42
3:C:3135:VAL:HG13	3:C:3136:ALA:N	2.35	0.42
3:C:3356:ARG:HA	3:C:3360:ILE:HD12	2.01	0.42
3:C:3645:LEU:CD2	3:C:3653:MET:HE1	2.49	0.42
2:N:51:ASP:HB3	2:N:54:ALA:HB3	2.01	0.42
2:M:29:LEU:HB2	2:M:70:VAL:HB	2.01	0.42
2:I:62:LEU:HD21	2:I:70:VAL:HG11	2.01	0.42
2:J:62:LEU:HD12	2:J:70:VAL:HG11	2.00	0.42
1:F:60:TRP:O	1:F:61:GLU:C	2.63	0.42
3:D:169:ASP:OD2	3:C:385:MET:HE1	2.18	0.42
3:D:2883:TYR:HB2	3:D:2920:ASP:OD2	2.19	0.42
3:D:2918:ALA:O	3:D:2922:GLU:CD	2.62	0.42
3:D:3086:PRO:O	3:D:3089:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3135:VAL:HG13	3:D:3136:ALA:N	2.35	0.42
3:A:2868:LEU:HD22	3:A:2872:LEU:HB3	2.02	0.42
3:A:3722:LEU:HD11	3:A:3726:TYR:HE2	1.84	0.42
3:B:351:HIS:O	3:B:355:GLY:N	2.44	0.42
3:B:352:VAL:HG23	3:B:353:ALA:N	2.34	0.42
3:B:1496:VAL:HG12	3:B:1539:THR:HG21	2.00	0.42
3:B:3526:CYS:SG	3:B:3527:ALA:N	2.92	0.42
3:C:102:LEU:HD12	3:C:151:MET:SD	2.60	0.42
3:C:1496:VAL:HG12	3:C:1539:THR:HG21	2.00	0.42
3:C:2160:LEU:HD13	3:C:2204:MET:HG2	2.02	0.42
2:L:14:ASN:O	2:L:17:HIS:ND1	2.52	0.42
2:L:62:LEU:HD12	2:L:70:VAL:HG11	2.01	0.42
2:N:62:LEU:HD12	2:N:70:VAL:HG11	2.01	0.42
3:D:988:ARG:NH1	3:D:1059:GLN:OE1	2.53	0.42
3:D:3405:ASP:O	3:D:3409:LEU:HD23	2.19	0.42
3:D:3994:GLY:O	3:D:3998:VAL:HG23	2.20	0.42
3:A:914:LEU:O	3:A:919:ARG:NH2	2.53	0.42
3:A:3405:ASP:O	3:A:3409:LEU:HD23	2.19	0.42
3:A:3440:GLY:O	3:A:3444:ILE:HG12	2.19	0.42
3:A:3724:MET:HE2	3:A:3795:ALA:HB1	2.02	0.42
3:A:3847:LEU:CD1	3:B:77:ARG:HE	2.33	0.42
3:A:4220:PHE:CZ	3:A:4237:PHE:HA	2.55	0.42
3:B:914:LEU:O	3:B:919:ARG:NH2	2.53	0.42
3:B:1090:TYR:HD1	3:B:1153:MET:HG2	1.84	0.42
3:B:2679:LEU:HD23	3:B:2679:LEU:C	2.45	0.42
3:B:2695:GLU:OE2	2:K:27:TYR:OH	2.37	0.42
3:B:3937:TYR:HD1	3:B:4002:MET:HE3	1.83	0.42
3:C:2698:ARG:NH2	2:M:17:HIS:CG	2.88	0.42
3:C:3405:ASP:O	3:C:3409:LEU:HD23	2.19	0.42
3:C:4220:PHE:CZ	3:C:4237:PHE:HA	2.55	0.42
2:L:51:ASP:HB3	2:L:54:ALA:HB3	2.01	0.42
3:D:914:LEU:O	3:D:919:ARG:NH2	2.53	0.42
3:D:1521:VAL:O	3:D:1521:VAL:HG23	2.19	0.42
3:D:2204:MET:O	3:D:2207:THR:N	2.53	0.42
3:D:2698:ARG:NH2	2:O:17:HIS:CG	2.88	0.42
3:A:15:LEU:HD12	3:A:166:VAL:HG22	2.02	0.42
3:A:649:ILE:HG23	3:A:815:ALA:HB3	2.02	0.42
3:A:2281:VAL:O	3:A:2281:VAL:HG22	2.20	0.42
3:A:3135:VAL:HG13	3:A:3136:ALA:N	2.35	0.42
3:A:3946:ILE:HD11	3:A:4005:LYS:HE3	2.02	0.42
3:B:2654:LYS:HD2	3:B:2658:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2918:ALA:O	3:B:2922:GLU:CD	2.62	0.42
3:B:3587:ALA:HA	3:B:3593:ILE:HD11	2.02	0.42
3:B:3946:ILE:HD11	3:B:4005:LYS:HE3	2.02	0.42
3:B:4678:LYS:HD3	3:B:4684:LEU:HD22	2.02	0.42
2:O:84:VAL:CG1	2:P:72:PHE:HE2	2.23	0.42
3:D:243:ARG:NH1	3:D:482:GLU:OE2	2.48	0.42
3:D:914:LEU:HD23	3:D:919:ARG:HA	2.01	0.42
3:D:1437:SER:OG	3:D:1566:GLU:HB2	2.19	0.42
3:D:3638:ARG:CZ	2:O:61:GLU:O	2.67	0.42
3:D:4096:PHE:CZ	3:D:4100:MET:HE3	2.55	0.42
3:A:2438:ALA:HB2	3:A:2510:VAL:HG22	2.01	0.42
3:A:2939:THR:HG22	3:A:2941:GLY:H	1.85	0.42
3:A:3607:LEU:O	3:A:3607:LEU:HD23	2.19	0.42
3:A:3936:PHE:CD2	3:A:3954:PHE:HE1	2.38	0.42
3:B:2939:THR:HG22	3:B:2941:GLY:H	1.85	0.42
3:B:3937:TYR:HD1	3:B:4002:MET:CE	2.33	0.42
3:B:4993:LEU:HA	3:B:4993:LEU:HD23	1.83	0.42
3:C:352:VAL:HG23	3:C:353:ALA:N	2.35	0.42
3:C:940:VAL:HG12	3:C:1054:ILE:HG22	2.02	0.42
3:C:2918:ALA:O	3:C:2922:GLU:CD	2.62	0.42
3:C:3551:ARG:HD3	3:C:3598:GLN:HG3	2.02	0.42
3:C:3587:ALA:HA	3:C:3593:ILE:HD11	2.02	0.42
2:L:29:LEU:CD1	2:L:33:GLU:HB3	2.50	0.42
2:L:75:TYR:O	2:L:76:VAL:C	2.62	0.42
3:D:2420:GLY:O	3:D:2423:ILE:HG22	2.20	0.41
3:D:2679:LEU:C	3:D:2679:LEU:HD23	2.45	0.41
3:D:2939:THR:HG22	3:D:2941:GLY:H	1.85	0.41
3:D:3343:ALA:O	3:D:3346:ILE:HG12	2.20	0.41
3:D:4678:LYS:HD3	3:D:4684:LEU:HD22	2.02	0.41
3:A:1521:VAL:O	3:A:1521:VAL:HG23	2.19	0.41
3:B:1521:VAL:HG23	3:B:1521:VAL:O	2.19	0.41
3:B:2978:LEU:HA	3:B:2981:VAL:HG22	2.02	0.41
3:B:3440:GLY:O	3:B:3444:ILE:HG12	2.19	0.41
3:C:649:ILE:HG23	3:C:815:ALA:HB3	2.02	0.41
3:C:867:HIS:O	3:C:1052:TYR:OH	2.38	0.41
3:C:2694:GLN:CD	2:N:87:ASN:HD21	2.28	0.41
3:C:2949:THR:O	3:C:2950:SER:C	2.62	0.41
3:C:3937:TYR:HD1	3:C:4002:MET:CE	2.33	0.41
3:D:157:GLN:H	3:C:228:MET:HE1	1.85	0.41
3:D:905:HIS:NE2	3:D:907:CYS:HB2	2.35	0.41
3:D:984:THR:C	3:D:988:ARG:HE	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2694:GLN:CD	2:P:87:ASN:HD21	2.28	0.41
3:D:3355:LEU:HD11	3:D:3431:ASN:ND2	2.35	0.41
3:D:4220:PHE:CZ	3:D:4237:PHE:HA	2.55	0.41
3:A:988:ARG:NH1	3:A:1059:GLN:OE1	2.53	0.41
3:A:3587:ALA:HA	3:A:3593:ILE:HD11	2.02	0.41
3:A:3730:MET:O	3:A:3733:SER:OG	2.31	0.41
3:A:3974:GLY:N	3:A:3975:PRO:HA	2.35	0.41
3:A:4942:ARG:NE	3:B:4936:ASP:OD1	2.52	0.41
3:B:243:ARG:NH1	3:B:482:GLU:OE2	2.48	0.41
3:B:310:THR:HG23	3:B:311:LYS:N	2.35	0.41
3:B:2438:ALA:HB2	3:B:2510:VAL:HG22	2.01	0.41
3:B:3513:ALA:O	3:B:3517:LYS:HG2	2.20	0.41
3:B:3724:MET:HE2	3:B:3795:ALA:HB1	2.02	0.41
3:C:1090:TYR:HD1	3:C:1153:MET:HG2	1.84	0.41
3:D:221:LEU:HD21	3:D:263:LEU:HD11	2.02	0.41
3:D:310:THR:HG23	3:D:311:LYS:N	2.35	0.41
3:D:2949:THR:O	3:D:2950:SER:C	2.62	0.41
3:D:2978:LEU:HA	3:D:2981:VAL:HG22	2.02	0.41
3:D:3131:THR:O	3:D:3135:VAL:HG12	2.21	0.41
3:A:1304:CYS:O	3:A:1305:THR:OG1	2.36	0.41
3:A:2654:LYS:HD2	3:A:2658:LEU:HD11	2.02	0.41
3:A:2768:ALA:HB3	3:A:2858:PRO:HB3	2.03	0.41
3:A:2949:THR:O	3:A:2950:SER:C	2.62	0.41
3:A:3355:LEU:HD11	3:A:3431:ASN:ND2	2.35	0.41
3:A:3994:GLY:O	3:A:3998:VAL:HG23	2.20	0.41
3:B:228:MET:HE1	3:C:157:GLN:H	1.86	0.41
3:B:760:ILE:HG23	3:B:760:ILE:O	2.20	0.41
3:B:986:VAL:CG2	3:B:1044:VAL:HG11	2.50	0.41
3:B:2698:ARG:NH2	2:K:17:HIS:CG	2.88	0.41
3:C:986:VAL:CG2	3:C:1044:VAL:HG11	2.50	0.41
3:C:1521:VAL:HG23	3:C:1521:VAL:O	2.19	0.41
3:C:1927:LEU:HB3	3:C:1940:MET:HE3	2.03	0.41
3:C:2281:VAL:O	3:C:2281:VAL:HG22	2.20	0.41
3:C:2791:MET:SD	3:C:2791:MET:O	2.79	0.41
3:C:2978:LEU:HA	3:C:2981:VAL:HG22	2.02	0.41
3:C:3343:ALA:O	3:C:3346:ILE:HG12	2.20	0.41
3:C:3638:ARG:CZ	2:M:61:GLU:O	2.67	0.41
2:M:62:LEU:HD21	2:M:70:VAL:HG11	2.01	0.41
2:M:73:LYS:O	2:M:76:VAL:HG22	2.21	0.41
2:J:87:ASN:HD21	3:A:2694:GLN:CD	2.28	0.41
3:D:1927:LEU:HB3	3:D:1940:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2925:GLN:OE1	3:D:2929:LYS:CE	2.68	0.41
3:D:3683:GLU:OE1	3:D:3683:GLU:O	2.39	0.41
3:D:4090:LEU:HD13	3:D:4127:ASN:HA	2.02	0.41
3:A:760:ILE:HG23	3:A:760:ILE:O	2.20	0.41
3:A:2420:GLY:O	3:A:2423:ILE:HG22	2.20	0.41
3:A:3847:LEU:HD11	3:A:3935:ASP:HB3	2.03	0.41
3:B:15:LEU:HD12	3:B:166:VAL:HG22	2.02	0.41
3:B:221:LEU:HD21	3:B:263:LEU:HD11	2.02	0.41
3:B:940:VAL:HG12	3:B:1054:ILE:HG22	2.02	0.41
3:B:988:ARG:NH1	3:B:1059:GLN:OE1	2.53	0.41
3:B:2281:VAL:HG22	3:B:2281:VAL:O	2.20	0.41
3:B:2698:ARG:HH21	2:K:17:HIS:CE1	2.38	0.41
3:B:3637:PHE:HE2	2:K:82:LEU:HD22	1.86	0.41
3:B:4552:TYR:O	3:B:4556:ASN:ND2	2.52	0.41
3:C:2420:GLY:O	3:C:2423:ILE:HG22	2.20	0.41
3:C:2654:LYS:HD2	3:C:2658:LEU:HD11	2.02	0.41
3:C:2939:THR:HG22	3:C:2941:GLY:H	1.85	0.41
3:C:3724:MET:HE2	3:C:3795:ALA:HB1	2.02	0.41
3:C:4019:LEU:HD23	3:C:4019:LEU:C	2.46	0.41
3:C:4096:PHE:CZ	3:C:4100:MET:HE3	2.55	0.41
2:K:62:LEU:HD21	2:K:70:VAL:HG11	2.01	0.41
2:I:61:GLU:O	3:A:3638:ARG:CZ	2.67	0.41
3:D:2940:ARG:NH1	3:D:2942:LEU:HD11	2.36	0.41
3:D:3946:ILE:HD11	3:D:4005:LYS:HE3	2.02	0.41
3:D:4837:MET:HE3	3:C:4821:LEU:HG	2.03	0.41
3:A:905:HIS:NE2	3:A:907:CYS:HB2	2.36	0.41
3:A:914:LEU:HD23	3:A:919:ARG:HA	2.01	0.41
3:A:2204:MET:O	3:A:2207:THR:N	2.53	0.41
3:A:2925:GLN:OE1	3:A:2929:LYS:NZ	2.51	0.41
3:A:2978:LEU:HA	3:A:2981:VAL:HG22	2.02	0.41
3:A:3551:ARG:HD3	3:A:3598:GLN:HG3	2.02	0.41
3:A:3683:GLU:OE1	3:A:3683:GLU:O	2.39	0.41
3:A:4090:LEU:HD13	3:A:4127:ASN:HA	2.02	0.41
3:A:4678:LYS:HD3	3:A:4684:LEU:HD22	2.02	0.41
8:A:8006:PCW:H41	8:A:8006:PCW:H63	1.83	0.41
3:B:649:ILE:HG23	3:B:815:ALA:HB3	2.02	0.41
3:B:1435:TYR:HD1	3:B:1573:ILE:HG21	1.86	0.41
3:B:2204:MET:O	3:B:2207:THR:N	2.53	0.41
3:B:2254:HIS:O	3:B:2255:LEU:C	2.64	0.41
3:B:2322:ILE:O	3:B:2322:ILE:HG22	2.21	0.41
3:B:2768:ALA:HB3	3:B:2858:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3936:PHE:CD2	3:B:3954:PHE:HE1	2.38	0.41
3:B:4090:LEU:HD13	3:B:4127:ASN:HA	2.02	0.41
3:C:1464:SER:O	3:C:1469:LYS:NZ	2.46	0.41
3:C:2698:ARG:HH21	2:M:17:HIS:CE1	2.38	0.41
1:E:60:TRP:O	1:E:61:GLU:C	2.62	0.41
2:I:17:HIS:CG	3:A:2698:ARG:NH2	2.88	0.41
2:J:75:TYR:O	2:J:76:VAL:C	2.62	0.41
1:H:26:HIS:HB3	1:H:41:ARG:NE	2.36	0.41
3:D:15:LEU:HD12	3:D:166:VAL:HG22	2.02	0.41
3:D:1435:TYR:HD1	3:D:1573:ILE:HG21	1.86	0.41
3:D:3637:PHE:HE2	2:O:82:LEU:HD22	1.86	0.41
3:A:940:VAL:HG12	3:A:1054:ILE:HG22	2.02	0.41
3:A:1236:THR:OG1	3:A:1703:ARG:NH1	2.54	0.41
3:A:2247:ASN:O	3:A:2250:SER:OG	2.28	0.41
3:A:2703:CYS:O	3:A:2707:ILE:CD1	2.68	0.41
3:A:3343:ALA:O	3:A:3346:ILE:HG12	2.20	0.41
3:A:4096:PHE:CZ	3:A:4100:MET:HE3	2.55	0.41
3:A:4154:SER:HB2	3:A:4167:LEU:HD11	2.02	0.41
3:A:4552:TYR:O	3:A:4556:ASN:ND2	2.52	0.41
3:B:984:THR:C	3:B:988:ARG:HE	2.27	0.41
3:B:1236:THR:OG1	3:B:1703:ARG:NH1	2.54	0.41
3:B:1930:MET:HG2	3:B:1930:MET:O	2.21	0.41
3:B:2925:GLN:OE1	3:B:2929:LYS:CE	2.68	0.41
3:B:3131:THR:O	3:B:3135:VAL:HG12	2.21	0.41
3:B:4019:LEU:C	3:B:4019:LEU:HD23	2.46	0.41
3:C:1236:THR:OG1	3:C:1703:ARG:NH1	2.54	0.41
3:C:1930:MET:HG2	3:C:1930:MET:O	2.21	0.41
3:C:2322:ILE:O	3:C:2322:ILE:HG22	2.21	0.41
3:C:3231:LEU:HB2	3:C:3233:LEU:HD23	2.03	0.41
3:C:3946:ILE:HD11	3:C:4005:LYS:HE3	2.02	0.41
2:K:12:LEU:O	2:K:15:VAL:HG12	2.21	0.41
1:E:59:GLY:CA	1:E:77:ILE:HD12	2.51	0.41
3:D:1462:ASP:OD2	3:D:1469:LYS:NZ	2.47	0.41
3:D:2281:VAL:O	3:D:2281:VAL:HG22	2.20	0.41
3:D:3551:ARG:HD3	3:D:3598:GLN:HG3	2.02	0.41
3:A:221:LEU:HD21	3:A:263:LEU:HD11	2.03	0.41
3:A:3254:ILE:HD11	3:A:3275:LEU:HD11	2.03	0.41
3:A:3267:MET:HG3	3:A:3271:ILE:CD1	2.51	0.41
3:A:3631:ARG:HA	3:A:3634:VAL:HG12	2.03	0.41
3:A:4019:LEU:C	3:A:4019:LEU:HD23	2.46	0.41
3:B:634:LEU:HB3	3:B:1640:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3267:MET:HG3	3:B:3271:ILE:CD1	2.51	0.41
3:B:3355:LEU:HD11	3:B:3431:ASN:ND2	2.35	0.41
3:C:784:PHE:HB3	3:C:788:ILE:HD13	2.03	0.41
3:C:1695:LEU:O	3:C:1699:LEU:HG	2.21	0.41
3:C:2254:HIS:O	3:C:2255:LEU:C	2.64	0.41
3:C:2940:ARG:NH1	3:C:2942:LEU:HD11	2.36	0.41
3:C:3254:ILE:HD11	3:C:3275:LEU:HD11	2.03	0.41
3:C:3355:LEU:HD11	3:C:3431:ASN:ND2	2.35	0.41
3:C:3994:GLY:O	3:C:3998:VAL:HG23	2.20	0.41
3:C:4678:LYS:HD3	3:C:4684:LEU:HD22	2.02	0.41
2:K:8:ALA:O	2:K:11:THR:OG1	2.37	0.41
2:L:5:LEU:HD23	2:L:9:MET:CE	2.44	0.41
2:O:8:ALA:O	2:O:11:THR:OG1	2.37	0.41
2:I:12:LEU:O	2:I:15:VAL:HG12	2.21	0.41
2:J:29:LEU:CD1	2:J:33:GLU:HB3	2.50	0.41
3:D:215:VAL:HG12	3:D:275:LEU:HD12	2.03	0.41
3:D:1244:PRO:O	3:D:1459:HIS:ND1	2.54	0.41
3:D:3185:GLU:HA	3:D:3188:ARG:HG3	2.03	0.41
3:D:3254:ILE:HD11	3:D:3275:LEU:HD11	2.03	0.41
3:D:3847:LEU:HD11	3:D:3935:ASP:HB3	2.03	0.41
3:D:3974:GLY:N	3:D:3975:PRO:HA	2.35	0.41
3:D:4019:LEU:HD23	3:D:4019:LEU:C	2.46	0.41
3:A:215:VAL:HG12	3:A:275:LEU:HD12	2.03	0.41
3:A:2940:ARG:NH1	3:A:2942:LEU:HD11	2.36	0.41
3:A:3513:ALA:O	3:A:3517:LYS:HG2	2.20	0.41
3:B:2249:ARG:HD3	3:B:2287:LEU:HD21	2.03	0.41
3:B:2420:GLY:O	3:B:2423:ILE:HG22	2.20	0.41
3:B:2694:GLN:CD	2:L:87:ASN:HD21	2.28	0.41
3:B:3356:ARG:HA	3:B:3360:ILE:HD12	2.01	0.41
3:B:4154:SER:HB2	3:B:4167:LEU:HD11	2.02	0.41
3:B:4821:LEU:HG	3:C:4837:MET:HE3	2.03	0.41
3:C:988:ARG:NH1	3:C:1059:GLN:OE1	2.53	0.41
3:C:2417:VAL:HG23	3:C:2417:VAL:O	2.21	0.41
3:C:3637:PHE:HE2	2:M:82:LEU:HD22	1.86	0.41
2:I:6:GLU:CD	2:J:42:LEU:HD13	2.40	0.41
2:I:82:LEU:HD22	3:A:3637:PHE:HE2	1.86	0.41
1:G:26:HIS:HB3	1:G:41:ARG:NE	2.36	0.41
3:D:610:CYS:O	3:D:613:VAL:HG22	2.21	0.41
3:D:940:VAL:HG12	3:D:1054:ILE:HG22	2.02	0.41
3:D:986:VAL:CG2	3:D:1044:VAL:HG11	2.50	0.41
3:D:1021:ARG:HE	7:D:8005:ATP:N6	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1695:LEU:O	3:D:1699:LEU:HG	2.21	0.41
3:D:2171:MET:SD	3:D:2229:MET:CE	3.09	0.41
3:D:2791:MET:SD	3:D:2791:MET:O	2.79	0.41
3:D:2868:LEU:HD22	3:D:2872:LEU:HB3	2.02	0.41
3:D:2925:GLN:OE1	3:D:2929:LYS:NZ	2.51	0.41
3:D:3587:ALA:HA	3:D:3593:ILE:HD11	2.02	0.41
3:A:610:CYS:O	3:A:613:VAL:HG22	2.21	0.41
3:A:986:VAL:CG2	3:A:1044:VAL:HG11	2.50	0.41
3:A:1435:TYR:HB3	3:A:1520:LEU:HG	2.03	0.41
3:A:1435:TYR:HD1	3:A:1573:ILE:HG21	1.86	0.41
3:A:1752:GLY:H	3:A:1756:GLU:HA	1.86	0.41
3:A:2160:LEU:HD13	3:A:2204:MET:HG2	2.02	0.41
3:A:2254:HIS:O	3:A:2255:LEU:C	2.64	0.41
3:A:2940:ARG:HG2	3:A:2942:LEU:HD22	2.03	0.41
3:A:3862:VAL:HG13	3:A:3863:ASN:N	2.36	0.41
3:B:215:VAL:HG12	3:B:275:LEU:HD12	2.03	0.41
3:B:1980:LEU:HD23	3:B:1980:LEU:C	2.46	0.41
3:B:2160:LEU:HD13	3:B:2204:MET:HG2	2.02	0.41
3:B:2207:THR:O	3:B:2211:VAL:HG23	2.21	0.41
3:B:2417:VAL:O	3:B:2417:VAL:HG23	2.21	0.41
3:B:2578:ILE:HG23	3:B:2579:MET:N	2.36	0.41
3:B:2791:MET:SD	3:B:2791:MET:O	2.79	0.41
3:B:2868:LEU:HD22	3:B:2872:LEU:HB3	2.02	0.41
3:B:3231:LEU:HB2	3:B:3233:LEU:HD23	2.03	0.41
3:B:3263:ARG:NH2	3:B:3330:ILE:HD12	2.36	0.41
3:B:3343:ALA:O	3:B:3346:ILE:HG12	2.20	0.41
3:B:3631:ARG:HA	3:B:3634:VAL:HG12	2.03	0.41
3:B:3683:GLU:OE1	3:B:3683:GLU:O	2.39	0.41
3:B:3994:GLY:O	3:B:3998:VAL:HG23	2.20	0.41
3:B:4096:PHE:CZ	3:B:4100:MET:HE3	2.55	0.41
3:C:215:VAL:HG12	3:C:275:LEU:HD12	2.03	0.41
3:C:310:THR:HG23	3:C:311:LYS:N	2.35	0.41
3:C:1435:TYR:HD1	3:C:1573:ILE:HG21	1.86	0.41
3:C:2171:MET:SD	3:C:2229:MET:CE	3.09	0.41
3:C:2578:ILE:HG23	3:C:2579:MET:N	2.36	0.41
3:C:2768:ALA:HB3	3:C:2858:PRO:HB3	2.03	0.41
3:C:2925:GLN:OE1	3:C:2929:LYS:NZ	2.51	0.41
3:C:2940:ARG:HG2	3:C:2942:LEU:HD22	2.03	0.41
3:C:3219:VAL:HG13	3:C:3220:TYR:N	2.36	0.41
3:C:3457:GLN:HA	3:C:3460:VAL:HG12	2.03	0.41
3:C:3513:ALA:O	3:C:3517:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3862:VAL:HG13	3:C:3863:ASN:N	2.36	0.41
3:C:3974:GLY:N	3:C:3975:PRO:HA	2.35	0.41
2:O:73:LYS:O	2:O:76:VAL:HG22	2.21	0.41
2:P:29:LEU:CD1	2:P:33:GLU:HB3	2.50	0.41
2:P:75:TYR:O	2:P:76:VAL:C	2.62	0.41
3:D:649:ILE:HG23	3:D:815:ALA:HB3	2.02	0.41
3:D:1930:MET:HG2	3:D:1930:MET:O	2.21	0.41
3:D:2226:PHE:N	3:D:2227:PRO:HD3	2.36	0.41
3:D:2564:THR:HG22	3:D:2607:CYS:CA	2.45	0.41
3:D:3513:ALA:O	3:D:3517:LYS:HG2	2.20	0.41
3:D:4154:SER:HB2	3:D:4167:LEU:HD11	2.02	0.41
3:D:4763:LEU:HD12	3:D:4764:THR:N	2.36	0.41
3:A:984:THR:C	3:A:988:ARG:HE	2.28	0.41
3:A:1217:ILE:HD12	3:A:1217:ILE:H	1.86	0.41
3:A:1244:PRO:O	3:A:1459:HIS:ND1	2.54	0.41
3:A:1980:LEU:HD23	3:A:1980:LEU:C	2.46	0.41
3:A:2207:THR:O	3:A:2211:VAL:HG23	2.21	0.41
3:A:2771:LYS:O	3:A:2776:TRP:N	2.53	0.41
3:B:664:TYR:OH	3:B:666:GLU:OE2	2.27	0.41
3:B:1244:PRO:O	3:B:1459:HIS:ND1	2.54	0.41
3:B:1464:SER:O	3:B:1469:LYS:NZ	2.46	0.41
3:B:1927:LEU:HB3	3:B:1940:MET:HE3	2.03	0.41
3:B:2314:LEU:HD12	3:B:2319:TYR:CD2	2.56	0.41
3:B:2940:ARG:NH1	3:B:2942:LEU:HD11	2.36	0.41
3:B:3457:GLN:HA	3:B:3460:VAL:HG12	2.03	0.41
3:C:221:LEU:HD21	3:C:263:LEU:HD11	2.02	0.41
3:C:610:CYS:O	3:C:613:VAL:HG22	2.21	0.41
3:C:634:LEU:HB3	3:C:1640:LEU:HD11	2.03	0.41
3:C:905:HIS:NE2	3:C:907:CYS:HB2	2.35	0.41
3:C:1244:PRO:O	3:C:1459:HIS:ND1	2.54	0.41
3:C:1980:LEU:HD23	3:C:1980:LEU:C	2.46	0.41
3:C:2226:PHE:N	3:C:2227:PRO:HD3	2.36	0.41
3:C:3847:LEU:HD11	3:C:3935:ASP:HB3	2.03	0.41
3:C:4090:LEU:HD13	3:C:4127:ASN:HA	2.02	0.41
1:F:59:GLY:CA	1:F:77:ILE:HD12	2.51	0.40
3:D:284:ARG:NH1	3:D:291:TYR:OH	2.54	0.40
3:D:1217:ILE:H	3:D:1217:ILE:HD12	1.86	0.40
3:D:1236:THR:OG1	3:D:1703:ARG:NH1	2.54	0.40
3:D:1435:TYR:HB3	3:D:1520:LEU:HG	2.03	0.40
3:D:2654:LYS:HD2	3:D:2658:LEU:HD11	2.02	0.40
3:D:2768:ALA:HB3	3:D:2858:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3219:VAL:HG13	3:D:3220:TYR:N	2.36	0.40
3:D:3862:VAL:HG13	3:D:3863:ASN:N	2.36	0.40
3:D:4942:ARG:NE	3:A:4936:ASP:OD1	2.51	0.40
3:A:263:LEU:HB3	3:A:281:LEU:HD12	2.04	0.40
3:A:2171:MET:SD	3:A:2229:MET:CE	3.09	0.40
3:A:2322:ILE:HG22	3:A:2322:ILE:O	2.21	0.40
3:A:3263:ARG:NH2	3:A:3330:ILE:HD12	2.36	0.40
3:B:102:LEU:HD12	3:B:151:MET:SD	2.60	0.40
3:B:263:LEU:HB3	3:B:281:LEU:HD12	2.04	0.40
3:B:784:PHE:HB3	3:B:788:ILE:HD13	2.03	0.40
3:B:1821:VAL:HG22	3:B:1927:LEU:HD21	2.04	0.40
3:B:2432:ASP:O	3:B:2436:ARG:HG2	2.21	0.40
3:B:2625:ARG:HA	3:B:2675:LEU:HD23	2.03	0.40
3:B:4763:LEU:HD12	3:B:4764:THR:N	2.36	0.40
8:B:8007:PCW:H20	8:B:8007:PCW:H232	1.76	0.40
3:C:15:LEU:HD12	3:C:166:VAL:HG22	2.02	0.40
3:C:1041:CYS:O	3:C:1044:VAL:HG12	2.22	0.40
3:C:1567:LEU:HD12	3:C:1567:LEU:N	2.36	0.40
3:C:2204:MET:O	3:C:2207:THR:N	2.53	0.40
3:C:2249:ARG:HD3	3:C:2287:LEU:HD21	2.03	0.40
3:C:3683:GLU:OE1	3:C:3683:GLU:O	2.39	0.40
2:N:29:LEU:CD1	2:N:33:GLU:HB3	2.50	0.40
2:M:59:MET:SD	2:M:63:ASP:OD2	2.79	0.40
2:O:6:GLU:CD	2:P:42:LEU:HD13	2.40	0.40
2:I:59:MET:SD	2:I:63:ASP:OD2	2.79	0.40
3:D:2207:THR:O	3:D:2211:VAL:HG23	2.21	0.40
3:D:2260:GLU:OE2	3:D:2298:LYS:NZ	2.22	0.40
3:D:3631:ARG:HA	3:D:3634:VAL:HG12	2.03	0.40
3:D:4883:PHE:CE2	3:D:4895:ILE:HD11	2.57	0.40
3:A:77:ARG:O	3:A:81:GLU:HG2	2.22	0.40
3:A:673:ALA:O	3:A:681:THR:OG1	2.35	0.40
3:A:1930:MET:HG2	3:A:1930:MET:O	2.21	0.40
3:A:1932:LEU:HG	3:A:1936:VAL:HG11	2.03	0.40
3:A:3131:THR:O	3:A:3135:VAL:HG12	2.21	0.40
3:A:4883:PHE:CE2	3:A:4895:ILE:HD11	2.57	0.40
3:B:180:TYR:HB2	3:B:197:MET:O	2.22	0.40
3:B:867:HIS:O	3:B:1052:TYR:OH	2.38	0.40
3:B:905:HIS:NE2	3:B:907:CYS:HB2	2.35	0.40
3:B:2940:ARG:HG2	3:B:2942:LEU:HD22	2.03	0.40
3:B:3861:MET:HG2	3:B:3863:ASN:O	2.21	0.40
3:C:1932:LEU:HG	3:C:1936:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2868:LEU:HD22	3:C:2872:LEU:HB3	2.02	0.40
3:C:2925:GLN:OE1	3:C:2929:LYS:CE	2.68	0.40
3:C:4154:SER:HB2	3:C:4167:LEU:HD11	2.02	0.40
3:C:4552:TYR:O	3:C:4556:ASN:ND2	2.52	0.40
2:N:75:TYR:O	2:N:76:VAL:C	2.62	0.40
2:M:12:LEU:O	2:M:15:VAL:HG12	2.21	0.40
3:D:77:ARG:O	3:D:81:GLU:HG2	2.22	0.40
3:D:3322:ARG:O	3:D:3325:VAL:HG12	2.21	0.40
3:D:3454:ARG:O	3:D:3458:ASN:OD1	2.40	0.40
3:D:3936:PHE:CD2	3:D:3954:PHE:HE1	2.38	0.40
3:A:1116:LEU:HD12	3:A:1194:SER:CB	2.51	0.40
3:B:619:GLN:OE1	3:B:1679:ASN:ND2	2.49	0.40
3:B:1752:GLY:H	3:B:1756:GLU:HA	1.86	0.40
3:B:2908:PRO:O	3:B:2911:THR:OG1	2.30	0.40
3:C:180:TYR:HB2	3:C:197:MET:O	2.22	0.40
3:C:1021:ARG:HE	7:C:5106:ATP:N6	2.16	0.40
3:C:1821:VAL:HG22	3:C:1927:LEU:HD21	2.04	0.40
3:C:2224:ILE:HD12	3:C:2268:MET:CE	2.52	0.40
3:C:2314:LEU:HD12	3:C:2319:TYR:CD2	2.56	0.40
3:C:3263:ARG:NH2	3:C:3330:ILE:HD12	2.36	0.40
3:C:3861:MET:HG2	3:C:3863:ASN:O	2.21	0.40
2:K:59:MET:SD	2:K:63:ASP:OD2	2.79	0.40
2:O:59:MET:SD	2:O:63:ASP:OD2	2.79	0.40
3:D:1567:LEU:HD12	3:D:1567:LEU:N	2.36	0.40
3:D:1821:VAL:HG22	3:D:1927:LEU:HD21	2.04	0.40
3:D:3263:ARG:NH2	3:D:3330:ILE:HD12	2.36	0.40
3:D:3267:MET:HG3	3:D:3271:ILE:CD1	2.51	0.40
3:A:284:ARG:NH1	3:A:291:TYR:OH	2.54	0.40
3:A:1194:SER:C	3:A:1195:LEU:HD12	2.47	0.40
3:A:1695:LEU:O	3:A:1699:LEU:HG	2.21	0.40
3:A:1927:LEU:HB3	3:A:1940:MET:HE3	2.02	0.40
3:A:2314:LEU:HD12	3:A:2319:TYR:CD2	2.56	0.40
3:A:3317:LEU:O	3:A:3321:LEU:HD23	2.22	0.40
3:A:3322:ARG:O	3:A:3325:VAL:HG12	2.21	0.40
3:B:1695:LEU:O	3:B:1699:LEU:HG	2.21	0.40
3:B:1964:GLU:HA	3:B:3651:CYS:SG	2.62	0.40
3:B:2171:MET:SD	3:B:2229:MET:CE	3.09	0.40
3:B:2224:ILE:HD12	3:B:2268:MET:CE	2.52	0.40
3:B:3181:ASN:HB2	3:B:3184:VAL:CG2	2.52	0.40
3:B:3454:ARG:O	3:B:3458:ASN:OD1	2.40	0.40
3:B:3974:GLY:N	3:B:3975:PRO:HA	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:284:ARG:NH1	3:C:291:TYR:OH	2.54	0.40
3:C:1964:GLU:HA	3:C:3651:CYS:SG	2.62	0.40
3:C:2179:MET:HE2	3:C:2233:CYS:SG	2.61	0.40
3:C:3185:GLU:HA	3:C:3188:ARG:HG3	2.03	0.40
3:C:3267:MET:HG3	3:C:3271:ILE:CD1	2.51	0.40
3:C:3936:PHE:CD2	3:C:3954:PHE:CE1	3.10	0.40
2:N:53:ASP:OD2	2:N:53:ASP:C	2.65	0.40
2:I:17:HIS:CE1	3:A:2698:ARG:HH21	2.39	0.40
2:I:73:LYS:O	2:I:76:VAL:HG22	2.21	0.40
3:D:760:ILE:O	3:D:760:ILE:HG23	2.20	0.40
3:D:2417:VAL:O	3:D:2417:VAL:HG23	2.21	0.40
3:D:3317:LEU:O	3:D:3321:LEU:HD23	2.22	0.40
3:D:3724:MET:HE2	3:D:3795:ALA:HB1	2.02	0.40
3:D:3936:PHE:CD2	3:D:3954:PHE:CE1	3.10	0.40
3:A:1041:CYS:O	3:A:1044:VAL:HG12	2.22	0.40
3:A:1449:VAL:HG22	3:A:1555:VAL:HG23	2.04	0.40
3:A:1481:GLN:O	3:A:1481:GLN:HG2	2.21	0.40
3:A:2179:MET:HE2	3:A:2233:CYS:SG	2.61	0.40
3:A:2578:ILE:HG23	3:A:2579:MET:N	2.36	0.40
3:A:2625:ARG:HA	3:A:2675:LEU:HD23	2.03	0.40
3:A:2701:MET:HE3	3:A:2702:PRO:HD3	2.04	0.40
3:A:2748:ILE:O	3:A:2748:ILE:HG23	2.21	0.40
3:A:2791:MET:SD	3:A:2791:MET:O	2.79	0.40
3:A:2958:PHE:CE2	3:A:3039:MET:HE1	2.57	0.40
3:A:3181:ASN:HB2	3:A:3184:VAL:CG2	2.52	0.40
3:B:1041:CYS:O	3:B:1044:VAL:HG12	2.22	0.40
3:B:1116:LEU:HD12	3:B:1194:SER:CB	2.51	0.40
3:B:1194:SER:C	3:B:1195:LEU:HD12	2.47	0.40
3:B:1567:LEU:N	3:B:1567:LEU:HD12	2.36	0.40
3:B:3551:ARG:HD3	3:B:3598:GLN:HG3	2.02	0.40
3:B:3847:LEU:HD11	3:B:3935:ASP:HB3	2.03	0.40
3:B:3862:VAL:HG13	3:B:3863:ASN:N	2.36	0.40
3:C:1435:TYR:HB3	3:C:1520:LEU:HG	2.03	0.40
3:C:2958:PHE:CE2	3:C:3039:MET:HE1	2.57	0.40
3:C:3131:THR:O	3:C:3135:VAL:HG12	2.21	0.40
2:K:73:LYS:O	2:K:76:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
1	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
1	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	I	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	J	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	K	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	L	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	M	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	N	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	O	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	P	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
3	A	4351/5035 (86%)	4238 (97%)	113 (3%)	0	100	100
3	B	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
3	C	4351/5035 (86%)	4241 (98%)	110 (2%)	0	100	100
3	D	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
All	All	18552/21324 (87%)	18032 (97%)	520 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	89/90 (99%)	89 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	H	89/90 (99%)	89 (100%)	0	100	100
2	I	80/81 (99%)	80 (100%)	0	100	100
2	J	80/81 (99%)	80 (100%)	0	100	100
2	K	80/81 (99%)	80 (100%)	0	100	100
2	L	80/81 (99%)	80 (100%)	0	100	100
2	M	80/81 (99%)	80 (100%)	0	100	100
2	N	80/81 (99%)	80 (100%)	0	100	100
2	O	80/81 (99%)	80 (100%)	0	100	100
2	P	80/81 (99%)	80 (100%)	0	100	100
3	A	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87
3	B	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87
3	C	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87
3	D	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87
All	All	16240/18192 (89%)	16232 (100%)	8 (0%)	100	100

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	3757	GLU
3	D	5011	MET
3	A	3757	GLU
3	A	5011	MET
3	B	3757	GLU
3	B	5011	MET
3	C	3757	GLU
3	C	5011	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	66	GLN
2	J	87	ASN
1	F	66	GLN

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Mol	Chain	Res	Type
1	G	66	GLN
1	H	66	GLN
3	D	106	HIS
3	D	544	ASN
3	D	726	HIS
3	D	766	GLN
3	D	890	GLN
3	D	1042	GLN
3	D	1063	GLN
3	D	1202	HIS
3	D	1221	GLN
3	D	1430	ASN
3	D	1485	HIS
3	D	1564	GLN
3	D	1954	HIS
3	D	2046	GLN
3	D	2162	GLN
3	D	2476	GLN
3	D	2488	GLN
3	D	2694	GLN
3	D	2977	HIS
3	D	3067	ASN
3	D	3181	ASN
3	D	3457	GLN
3	D	3612	HIS
3	D	3817	GLN
3	D	3848	ASN
3	D	3885	GLN
3	D	3917	ASN
3	D	3930	GLN
3	D	3963	GLN
3	D	4057	ASN
3	D	4219	GLN
3	D	4804	ASN
3	A	106	HIS
3	A	544	ASN
3	A	625	ASN
3	A	726	HIS
3	A	766	GLN
3	A	813	HIS
3	A	890	GLN
3	A	1042	GLN

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Mol	Chain	Res	Type
3	A	1063	GLN
3	A	1202	HIS
3	A	1221	GLN
3	A	1430	ASN
3	A	1485	HIS
3	A	1664	HIS
3	A	1954	HIS
3	A	2046	GLN
3	A	2162	GLN
3	A	2476	GLN
3	A	2488	GLN
3	A	2694	GLN
3	A	2977	HIS
3	A	3067	ASN
3	A	3147	HIS
3	A	3181	ASN
3	A	3457	GLN
3	A	3612	HIS
3	A	3817	GLN
3	A	3848	ASN
3	A	3885	GLN
3	A	3917	ASN
3	A	3930	GLN
3	A	3963	GLN
3	A	3973	GLN
3	A	4057	ASN
3	A	4219	GLN
3	B	106	HIS
3	B	414	GLN
3	B	544	ASN
3	B	726	HIS
3	B	766	GLN
3	B	813	HIS
3	B	890	GLN
3	B	1042	GLN
3	B	1063	GLN
3	B	1202	HIS
3	B	1430	ASN
3	B	1485	HIS
3	B	1506	GLN
3	B	1564	GLN
3	B	1954	HIS

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Mol	Chain	Res	Type
3	B	2046	GLN
3	B	2162	GLN
3	B	2476	GLN
3	B	2488	GLN
3	B	2694	GLN
3	B	2774	ASN
3	B	2977	HIS
3	B	3067	ASN
3	B	3147	HIS
3	B	3181	ASN
3	B	3457	GLN
3	B	3612	HIS
3	B	3817	GLN
3	B	3885	GLN
3	B	3917	ASN
3	B	3930	GLN
3	B	3963	GLN
3	B	4057	ASN
3	B	4219	GLN
3	B	4804	ASN
3	B	5001	HIS
3	C	106	HIS
3	C	414	GLN
3	C	544	ASN
3	C	726	HIS
3	C	766	GLN
3	C	813	HIS
3	C	890	GLN
3	C	1042	GLN
3	C	1063	GLN
3	C	1202	HIS
3	C	1221	GLN
3	C	1430	ASN
3	C	1485	HIS
3	C	1564	GLN
3	C	1591	GLN
3	C	2046	GLN
3	C	2162	GLN
3	C	2476	GLN
3	C	2488	GLN
3	C	2694	GLN
3	C	2977	HIS

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Mol	Chain	Res	Type
3	C	3067	ASN
3	C	3147	HIS
3	C	3181	ASN
3	C	3457	GLN
3	C	3612	HIS
3	C	3817	GLN
3	C	3848	ASN
3	C	3885	GLN
3	C	3917	ASN
3	C	3930	GLN
3	C	3963	GLN
3	C	4057	ASN
3	C	4219	GLN
3	C	4804	ASN
2	L	87	ASN
2	N	87	ASN
2	P	87	ASN

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 44 ligands modelled in this entry, 24 are monoatomic - leaving 20 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
8	PCW	C	5107	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
8	PCW	A	8007	-	53,53,53	1.17	5 (9%)	59,61,61	2.30	9 (15%)
7	ATP	B	8003	-	32,33,33	0.54	0	48,52,52	0.55	0
6	CFF	A	8002	-	15,15,15	0.32	0	23,23,23	0.46	0
8	PCW	B	8006	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
7	ATP	B	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
8	PCW	A	8006	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
7	ATP	A	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
8	PCW	D	8007	-	53,53,53	1.17	4 (7%)	59,61,61	2.30	9 (15%)
8	PCW	D	8006	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
7	ATP	C	5106	-	32,33,33	0.27	0	48,52,52	0.68	0
8	PCW	B	8007	-	53,53,53	1.17	5 (9%)	59,61,61	2.30	9 (15%)
6	CFF	D	8002	-	15,15,15	0.33	0	23,23,23	0.46	0
7	ATP	A	8003	-	32,33,33	0.53	0	48,52,52	0.54	0
6	CFF	C	5103	-	15,15,15	0.33	0	23,23,23	0.46	0
7	ATP	D	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
7	ATP	C	5104	-	32,33,33	0.54	0	48,52,52	0.55	0
8	PCW	C	5101	-	53,53,53	1.17	5 (9%)	59,61,61	2.30	9 (15%)
6	CFF	B	8002	-	15,15,15	0.33	0	23,23,23	0.46	0
7	ATP	D	8003	-	32,33,33	0.53	0	48,52,52	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PCW	C	5107	-	-	21/57/57/57	-
8	PCW	A	8007	-	-	19/57/57/57	-
7	ATP	B	8003	-	-	6/22/38/38	0/3/3/3
6	CFF	A	8002	-	-	-	0/2/2/2
8	PCW	B	8006	-	-	21/57/57/57	-
7	ATP	B	8005	-	-	6/22/38/38	0/3/3/3
8	PCW	A	8006	-	-	21/57/57/57	-
7	ATP	A	8005	-	-	6/22/38/38	0/3/3/3
8	PCW	D	8007	-	-	19/57/57/57	-
8	PCW	D	8006	-	-	21/57/57/57	-
7	ATP	C	5106	-	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PCW	B	8007	-	-	19/57/57/57	-
6	CFF	D	8002	-	-	-	0/2/2/2
7	ATP	A	8003	-	-	6/22/38/38	0/3/3/3
6	CFF	C	5103	-	-	-	0/2/2/2
7	ATP	D	8005	-	-	6/22/38/38	0/3/3/3
7	ATP	C	5104	-	-	6/22/38/38	0/3/3/3
8	PCW	C	5101	-	-	19/57/57/57	-
6	CFF	B	8002	-	-	-	0/2/2/2
7	ATP	D	8003	-	-	6/22/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	8006	PCW	O3-C11	3.07	1.42	1.33
8	A	8006	PCW	O3-C11	3.07	1.42	1.33
8	B	8006	PCW	O3-C11	3.07	1.42	1.33
8	C	5107	PCW	O3-C11	3.07	1.42	1.33
8	A	8007	PCW	O3-C11	3.03	1.42	1.33
8	B	8007	PCW	O3-C11	3.03	1.42	1.33
8	C	5101	PCW	O3-C11	3.03	1.42	1.33
8	D	8007	PCW	O3-C11	3.01	1.42	1.33
8	D	8006	PCW	O2-C31	2.88	1.42	1.34
8	C	5107	PCW	O2-C31	2.88	1.42	1.34
8	D	8007	PCW	O2-C2	-2.87	1.39	1.46
8	A	8006	PCW	O2-C31	2.86	1.42	1.34
8	B	8006	PCW	O2-C31	2.85	1.42	1.34
8	A	8007	PCW	O2-C2	-2.84	1.39	1.46
8	B	8007	PCW	O2-C2	-2.84	1.39	1.46
8	C	5101	PCW	O2-C2	-2.84	1.39	1.46
8	A	8007	PCW	O2-C31	2.76	1.42	1.34
8	B	8007	PCW	O2-C31	2.76	1.42	1.34
8	C	5101	PCW	O2-C31	2.76	1.42	1.34
8	D	8007	PCW	O2-C31	2.75	1.42	1.34
8	D	8006	PCW	O2-C2	-2.68	1.40	1.46
8	B	8006	PCW	O2-C2	-2.68	1.40	1.46
8	C	5107	PCW	O2-C2	-2.68	1.40	1.46
8	A	8006	PCW	O2-C2	-2.68	1.40	1.46
8	D	8007	PCW	P-O4P	2.10	1.67	1.59
8	A	8007	PCW	P-O4P	2.09	1.67	1.59
8	B	8007	PCW	P-O4P	2.09	1.67	1.59
8	C	5101	PCW	P-O4P	2.09	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	8006	PCW	C5-C4	2.04	1.57	1.51
8	C	5107	PCW	C5-C4	2.04	1.57	1.51
8	D	8006	PCW	C5-C4	2.04	1.57	1.51
8	B	8006	PCW	C5-C4	2.04	1.57	1.51
8	A	8006	PCW	P-O4P	2.02	1.67	1.59
8	D	8006	PCW	P-O4P	2.01	1.67	1.59
8	B	8006	PCW	P-O4P	2.01	1.67	1.59
8	C	5107	PCW	P-O4P	2.01	1.67	1.59
8	A	8007	PCW	C5-C4	2.00	1.57	1.51
8	B	8007	PCW	C5-C4	2.00	1.57	1.51
8	C	5101	PCW	C5-C4	2.00	1.57	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	8006	PCW	C8-N-C6	11.60	139.44	108.98
8	C	5107	PCW	C8-N-C6	11.60	139.44	108.98
8	D	8006	PCW	C8-N-C6	11.59	139.42	108.98
8	B	8006	PCW	C8-N-C6	11.59	139.42	108.98
8	B	8007	PCW	C8-N-C6	10.98	137.81	108.98
8	A	8007	PCW	C8-N-C6	10.97	137.78	108.98
8	C	5101	PCW	C8-N-C6	10.97	137.78	108.98
8	D	8007	PCW	C8-N-C6	10.96	137.78	108.98
8	D	8007	PCW	C7-N-C5	7.71	140.54	109.91
8	A	8007	PCW	C7-N-C5	7.70	140.51	109.91
8	C	5101	PCW	C7-N-C5	7.70	140.51	109.91
8	B	8007	PCW	C7-N-C5	7.69	140.47	109.91
8	D	8006	PCW	C7-N-C5	7.32	139.00	109.91
8	B	8006	PCW	C7-N-C5	7.32	139.00	109.91
8	C	5107	PCW	C7-N-C5	7.32	139.00	109.91
8	A	8006	PCW	C7-N-C5	7.31	138.96	109.91
8	A	8006	PCW	C8-N-C7	-5.67	94.08	108.98
8	D	8006	PCW	C8-N-C7	-5.67	94.09	108.98
8	B	8006	PCW	C8-N-C7	-5.67	94.09	108.98
8	C	5107	PCW	C8-N-C7	-5.67	94.09	108.98
8	B	8007	PCW	C7-N-C6	-5.16	95.43	108.98
8	A	8007	PCW	C7-N-C6	-5.15	95.44	108.98
8	C	5101	PCW	C7-N-C6	-5.15	95.44	108.98
8	D	8007	PCW	C7-N-C6	-5.15	95.45	108.98
8	D	8007	PCW	C8-N-C7	-5.01	95.82	108.98
8	A	8007	PCW	C8-N-C7	-5.00	95.83	108.98
8	B	8007	PCW	C8-N-C7	-5.00	95.83	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	5101	PCW	C8-N-C7	-5.00	95.83	108.98
8	A	8006	PCW	C7-N-C6	-4.98	95.88	108.98
8	D	8006	PCW	C7-N-C6	-4.98	95.89	108.98
8	B	8006	PCW	C7-N-C6	-4.98	95.89	108.98
8	C	5107	PCW	C7-N-C6	-4.97	95.91	108.98
8	D	8006	PCW	C21-C20-C19	3.98	154.63	124.83
8	B	8006	PCW	C21-C20-C19	3.98	154.63	124.83
8	C	5107	PCW	C21-C20-C19	3.98	154.63	124.83
8	A	8006	PCW	C21-C20-C19	3.98	154.63	124.83
8	A	8007	PCW	C21-C20-C19	3.88	153.88	124.83
8	B	8007	PCW	C21-C20-C19	3.88	153.88	124.83
8	C	5101	PCW	C21-C20-C19	3.88	153.88	124.83
8	D	8007	PCW	C21-C20-C19	3.87	153.83	124.83
8	A	8006	PCW	O2-C31-C32	3.57	119.20	111.48
8	D	8006	PCW	O2-C31-C32	3.56	119.18	111.48
8	C	5107	PCW	O2-C31-C32	3.56	119.18	111.48
8	B	8006	PCW	O2-C31-C32	3.55	119.17	111.48
8	D	8007	PCW	O2-C31-C32	3.49	119.02	111.48
8	A	8007	PCW	O2-C31-C32	3.47	118.98	111.48
8	B	8007	PCW	O2-C31-C32	3.47	118.98	111.48
8	C	5101	PCW	O2-C31-C32	3.47	118.98	111.48
8	B	8007	PCW	C8-N-C5	-3.37	96.51	109.91
8	D	8007	PCW	C8-N-C5	-3.37	96.51	109.91
8	A	8007	PCW	C8-N-C5	-3.37	96.52	109.91
8	C	5101	PCW	C8-N-C5	-3.37	96.52	109.91
8	D	8006	PCW	C8-N-C5	-3.04	97.84	109.91
8	B	8006	PCW	C8-N-C5	-3.04	97.84	109.91
8	C	5107	PCW	C8-N-C5	-3.04	97.84	109.91
8	A	8006	PCW	C8-N-C5	-3.03	97.85	109.91
8	C	5107	PCW	C6-N-C5	-2.52	99.89	109.91
8	D	8006	PCW	C6-N-C5	-2.51	99.93	109.91
8	B	8006	PCW	C6-N-C5	-2.51	99.93	109.91
8	A	8006	PCW	C6-N-C5	-2.51	99.93	109.91
8	D	8007	PCW	C6-N-C5	-2.47	100.07	109.91
8	A	8007	PCW	C6-N-C5	-2.47	100.08	109.91
8	C	5101	PCW	C6-N-C5	-2.47	100.08	109.91
8	B	8007	PCW	C6-N-C5	-2.47	100.11	109.91
8	A	8006	PCW	O3-C11-C12	2.42	119.23	111.83
8	D	8006	PCW	O3-C11-C12	2.42	119.22	111.83
8	B	8006	PCW	O3-C11-C12	2.42	119.22	111.83
8	C	5107	PCW	O3-C11-C12	2.42	119.22	111.83
8	D	8007	PCW	O3-C11-C12	2.41	119.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	8007	PCW	O3-C11-C12	2.41	119.19	111.83
8	C	5101	PCW	O3-C11-C12	2.41	119.19	111.83
8	B	8007	PCW	O3-C11-C12	2.41	119.18	111.83

There are no chirality outliers.

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	8003	ATP	C5'-O5'-PA-O1A
7	D	8003	ATP	C5'-O5'-PA-O3A
7	D	8005	ATP	C5'-O5'-PA-O1A
7	A	8003	ATP	C5'-O5'-PA-O1A
7	A	8003	ATP	C5'-O5'-PA-O3A
7	A	8005	ATP	C5'-O5'-PA-O1A
7	B	8003	ATP	C5'-O5'-PA-O1A
7	B	8003	ATP	C5'-O5'-PA-O3A
7	B	8005	ATP	C5'-O5'-PA-O1A
7	C	5104	ATP	C5'-O5'-PA-O1A
7	C	5104	ATP	C5'-O5'-PA-O3A
7	C	5106	ATP	C5'-O5'-PA-O1A
8	D	8006	PCW	C1-O3P-P-O2P
8	D	8006	PCW	C1-O3P-P-O4P
8	D	8007	PCW	O4P-C4-C5-N
8	A	8006	PCW	C1-O3P-P-O2P
8	A	8006	PCW	C1-O3P-P-O4P
8	A	8007	PCW	O4P-C4-C5-N
8	B	8006	PCW	C1-O3P-P-O2P
8	B	8006	PCW	C1-O3P-P-O4P
8	B	8007	PCW	O4P-C4-C5-N
8	C	5101	PCW	O4P-C4-C5-N
8	C	5107	PCW	C1-O3P-P-O2P
8	C	5107	PCW	C1-O3P-P-O4P
8	D	8007	PCW	C23-C24-C25-C26
8	B	8007	PCW	C23-C24-C25-C26
8	C	5101	PCW	C23-C24-C25-C26
8	A	8007	PCW	C23-C24-C25-C26
8	D	8006	PCW	C43-C44-C45-C46
8	A	8006	PCW	C43-C44-C45-C46
8	B	8006	PCW	C43-C44-C45-C46
8	C	5107	PCW	C43-C44-C45-C46
8	D	8006	PCW	C15-C16-C17-C18
8	A	8006	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	B	8006	PCW	C15-C16-C17-C18
8	C	5107	PCW	C15-C16-C17-C18
8	D	8007	PCW	C13-C14-C15-C16
8	A	8007	PCW	C13-C14-C15-C16
8	B	8007	PCW	C13-C14-C15-C16
8	C	5101	PCW	C13-C14-C15-C16
8	D	8007	PCW	C21-C22-C23-C24
8	A	8007	PCW	C21-C22-C23-C24
8	B	8007	PCW	C21-C22-C23-C24
8	C	5101	PCW	C21-C22-C23-C24
8	D	8007	PCW	C11-C12-C13-C14
8	A	8007	PCW	C11-C12-C13-C14
8	B	8007	PCW	C11-C12-C13-C14
8	C	5101	PCW	C11-C12-C13-C14
8	D	8006	PCW	C17-C18-C19-C20
8	A	8006	PCW	C17-C18-C19-C20
8	B	8006	PCW	C17-C18-C19-C20
8	C	5107	PCW	C17-C18-C19-C20
8	D	8006	PCW	C32-C31-O2-C2
8	A	8006	PCW	C32-C31-O2-C2
8	B	8006	PCW	C32-C31-O2-C2
8	C	5107	PCW	C32-C31-O2-C2
8	D	8007	PCW	C25-C26-C27-C28
8	A	8007	PCW	C25-C26-C27-C28
8	B	8007	PCW	C25-C26-C27-C28
8	C	5101	PCW	C25-C26-C27-C28
7	D	8005	ATP	C3'-C4'-C5'-O5'
7	A	8005	ATP	C3'-C4'-C5'-O5'
7	B	8005	ATP	C3'-C4'-C5'-O5'
7	C	5106	ATP	C3'-C4'-C5'-O5'
8	D	8007	PCW	C14-C15-C16-C17
8	A	8007	PCW	C14-C15-C16-C17
8	B	8007	PCW	C14-C15-C16-C17
8	C	5101	PCW	C14-C15-C16-C17
8	D	8006	PCW	O31-C31-O2-C2
8	A	8006	PCW	O31-C31-O2-C2
8	B	8006	PCW	O31-C31-O2-C2
8	C	5107	PCW	O31-C31-O2-C2
8	D	8007	PCW	C15-C16-C17-C18
8	A	8007	PCW	C15-C16-C17-C18
8	B	8007	PCW	C15-C16-C17-C18
8	C	5101	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	D	8005	ATP	O4'-C4'-C5'-O5'
7	A	8005	ATP	O4'-C4'-C5'-O5'
7	B	8005	ATP	O4'-C4'-C5'-O5'
7	C	5106	ATP	O4'-C4'-C5'-O5'
8	D	8007	PCW	C40-C41-C42-C43
8	A	8007	PCW	C40-C41-C42-C43
8	B	8007	PCW	C40-C41-C42-C43
8	C	5101	PCW	C40-C41-C42-C43
8	D	8006	PCW	C40-C41-C42-C43
8	A	8006	PCW	C40-C41-C42-C43
8	B	8006	PCW	C40-C41-C42-C43
8	C	5107	PCW	C40-C41-C42-C43
8	D	8007	PCW	C44-C45-C46-C47
8	A	8007	PCW	C44-C45-C46-C47
8	B	8007	PCW	C44-C45-C46-C47
8	C	5101	PCW	C44-C45-C46-C47
8	D	8006	PCW	C19-C20-C21-C22
8	A	8006	PCW	C19-C20-C21-C22
8	B	8006	PCW	C19-C20-C21-C22
8	C	5107	PCW	C19-C20-C21-C22
7	D	8005	ATP	C4'-C5'-O5'-PA
7	A	8005	ATP	C4'-C5'-O5'-PA
7	B	8005	ATP	C4'-C5'-O5'-PA
7	C	5106	ATP	C4'-C5'-O5'-PA
8	D	8006	PCW	C23-C24-C25-C26
8	A	8006	PCW	C23-C24-C25-C26
8	B	8006	PCW	C23-C24-C25-C26
8	C	5107	PCW	C23-C24-C25-C26
8	A	8007	PCW	C45-C46-C47-C48
8	B	8007	PCW	C45-C46-C47-C48
8	C	5101	PCW	C45-C46-C47-C48
8	D	8007	PCW	C45-C46-C47-C48
8	D	8006	PCW	C14-C15-C16-C17
8	A	8006	PCW	C14-C15-C16-C17
8	B	8006	PCW	C14-C15-C16-C17
8	C	5107	PCW	C14-C15-C16-C17
8	D	8006	PCW	C1-C2-C3-O3
8	A	8006	PCW	C1-C2-C3-O3
8	B	8006	PCW	C1-C2-C3-O3
8	C	5107	PCW	C1-C2-C3-O3
8	D	8006	PCW	C21-C22-C23-C24
8	A	8006	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	B	8006	PCW	C21-C22-C23-C24
8	C	5107	PCW	C21-C22-C23-C24
8	D	8006	PCW	C33-C34-C35-C36
8	A	8006	PCW	C33-C34-C35-C36
8	B	8006	PCW	C33-C34-C35-C36
8	C	5107	PCW	C33-C34-C35-C36
8	D	8006	PCW	O2-C2-C3-O3
8	A	8006	PCW	O2-C2-C3-O3
8	B	8006	PCW	O2-C2-C3-O3
8	C	5107	PCW	O2-C2-C3-O3
8	D	8006	PCW	C25-C26-C27-C28
8	A	8006	PCW	C25-C26-C27-C28
8	C	5107	PCW	C25-C26-C27-C28
8	B	8006	PCW	C25-C26-C27-C28
8	D	8007	PCW	O3P-C1-C2-C3
8	A	8007	PCW	O3P-C1-C2-C3
8	B	8007	PCW	O3P-C1-C2-C3
8	C	5101	PCW	O3P-C1-C2-C3
8	D	8007	PCW	C32-C31-O2-C2
8	A	8007	PCW	C32-C31-O2-C2
8	B	8007	PCW	C32-C31-O2-C2
8	C	5101	PCW	C32-C31-O2-C2
8	D	8007	PCW	C4-C5-N-C8
8	A	8007	PCW	C4-C5-N-C8
8	B	8007	PCW	C4-C5-N-C8
8	C	5101	PCW	C4-C5-N-C8
8	D	8007	PCW	C2-C1-O3P-P
8	A	8007	PCW	C2-C1-O3P-P
8	B	8007	PCW	C2-C1-O3P-P
8	C	5101	PCW	C2-C1-O3P-P
7	D	8003	ATP	PG-O3B-PB-O2B
7	A	8003	ATP	PG-O3B-PB-O2B
7	B	8003	ATP	PG-O3B-PB-O2B
7	C	5104	ATP	PG-O3B-PB-O2B
8	D	8006	PCW	O4P-C4-C5-N
8	A	8006	PCW	O4P-C4-C5-N
8	B	8006	PCW	O4P-C4-C5-N
8	C	5107	PCW	O4P-C4-C5-N
8	D	8007	PCW	O31-C31-O2-C2
8	A	8007	PCW	O31-C31-O2-C2
8	B	8007	PCW	O31-C31-O2-C2
8	C	5101	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
8	D	8007	PCW	O3P-C1-C2-O2
8	A	8007	PCW	O3P-C1-C2-O2
8	B	8007	PCW	O3P-C1-C2-O2
8	C	5101	PCW	O3P-C1-C2-O2
8	D	8007	PCW	C36-C37-C38-C39
8	A	8007	PCW	C36-C37-C38-C39
8	B	8007	PCW	C36-C37-C38-C39
8	C	5101	PCW	C36-C37-C38-C39
8	D	8006	PCW	C44-C45-C46-C47
8	C	5107	PCW	C44-C45-C46-C47
8	B	8006	PCW	C44-C45-C46-C47
8	A	8006	PCW	C44-C45-C46-C47
7	D	8003	ATP	C5'-O5'-PA-O2A
7	A	8003	ATP	C5'-O5'-PA-O2A
7	B	8003	ATP	C5'-O5'-PA-O2A
7	C	5104	ATP	C5'-O5'-PA-O2A
8	D	8007	PCW	C1-C2-O2-C31
8	A	8007	PCW	C1-C2-O2-C31
8	B	8007	PCW	C1-C2-O2-C31
8	C	5101	PCW	C1-C2-O2-C31
7	D	8003	ATP	PG-O3B-PB-O1B
7	D	8005	ATP	PG-O3B-PB-O2B
7	A	8003	ATP	PG-O3B-PB-O1B
7	A	8005	ATP	PG-O3B-PB-O2B
7	B	8003	ATP	PG-O3B-PB-O1B
7	B	8005	ATP	PG-O3B-PB-O2B
7	C	5104	ATP	PG-O3B-PB-O1B
7	C	5106	ATP	PG-O3B-PB-O2B
7	D	8003	ATP	C4'-C5'-O5'-PA
7	A	8003	ATP	C4'-C5'-O5'-PA
7	B	8003	ATP	C4'-C5'-O5'-PA
7	C	5104	ATP	C4'-C5'-O5'-PA
8	A	8006	PCW	C42-C43-C44-C45
8	D	8006	PCW	C42-C43-C44-C45
8	B	8006	PCW	C42-C43-C44-C45
8	C	5107	PCW	C42-C43-C44-C45
8	D	8006	PCW	C2-C1-O3P-P
8	A	8006	PCW	C2-C1-O3P-P
8	B	8006	PCW	C2-C1-O3P-P
8	C	5107	PCW	C2-C1-O3P-P
8	D	8006	PCW	C13-C14-C15-C16
8	B	8006	PCW	C13-C14-C15-C16

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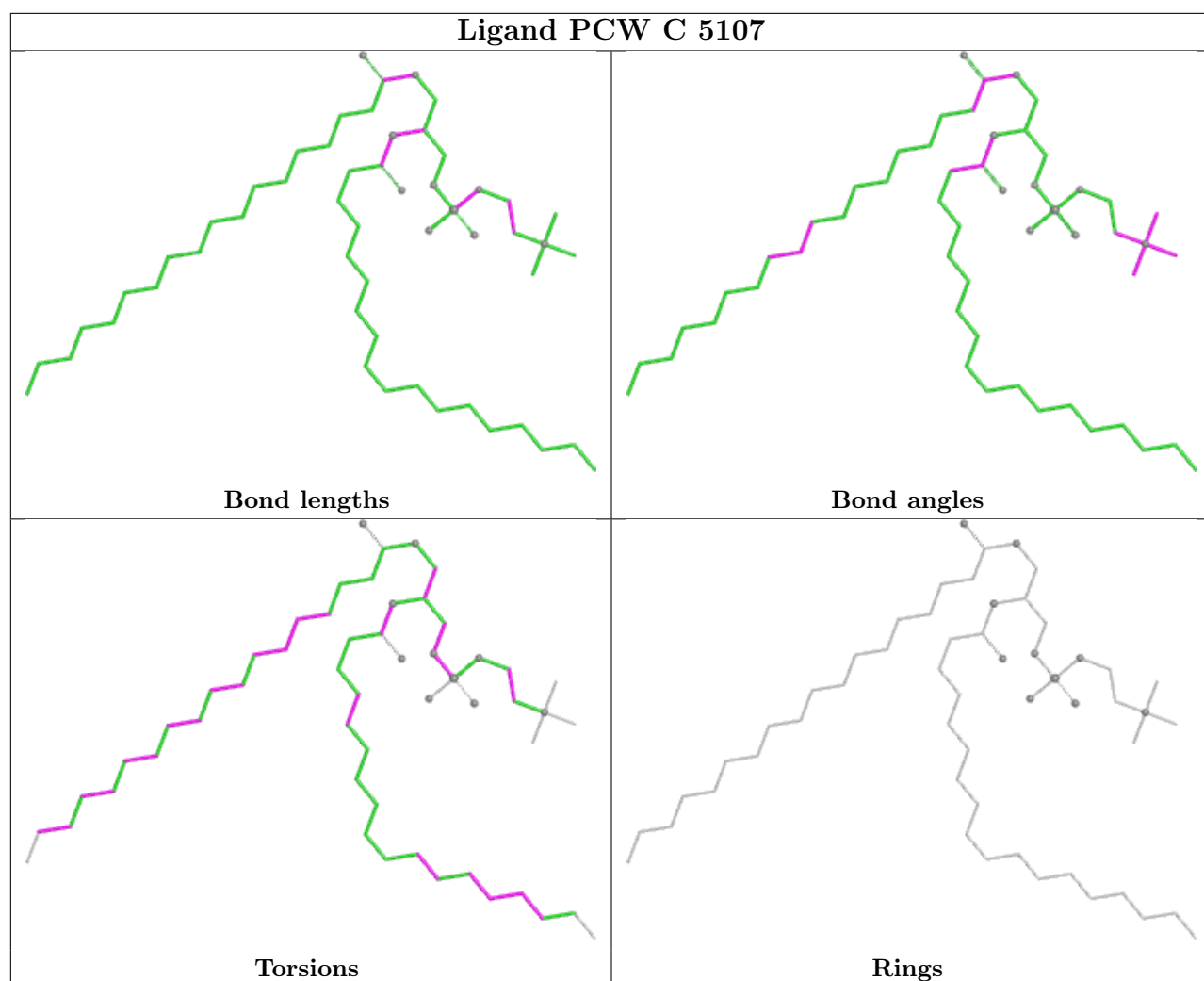
Mol	Chain	Res	Type	Atoms
8	C	5107	PCW	C13-C14-C15-C16
8	A	8006	PCW	C13-C14-C15-C16
7	D	8005	ATP	PG-O3B-PB-O1B
7	A	8005	ATP	PG-O3B-PB-O1B
7	B	8005	ATP	PG-O3B-PB-O1B
7	C	5106	ATP	PG-O3B-PB-O1B

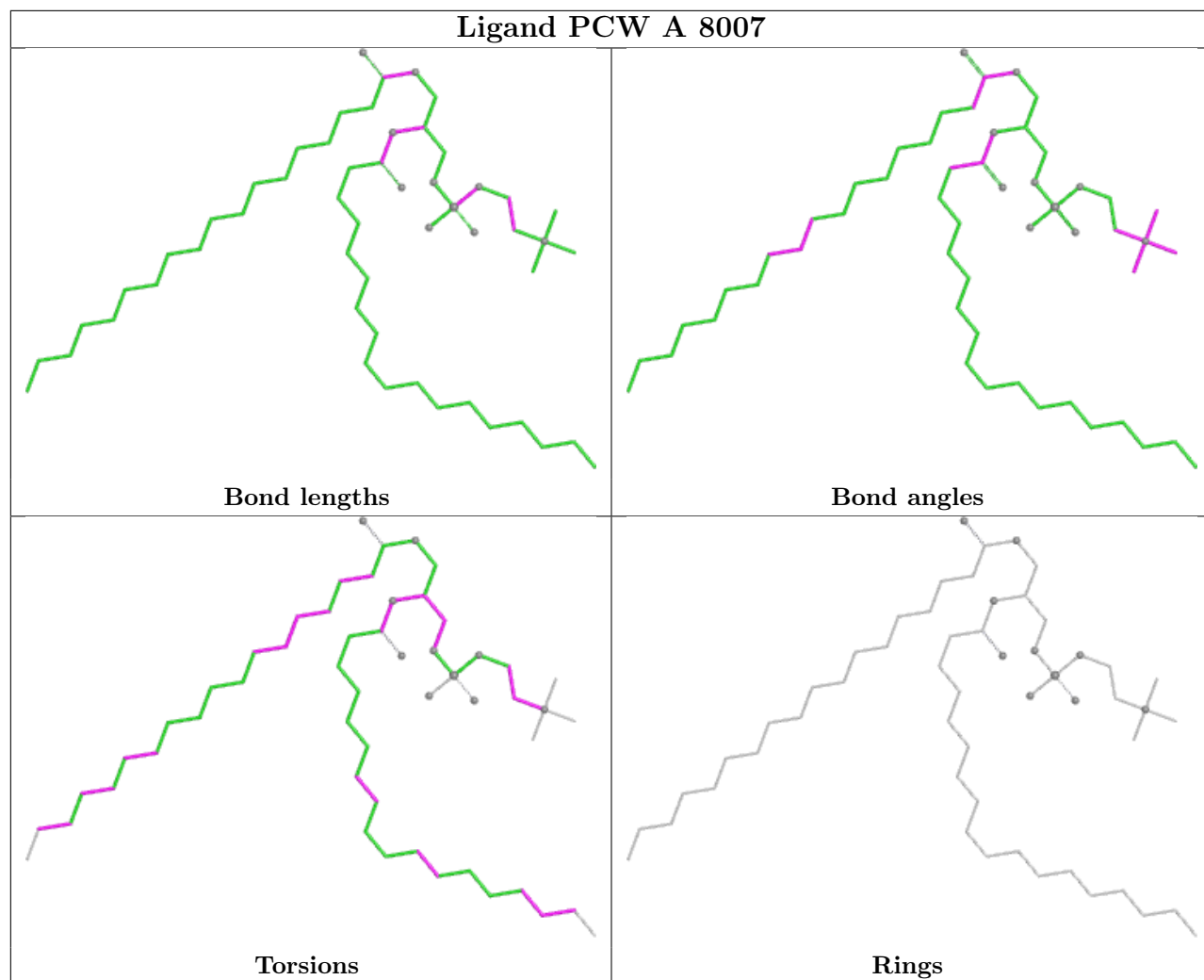
There are no ring outliers.

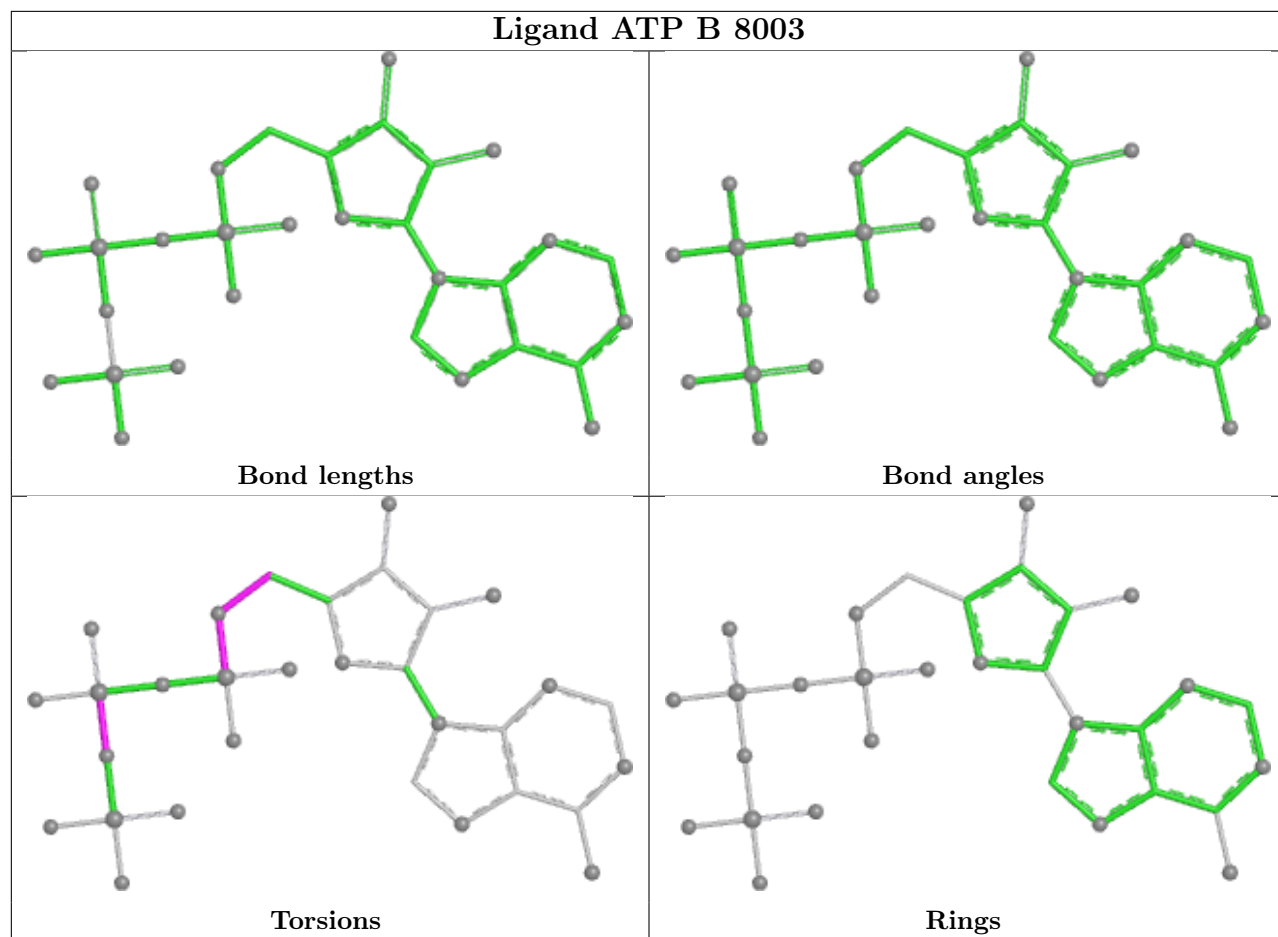
12 monomers are involved in 31 short contacts:

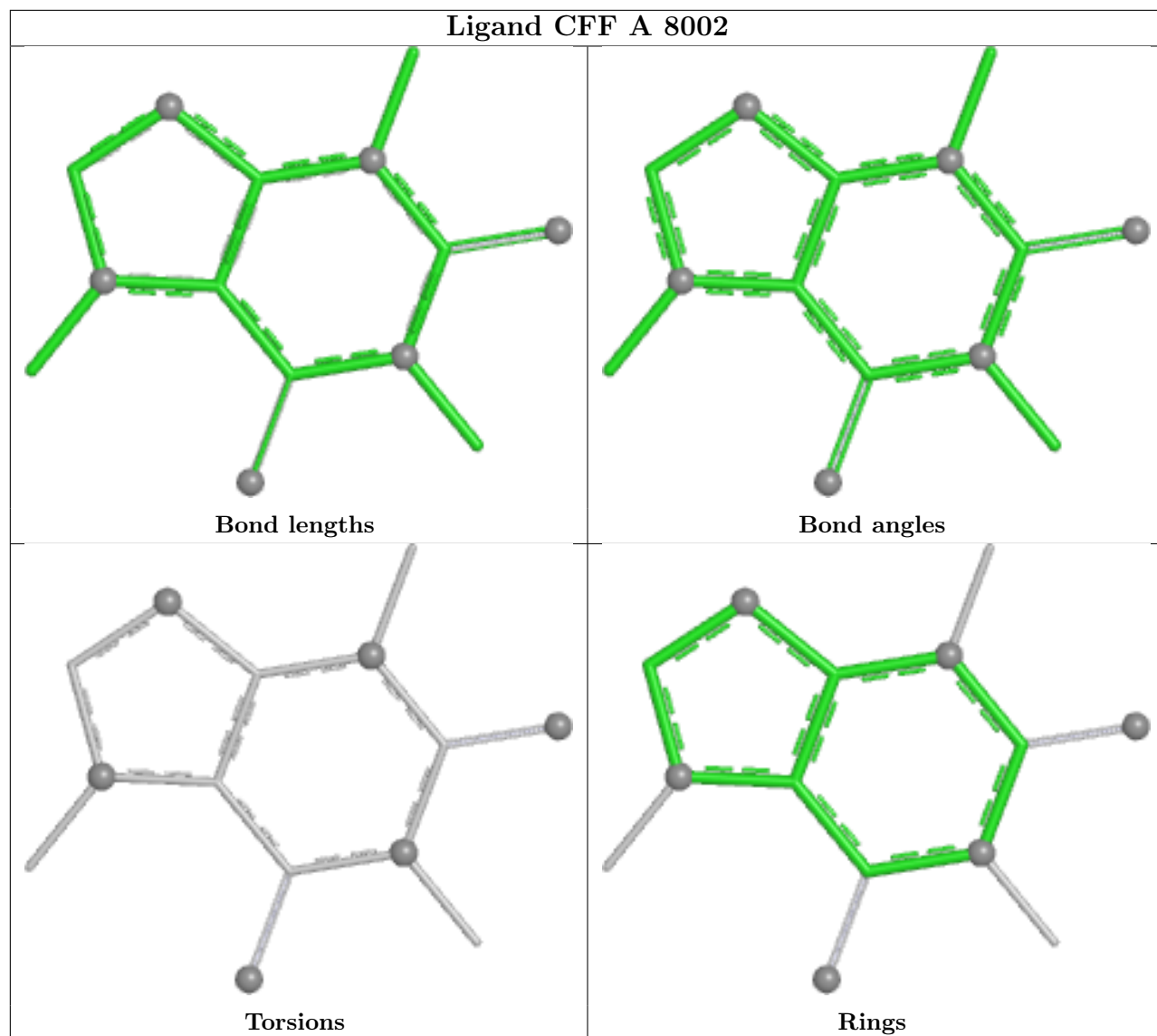
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	5107	PCW	1	0
8	A	8007	PCW	4	0
8	B	8006	PCW	1	0
7	B	8005	ATP	4	0
8	A	8006	PCW	2	0
7	A	8005	ATP	3	0
8	D	8007	PCW	4	0
8	D	8006	PCW	1	0
7	C	5106	ATP	4	0
8	B	8007	PCW	4	0
7	D	8005	ATP	4	0
8	C	5101	PCW	3	0

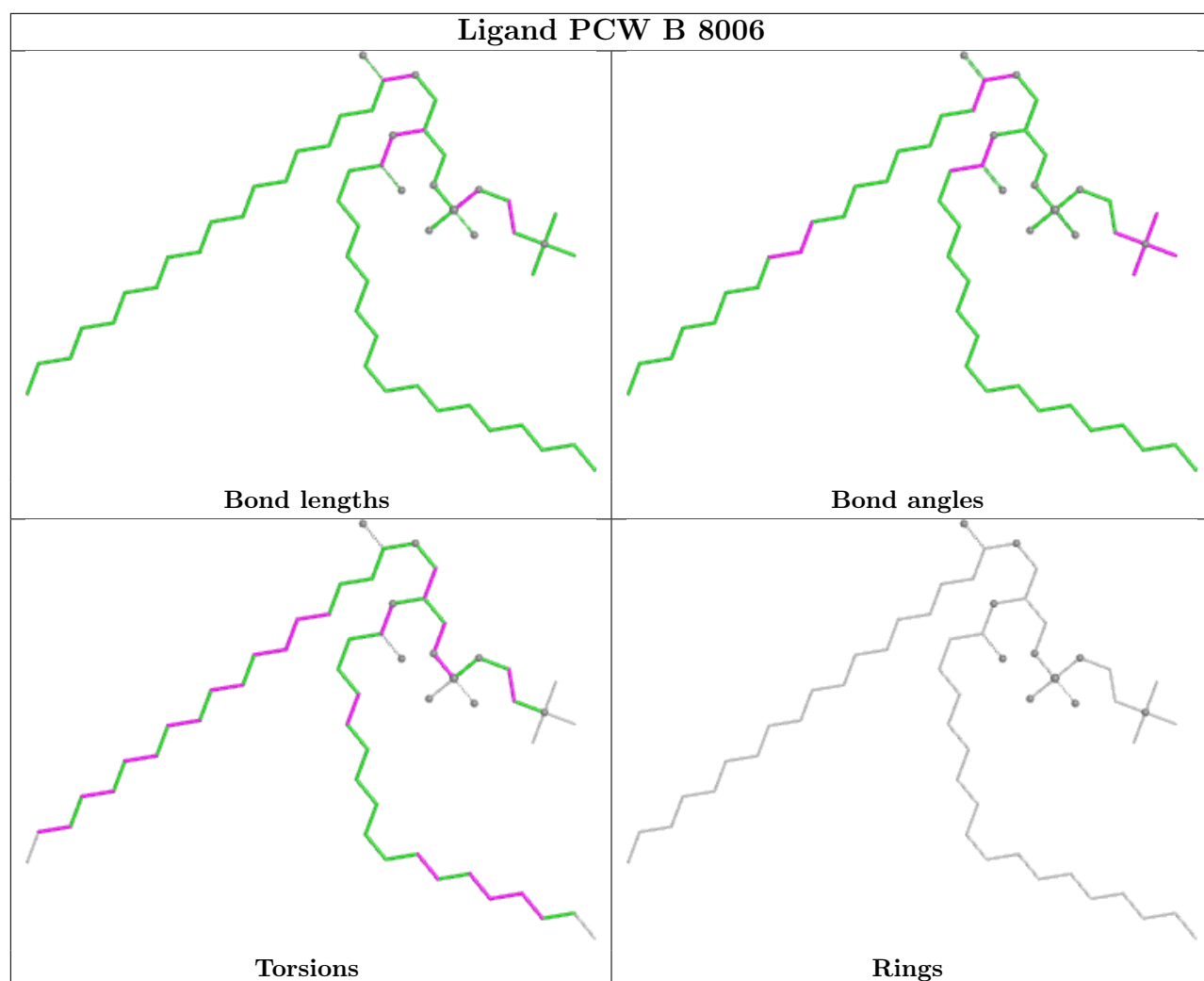
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

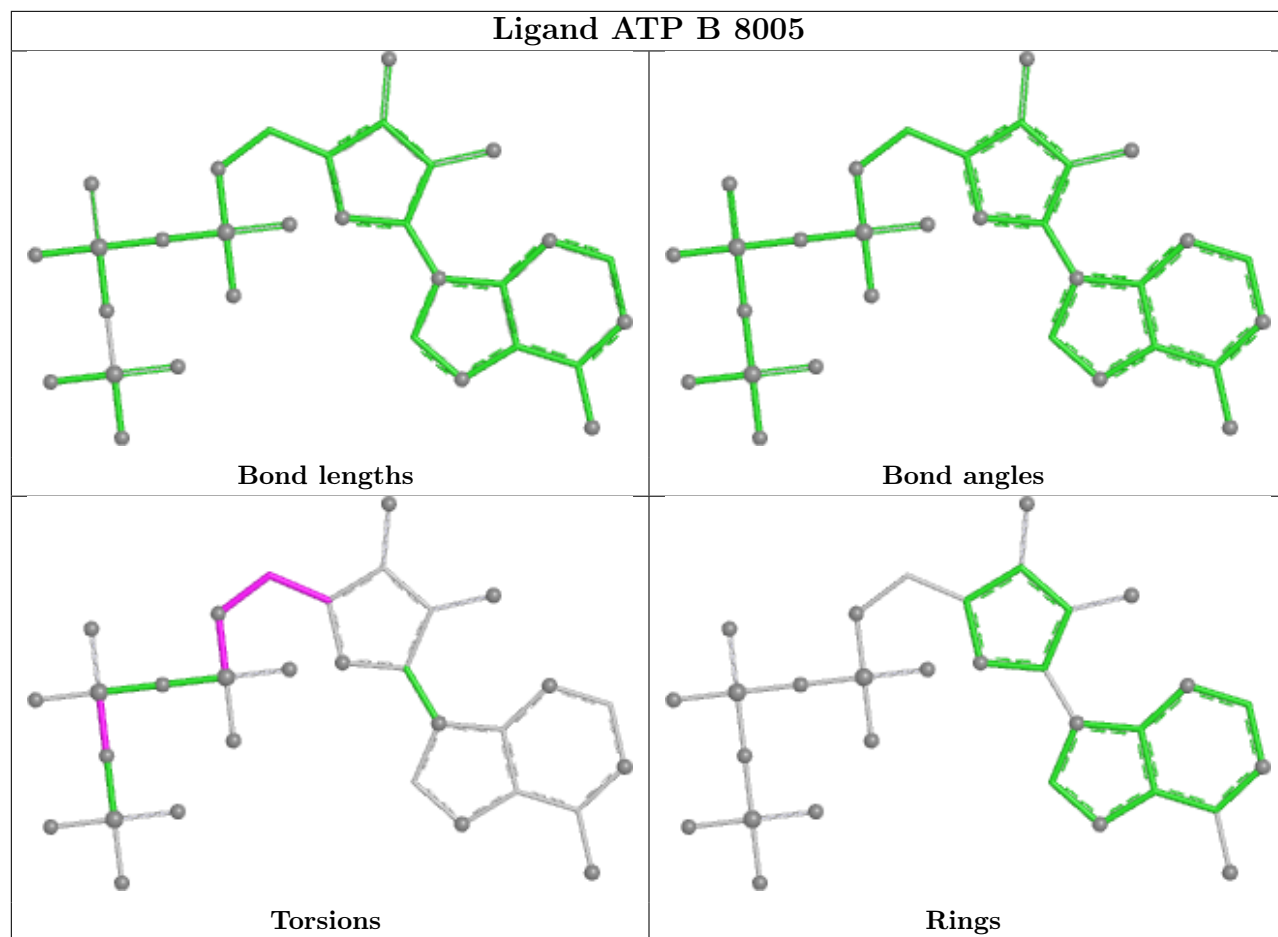


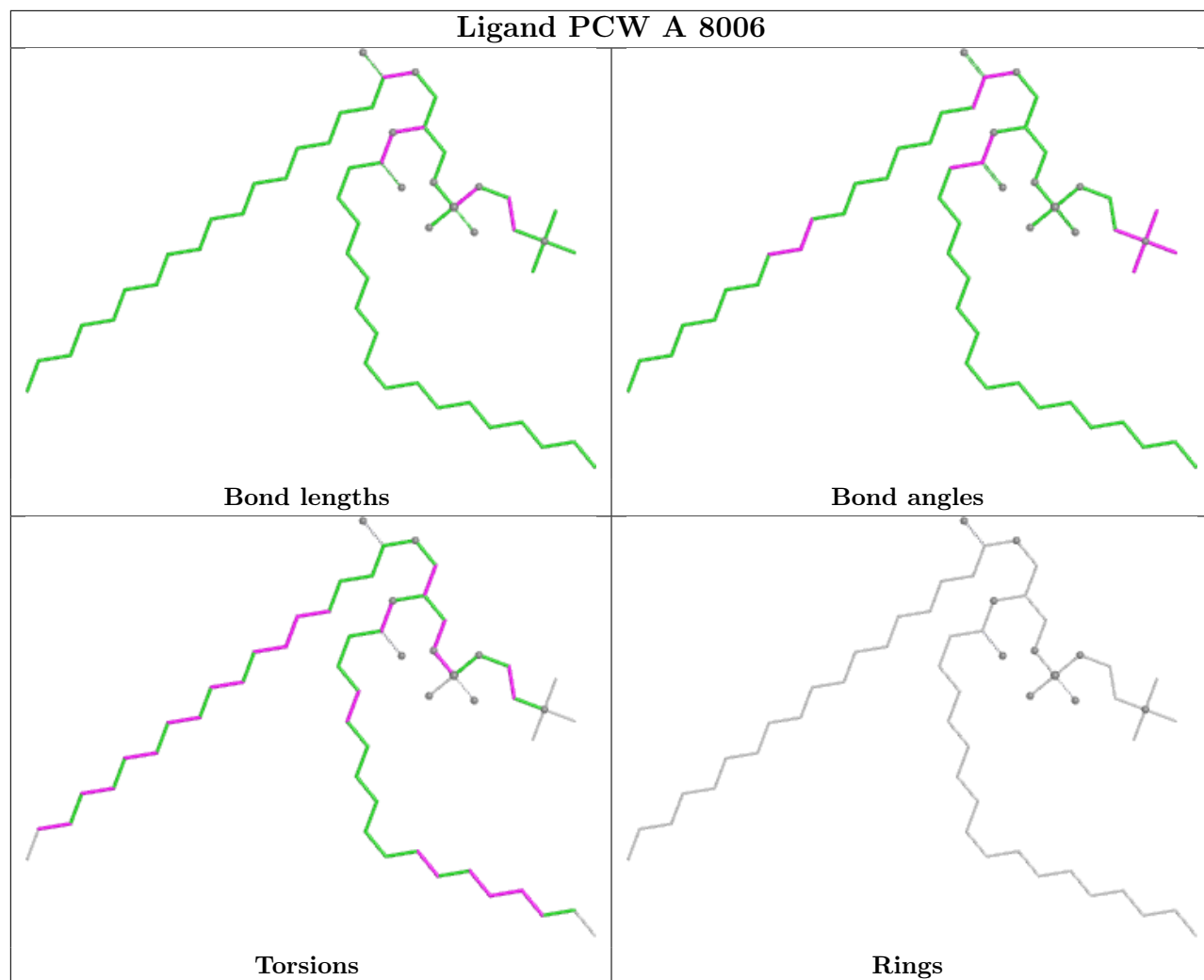


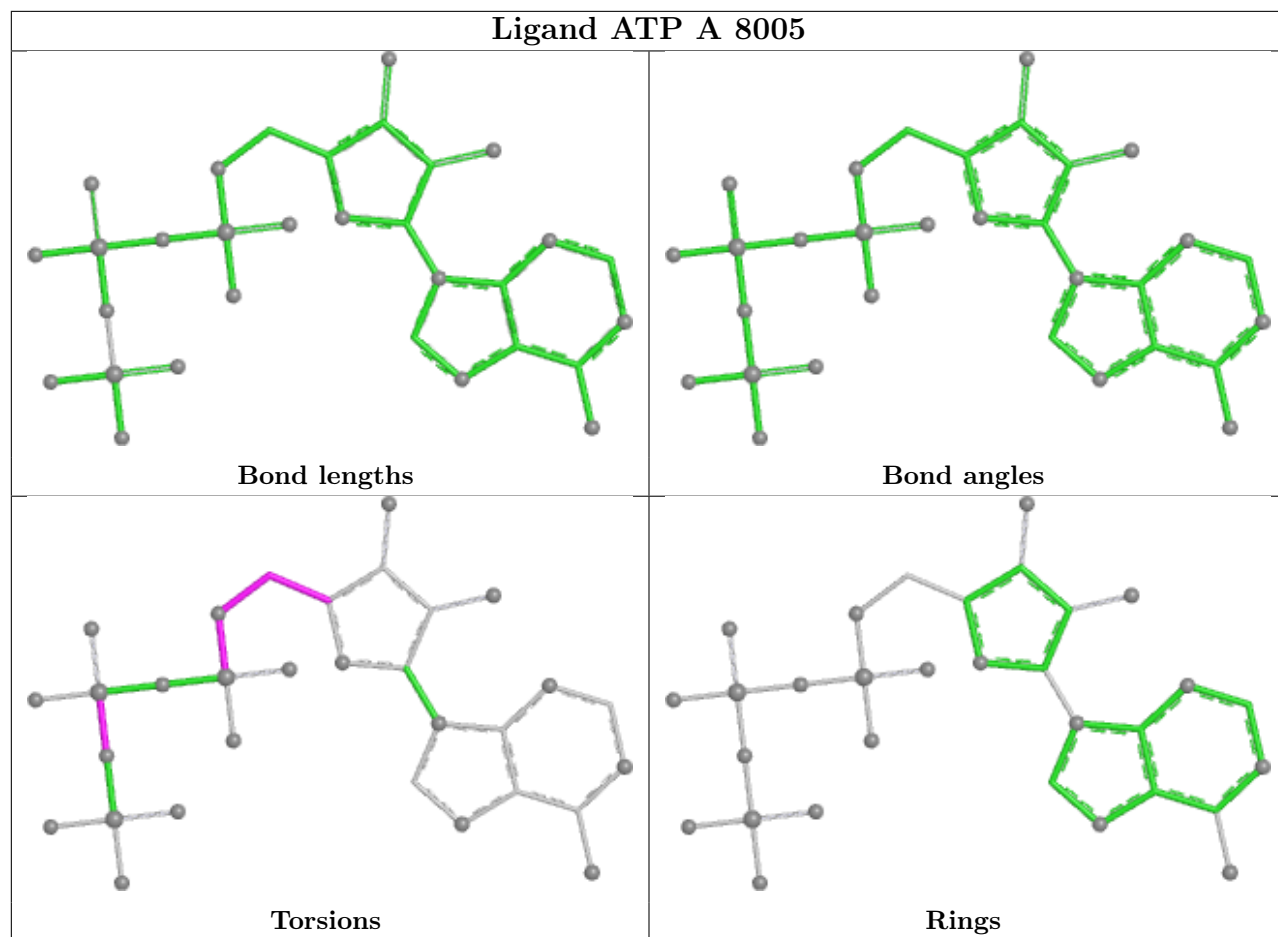


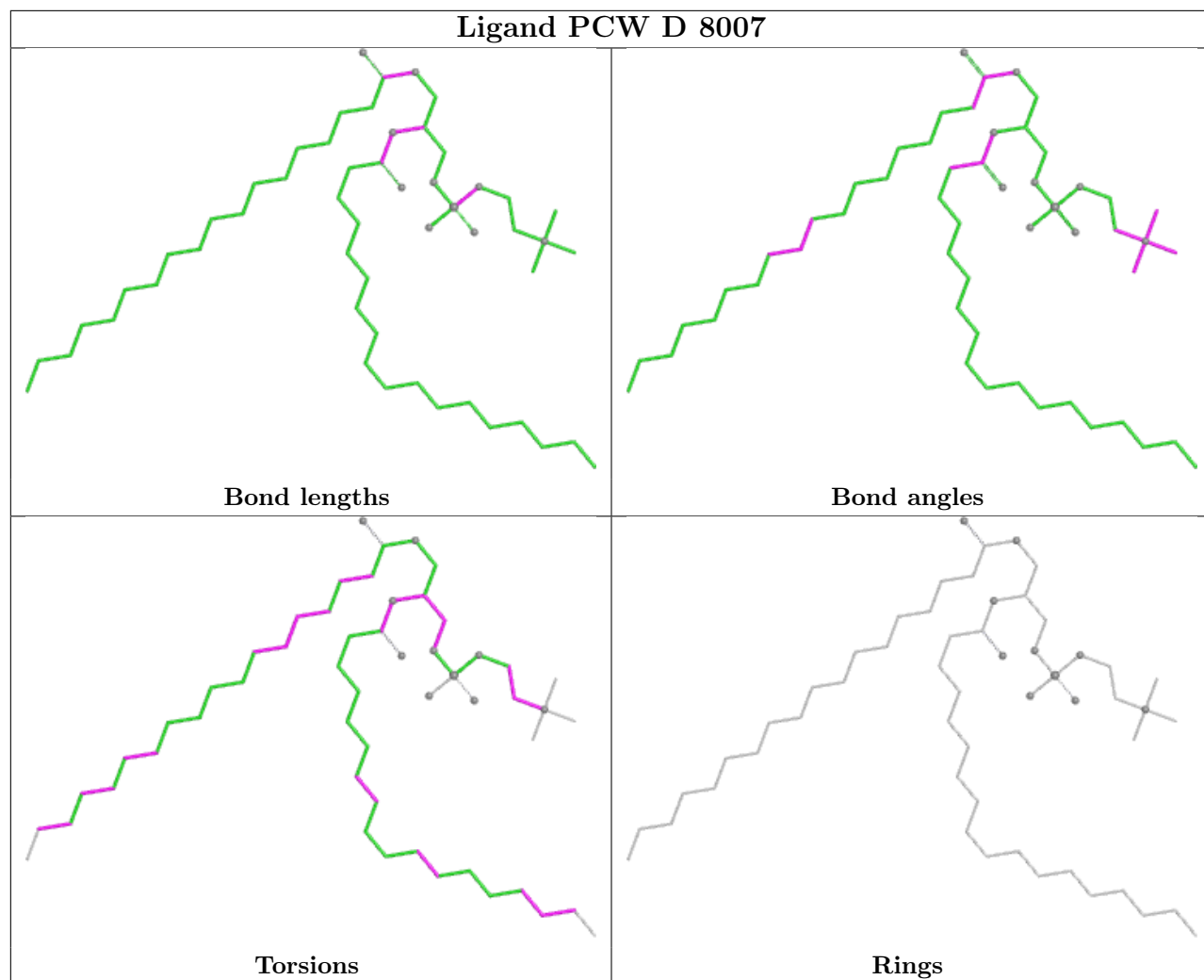


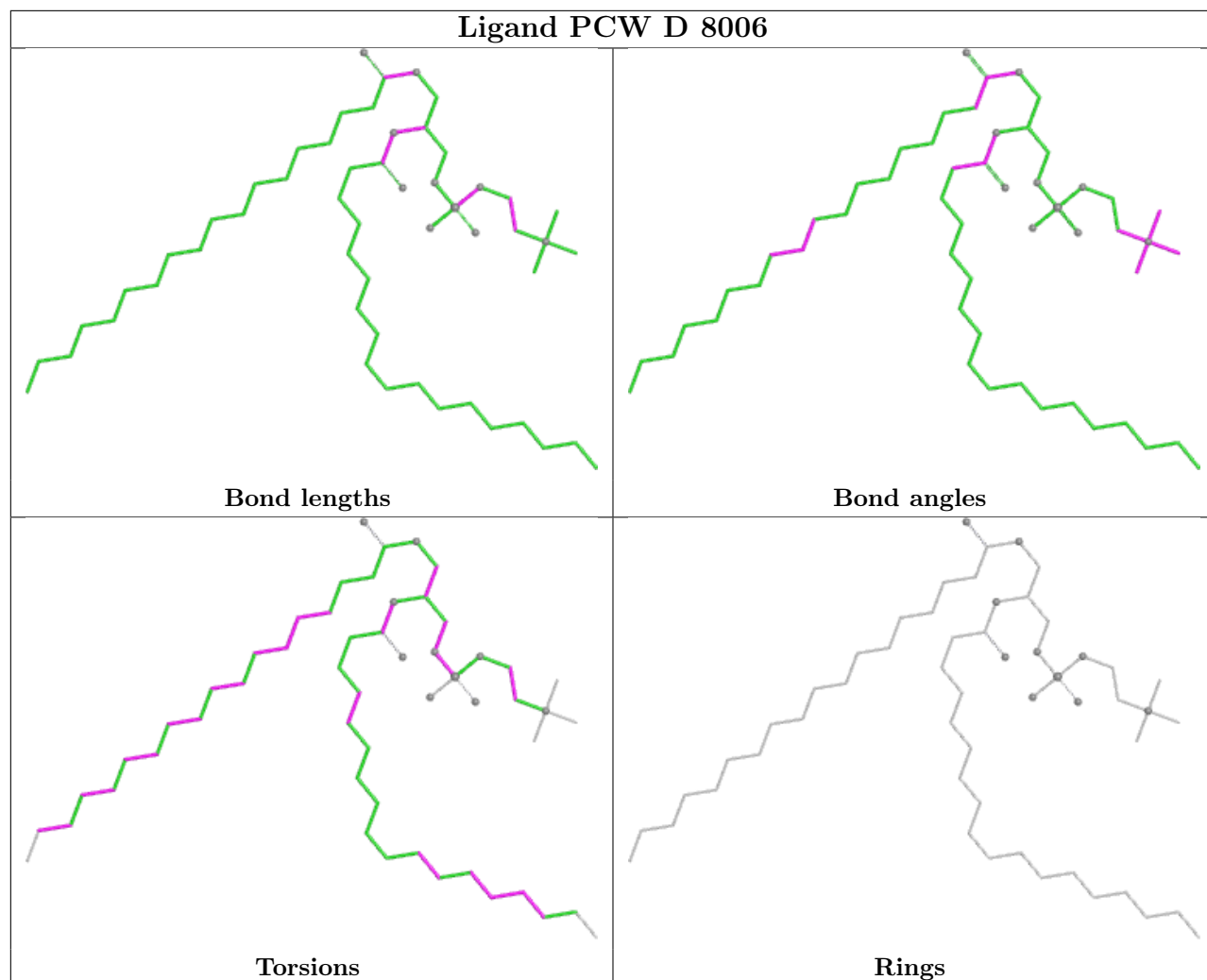


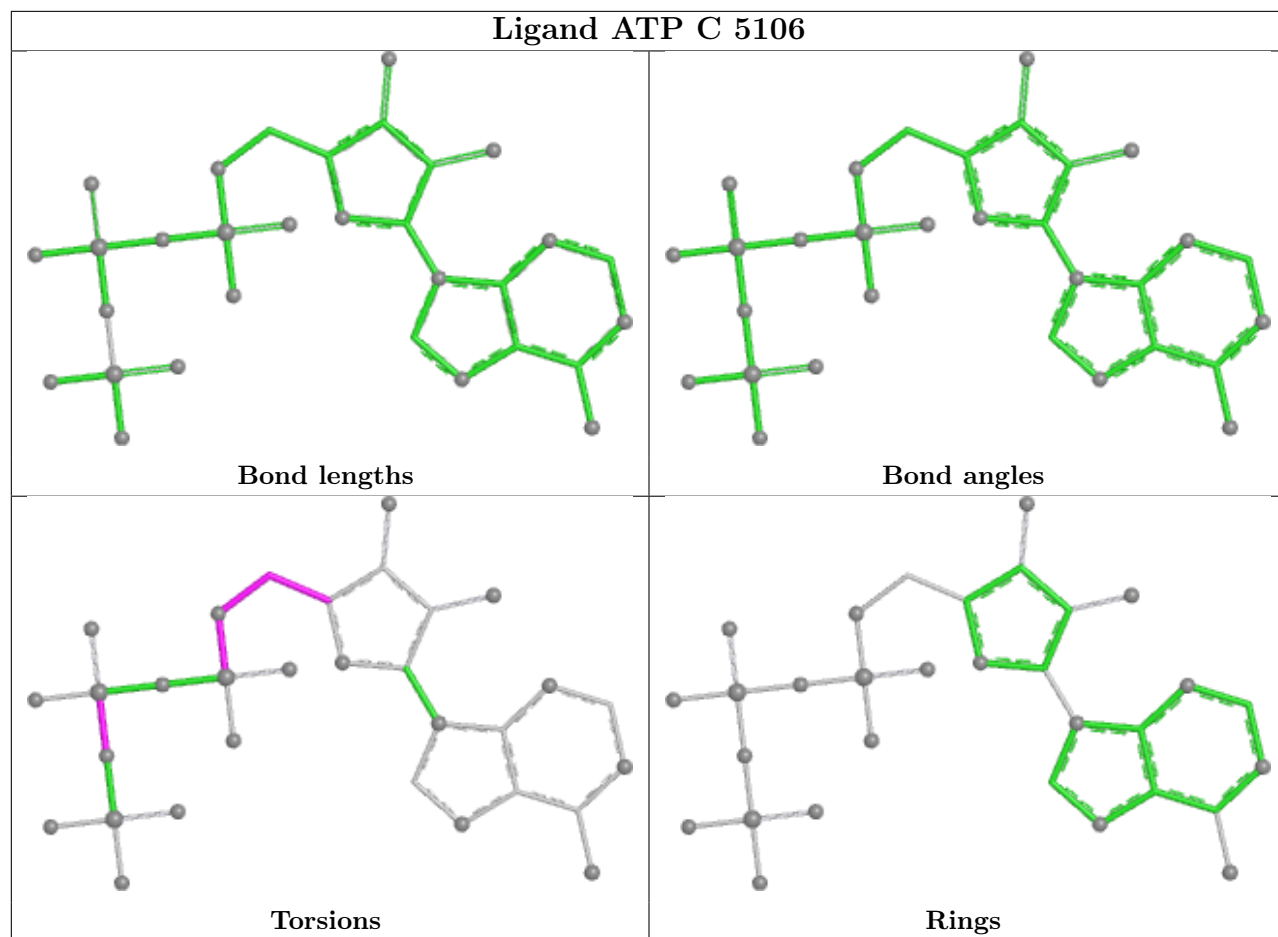


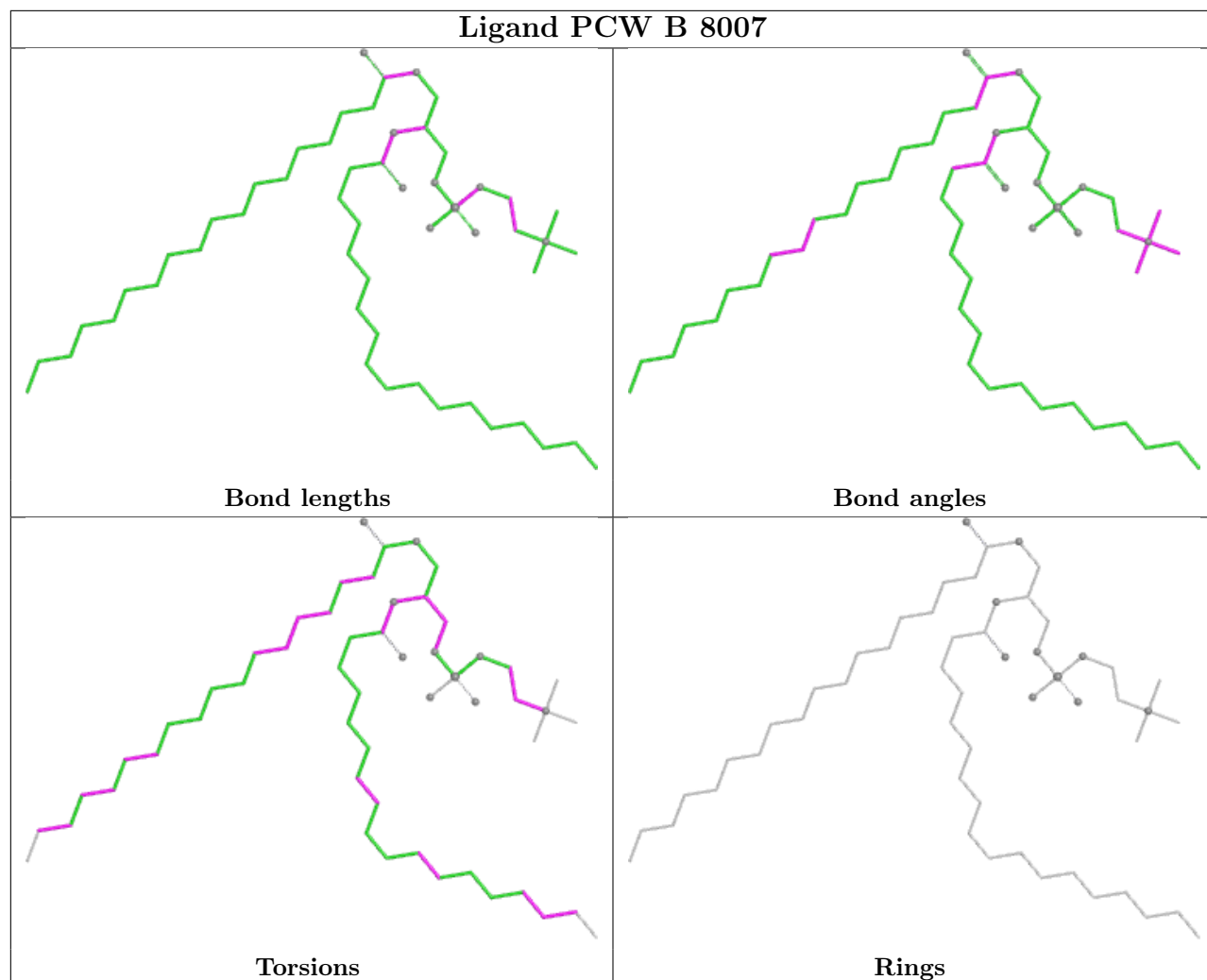


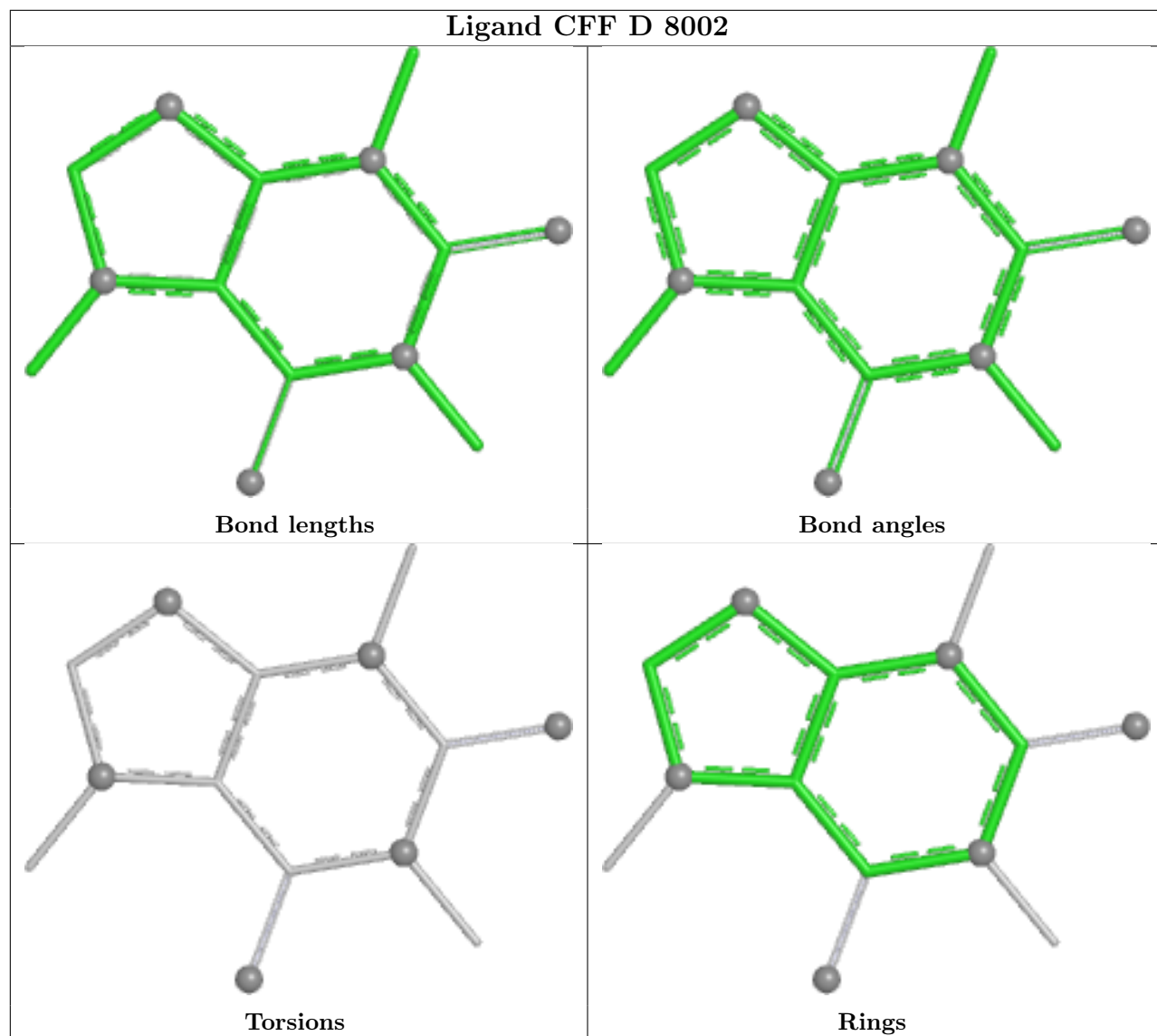


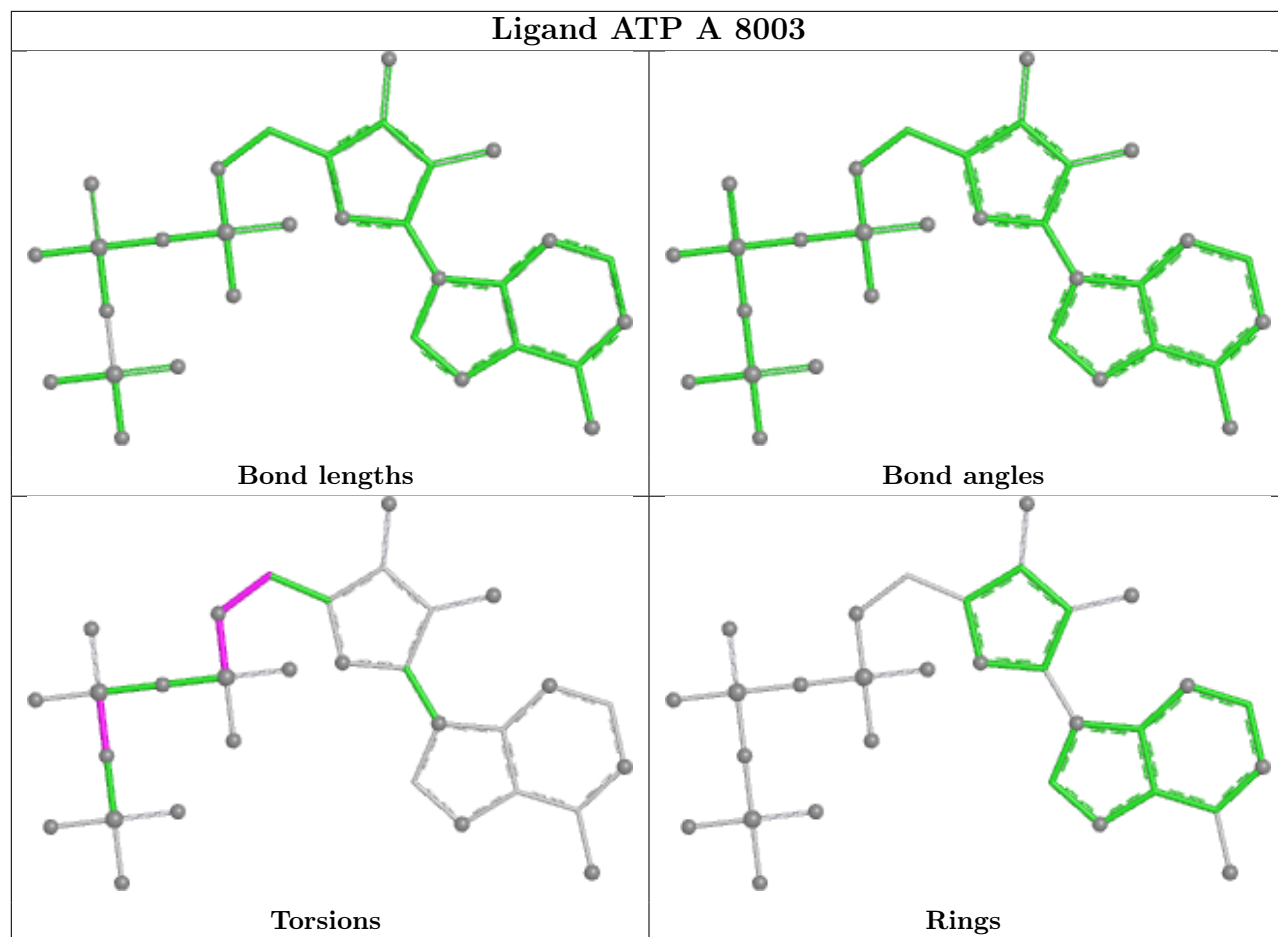


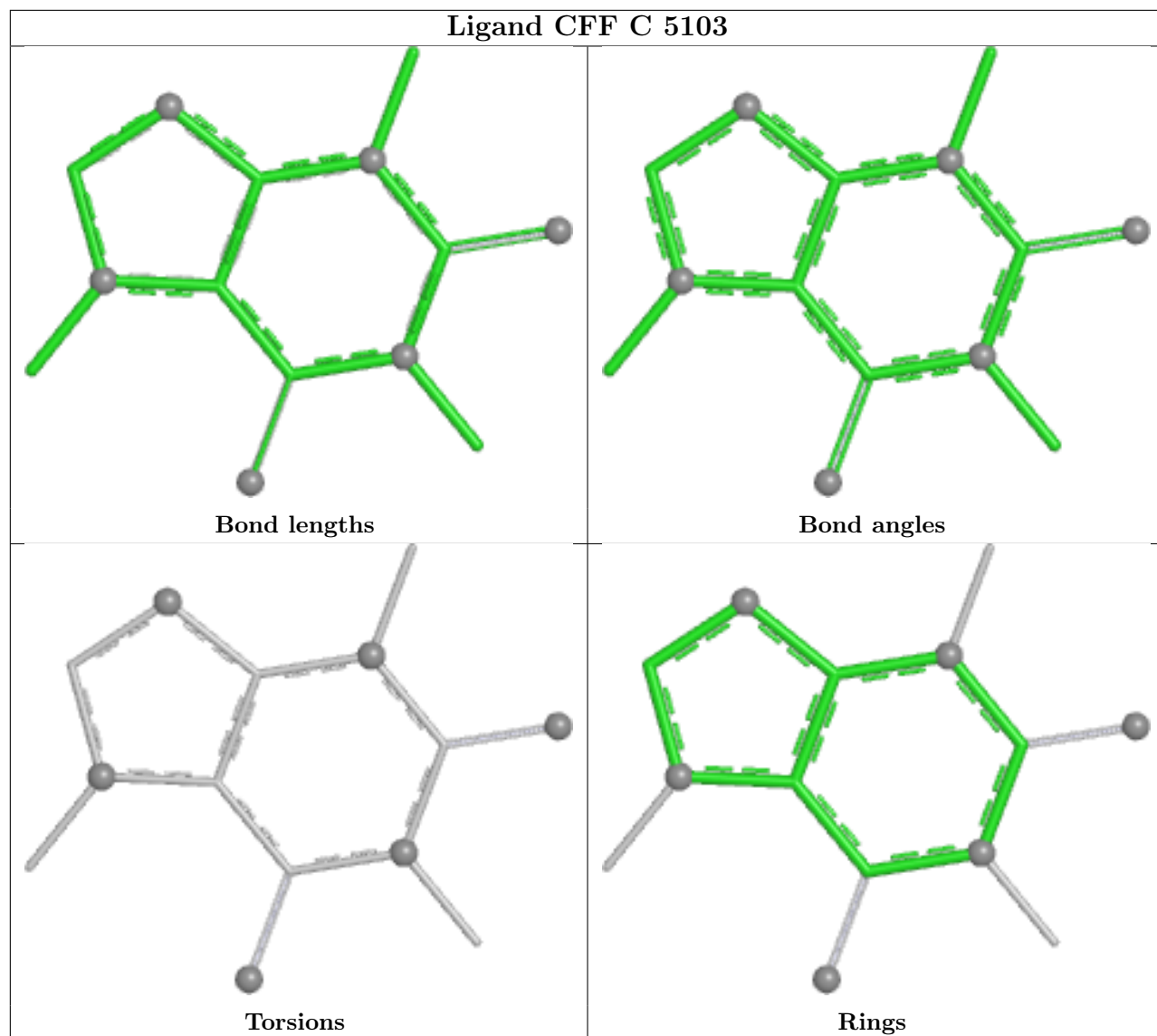


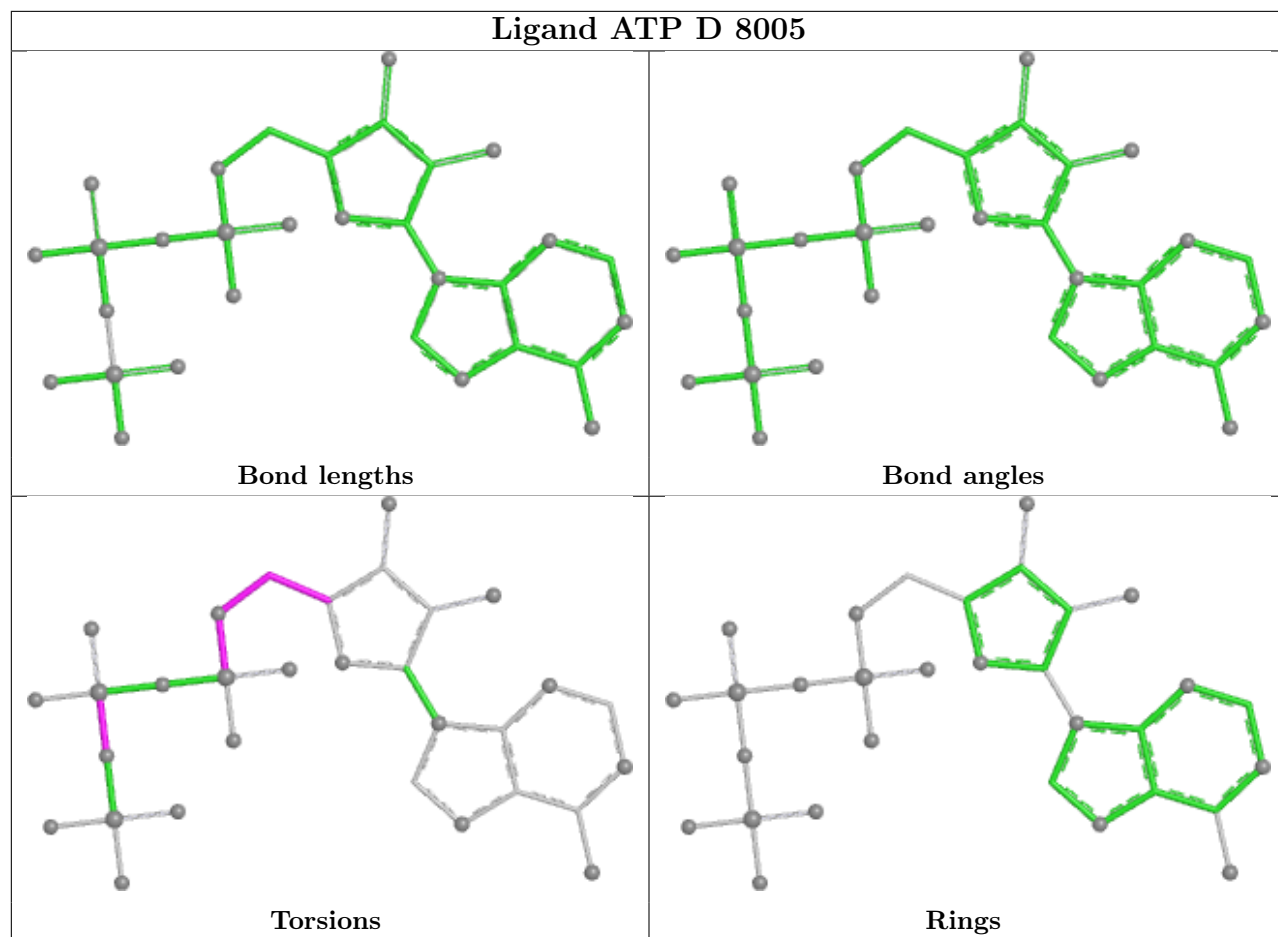


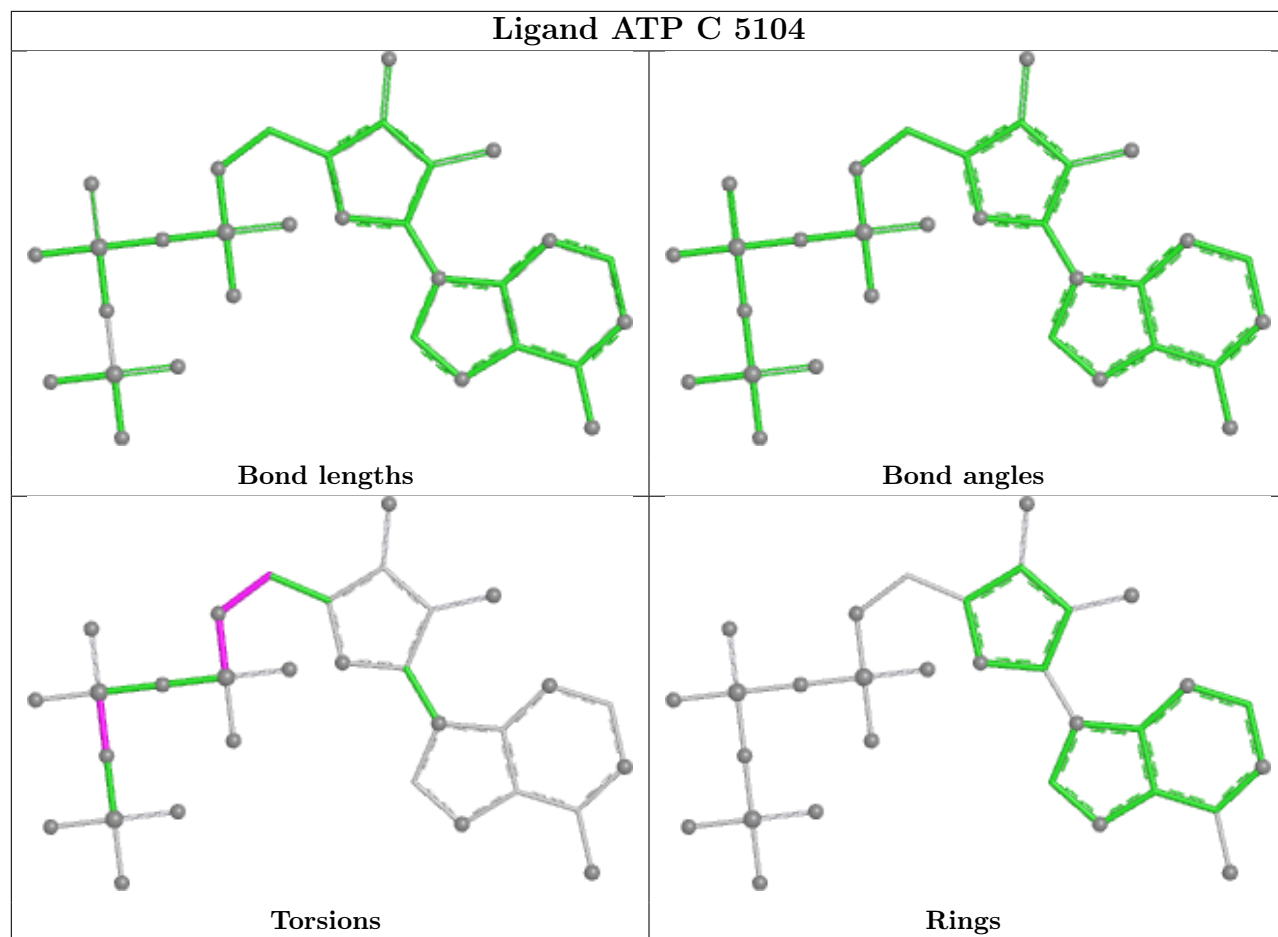


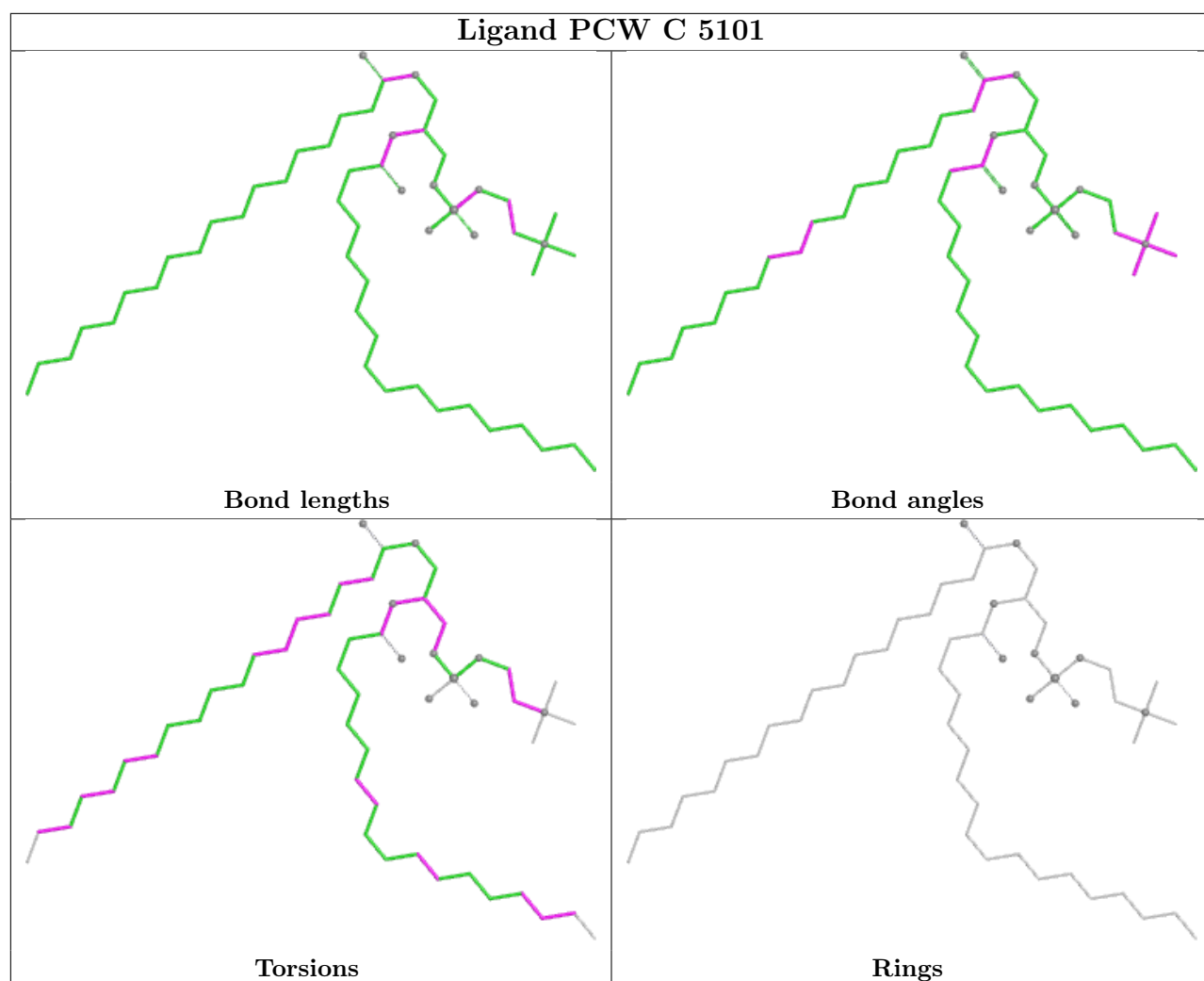


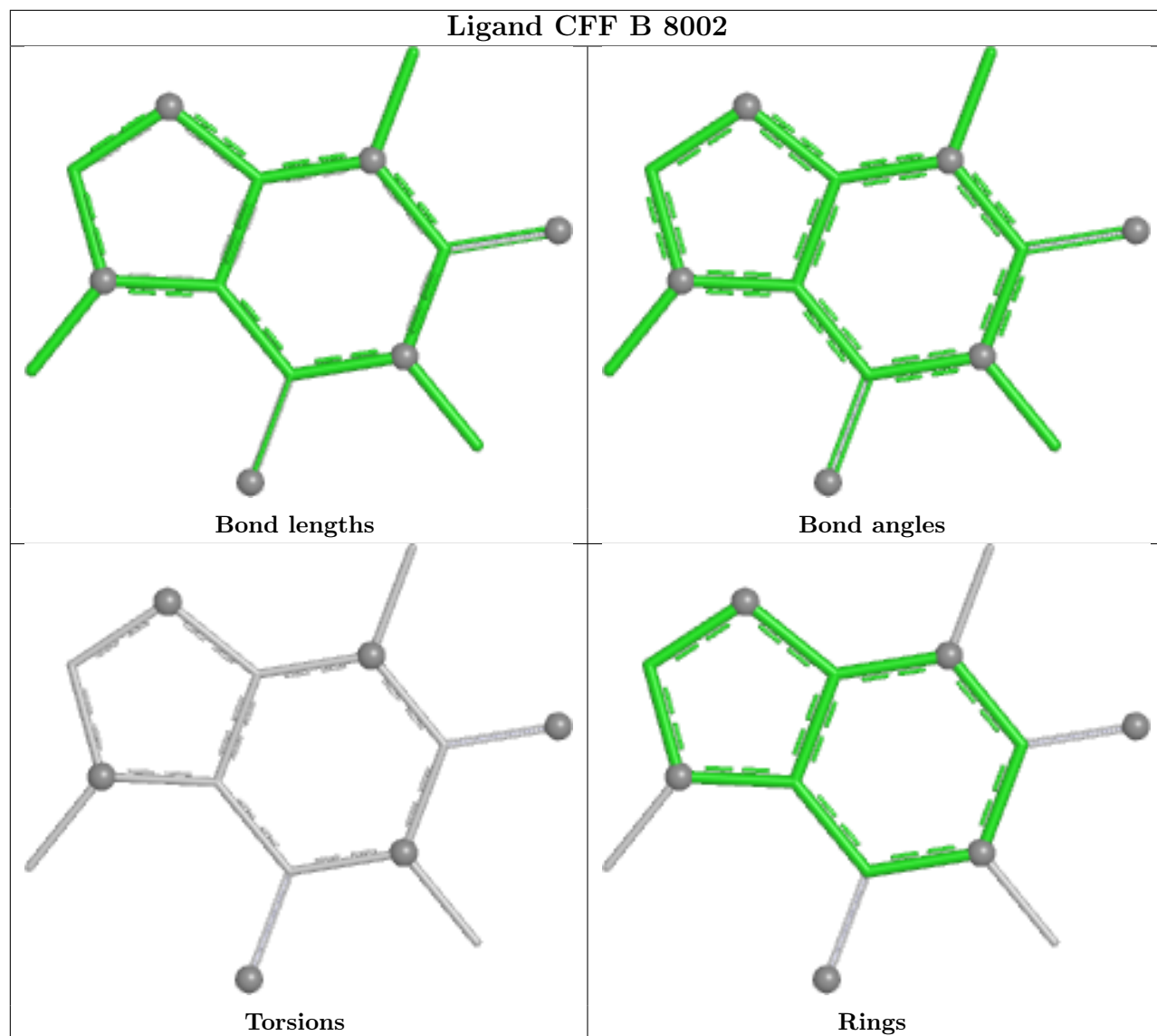


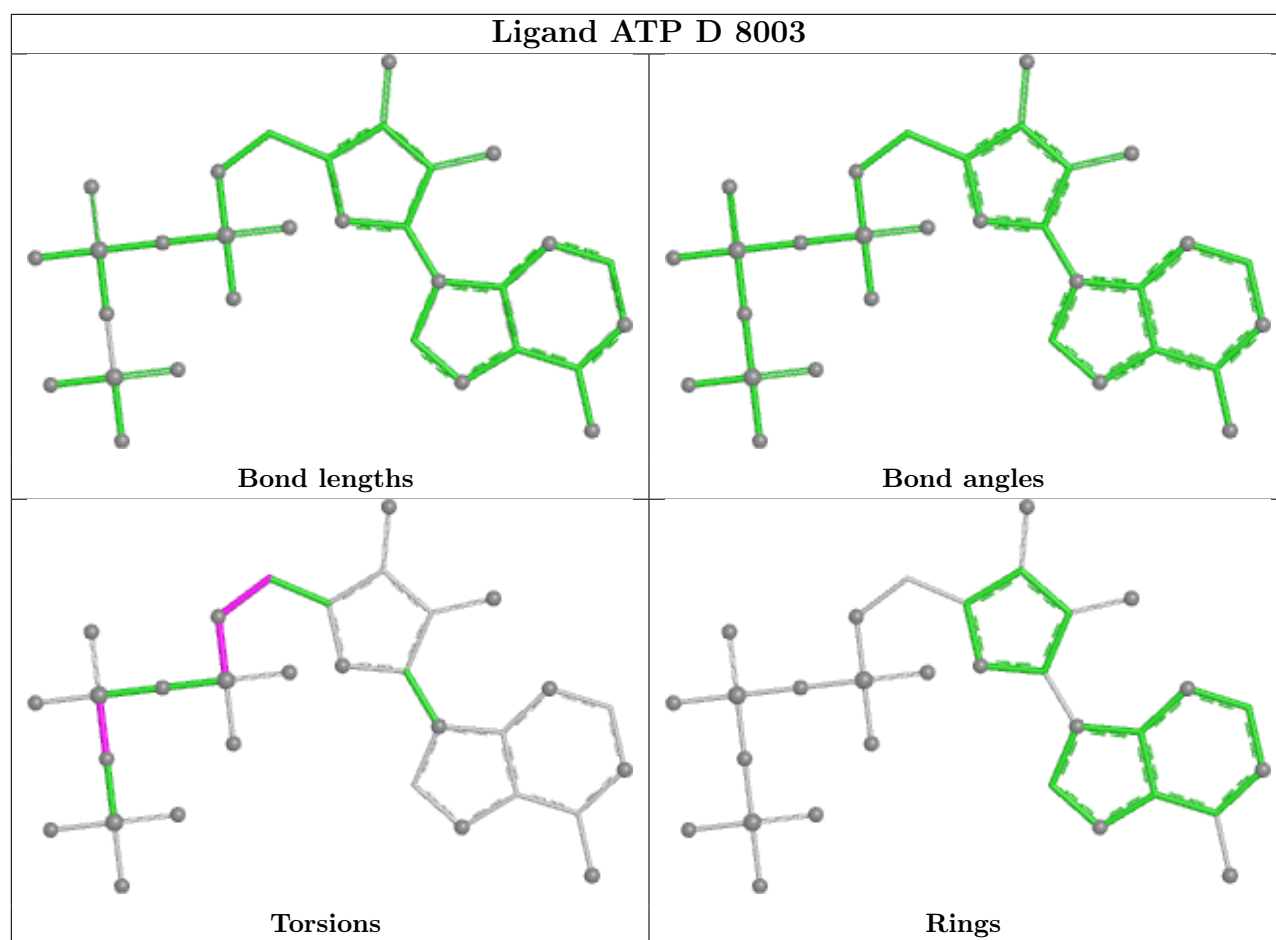












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

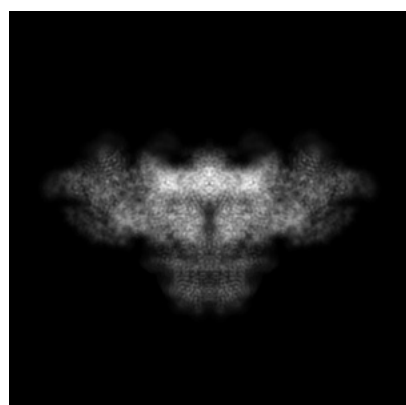
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43304. These allow visual inspection of the internal detail of the map and identification of artifacts.

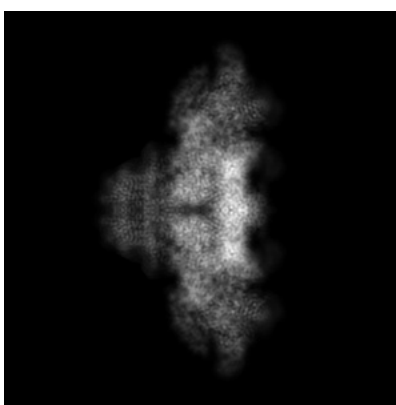
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

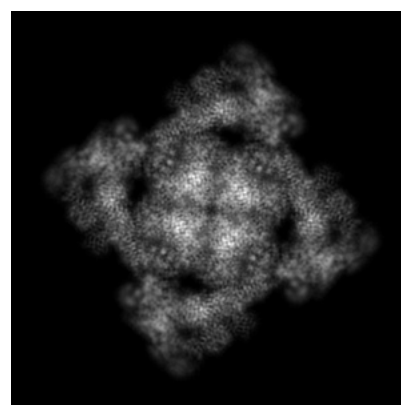
6.1.1 Primary map



X



Y



Z

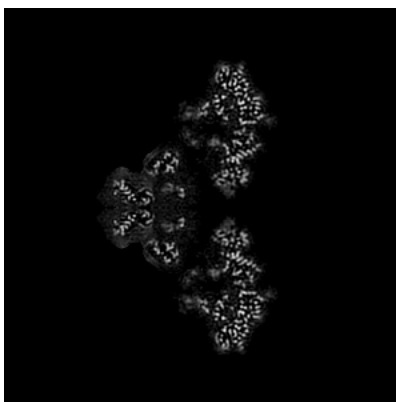
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

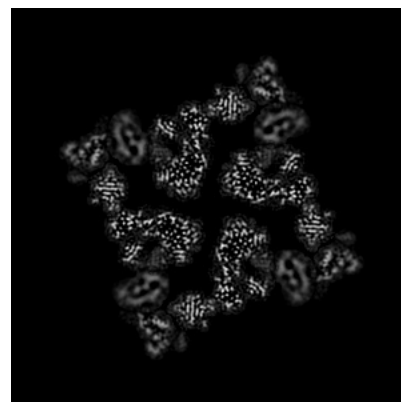
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

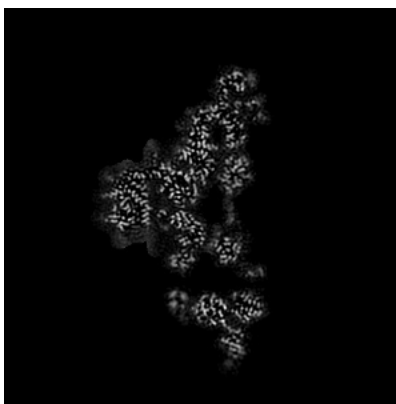
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

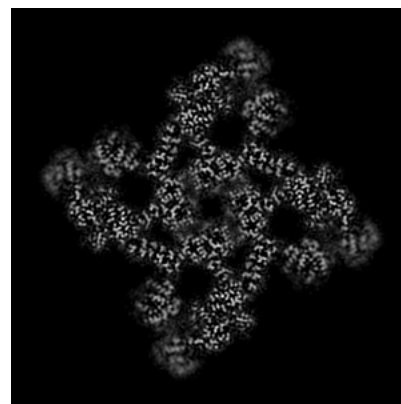
6.3.1 Primary map



X Index: 274



Y Index: 274

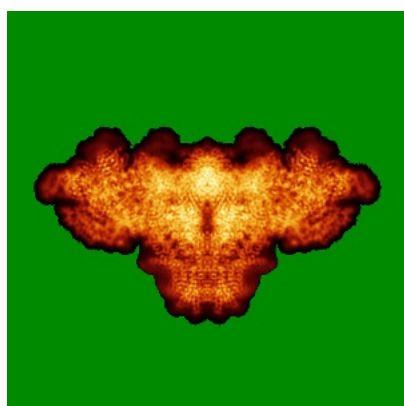


Z Index: 285

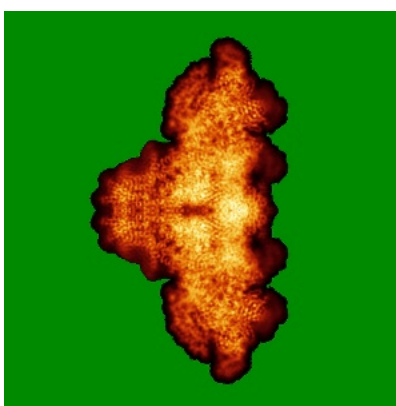
The images above show the largest variance slices of the map in three orthogonal directions.

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

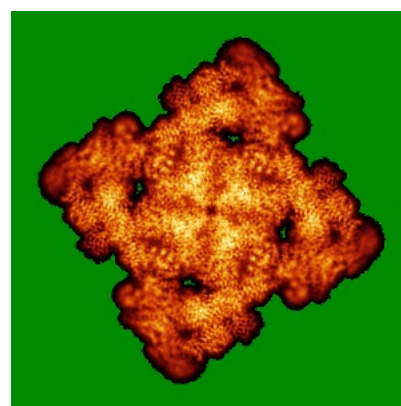
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

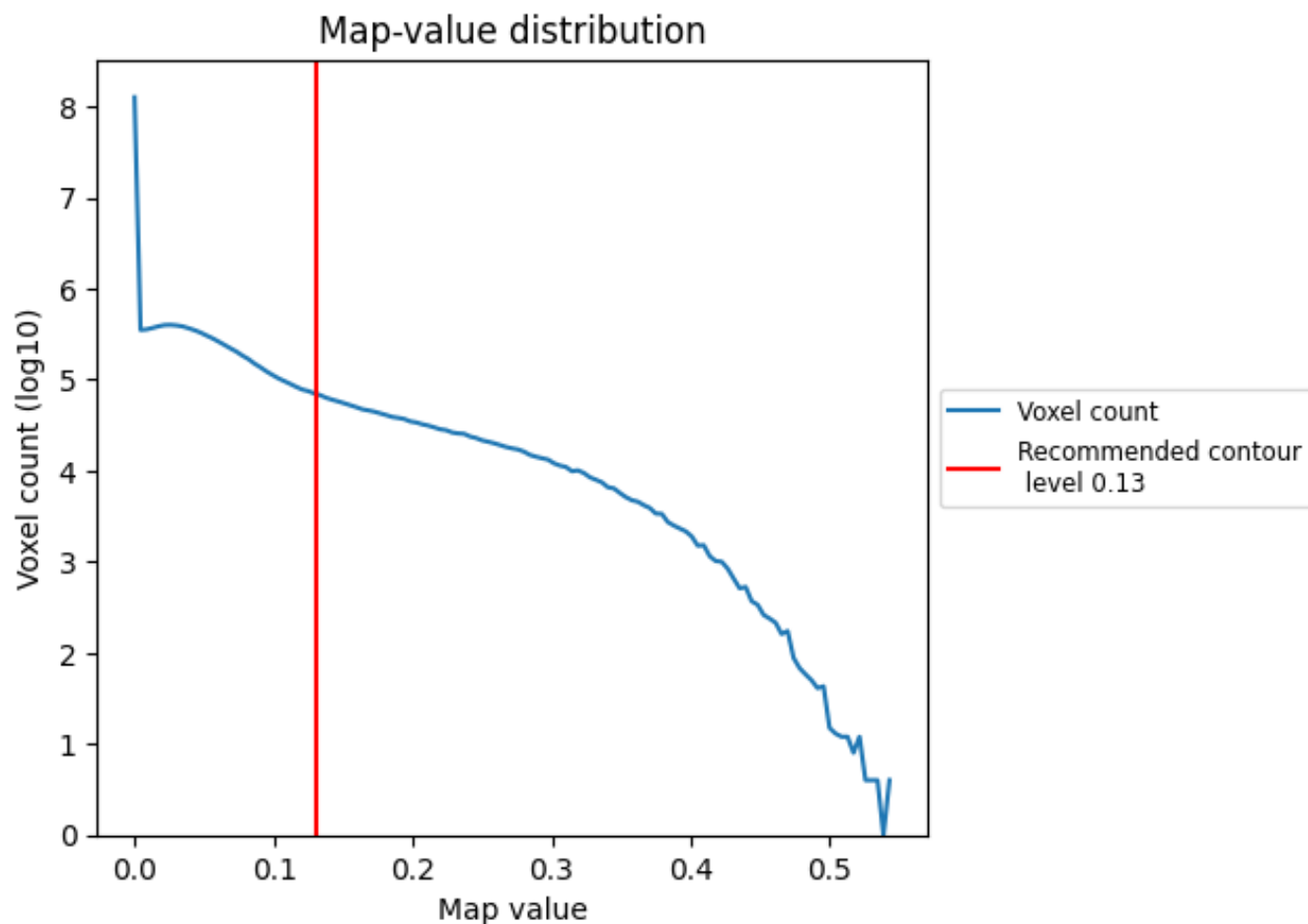
6.6 Mask visualisation

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

7 Map analysis [i](#)

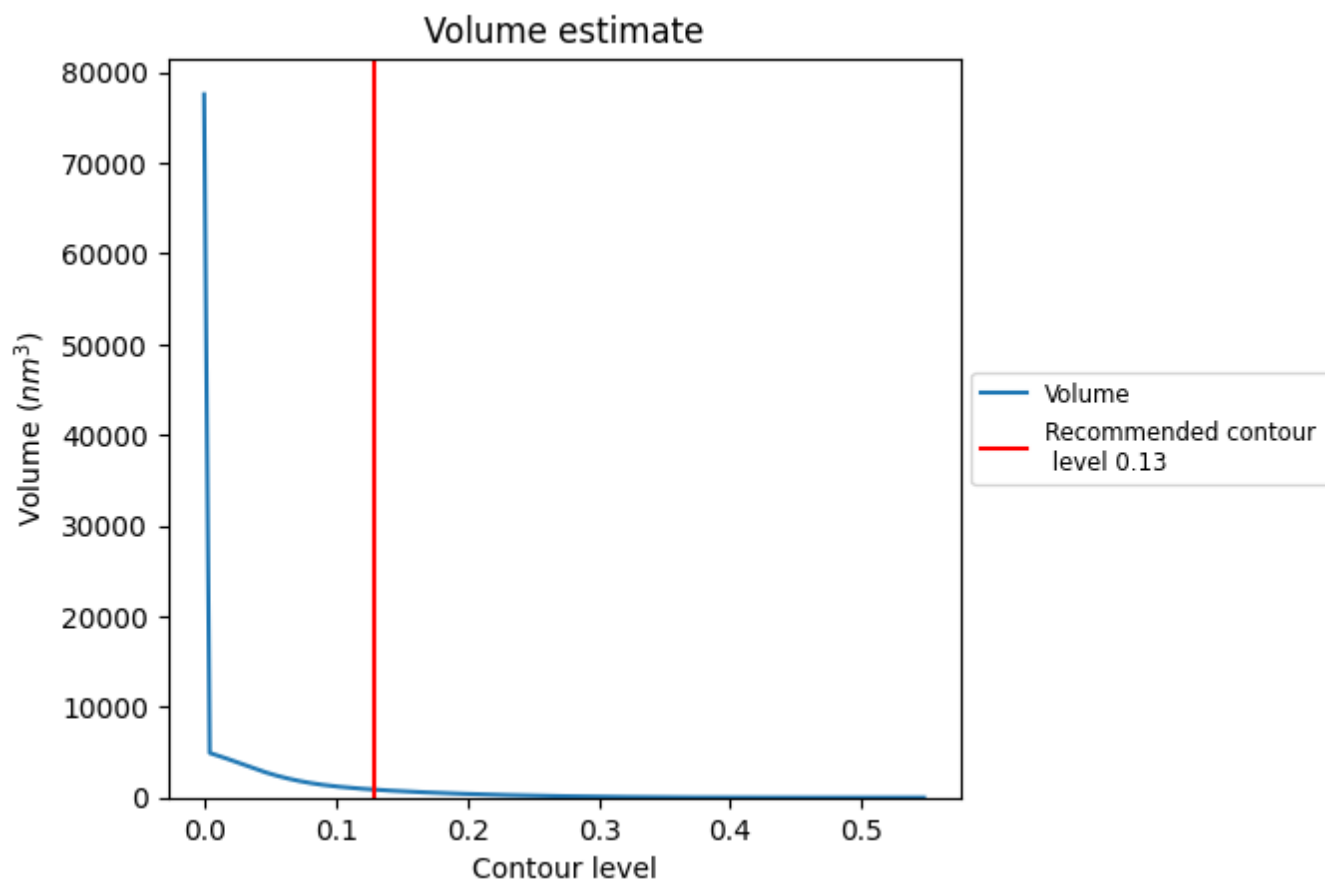
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

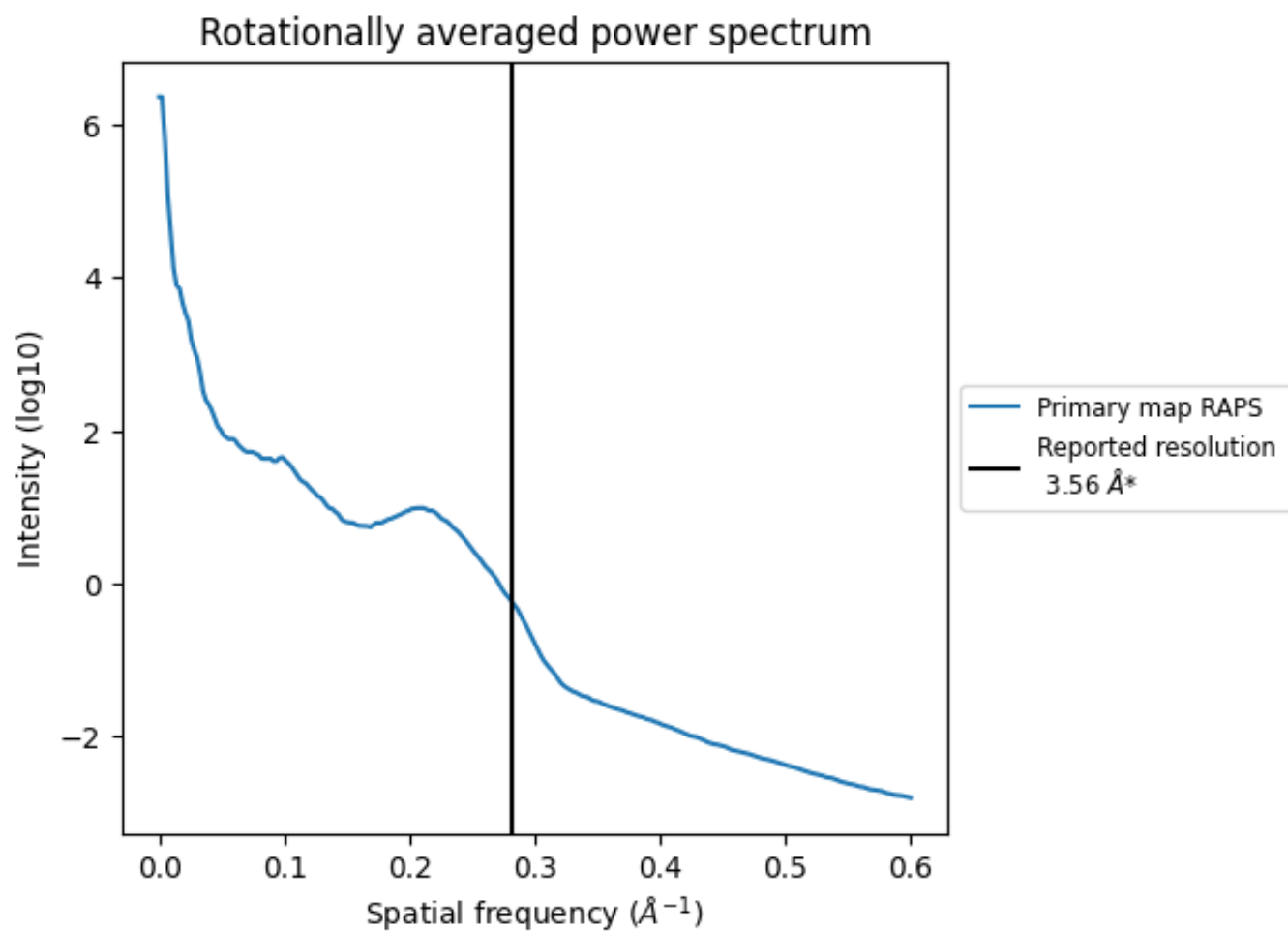
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 870 nm³; this corresponds to an approximate mass of 786 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 0.281 Å⁻¹

8 Fourier-Shell correlation

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

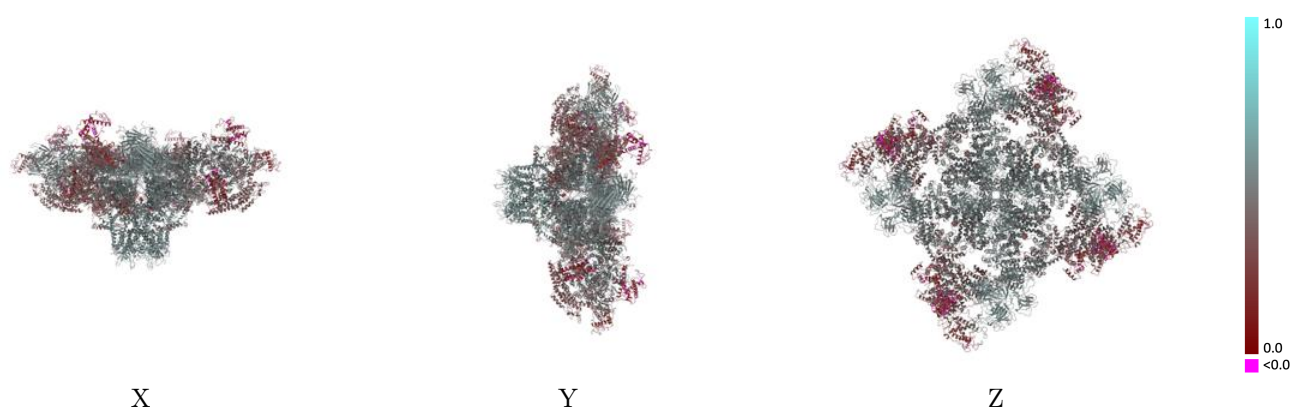
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43304 and PDB model 8VK4. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

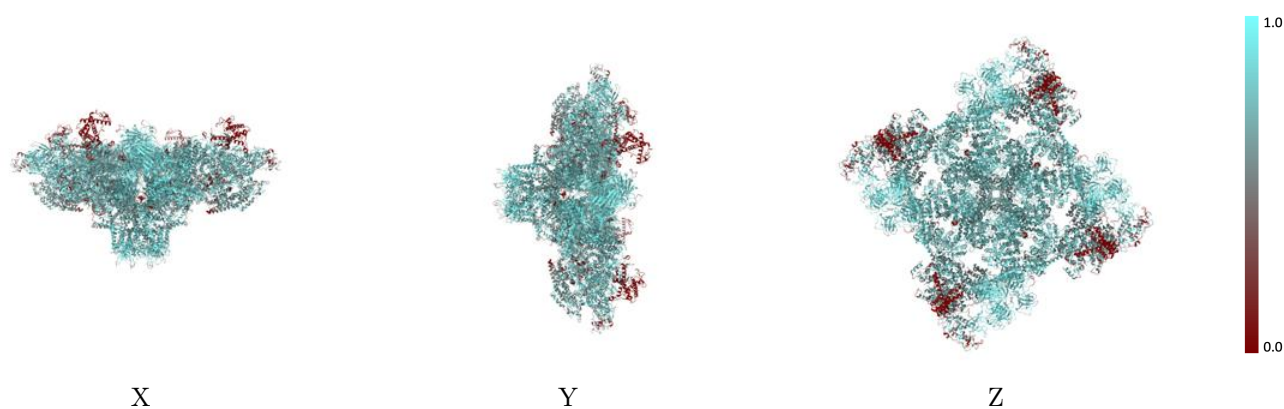
This section was not generated.

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



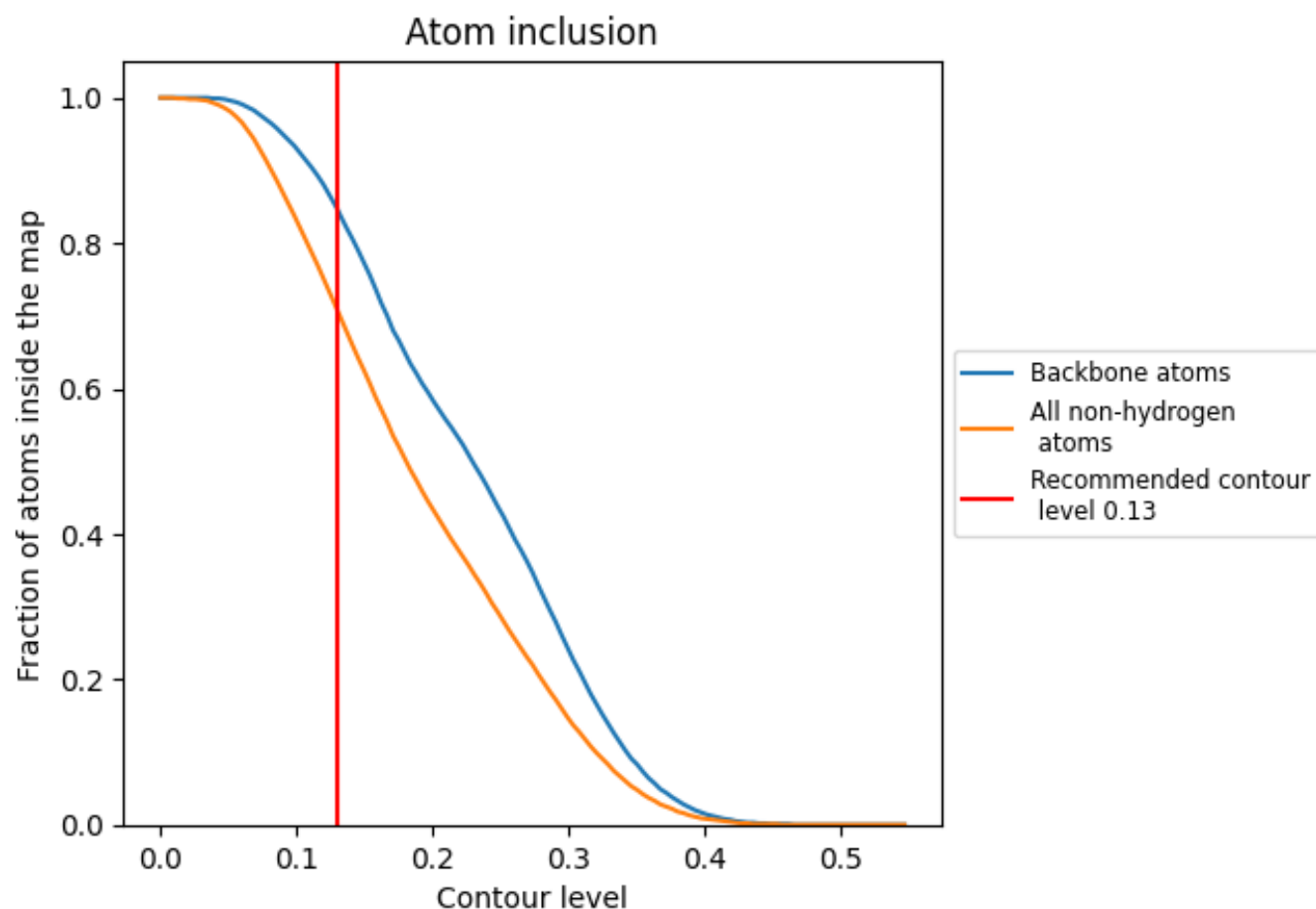
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.4400
A	 0.7140	 0.4500
B	 0.7140	 0.4490
C	 0.7140	 0.4500
D	 0.7140	 0.4500
E	 0.7630	 0.5070
F	 0.7700	 0.5060
G	 0.7670	 0.5050
H	 0.7690	 0.5070
I	 0.4960	 0.1660
J	 0.5800	 0.1760
K	 0.4990	 0.1680
L	 0.5820	 0.1770
M	 0.5000	 0.1690
N	 0.5820	 0.1790
O	 0.4970	 0.1650
P	 0.5810	 0.1770

