



Full wwPDB EM Validation Report ⓘ

Sep 22, 2026 – 08:50 PM EDT

PDB ID : 9ZO8 / pdb_00009zo8
EMDB ID : EMD-74471
Title : Structure of RyR1 in presence of rosuvastatin (including auxiliary transmembrane helices TMx1 and TMx2; Ca²⁺/CFF/ATP dataset; closed pore)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-12-15
Resolution : 2.70 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:

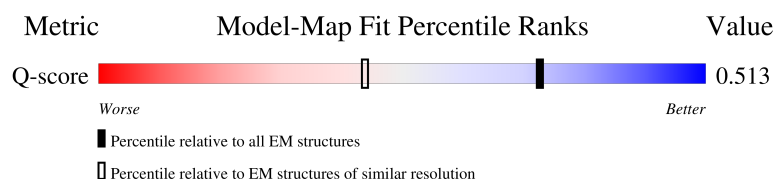
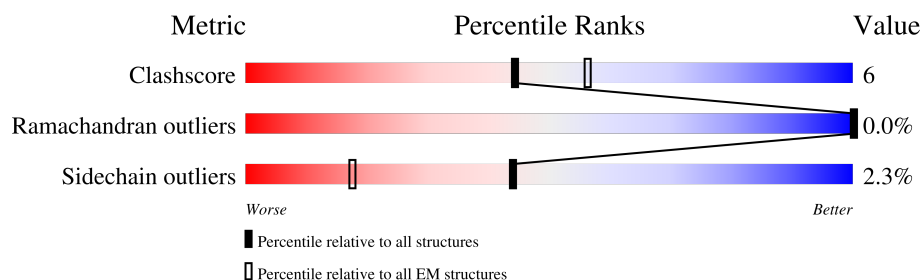
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.70 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	10327 (2.20 - 3.20)

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	A	5037	9% 74% 13% 12%
2	B	5037	9% 75% 13% 12%
2	C	5037	9% 74% 13% 12%
2	D	5037	9% 74% 13% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144732 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
			831	527	146	154	4		
1	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
1	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
1	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4433	Total	C	N	O	S	6	0
			35197	22383	6068	6509	237		
2	B	4433	Total	C	N	O	S	6	0
			35197	22383	6068	6509	237		
2	D	4433	Total	C	N	O	S	6	0
			35197	22383	6068	6509	237		
2	C	4433	Total	C	N	O	S	6	0
			35197	22383	6068	6509	237		

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4279	UNK	ALA	conflict	UNP P11716
A	4280	UNK	GLY	conflict	UNP P11716
A	4281	UNK	ALA	conflict	UNP P11716
A	4282	UNK	GLU	conflict	UNP P11716
A	4283	UNK	GLY	conflict	UNP P11716
A	4284	UNK	ALA	conflict	UNP P11716
A	4285	UNK	ALA	conflict	UNP P11716
A	4286	UNK	GLY	conflict	UNP P11716
A	4287	UNK	THR	conflict	UNP P11716

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4288	UNK	VAL	conflict	UNP P11716
A	4289	UNK	ALA	conflict	UNP P11716
A	4290	UNK	ALA	conflict	UNP P11716
A	4291	UNK	GLY	conflict	UNP P11716
A	4292	UNK	ALA	conflict	UNP P11716
A	4293	UNK	THR	conflict	UNP P11716
A	4294	UNK	ALA	conflict	UNP P11716
A	4295	UNK	ARG	conflict	UNP P11716
A	4296	UNK	LEU	conflict	UNP P11716
A	4297	UNK	ALA	conflict	UNP P11716
A	4298	UNK	ALA	conflict	UNP P11716
A	4299	UNK	ALA	conflict	UNP P11716
A	4300	UNK	ALA	conflict	UNP P11716
A	4301	UNK	ALA	conflict	UNP P11716
A	4302	UNK	ARG	conflict	UNP P11716
A	4318	UNK	ARG	conflict	UNP P11716
A	4319	UNK	LEU	conflict	UNP P11716
A	4320	UNK	ARG	conflict	UNP P11716
A	4321	UNK	ARG	conflict	UNP P11716
A	4322	UNK	LEU	conflict	UNP P11716
A	4323	UNK	THR	conflict	UNP P11716
A	4324	UNK	ALA	conflict	UNP P11716
A	4325	UNK	ARG	conflict	UNP P11716
A	4326	UNK	GLU	conflict	UNP P11716
A	4327	UNK	ALA	conflict	UNP P11716
A	4328	UNK	ALA	conflict	UNP P11716
A	4329	UNK	THR	conflict	UNP P11716
A	4330	UNK	ALA	conflict	UNP P11716
A	4331	UNK	LEU	conflict	UNP P11716
A	4332	UNK	ALA	conflict	UNP P11716
A	4333	UNK	ALA	conflict	UNP P11716
A	4334	UNK	LEU	conflict	UNP P11716
A	4335	UNK	LEU	conflict	UNP P11716
A	4336	UNK	TRP	conflict	UNP P11716
A	4337	UNK	ALA	conflict	UNP P11716
A	4338	UNK	VAL	conflict	UNP P11716
A	4339	UNK	VAL	conflict	UNP P11716
A	4340	UNK	ALA	conflict	UNP P11716
A	4341	UNK	ARG	conflict	UNP P11716
A	4342	UNK	ALA	conflict	UNP P11716
A	4343	UNK	GLY	conflict	UNP P11716
B	4279	UNK	ALA	conflict	UNP P11716

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4280	UNK	GLY	conflict	UNP P11716
B	4281	UNK	ALA	conflict	UNP P11716
B	4282	UNK	GLU	conflict	UNP P11716
B	4283	UNK	GLY	conflict	UNP P11716
B	4284	UNK	ALA	conflict	UNP P11716
B	4285	UNK	ALA	conflict	UNP P11716
B	4286	UNK	GLY	conflict	UNP P11716
B	4287	UNK	THR	conflict	UNP P11716
B	4288	UNK	VAL	conflict	UNP P11716
B	4289	UNK	ALA	conflict	UNP P11716
B	4290	UNK	ALA	conflict	UNP P11716
B	4291	UNK	GLY	conflict	UNP P11716
B	4292	UNK	ALA	conflict	UNP P11716
B	4293	UNK	THR	conflict	UNP P11716
B	4294	UNK	ALA	conflict	UNP P11716
B	4295	UNK	ARG	conflict	UNP P11716
B	4296	UNK	LEU	conflict	UNP P11716
B	4297	UNK	ALA	conflict	UNP P11716
B	4298	UNK	ALA	conflict	UNP P11716
B	4299	UNK	ALA	conflict	UNP P11716
B	4300	UNK	ALA	conflict	UNP P11716
B	4301	UNK	ALA	conflict	UNP P11716
B	4302	UNK	ARG	conflict	UNP P11716
B	4318	UNK	ARG	conflict	UNP P11716
B	4319	UNK	LEU	conflict	UNP P11716
B	4320	UNK	ARG	conflict	UNP P11716
B	4321	UNK	ARG	conflict	UNP P11716
B	4322	UNK	LEU	conflict	UNP P11716
B	4323	UNK	THR	conflict	UNP P11716
B	4324	UNK	ALA	conflict	UNP P11716
B	4325	UNK	ARG	conflict	UNP P11716
B	4326	UNK	GLU	conflict	UNP P11716
B	4327	UNK	ALA	conflict	UNP P11716
B	4328	UNK	ALA	conflict	UNP P11716
B	4329	UNK	THR	conflict	UNP P11716
B	4330	UNK	ALA	conflict	UNP P11716
B	4331	UNK	LEU	conflict	UNP P11716
B	4332	UNK	ALA	conflict	UNP P11716
B	4333	UNK	ALA	conflict	UNP P11716
B	4334	UNK	LEU	conflict	UNP P11716
B	4335	UNK	LEU	conflict	UNP P11716
B	4336	UNK	TRP	conflict	UNP P11716

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4337	UNK	ALA	conflict	UNP P11716
B	4338	UNK	VAL	conflict	UNP P11716
B	4339	UNK	VAL	conflict	UNP P11716
B	4340	UNK	ALA	conflict	UNP P11716
B	4341	UNK	ARG	conflict	UNP P11716
B	4342	UNK	ALA	conflict	UNP P11716
B	4343	UNK	GLY	conflict	UNP P11716
D	4279	UNK	ALA	conflict	UNP P11716
D	4280	UNK	GLY	conflict	UNP P11716
D	4281	UNK	ALA	conflict	UNP P11716
D	4282	UNK	GLU	conflict	UNP P11716
D	4283	UNK	GLY	conflict	UNP P11716
D	4284	UNK	ALA	conflict	UNP P11716
D	4285	UNK	ALA	conflict	UNP P11716
D	4286	UNK	GLY	conflict	UNP P11716
D	4287	UNK	THR	conflict	UNP P11716
D	4288	UNK	VAL	conflict	UNP P11716
D	4289	UNK	ALA	conflict	UNP P11716
D	4290	UNK	ALA	conflict	UNP P11716
D	4291	UNK	GLY	conflict	UNP P11716
D	4292	UNK	ALA	conflict	UNP P11716
D	4293	UNK	THR	conflict	UNP P11716
D	4294	UNK	ALA	conflict	UNP P11716
D	4295	UNK	ARG	conflict	UNP P11716
D	4296	UNK	LEU	conflict	UNP P11716
D	4297	UNK	ALA	conflict	UNP P11716
D	4298	UNK	ALA	conflict	UNP P11716
D	4299	UNK	ALA	conflict	UNP P11716
D	4300	UNK	ALA	conflict	UNP P11716
D	4301	UNK	ALA	conflict	UNP P11716
D	4302	UNK	ARG	conflict	UNP P11716
D	4318	UNK	ARG	conflict	UNP P11716
D	4319	UNK	LEU	conflict	UNP P11716
D	4320	UNK	ARG	conflict	UNP P11716
D	4321	UNK	ARG	conflict	UNP P11716
D	4322	UNK	LEU	conflict	UNP P11716
D	4323	UNK	THR	conflict	UNP P11716
D	4324	UNK	ALA	conflict	UNP P11716
D	4325	UNK	ARG	conflict	UNP P11716
D	4326	UNK	GLU	conflict	UNP P11716
D	4327	UNK	ALA	conflict	UNP P11716
D	4328	UNK	ALA	conflict	UNP P11716

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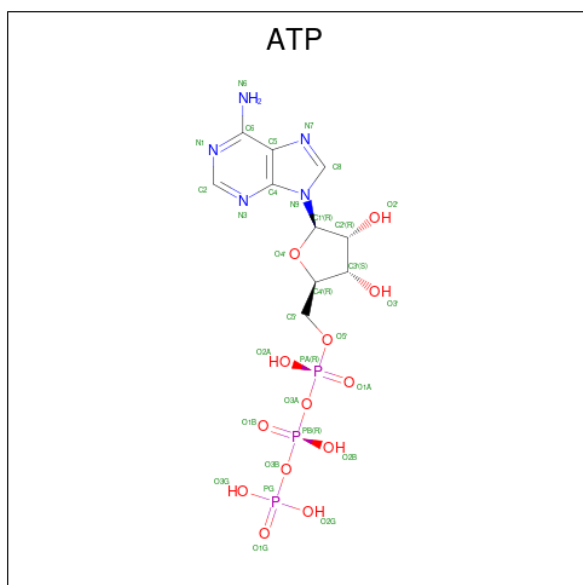
Chain	Residue	Modelled	Actual	Comment	Reference
D	4329	UNK	THR	conflict	UNP P11716
D	4330	UNK	ALA	conflict	UNP P11716
D	4331	UNK	LEU	conflict	UNP P11716
D	4332	UNK	ALA	conflict	UNP P11716
D	4333	UNK	ALA	conflict	UNP P11716
D	4334	UNK	LEU	conflict	UNP P11716
D	4335	UNK	LEU	conflict	UNP P11716
D	4336	UNK	TRP	conflict	UNP P11716
D	4337	UNK	ALA	conflict	UNP P11716
D	4338	UNK	VAL	conflict	UNP P11716
D	4339	UNK	VAL	conflict	UNP P11716
D	4340	UNK	ALA	conflict	UNP P11716
D	4341	UNK	ARG	conflict	UNP P11716
D	4342	UNK	ALA	conflict	UNP P11716
D	4343	UNK	GLY	conflict	UNP P11716
C	4279	UNK	ALA	conflict	UNP P11716
C	4280	UNK	GLY	conflict	UNP P11716
C	4281	UNK	ALA	conflict	UNP P11716
C	4282	UNK	GLU	conflict	UNP P11716
C	4283	UNK	GLY	conflict	UNP P11716
C	4284	UNK	ALA	conflict	UNP P11716
C	4285	UNK	ALA	conflict	UNP P11716
C	4286	UNK	GLY	conflict	UNP P11716
C	4287	UNK	THR	conflict	UNP P11716
C	4288	UNK	VAL	conflict	UNP P11716
C	4289	UNK	ALA	conflict	UNP P11716
C	4290	UNK	ALA	conflict	UNP P11716
C	4291	UNK	GLY	conflict	UNP P11716
C	4292	UNK	ALA	conflict	UNP P11716
C	4293	UNK	THR	conflict	UNP P11716
C	4294	UNK	ALA	conflict	UNP P11716
C	4295	UNK	ARG	conflict	UNP P11716
C	4296	UNK	LEU	conflict	UNP P11716
C	4297	UNK	ALA	conflict	UNP P11716
C	4298	UNK	ALA	conflict	UNP P11716
C	4299	UNK	ALA	conflict	UNP P11716
C	4300	UNK	ALA	conflict	UNP P11716
C	4301	UNK	ALA	conflict	UNP P11716
C	4302	UNK	ARG	conflict	UNP P11716
C	4318	UNK	ARG	conflict	UNP P11716
C	4319	UNK	LEU	conflict	UNP P11716
C	4320	UNK	ARG	conflict	UNP P11716

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4321	UNK	ARG	conflict	UNP P11716
C	4322	UNK	LEU	conflict	UNP P11716
C	4323	UNK	THR	conflict	UNP P11716
C	4324	UNK	ALA	conflict	UNP P11716
C	4325	UNK	ARG	conflict	UNP P11716
C	4326	UNK	GLU	conflict	UNP P11716
C	4327	UNK	ALA	conflict	UNP P11716
C	4328	UNK	ALA	conflict	UNP P11716
C	4329	UNK	THR	conflict	UNP P11716
C	4330	UNK	ALA	conflict	UNP P11716
C	4331	UNK	LEU	conflict	UNP P11716
C	4332	UNK	ALA	conflict	UNP P11716
C	4333	UNK	ALA	conflict	UNP P11716
C	4334	UNK	LEU	conflict	UNP P11716
C	4335	UNK	LEU	conflict	UNP P11716
C	4336	UNK	TRP	conflict	UNP P11716
C	4337	UNK	ALA	conflict	UNP P11716
C	4338	UNK	VAL	conflict	UNP P11716
C	4339	UNK	VAL	conflict	UNP P11716
C	4340	UNK	ALA	conflict	UNP P11716
C	4341	UNK	ARG	conflict	UNP P11716
C	4342	UNK	ALA	conflict	UNP P11716
C	4343	UNK	GLY	conflict	UNP P11716

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



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

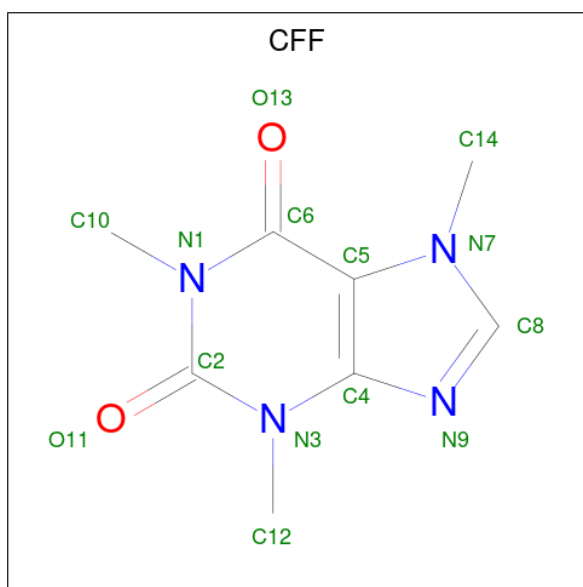
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

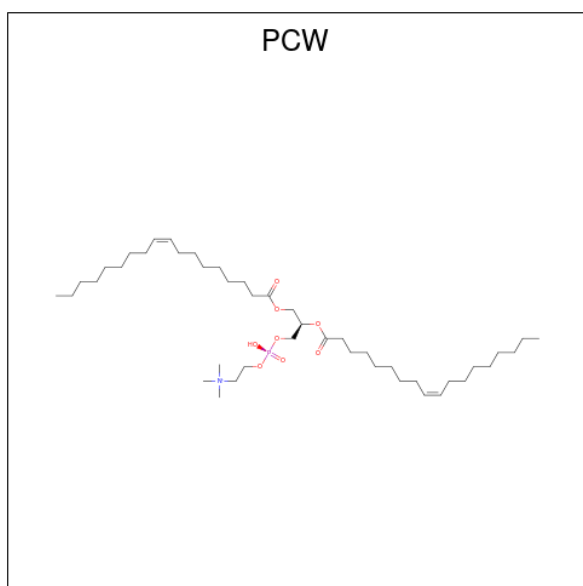
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
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	D	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 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).

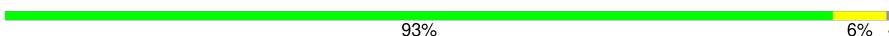


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	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: 

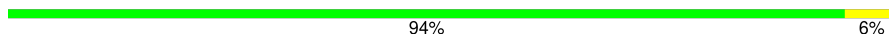


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 

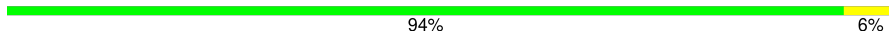


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 



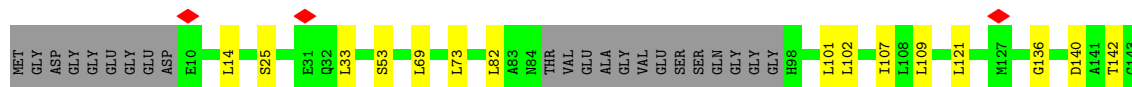
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 



- Molecule 2: Ryanodine receptor 1

Chain A: 



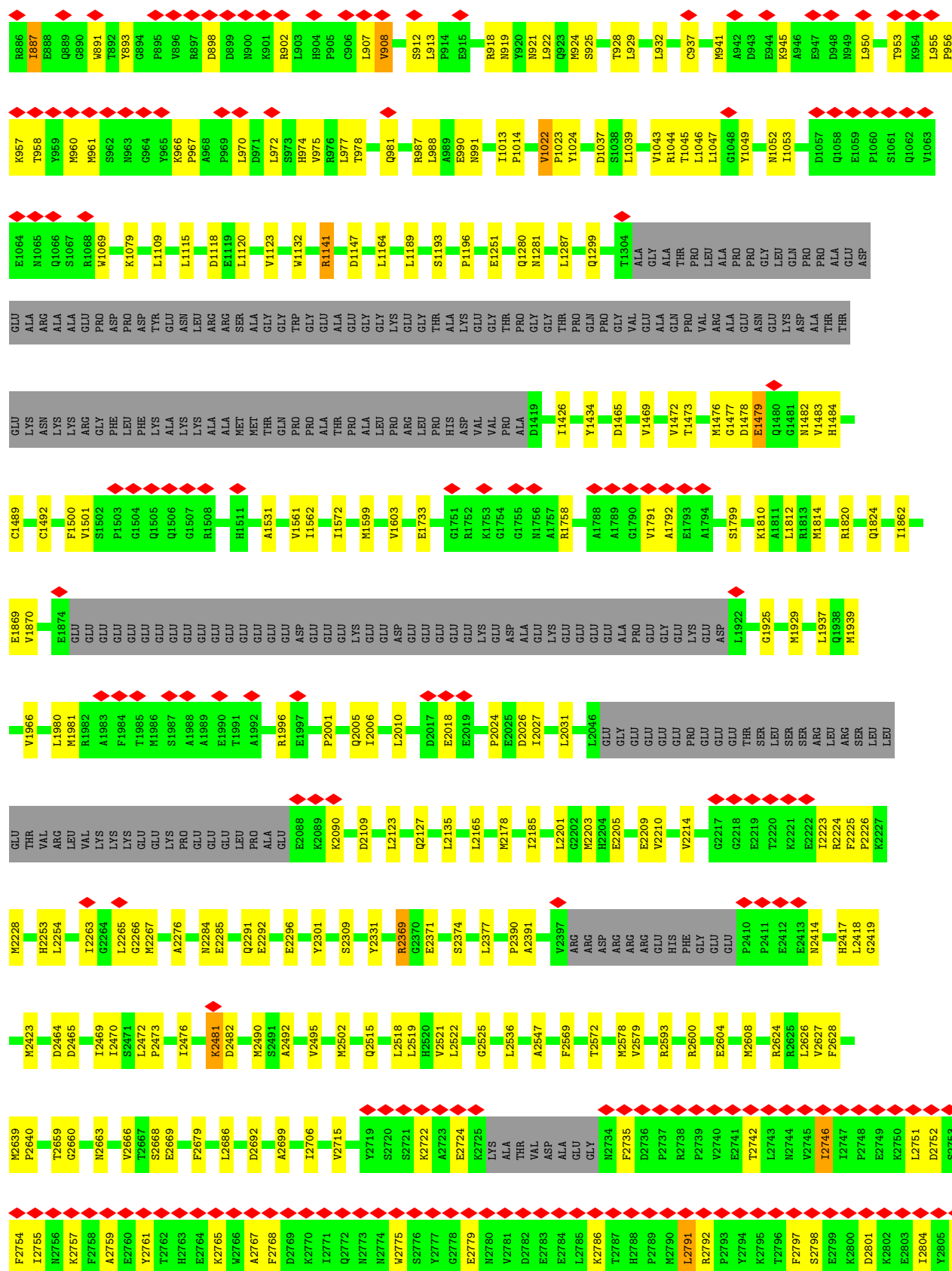




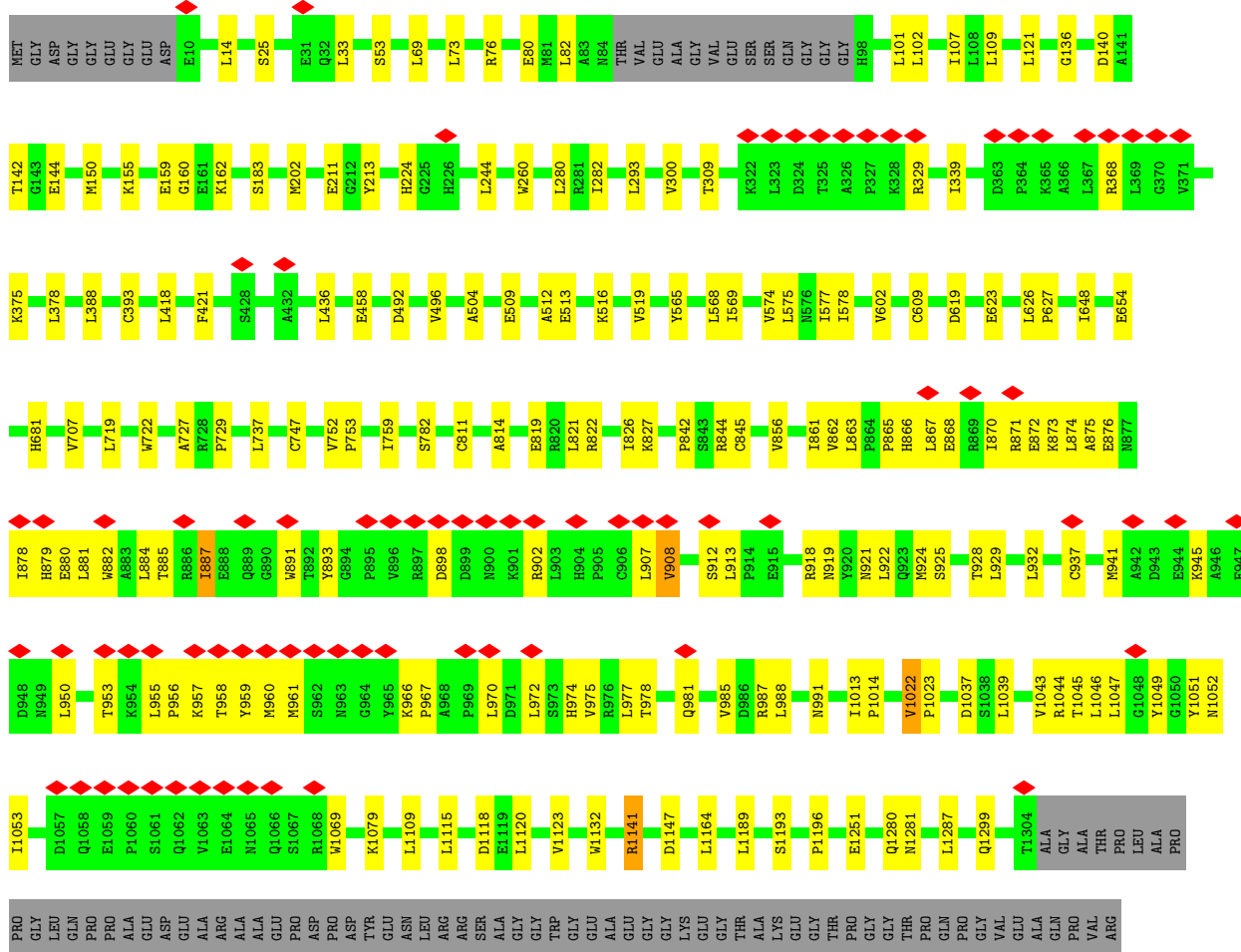


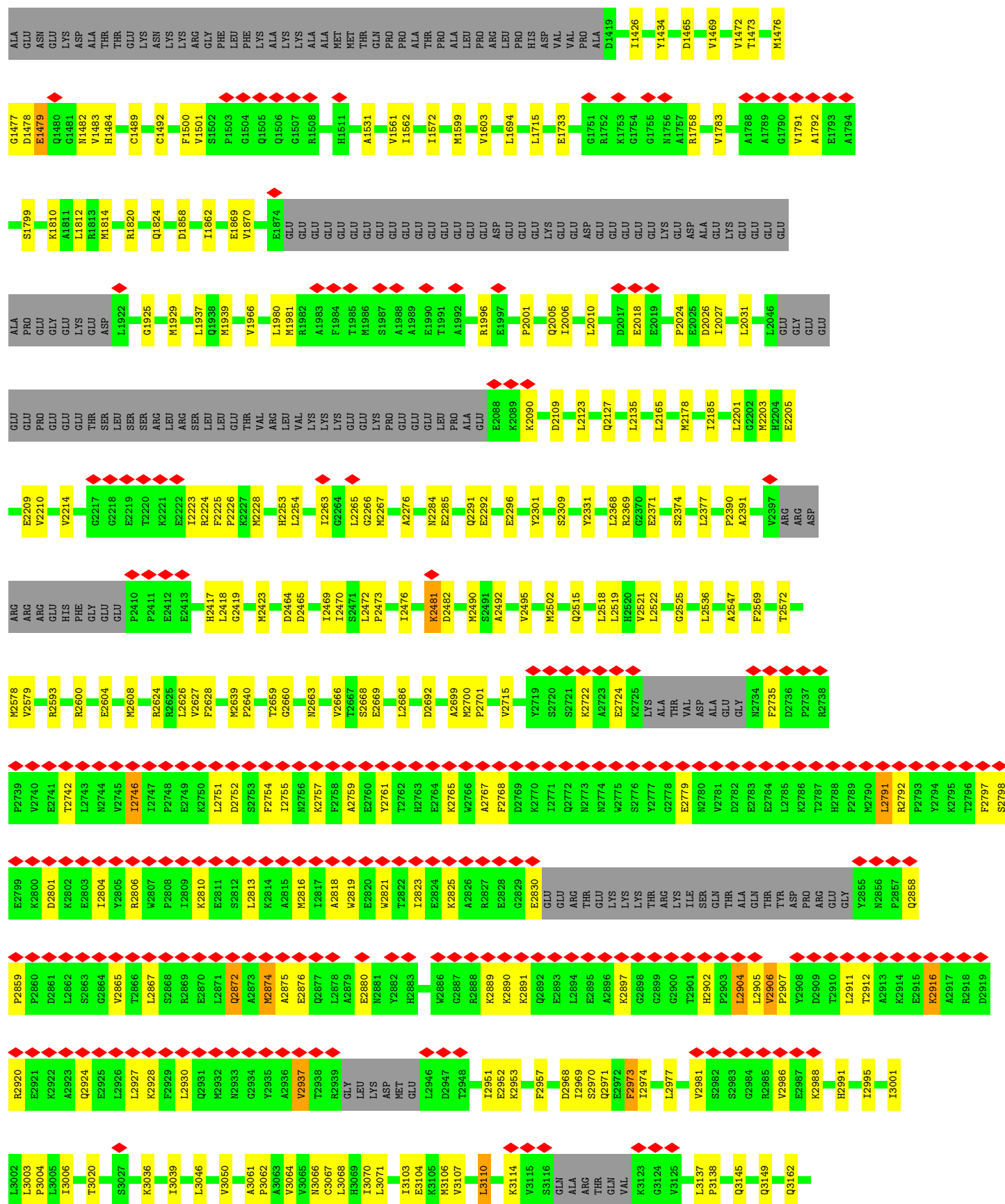
Frequency	Percentage
Very often	9%
Often	75%
Sometimes	13%
Never	12%













Chain C:



R3498	R3499	G3500	D3501	R3502	Y3503	S3504	V3505	G3506	T3507	S3508	L3509	I3510	T3513	M3517	L3518	G3521	L3522	R3523	R3524	T3528	R3529	L3532	R3539	V3540	T3545	E3547	V3549	R3550	E3551	F3552	Q3554	Q3560	G3561	K3562	G3565	S3568	W3571	K3572	K3573	Y3576	G3581	R3582	E3583																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
R3403	D3404	L3405	Y3409	L3412	L3413	R3414	Y3415	V3416	E3433	L3434	M3437	V3438	G3439	I3443	R3453	E3454	V3459	V3460	Q3461	N3465	R3466	M3467	L3470	T3471	A3472	S3473	K3474	K3475	S3476	M3477	K3478	A3479	LYS	ALA	GLY	ASP	ALA	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G3299	A3300	P3301	C3304	T3305	L3312	L3316	L3319	R3320	R3321	T3322	L3323	V3324	N3325	N3326	T3329	K3336	V3340	Q3343	V3346	R3350	P3351	E3352	L3359	P3360	L3365	R3366	K3367	K3371	A3374	E3377	R3380	L3381	L3382	M3266	M3276	E3290	P3294	A3295	L3296	P3297	Y3400																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
K2988	Q3145	Q3149	Q3162	Y3166	L3169	C3170	L3175	Y3182	V3183	E3184	L3194	V3203	L3210	N3211	N3214	V3218	Y3219	S3223	P3324	R3325	E3226	R3327	L3332	V3336	V3337	L3341	D3346	E3353	E3354	E3355	E3356	E3357	E3358	E3359	E3360	E3361	E3362	E3363	E3364	E3365	E3366	E3367	E3368	E3369	E3370	E3371	E3372	E3373	E3374	E3375	E3376	E3377	E3378	E3379	E3380	E3381	E3382	E3383	E3384	E3385	E3386	E3387	E3388	E3389	E3390	E3391	E3392	E3393	E3394	E3395	E3396	E3397	E3398	E3399	E3400	E3401	E3402	E3403	E3404	E3405	E3406	E3407	E3408	E3409	E3410	E3411	E3412	E3413	E3414	E3415	E3416	E3417	E3418	E3419	E3420	E3421	E3422	E3423	E3424	E3425	E3426	E3427	E3428	E3429	E3430	E3431	E3432	E3433	E3434	E3435	E3436	E3437	E3438	E3439	E3440	E3441	E3442	E3443	E3444	E3445	E3446	E3447	E3448	E3449	E3450	E3451	E3452	E3453	E3454	E3455	E3456	E3457	E3458	E3459	E3460	E3461	E3462	E3463	E3464	E3465	E3466	E3467	E3468	E3469	E3470	E3471	E3472	E3473	E3474	E3475	E3476	E3477	E3478	E3479	E3480	E3481	E3482	E3483	E3484	E3485	E3486	E3487	E3488	E3489	E3490	E3491	E3492	E3493	E3494	E3495	E3496	E3497	E3498	E3499	E3500	E3501	E3502	E3503	E3504	E3505	E3506	E3507	E3508	E3509	E3510	E3511	E3512	E3513	E3514	E3515	E3516	E3517	E3518	E3519	E3520	E3521	E3522	E3523	E3524	E3525	E3526	E3527	E3528	E3529	E3530	E3531	E3532	E3533	E3534	E3535	E3536	E3537	E3538	E3539	E3540	E3541	E3542	E3543	E3544	E3545	E3546	E3547	E3548	E3549	E3550	E3551	E3552	E3553	E3554	E3555	E3556	E3557	E3558	E3559	E3560	E3561	E3562	E3563	E3564	E3565	E3566	E3567	E3568	E3569	E3570	E3571	E3572	E3573	E3574	E3575	E3576	E3577	E3578	E3579	E3580	E3581	E3582	E3583	E3584	E3585	E3586	E3587	E3588	E3589	E3590	E3591	E3592	E3593	E3594	E3595	E3596	E3597	E3598	E3599	E3600	E3601	E3602	E3603	E3604	E3605	E3606	E3607	E3608	E3609	E3610	E3611	E3612	E3613	E3614	E3615	E3616	E3617	E3618	E3619	E3620	E3621	E3622	E3623	E3624	E3625	E3626	E3627	E3628	E3629	E3630	E3631	E3632	E3633	E3634	E3635	E3636	E3637	E3638	E3639	E3640	E3641	E3642	E3643	E3644	E3645	E3646	E3647	E3648	E3649	E3650	E3651	E3652	E3653	E3654	E3655	E3656	E3657	E3658	E3659	E3660	E3661	E3662	E3663	E3664	E3665	E3666	E3667	E3668	E3669	E3670	E3671	E3672	E3673	E3674	E3675	E3676	E3677	E3678	E3679	E3680	E3681	E3682	E3683	E3684	E3685	E3686	E3687	E3688	E3689	E3690	E3691	E3692	E3693	E3694	E3695	E3696	E3697	E3698	E3699	E3700	E3701	E3702	E3703	E3704	E3705	E3706	E3707	E3708	E3709	E3710	E3711	E3712	E3713	E3714	E3715	E3716	E3717	E3718	E3719	E3720	E3721	E3722	E3723	E3724	E3725	E3726	E3727	E3728	E3729	E3730	E3731	E3732	E3733	E3734	E3735	E3736	E3737	E3738	E3739	E3740	E3741	E3742	E3743	E3744	E3745	E3746	E3747	E3748	E3749	E3750	E3751	E3752	E3753	E3754	E3755	E3756	E3757	E3758	E3759	E3760	E3761	E3762	E3763	E3764	E3765	E3766	E3767	E3768	E3769	E3770	E3771	E3772	E3773	E3774	E3775	E3776	E3777	E3778	E3779	E3780	E3781	E3782	E3783	E3784	E3785	E3786	E3787	E3788	E3789	E3790	E3791	E3792	E3793	E3794	E3795	E3796	E3797	E3798	E3799	E3800	E3801	E3802	E3803	E3804	E3805	E3806	E3807	E3808	E3809	E3810	E3811	E3812	E3813	E3814	E3815	E3816	E3817	E3818	E3819	E3820	E3821	E3822	E3823	E3824	E3825	E3826	E3827	E3828	E3829	E3830	E3831	E3832	E3833	E3834	E3835	E3836	E3837	E3838	E3839	E3840	E3841	E3842	E3843	E3844	E3845	E3846	E3847	E3848	E3849	E3850	E3851	E3852	E3853	E3854	E3855	E3856	E3857	E3858	E3859	E3860	E3861	E3862	E3863	E3864	E3865	E3866	E3867	E3868	E3869	E3870	E3871	E3872	E3873	E3874	E3875	E3876	E3877	E3878	E3879	E3880	E3881	E3882	E3883	E3884	E3885	E3886	E3887	E3888	E3889	E3890	E3891	E3892	E3893	E3894	E3895	E3896	E3897	E3898	E3899	E3900	E3901	E3902	E3903	E3904	E3905	E3906	E3907	E3908	E3909	E3910	E3911	E3912	E3913	E3914	E3915	E3916	E3917	E3918	E3919	E3920	E3921	E3922	E3923	E3924	E3925	E3926	E3927	E3928	E3929	E3930	E3931	E3932	E3933	E3934	E3935	E3936	E3937	E3938	E3939	E3940	E3941	E3942	E3943	E3944	E3945	E3946	E3947	E3948	E3949	E3950	E3951	E3952	E3953	E3954	E3955	E3956	E3957	E3958	E3959	E3960	E3961	E3962	E3963	E3964	E3965	E3966	E3967	E3968	E3969	E3970	E3971	E3972	E3973	E3974	E3975	E3976	E3977	E3978	E3979	E3980	E3981	E3982	E3983	E3984	E3985	E3986	E3987	E3988	E3989	E3990	E3991	E3992	E3993	E3994	E3995	E3996	E3997	E3998	E3999	E4000	E4001	E4002	E4003	E4004	E4005	E4006	E4007	E4008	E4009	E4010	E4011	E4012	E4013	E4014	E4015	E4016	E4017	E4018	E4019	E4020	E4021	E4022	E4023	E4024	E4025	E4026	E4027	E4028	E4029	E4030	E4031	E4032	E4033	E4034	E4035	E4036	E4037	E4038	E4039	E4040	E4041	E4042	E4043	E4044	E4045	E4046	E4047	E4048	E4049	E4050	E4051	E4052	E4053	E4054	E4055	E4056	E4057	E4058	E4059	E4060	E4061	E4062	E4063	E4064	E4065	E4066	E4067	E4068	E4069	E4070	E4071	E4072	E4073	E4074	E4075	E4076	E4077	E4078	E4079	E4080	E4081	E4082	E4083	E4084	E4085	E4086	E4087	E4088	E4089	E4090	E4091	E4092	E4093	E4094	E4095	E4096	E4097	E4098	E4099	E4100	E4101	E4102	E4103	E4104	E4105	E4106	E4107	E4108	E4109	E4110	E4111	E4112	E4113	E4114	E4115	E4116	E4117	E4118	E4119	E4120	E4121	E4122	E4123	E4124	E4125	E4126	E4127	E4128	E4129	E4130	E4131	E4132	E4133	E4134	E4135	E4136	E4137	E4138	E4139	E4140	E4141	E4142	E4143	E4144	E4145	E4146	E4147	E4148	E4149	E4150	E4151	E4152	E4153	E4154	E4155	E4156	E4157	E4158	E4159	E4160	E4161	E4162	E4163	E4164	E4165	E4166	E4167	E4168	E4169	E4170	E4171	E4172	E4173	E4174	E4175	E4176	E4177	E4178	E4179	E4180	E4181	E4182	E4183	E4184	E4185	E4186	E4187	E4188	E4189	E4190	E4191	E4192	E4193	E4194	E4195	E4196	E4197	E4198	E4199	E4200	E4201	E4202	E4203	E4204	E4205	E4206	E4207	E4208	E4209	E4210	E4211	E4212	E4213	E4214	E4215	E4216	E4217	E4218	E4219	E4220	E4221	E4222	E4223	E4224	E4225	E4226	E4227	E4228	E4229	E4230	E4231	E4232	E4233	E4234	E4235	E4236	E4237	E4238	E4239	E4240	E4241	E4242	E4243	E4244	E4245	E4246	E4247	E4248	E4249	E4250	E4251	E4252	E4253	E4254	E4255	E4256	E4257	E4258	E4259	E4260	E4261	E4262	E4263	E4264	E4265	E4266	E4267	E4268	E4269	E4270	E4271	E4272	E4273	E4274	E4275	E4276	E4277	E4278	E4279	E4280	E4281	E4282	E4283	E4284	E4285	E4286	E4287	E4288	E4289	E4290	E4291	E4292	E4293	E4294	E4295	E4296	E4297	E4298	E4299	E4300	E4301	E4302	E4303	E4304	E4305	E4306	E4307	E4308	E4309	E4310	E4311	E4312	E4313	E4314	E4315	E4316	E4317	E4318	E4319	E4320	E4321	E4322	E4323	E4324	E4325	E4326	E4327	E4328	E4329	E4330	E4331	E4332	E4333	E4334	E4335	E4336	E4337	E4338	E4339	E4340	E4341	E4342	E4343	E4344	E4345	E4346	E4347	E4348	E4349	E4350	E4351	E4352	E4353	E4354	E4355	E4356	E4357	E4358	E4359	E4360	E4361	E4362	E4363	E4364	E4365	E4366	E4367	E4368	E4369	E4370	E4371	E4372	E4373	E4374	E4375	E4376	E4377	E4378	E4379	E4380	E4381	E4382	E4383	E4384	E4385	E4386	E4387	E4388	E4389	E4390	E4391	E4392	E4393	E4394	E4395	E4396	E4397	E4398	E4399	E4400	E4401	E4402	E4403	E4404	E4405	E4406	E4407	E4408	E4409	E4410	E4411	E4412	E4413	E4414	E4415	E4416	E4417	E4418	E4419	E4420	E4421	E4422	E4423	E4424	E4425	E4426	E4427	E4428	E4429	E4430	E4431	E4432	E4433	E4434	E4435	E4436	E4437	E4438	E4439	E4440	E4441	E4442	E4443	E4444	E4445	E4446	E4447	E4448	E4449	E4450	E4451	E4452	E4453	E4454	E4455	E4456	E4457	E4458	E4459	E4460	E4461	E4462	E4463	E4464	E4465	E4466	E4467	E4468	E4469	E4470	E4471	E4472	E4473	E4474	E4475	E4476	E4477	E4478	E4479	E4480	E4481	E4482	E4483	E4484	E4485	E4486	E4487	E4488	E4489	E4490	E4491	E4492	E4493	E4494	E4495	E4496	E4497	E4498	E4499	E4500	E4501	E4502	E4503	E4504	E4505	E4506	E4507	E4508	E4509	E4510	E4511	E4512	E4513	E4514	E4515	E4516	E4517	E4518	E4519	E4520	E4521	E4522	E4523	E4524	E4525	E4526	E4527	E4528	E4529	E4530	E4531	E4532	E4533	E4534	E4535	E4536	E4537	E4538	E4539	E4540	E4541	E4542	E4543	E4544	E4545	E4546	E4547	E4548	E4549	E4550</



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.95	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	0.613	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, CA, ZN, 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	0.13	0/850	0.34	0/1146
1	F	0.13	0/850	0.34	0/1146
1	G	0.13	0/850	0.34	0/1146
1	H	0.13	0/850	0.34	0/1146
2	A	0.15	0/35759	0.38	1/48435 (0.0%)
2	B	0.16	0/35759	0.38	1/48435 (0.0%)
2	C	0.16	0/35759	0.38	1/48435 (0.0%)
2	D	0.16	0/35759	0.38	1/48435 (0.0%)
All	All	0.15	0/146436	0.38	4/198324 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3240	CYS	CA-CB-SG	5.48	127.00	114.40
2	A	3240	CYS	CA-CB-SG	5.47	126.99	114.40
2	B	3240	CYS	CA-CB-SG	5.46	126.95	114.40
2	D	3240	CYS	CA-CB-SG	5.46	126.95	114.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	831	0	828	5	0
1	F	831	0	828	4	0
1	G	831	0	828	3	0
1	H	831	0	828	3	0
2	A	35197	0	34615	455	0
2	B	35197	0	34615	447	0
2	C	35197	0	34615	457	0
2	D	35197	0	34615	453	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
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	162	0	252	6	0
7	B	108	0	168	4	0
7	C	108	0	168	5	0
7	D	54	0	84	1	0
All	All	144732	0	142532	1827	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 6.

All (1827) 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:C:2178:MET:HE3	2:C:2210:VAL:HG11	1.56	0.87
2:B:2178:MET:HE3	2:B:2210:VAL:HG11	1.56	0.86
2:A:2178:MET:HE3	2:A:2210:VAL:HG11	1.56	0.85
2:D:2178:MET:HE3	2:D:2210:VAL:HG11	1.56	0.85
2:A:955:LEU:HD22	2:A:956:PRO:HD2	1.60	0.83
2:C:955:LEU:HD22	2:C:956:PRO:HD2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:LEU:HD22	2:B:956:PRO:HD2	1.59	0.83
2:D:955:LEU:HD22	2:D:956:PRO:HD2	1.59	0.83
2:C:861:ILE:HD12	2:C:861:ILE:O	1.80	0.82
2:B:861:ILE:HD12	2:B:861:ILE:O	1.80	0.82
2:D:861:ILE:O	2:D:861:ILE:HD12	1.80	0.81
2:A:861:ILE:HD12	2:A:861:ILE:O	1.80	0.81
2:D:3605:HIS:O	2:D:3609:THR:HG23	1.84	0.78
2:A:3605:HIS:O	2:A:3609:THR:HG23	1.84	0.78
2:D:2519:LEU:HD12	2:D:2578:MET:HE1	1.67	0.77
2:B:3605:HIS:O	2:B:3609:THR:HG23	1.84	0.76
2:C:2519:LEU:HD12	2:C:2578:MET:HE1	1.67	0.76
2:C:3605:HIS:O	2:C:3609:THR:HG23	1.84	0.76
2:C:884:LEU:HD13	2:C:955:LEU:HD23	1.68	0.76
2:A:2519:LEU:HD12	2:A:2578:MET:HE1	1.67	0.75
2:D:874:LEU:O	2:D:878:ILE:HG23	1.87	0.75
2:B:884:LEU:HD13	2:B:955:LEU:HD23	1.68	0.75
2:C:874:LEU:O	2:C:878:ILE:HG23	1.87	0.75
2:B:2214:VAL:HG21	2:B:2228:MET:HE2	1.70	0.74
2:A:884:LEU:HD13	2:A:955:LEU:HD23	1.68	0.74
2:B:2519:LEU:HD12	2:B:2578:MET:HE1	1.67	0.74
2:D:884:LEU:HD13	2:D:955:LEU:HD23	1.68	0.74
2:C:2214:VAL:HG21	2:C:2228:MET:HE2	1.70	0.74
2:A:874:LEU:O	2:A:878:ILE:HG23	1.87	0.74
2:B:874:LEU:O	2:B:878:ILE:HG23	1.87	0.74
2:A:2214:VAL:HG21	2:A:2228:MET:HE2	1.70	0.73
2:D:2214:VAL:HG21	2:D:2228:MET:HE2	1.70	0.73
2:B:887:ILE:HG21	2:B:955:LEU:HD21	1.71	0.73
2:C:4097:MET:HA	2:C:4097:MET:HE3	1.71	0.72
2:D:4097:MET:HA	2:D:4097:MET:HE3	1.71	0.72
2:A:887:ILE:HG21	2:A:955:LEU:HD21	1.71	0.72
2:A:4097:MET:HA	2:A:4097:MET:HE3	1.71	0.72
2:B:3336:LYS:O	2:B:3340:VAL:HG23	1.90	0.71
2:D:887:ILE:HG21	2:D:955:LEU:HD21	1.71	0.71
2:A:3336:LYS:O	2:A:3340:VAL:HG23	1.91	0.71
2:C:2746:ILE:HD12	2:C:2746:ILE:O	1.91	0.71
2:B:2746:ILE:HD12	2:B:2746:ILE:O	1.91	0.71
2:D:2746:ILE:HD12	2:D:2746:ILE:O	1.91	0.71
2:C:3336:LYS:O	2:C:3340:VAL:HG23	1.91	0.71
2:C:4885:PHE:O	2:C:4889:VAL:HG22	1.91	0.71
2:A:4655:PHE:CE2	2:A:4659:ILE:HD11	2.26	0.71
2:A:4885:PHE:O	2:A:4889:VAL:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4097:MET:HA	2:B:4097:MET:HE3	1.71	0.71
2:B:4885:PHE:O	2:B:4889:VAL:HG22	1.90	0.71
2:D:4655:PHE:CE2	2:D:4659:ILE:HD11	2.26	0.71
2:C:887:ILE:HG21	2:C:955:LEU:HD21	1.71	0.71
2:A:2746:ILE:HD12	2:A:2746:ILE:O	1.91	0.70
2:D:3336:LYS:O	2:D:3340:VAL:HG23	1.90	0.70
2:D:3319:ILE:O	2:D:3323:ILE:HD12	1.91	0.70
2:D:4885:PHE:O	2:D:4889:VAL:HG22	1.90	0.70
2:C:4655:PHE:CE2	2:C:4659:ILE:HD11	2.26	0.70
2:B:4655:PHE:CE2	2:B:4659:ILE:HD11	2.26	0.70
2:C:3319:ILE:O	2:C:3323:ILE:HD12	1.92	0.70
2:C:2906:VAL:HG12	2:C:2907:PRO:HD2	1.74	0.70
2:A:3319:ILE:O	2:A:3323:ILE:HD12	1.91	0.69
2:B:3319:ILE:O	2:B:3323:ILE:HD12	1.91	0.69
2:B:2906:VAL:HG12	2:B:2907:PRO:HD2	1.74	0.69
2:C:2214:VAL:HG21	2:C:2228:MET:CE	2.23	0.69
2:A:2214:VAL:HG21	2:A:2228:MET:CE	2.23	0.69
2:B:2214:VAL:HG21	2:B:2228:MET:CE	2.23	0.69
2:B:3414:ARG:HH21	2:B:3472:ALA:HB1	1.58	0.69
2:D:2906:VAL:HG12	2:D:2907:PRO:HD2	1.74	0.68
2:D:2214:VAL:HG21	2:D:2228:MET:CE	2.23	0.68
2:A:3414:ARG:HH21	2:A:3472:ALA:HB1	1.58	0.68
2:B:3528:THR:HG23	2:B:3573:MET:CE	2.24	0.68
2:A:2906:VAL:HG12	2:A:2907:PRO:HD2	1.74	0.68
2:D:3414:ARG:HH21	2:D:3472:ALA:HB1	1.58	0.68
2:C:3836:MET:HG3	2:C:3884:LEU:HD21	1.76	0.67
2:C:3528:THR:HG23	2:C:3573:MET:CE	2.24	0.67
2:B:3836:MET:HG3	2:B:3884:LEU:HD21	1.76	0.67
2:D:3528:THR:HG23	2:D:3573:MET:CE	2.24	0.67
2:A:3528:THR:HG23	2:A:3573:MET:CE	2.24	0.67
2:A:3836:MET:HG3	2:A:3884:LEU:HD21	1.76	0.66
2:C:3414:ARG:HH21	2:C:3472:ALA:HB1	1.58	0.66
2:D:3836:MET:HG3	2:D:3884:LEU:HD21	1.76	0.66
2:B:1046:LEU:C	2:B:1046:LEU:HD23	2.22	0.65
2:B:2490:MET:HE3	2:B:2495:VAL:HG12	1.79	0.65
2:C:2490:MET:HE3	2:C:2495:VAL:HG12	1.79	0.65
2:D:1046:LEU:HD23	2:D:1046:LEU:C	2.22	0.65
2:D:2490:MET:HE3	2:D:2495:VAL:HG12	1.79	0.65
2:A:2490:MET:HE3	2:A:2495:VAL:HG12	1.79	0.64
2:C:1046:LEU:HD23	2:C:1046:LEU:C	2.22	0.64
2:A:1046:LEU:HD23	2:A:1046:LEU:C	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3414:ARG:NH2	2:B:3472:ALA:HB1	2.13	0.64
2:D:3346:VAL:HG11	2:D:3414:ARG:CB	2.28	0.64
2:C:3103:ILE:O	2:C:3107:VAL:HG13	1.98	0.64
2:A:3346:VAL:HG11	2:A:3414:ARG:CB	2.28	0.63
2:C:2968:ASP:OD2	2:C:2969:ILE:HD12	1.98	0.63
2:B:2968:ASP:OD2	2:B:2969:ILE:HD12	1.98	0.63
2:C:4062:PHE:HB2	2:C:4170:ILE:HD11	1.80	0.63
2:C:3346:VAL:HG11	2:C:3414:ARG:CB	2.28	0.63
2:C:3414:ARG:NH2	2:C:3472:ALA:HB1	2.13	0.63
2:B:4062:PHE:HB2	2:B:4170:ILE:HD11	1.80	0.63
2:A:2968:ASP:OD2	2:A:2969:ILE:HD12	1.98	0.63
2:A:3414:ARG:NH2	2:A:3472:ALA:HB1	2.13	0.63
2:D:3103:ILE:O	2:D:3107:VAL:HG13	1.98	0.63
2:B:3103:ILE:O	2:B:3107:VAL:HG13	1.98	0.63
2:A:870:ILE:HD12	2:A:871:ARG:N	2.14	0.63
2:B:870:ILE:HD12	2:B:871:ARG:N	2.14	0.63
2:D:870:ILE:HD12	2:D:871:ARG:N	2.14	0.63
2:A:862:VAL:HG12	2:A:862:VAL:O	1.99	0.63
2:A:4062:PHE:HB2	2:A:4170:ILE:HD11	1.80	0.63
2:D:862:VAL:O	2:D:862:VAL:HG12	1.99	0.63
2:B:862:VAL:O	2:B:862:VAL:HG12	1.99	0.62
2:D:3834:ALA:O	2:D:3838:THR:HG23	1.99	0.62
2:C:870:ILE:HD12	2:C:871:ARG:N	2.14	0.62
2:C:3969:ILE:HG21	2:C:3980:LEU:HD12	1.81	0.62
2:A:3103:ILE:O	2:A:3107:VAL:HG13	1.98	0.62
2:D:2751:LEU:HD13	2:D:2813:LEU:HD12	1.81	0.62
2:C:4747:SER:O	2:C:4751:THR:HG23	1.99	0.62
2:A:3834:ALA:O	2:A:3838:THR:HG23	1.99	0.62
2:B:3346:VAL:HG11	2:B:3414:ARG:CB	2.28	0.62
2:B:3969:ILE:HG21	2:B:3980:LEU:HD12	1.81	0.62
2:D:4062:PHE:HB2	2:D:4170:ILE:HD11	1.80	0.62
2:D:4747:SER:O	2:D:4751:THR:HG23	1.99	0.62
2:A:3969:ILE:HG21	2:A:3980:LEU:HD12	1.81	0.62
2:D:3414:ARG:NH2	2:D:3472:ALA:HB1	2.13	0.62
2:D:4910:GLU:O	2:D:4914:VAL:HG13	2.00	0.62
2:C:3834:ALA:O	2:C:3838:THR:HG23	1.99	0.62
2:A:2751:LEU:HD13	2:A:2813:LEU:HD12	1.81	0.62
2:D:2968:ASP:OD2	2:D:2969:ILE:HD12	1.98	0.62
2:A:2292:GLU:O	2:A:2296:GLU:HG3	2.00	0.62
2:B:2292:GLU:O	2:B:2296:GLU:HG3	2.00	0.62
2:A:4850:LEU:HD22	7:A:5307:PCW:H411	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4747:SER:O	2:B:4751:THR:HG23	1.99	0.61
2:C:2292:GLU:O	2:C:2296:GLU:HG3	2.00	0.61
2:C:881:LEU:O	2:C:885:THR:HG23	2.00	0.61
2:C:4910:GLU:O	2:C:4914:VAL:HG13	2.00	0.61
2:B:881:LEU:O	2:B:885:THR:HG23	2.00	0.61
2:B:4241:THR:HG22	2:B:4245:MET:HE3	1.83	0.61
2:D:3439:GLY:O	2:D:3443:ILE:HG13	2.01	0.61
2:B:3834:ALA:O	2:B:3838:THR:HG23	1.99	0.61
2:D:881:LEU:O	2:D:885:THR:HG23	2.00	0.61
2:C:2265:LEU:HD12	2:C:2266:GLY:N	2.16	0.61
2:A:881:LEU:O	2:A:885:THR:HG23	2.00	0.61
2:A:4747:SER:O	2:A:4751:THR:HG23	1.99	0.61
2:C:2223:ILE:HD11	2:C:2263:ILE:CD1	2.31	0.61
2:C:2751:LEU:HD13	2:C:2813:LEU:HD12	1.81	0.61
2:A:4910:GLU:O	2:A:4914:VAL:HG13	2.00	0.61
2:D:3969:ILE:HG21	2:D:3980:LEU:HD12	1.81	0.61
2:C:3439:GLY:O	2:C:3443:ILE:HG13	2.01	0.61
2:A:3439:GLY:O	2:A:3443:ILE:HG13	2.01	0.61
2:A:4241:THR:HG22	2:A:4245:MET:HE3	1.83	0.61
2:B:2751:LEU:HD13	2:B:2813:LEU:HD12	1.81	0.61
2:D:2265:LEU:HD12	2:D:2266:GLY:N	2.16	0.61
2:C:862:VAL:O	2:C:862:VAL:HG12	1.99	0.61
2:C:4241:THR:HG22	2:C:4245:MET:HE3	1.83	0.61
2:D:2223:ILE:HD11	2:D:2263:ILE:CD1	2.31	0.60
2:A:2904:LEU:O	2:A:2904:LEU:HD13	2.01	0.60
2:B:2223:ILE:HD11	2:B:2263:ILE:CD1	2.31	0.60
2:B:2265:LEU:HD12	2:B:2266:GLY:N	2.16	0.60
2:B:2904:LEU:HD13	2:B:2904:LEU:O	2.01	0.60
2:D:2292:GLU:O	2:D:2296:GLU:HG3	2.00	0.60
2:D:2904:LEU:O	2:D:2904:LEU:HD13	2.01	0.60
2:B:4910:GLU:O	2:B:4914:VAL:HG13	2.00	0.60
2:C:2905:LEU:HD12	2:C:2905:LEU:O	2.02	0.60
2:A:2265:LEU:HD12	2:A:2266:GLY:N	2.16	0.60
7:B:5305:PCW:H411	2:C:4850:LEU:HD22	1.84	0.60
2:C:2904:LEU:O	2:C:2904:LEU:HD13	2.02	0.60
2:A:2905:LEU:HD12	2:A:2905:LEU:O	2.02	0.59
2:D:3061:ALA:HB3	2:D:3062:PRO:HD3	1.84	0.59
2:D:4241:THR:HG22	2:D:4245:MET:HE3	1.83	0.59
2:D:2905:LEU:O	2:D:2905:LEU:HD12	2.02	0.59
2:C:4694:ASP:OD1	2:C:4694:ASP:O	2.20	0.59
2:A:2223:ILE:HD11	2:A:2263:ILE:CD1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3439:GLY:O	2:B:3443:ILE:HG13	2.01	0.59
2:D:955:LEU:HD22	2:D:956:PRO:CD	2.32	0.59
2:D:4694:ASP:OD1	2:D:4694:ASP:O	2.20	0.59
2:A:2291:GLN:OE1	2:A:2291:GLN:HA	2.03	0.59
2:A:3061:ALA:HB3	2:A:3062:PRO:HD3	1.84	0.59
2:B:2905:LEU:HD12	2:B:2905:LEU:O	2.02	0.59
2:B:3061:ALA:HB3	2:B:3062:PRO:HD3	1.84	0.59
2:D:3460:VAL:HG23	2:D:3461:GLN:OE1	2.03	0.59
1:G:26:HIS:CD2	1:G:105:LEU:HD11	2.37	0.59
2:A:3460:VAL:HG23	2:A:3461:GLN:OE1	2.03	0.59
2:C:3460:VAL:HG23	2:C:3461:GLN:OE1	2.03	0.59
1:E:26:HIS:CD2	1:E:105:LEU:HD11	2.37	0.59
2:A:2481:LYS:HD2	2:A:2481:LYS:O	2.03	0.59
2:D:2481:LYS:HD2	2:D:2481:LYS:O	2.03	0.59
7:A:5305:PCW:H411	2:B:4850:LEU:HD22	1.85	0.59
2:B:4694:ASP:OD1	2:B:4694:ASP:O	2.20	0.59
2:C:3061:ALA:HB3	2:C:3062:PRO:HD3	1.84	0.59
1:F:26:HIS:CD2	1:F:105:LEU:HD11	2.37	0.59
2:A:4694:ASP:OD1	2:A:4694:ASP:O	2.20	0.58
2:B:2291:GLN:OE1	2:B:2291:GLN:HA	2.03	0.58
1:H:26:HIS:CD2	1:H:105:LEU:HD11	2.37	0.58
2:B:2481:LYS:O	2:B:2481:LYS:HD2	2.03	0.58
2:B:3460:VAL:HG23	2:B:3461:GLN:OE1	2.03	0.58
2:D:4850:LEU:HD22	7:C:5305:PCW:H411	1.84	0.58
2:B:3592:ILE:O	2:B:3596:VAL:HG13	2.04	0.58
2:D:2291:GLN:OE1	2:D:2291:GLN:HA	2.03	0.58
2:D:2624:ARG:O	2:D:2627:VAL:HG12	2.04	0.58
2:C:2624:ARG:O	2:C:2627:VAL:HG12	2.04	0.58
2:B:4245:MET:HE1	2:B:4989:MET:HE1	1.86	0.58
2:D:1980:LEU:O	2:D:1980:LEU:HD13	2.04	0.58
2:C:140:ASP:OD2	2:C:142:THR:HG22	2.04	0.58
2:B:4697:VAL:HG13	2:B:4698:LYS:HE2	1.86	0.58
2:C:101:LEU:HB3	2:C:150:MET:HE1	1.86	0.58
2:C:2291:GLN:OE1	2:C:2291:GLN:HA	2.03	0.58
2:C:3592:ILE:O	2:C:3596:VAL:HG13	2.04	0.58
2:D:101:LEU:HB3	2:D:150:MET:HE1	1.86	0.57
2:C:1980:LEU:O	2:C:1980:LEU:HD13	2.04	0.57
2:B:140:ASP:OD2	2:B:142:THR:HG22	2.04	0.57
2:C:2481:LYS:HD2	2:C:2481:LYS:O	2.03	0.57
2:A:1980:LEU:HD13	2:A:1980:LEU:O	2.04	0.57
2:A:2624:ARG:O	2:A:2627:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:LEU:HD22	2:B:956:PRO:CD	2.31	0.57
2:A:14:LEU:HD13	2:A:202:MET:HE2	1.87	0.57
2:A:4697:VAL:HG13	2:A:4698:LYS:HE2	1.86	0.57
2:B:2624:ARG:O	2:B:2627:VAL:HG12	2.04	0.57
2:D:140:ASP:OD2	2:D:142:THR:HG22	2.04	0.57
2:D:4245:MET:HE1	2:D:4989:MET:HE1	1.86	0.57
2:A:4245:MET:HE1	2:A:4989:MET:HE1	1.86	0.57
2:D:3312:LEU:H	2:D:3312:LEU:HD12	1.70	0.57
2:C:4245:MET:HE1	2:C:4989:MET:HE1	1.86	0.57
2:A:140:ASP:OD2	2:A:142:THR:HG22	2.04	0.57
2:B:14:LEU:HD13	2:B:202:MET:HE2	1.87	0.57
2:C:3312:LEU:HD12	2:C:3312:LEU:H	1.70	0.57
2:C:4697:VAL:HG13	2:C:4698:LYS:HE2	1.86	0.57
2:A:2754:PHE:CE2	2:A:2813:LEU:HD21	2.40	0.57
2:A:3592:ILE:O	2:A:3596:VAL:HG13	2.04	0.57
2:A:955:LEU:HD22	2:A:956:PRO:CD	2.32	0.57
2:B:1980:LEU:O	2:B:1980:LEU:HD13	2.04	0.57
2:D:14:LEU:HD13	2:D:202:MET:HE2	1.87	0.56
2:B:4062:PHE:CB	2:B:4170:ILE:HD11	2.36	0.56
2:D:3300:ALA:HB3	2:D:3301:PRO:HD3	1.87	0.56
2:D:3592:ILE:O	2:D:3596:VAL:HG13	2.04	0.56
2:C:4062:PHE:CB	2:C:4170:ILE:HD11	2.36	0.56
2:A:101:LEU:HB3	2:A:150:MET:HE1	1.86	0.56
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.86	0.56
2:B:2754:PHE:CE2	2:B:2813:LEU:HD21	2.40	0.56
2:D:2754:PHE:CE2	2:D:2813:LEU:HD21	2.40	0.56
2:D:4697:VAL:HG13	2:D:4698:LYS:HE2	1.86	0.56
2:C:2754:PHE:CE2	2:C:2813:LEU:HD21	2.40	0.56
2:B:3300:ALA:HB3	2:B:3301:PRO:HD3	1.87	0.56
2:C:1287:LEU:HD11	2:C:1599:MET:HE3	1.88	0.56
2:B:3864:THR:O	2:B:3866:ILE:HD12	2.06	0.56
2:D:1287:LEU:HD11	2:D:1599:MET:HE3	1.88	0.56
2:C:14:LEU:HD13	2:C:202:MET:HE2	1.87	0.56
2:A:3343:GLN:O	2:A:3346:VAL:HG12	2.06	0.55
2:A:4062:PHE:CB	2:A:4170:ILE:HD11	2.36	0.55
2:B:2519:LEU:HD12	2:B:2578:MET:CE	2.36	0.55
2:B:2476:ILE:HG23	2:B:2536:LEU:HD13	1.89	0.55
2:B:4222:VAL:HG11	2:B:4950:VAL:HA	1.88	0.55
2:D:3343:GLN:O	2:D:3346:VAL:HG12	2.06	0.55
2:A:2519:LEU:HD12	2:A:2578:MET:CE	2.36	0.55
2:D:4222:VAL:HG11	2:D:4950:VAL:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2476:ILE:HG23	2:C:2536:LEU:HD13	1.89	0.55
2:C:3864:THR:O	2:C:3866:ILE:HD12	2.06	0.55
2:A:3312:LEU:H	2:A:3312:LEU:HD12	1.69	0.55
2:B:2973:PHE:CD1	2:B:2973:PHE:C	2.85	0.55
2:B:3312:LEU:H	2:B:3312:LEU:HD12	1.70	0.55
2:D:880:GLU:O	2:D:884:LEU:HD23	2.07	0.55
2:D:4062:PHE:CB	2:D:4170:ILE:HD11	2.36	0.55
2:C:3300:ALA:HB3	2:C:3301:PRO:HD3	1.87	0.55
2:C:955:LEU:HD22	2:C:956:PRO:CD	2.31	0.55
2:C:3550:ARG:O	2:C:3554:GLN:HG3	2.07	0.55
2:D:3864:THR:O	2:D:3866:ILE:HD12	2.06	0.55
2:C:2973:PHE:CD1	2:C:2973:PHE:C	2.85	0.55
2:A:3300:ALA:HB3	2:A:3301:PRO:HD3	1.87	0.55
2:A:3864:THR:O	2:A:3866:ILE:HD12	2.06	0.55
2:A:4222:VAL:HG11	2:A:4950:VAL:HA	1.88	0.55
2:B:3343:GLN:O	2:B:3346:VAL:HG12	2.06	0.55
2:B:2911:LEU:HD11	2:B:2916:LYS:HB2	1.89	0.55
2:C:33:LEU:HD12	2:C:53:SER:HB2	1.88	0.55
2:A:880:GLU:O	2:A:884:LEU:HD23	2.07	0.54
2:D:2973:PHE:C	2:D:2973:PHE:CD1	2.85	0.54
2:C:880:GLU:O	2:C:884:LEU:HD23	2.07	0.54
2:A:159:GLU:OE1	2:A:159:GLU:C	2.50	0.54
2:B:3166:TYR:OH	2:B:3203:VAL:HG11	2.07	0.54
2:D:159:GLU:C	2:D:159:GLU:OE1	2.50	0.54
2:C:3166:TYR:OH	2:C:3203:VAL:HG11	2.07	0.54
2:A:2973:PHE:CD1	2:A:2973:PHE:C	2.85	0.54
2:B:1287:LEU:HD11	2:B:1599:MET:HE3	1.88	0.54
2:D:2519:LEU:HD12	2:D:2578:MET:CE	2.36	0.54
2:B:880:GLU:O	2:B:884:LEU:HD23	2.07	0.54
2:B:3550:ARG:O	2:B:3554:GLN:HG3	2.07	0.54
2:D:2476:ILE:HG23	2:D:2536:LEU:HD13	1.89	0.54
2:C:4222:VAL:HG11	2:C:4950:VAL:HA	1.89	0.54
2:A:3550:ARG:O	2:A:3554:GLN:HG3	2.07	0.54
2:D:3104:GLU:O	2:D:3107:VAL:HG22	2.08	0.54
2:C:159:GLU:C	2:C:159:GLU:OE1	2.50	0.54
2:A:1287:LEU:HD11	2:A:1599:MET:HE3	1.88	0.54
2:A:2476:ILE:HG23	2:A:2536:LEU:HD13	1.89	0.54
2:A:2911:LEU:HD11	2:A:2916:LYS:HB2	1.89	0.54
2:D:33:LEU:HD12	2:D:53:SER:HB2	1.89	0.54
2:C:2135:LEU:HD21	2:C:3663:LEU:HD13	1.90	0.54
2:C:3343:GLN:O	2:C:3346:VAL:HG12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3104:GLU:O	2:A:3107:VAL:HG22	2.08	0.54
2:A:1118:ASP:OD2	2:A:1120:LEU:HD12	2.08	0.54
2:A:3540:TYR:HB3	2:A:3604:TYR:CD2	2.43	0.54
2:B:159:GLU:C	2:B:159:GLU:OE1	2.50	0.54
2:D:2755:ILE:HG22	2:D:2813:LEU:HG	1.90	0.54
2:C:3104:GLU:O	2:C:3107:VAL:HG22	2.08	0.54
2:B:33:LEU:HD12	2:B:53:SER:HB2	1.88	0.53
2:B:1118:ASP:OD2	2:B:1120:LEU:HD12	2.08	0.53
2:C:2465:ASP:O	2:C:2469:ILE:HD12	2.08	0.53
2:C:2482:ASP:OD2	2:C:2482:ASP:C	2.52	0.53
2:A:33:LEU:HD12	2:A:53:SER:HB2	1.88	0.53
2:A:2482:ASP:C	2:A:2482:ASP:OD2	2.51	0.53
2:D:2991:HIS:O	2:D:2995:ILE:HD12	2.08	0.53
2:D:3550:ARG:O	2:D:3554:GLN:HG3	2.07	0.53
2:B:3684:GLU:HG2	2:B:3684:GLU:O	2.09	0.53
2:D:3684:GLU:O	2:D:3684:GLU:HG2	2.09	0.53
2:A:918:ARG:O	2:A:922:LEU:HD13	2.09	0.53
2:A:3166:TYR:OH	2:A:3203:VAL:HG11	2.07	0.53
2:B:2465:ASP:O	2:B:2469:ILE:HD12	2.08	0.53
2:D:2135:LEU:HD21	2:D:3663:LEU:HD13	1.90	0.53
2:D:2465:ASP:O	2:D:2469:ILE:HD12	2.08	0.53
2:C:1118:ASP:OD2	2:C:1120:LEU:HD12	2.08	0.53
2:A:2755:ILE:HG22	2:A:2813:LEU:HG	1.90	0.53
2:C:918:ARG:O	2:C:922:LEU:HD13	2.09	0.53
2:A:2465:ASP:O	2:A:2469:ILE:HD12	2.08	0.53
2:B:3702:VAL:HG22	2:B:3729:MET:HE1	1.90	0.53
2:D:1109:LEU:HA	2:D:1120:LEU:HD13	1.91	0.53
2:D:3540:TYR:HB3	2:D:3604:TYR:CD2	2.43	0.53
2:D:4199:GLU:OE1	2:D:4199:GLU:O	2.27	0.53
2:C:2911:LEU:HD11	2:C:2916:LYS:HB2	1.90	0.53
2:C:3684:GLU:O	2:C:3684:GLU:HG2	2.09	0.53
2:A:2970:SER:HA	2:A:2973:PHE:CD2	2.44	0.53
2:D:2911:LEU:HD11	2:D:2916:LYS:HB2	1.89	0.53
2:D:3166:TYR:OH	2:D:3203:VAL:HG11	2.07	0.53
2:C:2991:HIS:O	2:C:2995:ILE:HD12	2.09	0.53
2:A:1109:LEU:HA	2:A:1120:LEU:HD13	1.91	0.53
2:B:2135:LEU:HD21	2:B:3663:LEU:HD13	1.90	0.53
2:B:2755:ILE:HG22	2:B:2813:LEU:HG	1.90	0.53
2:B:3104:GLU:O	2:B:3107:VAL:HG22	2.08	0.53
2:B:4199:GLU:OE1	2:B:4199:GLU:O	2.27	0.53
2:C:3702:VAL:HG22	2:C:3729:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1109:LEU:HA	2:C:1120:LEU:HD13	1.91	0.53
2:C:3412:LEU:HD12	2:C:3412:LEU:O	2.09	0.53
2:C:4199:GLU:OE1	2:C:4199:GLU:O	2.27	0.53
2:B:1109:LEU:HA	2:B:1120:LEU:HD13	1.91	0.53
2:B:3384:LYS:H	2:B:3387:ALA:HB3	1.74	0.53
2:D:918:ARG:O	2:D:922:LEU:HD13	2.09	0.53
2:D:2970:SER:HA	2:D:2973:PHE:CD2	2.44	0.53
2:D:3412:LEU:O	2:D:3412:LEU:HD12	2.09	0.53
2:C:3540:TYR:HB3	2:C:3604:TYR:CD2	2.43	0.53
2:A:3384:LYS:H	2:A:3387:ALA:HB3	1.74	0.52
2:A:3702:VAL:HG22	2:A:3729:MET:HE1	1.90	0.52
2:A:4199:GLU:OE1	2:A:4199:GLU:O	2.27	0.52
2:B:2970:SER:HA	2:B:2973:PHE:CD2	2.44	0.52
2:D:1118:ASP:OD2	2:D:1120:LEU:HD12	2.08	0.52
2:A:2135:LEU:HD21	2:A:3663:LEU:HD13	1.90	0.52
2:B:2482:ASP:C	2:B:2482:ASP:OD2	2.51	0.52
2:D:224:HIS:HA	2:D:388:LEU:HD23	1.91	0.52
2:D:2482:ASP:C	2:D:2482:ASP:OD2	2.51	0.52
2:C:2911:LEU:HD12	2:C:2912:THR:O	2.10	0.52
2:A:1251:GLU:OE1	2:A:1251:GLU:HA	2.09	0.52
2:B:918:ARG:O	2:B:922:LEU:HD13	2.09	0.52
2:B:3540:TYR:HB3	2:B:3604:TYR:CD2	2.43	0.52
2:D:3070:ILE:H	2:D:3070:ILE:HD12	1.74	0.52
2:C:224:HIS:HA	2:C:388:LEU:HD23	1.91	0.52
2:A:3412:LEU:O	2:A:3412:LEU:HD12	2.09	0.52
2:B:3412:LEU:HD12	2:B:3412:LEU:O	2.10	0.52
2:A:2742:THR:OG1	2:A:2818:ALA:HB2	2.10	0.52
2:B:3465:ASN:HA	2:B:3502:ARG:HA	1.92	0.52
2:C:2519:LEU:HD12	2:C:2578:MET:CE	2.36	0.52
2:C:3384:LYS:H	2:C:3387:ALA:HB3	1.74	0.52
2:A:3684:GLU:O	2:A:3684:GLU:HG2	2.09	0.52
2:D:2911:LEU:HD12	2:D:2912:THR:O	2.10	0.52
2:D:3702:VAL:HG22	2:D:3729:MET:HE1	1.90	0.52
2:D:4244:GLU:HA	2:D:4244:GLU:OE2	2.10	0.52
2:C:2755:ILE:HG22	2:C:2813:LEU:HG	1.90	0.52
2:B:1251:GLU:OE1	2:B:1251:GLU:HA	2.09	0.52
2:B:2911:LEU:HD12	2:B:2912:THR:O	2.10	0.52
2:B:2991:HIS:O	2:B:2995:ILE:HD12	2.08	0.52
2:D:1251:GLU:HA	2:D:1251:GLU:OE1	2.09	0.52
2:D:3509:LEU:O	2:D:3513:THR:HG23	2.10	0.52
2:C:2742:THR:OG1	2:C:2818:ALA:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2911:LEU:HD12	2:A:2912:THR:O	2.10	0.52
2:A:2991:HIS:O	2:A:2995:ILE:HD12	2.08	0.52
2:B:3070:ILE:H	2:B:3070:ILE:HD12	1.74	0.52
2:C:1251:GLU:OE1	2:C:1251:GLU:HA	2.09	0.52
2:A:3465:ASN:HA	2:A:3502:ARG:HA	1.92	0.52
2:A:3509:LEU:O	2:A:3513:THR:HG23	2.10	0.52
2:B:957:LYS:O	2:B:960:MET:HE2	2.10	0.52
2:D:3381:LEU:HD23	2:D:3381:LEU:C	2.35	0.52
2:D:3384:LYS:H	2:D:3387:ALA:HB3	1.74	0.52
2:C:3070:ILE:H	2:C:3070:ILE:HD12	1.74	0.52
2:B:2968:ASP:OD2	2:B:2969:ILE:N	2.43	0.52
2:D:2165:LEU:HD12	2:D:2178:MET:HE2	1.92	0.52
2:C:2165:LEU:HD12	2:C:2178:MET:HE2	1.92	0.52
2:C:2968:ASP:OD2	2:C:2969:ILE:N	2.43	0.52
2:C:3381:LEU:C	2:C:3381:LEU:HD23	2.35	0.52
2:A:224:HIS:HA	2:A:388:LEU:HD23	1.91	0.51
2:D:2986:VAL:HG22	2:D:2988:LYS:H	1.75	0.51
2:C:3409:TYR:CD2	2:C:3513:THR:HG21	2.45	0.51
2:C:3465:ASN:HA	2:C:3502:ARG:HA	1.92	0.51
2:A:2968:ASP:OD2	2:A:2969:ILE:N	2.43	0.51
2:A:3070:ILE:H	2:A:3070:ILE:HD12	1.74	0.51
2:A:4056:GLU:HG2	2:A:4166:LEU:HD13	1.93	0.51
2:B:3509:LEU:O	2:B:3513:THR:HG23	2.10	0.51
2:D:2968:ASP:OD2	2:D:2969:ILE:N	2.43	0.51
2:C:955:LEU:O	2:C:966:LYS:HG2	2.10	0.51
2:C:3528:THR:HG23	2:C:3573:MET:HE3	1.92	0.51
2:A:957:LYS:O	2:A:960:MET:HE2	2.10	0.51
2:B:4244:GLU:HA	2:B:4244:GLU:OE2	2.10	0.51
2:D:4056:GLU:HG2	2:D:4166:LEU:HD13	1.93	0.51
2:C:4244:GLU:HA	2:C:4244:GLU:OE2	2.10	0.51
2:A:3409:TYR:CD2	2:A:3513:THR:HG21	2.45	0.51
2:B:224:HIS:HA	2:B:388:LEU:HD23	1.91	0.51
2:D:2742:THR:OG1	2:D:2818:ALA:HB2	2.10	0.51
2:C:2970:SER:HA	2:C:2973:PHE:CD2	2.44	0.51
2:A:972:LEU:HB3	2:A:1044:ARG:HG2	1.92	0.51
2:B:955:LEU:O	2:B:966:LYS:HG2	2.10	0.51
2:B:2742:THR:OG1	2:B:2818:ALA:HB2	2.10	0.51
2:B:3381:LEU:HD23	2:B:3381:LEU:C	2.35	0.51
2:B:3409:TYR:CD2	2:B:3513:THR:HG21	2.45	0.51
2:D:3211:ASN:OD1	2:D:3236:VAL:HG11	2.11	0.51
2:B:3211:ASN:OD1	2:B:3236:VAL:HG11	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3528:THR:HG23	2:B:3573:MET:HE3	1.92	0.51
2:B:4056:GLU:HG2	2:B:4166:LEU:HD13	1.93	0.51
2:C:3509:LEU:O	2:C:3513:THR:HG23	2.10	0.51
2:C:4056:GLU:HG2	2:C:4166:LEU:HD13	1.93	0.51
2:A:3211:ASN:OD1	2:A:3236:VAL:HG11	2.11	0.51
2:A:4244:GLU:OE2	2:A:4244:GLU:HA	2.10	0.51
2:B:1824:GLN:OE1	2:B:1824:GLN:HA	2.11	0.51
2:D:955:LEU:O	2:D:966:LYS:HG2	2.10	0.51
2:D:957:LYS:O	2:D:960:MET:HE2	2.10	0.51
2:B:893:TYR:H	2:B:961:MET:HB2	1.76	0.51
2:B:972:LEU:HB3	2:B:1044:ARG:HG2	1.92	0.51
2:C:893:TYR:H	2:C:961:MET:HB2	1.76	0.51
2:A:872:GLU:O	2:A:876:GLU:HG3	2.11	0.51
2:A:893:TYR:H	2:A:961:MET:HB2	1.76	0.51
2:A:1824:GLN:OE1	2:A:1824:GLN:HA	2.11	0.51
2:A:3381:LEU:HD23	2:A:3381:LEU:C	2.35	0.51
2:B:329:ARG:N	2:B:329:ARG:HD2	2.26	0.51
2:B:2165:LEU:HD12	2:B:2178:MET:HE2	1.92	0.51
2:D:972:LEU:HB3	2:D:1044:ARG:HG2	1.92	0.51
2:B:3504:SER:HB2	2:B:3507:THR:HG23	1.93	0.51
2:D:3409:TYR:CD2	2:D:3513:THR:HG21	2.45	0.51
2:D:3465:ASN:HA	2:D:3502:ARG:HA	1.92	0.51
2:C:329:ARG:HD2	2:C:329:ARG:N	2.26	0.51
2:C:2018:GLU:OE1	2:C:2018:GLU:HA	2.11	0.51
2:C:4634:GLU:HB2	2:C:4639:MET:HE2	1.93	0.51
2:A:2986:VAL:HG22	2:A:2988:LYS:H	1.75	0.50
2:D:872:GLU:O	2:D:876:GLU:HG3	2.11	0.50
2:C:458:GLU:N	2:C:458:GLU:OE2	2.45	0.50
2:A:492:ASP:O	2:A:496:VAL:HG13	2.11	0.50
2:A:2018:GLU:OE1	2:A:2018:GLU:HA	2.11	0.50
2:B:872:GLU:O	2:B:876:GLU:HG3	2.11	0.50
2:D:893:TYR:H	2:D:961:MET:HB2	1.76	0.50
2:D:4634:GLU:HB2	2:D:4639:MET:HE2	1.93	0.50
2:C:2986:VAL:HG22	2:C:2988:LYS:H	1.75	0.50
2:C:1824:GLN:OE1	2:C:1824:GLN:HA	2.11	0.50
2:A:619:ASP:O	2:A:623:GLU:HG3	2.12	0.50
2:A:821:LEU:HD23	2:A:822:ARG:N	2.27	0.50
2:A:2165:LEU:HD12	2:A:2178:MET:HE2	1.92	0.50
2:B:492:ASP:O	2:B:496:VAL:HG13	2.11	0.50
2:B:821:LEU:HD23	2:B:822:ARG:N	2.27	0.50
2:D:1022:VAL:HG22	2:D:1023:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3504:SER:HB2	2:D:3507:THR:HG23	1.93	0.50
2:C:870:ILE:HD12	2:C:870:ILE:C	2.37	0.50
2:C:2285:GLU:HG2	2:C:3858:MET:HG2	1.94	0.50
2:A:955:LEU:O	2:A:966:LYS:HG2	2.10	0.50
2:A:3412:LEU:HD12	2:A:3416:VAL:HG23	1.93	0.50
2:B:870:ILE:HD12	2:B:870:ILE:C	2.37	0.50
2:D:1824:GLN:HA	2:D:1824:GLN:OE1	2.11	0.50
2:C:957:LYS:O	2:C:960:MET:HE2	2.10	0.50
2:A:826:ILE:HG22	2:A:827:LYS:HG2	1.94	0.50
2:A:1022:VAL:HG22	2:A:1023:PRO:HD2	1.94	0.50
2:B:2986:VAL:HG22	2:B:2988:LYS:H	1.75	0.50
2:B:3316:LEU:HD11	2:B:3346:VAL:HG23	1.93	0.50
2:D:619:ASP:O	2:D:623:GLU:HG3	2.12	0.50
2:D:826:ILE:HG22	2:D:827:LYS:HG2	1.94	0.50
2:D:2377:LEU:HA	2:D:2469:ILE:HD11	1.94	0.50
2:D:3316:LEU:HD11	2:D:3346:VAL:HG23	1.93	0.50
7:A:5306:PCW:H483	7:A:5307:PCW:H461	1.93	0.50
2:B:3107:VAL:HG12	2:B:3175:LEU:HD22	1.94	0.50
2:D:870:ILE:HD12	2:D:870:ILE:C	2.37	0.50
2:D:1434:TYR:HB2	2:D:1572:ILE:HG21	1.94	0.50
2:D:2224:ARG:H	2:D:2224:ARG:HD3	1.77	0.50
2:D:3296:LEU:HB2	2:D:3297:PRO:HD3	1.94	0.50
2:C:821:LEU:HD23	2:C:822:ARG:N	2.27	0.50
2:C:972:LEU:HB3	2:C:1044:ARG:HG2	1.92	0.50
2:C:2224:ARG:HD3	2:C:2224:ARG:H	1.77	0.50
2:C:2626:LEU:HD22	2:C:2640:PRO:HB3	1.94	0.50
2:C:3211:ASN:OD1	2:C:3236:VAL:HG11	2.11	0.50
2:C:3412:LEU:HD12	2:C:3416:VAL:HG23	1.93	0.50
2:A:2377:LEU:HA	2:A:2469:ILE:HD11	1.94	0.50
2:A:3504:SER:HB2	2:A:3507:THR:HG23	1.93	0.50
2:A:4150:LEU:HB3	2:A:4160:LEU:HD21	1.94	0.50
2:B:458:GLU:N	2:B:458:GLU:OE2	2.45	0.50
2:B:619:ASP:O	2:B:623:GLU:HG3	2.12	0.50
2:B:2224:ARG:H	2:B:2224:ARG:HD3	1.77	0.50
2:D:458:GLU:N	2:D:458:GLU:OE2	2.45	0.50
2:C:1022:VAL:HG22	2:C:1023:PRO:HD2	1.94	0.50
2:A:329:ARG:HD2	2:A:329:ARG:N	2.26	0.50
2:A:2224:ARG:HD3	2:A:2224:ARG:H	1.77	0.50
2:D:1147:ASP:HB3	2:D:1164:LEU:HD11	1.94	0.50
2:C:872:GLU:O	2:C:876:GLU:HG3	2.11	0.50
2:A:870:ILE:HD12	2:A:870:ILE:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1147:ASP:HB3	2:A:1164:LEU:HD11	1.94	0.49
2:B:1022:VAL:HG22	2:B:1023:PRO:HD2	1.94	0.49
2:B:1299:GLN:OE1	2:B:1299:GLN:O	2.30	0.49
2:B:2018:GLU:OE1	2:B:2018:GLU:HA	2.11	0.49
2:B:2285:GLU:HG2	2:B:3858:MET:HG2	1.93	0.49
2:B:3352:GLU:OE1	2:B:3352:GLU:C	2.55	0.49
2:D:1939:MET:HA	2:D:1939:MET:HE3	1.94	0.49
2:D:2902:HIS:HB3	2:D:2905:LEU:HD23	1.95	0.49
2:C:3352:GLU:C	2:C:3352:GLU:OE1	2.55	0.49
2:A:458:GLU:OE2	2:A:458:GLU:N	2.45	0.49
2:A:957:LYS:O	2:A:960:MET:CE	2.60	0.49
2:A:1939:MET:HA	2:A:1939:MET:HE3	1.94	0.49
2:A:3352:GLU:C	2:A:3352:GLU:OE1	2.55	0.49
2:B:4150:LEU:HB3	2:B:4160:LEU:HD21	1.94	0.49
2:D:329:ARG:HD2	2:D:329:ARG:N	2.26	0.49
2:D:3352:GLU:C	2:D:3352:GLU:OE1	2.55	0.49
2:C:1434:TYR:HB2	2:C:1572:ILE:HG21	1.94	0.49
2:C:3296:LEU:HB2	2:C:3297:PRO:HD3	1.94	0.49
2:C:3504:SER:HB2	2:C:3507:THR:HG23	1.93	0.49
2:A:4634:GLU:HB2	2:A:4639:MET:HE2	1.93	0.49
2:B:1939:MET:HE3	2:B:1939:MET:HA	1.94	0.49
2:B:2178:MET:CE	2:B:2210:VAL:HG11	2.38	0.49
2:D:957:LYS:O	2:D:960:MET:CE	2.61	0.49
2:D:2626:LEU:HD22	2:D:2640:PRO:HB3	1.94	0.49
2:C:957:LYS:O	2:C:960:MET:CE	2.60	0.49
2:A:2626:LEU:HD22	2:A:2640:PRO:HB3	1.94	0.49
2:A:2902:HIS:HB3	2:A:2905:LEU:HD23	1.95	0.49
2:A:3316:LEU:HD11	2:A:3346:VAL:HG23	1.93	0.49
2:A:3528:THR:HG23	2:A:3573:MET:HE3	1.92	0.49
2:B:957:LYS:O	2:B:960:MET:CE	2.60	0.49
2:B:4634:GLU:HB2	2:B:4639:MET:HE2	1.93	0.49
2:D:821:LEU:HD23	2:D:822:ARG:N	2.27	0.49
2:C:2593:ARG:NH1	2:C:2593:ARG:HB2	2.28	0.49
2:C:3545:THR:HG22	2:C:3547:GLU:H	1.78	0.49
2:A:3107:VAL:HG12	2:A:3175:LEU:HD22	1.94	0.49
2:B:2377:LEU:HA	2:B:2469:ILE:HD11	1.94	0.49
2:D:2018:GLU:OE1	2:D:2018:GLU:HA	2.11	0.49
2:D:3412:LEU:HD12	2:D:3416:VAL:HG23	1.93	0.49
2:C:2377:LEU:HA	2:C:2469:ILE:HD11	1.94	0.49
2:B:1434:TYR:HB2	2:B:1572:ILE:HG21	1.94	0.49
2:D:2593:ARG:NH1	2:D:2593:ARG:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4150:LEU:HB3	2:D:4160:LEU:HD21	1.94	0.49
2:C:1939:MET:HA	2:C:1939:MET:HE3	1.94	0.49
2:A:2285:GLU:HG2	2:A:3858:MET:HG2	1.94	0.49
2:A:4071:ILE:HG21	2:A:4097:MET:HE1	1.94	0.49
2:B:1147:ASP:HB3	2:B:1164:LEU:HD11	1.94	0.49
2:B:2593:ARG:HB2	2:B:2593:ARG:NH1	2.28	0.49
2:B:2902:HIS:HB3	2:B:2905:LEU:HD23	1.94	0.49
2:C:492:ASP:O	2:C:496:VAL:HG13	2.11	0.49
2:C:826:ILE:HG22	2:C:827:LYS:HG2	1.94	0.49
2:B:3412:LEU:HD12	2:B:3416:VAL:HG23	1.93	0.49
2:D:492:ASP:O	2:D:496:VAL:HG13	2.11	0.49
2:C:1147:ASP:HB3	2:C:1164:LEU:HD11	1.94	0.49
2:C:4901:ILE:HG13	2:C:4913:ARG:NH2	2.28	0.49
2:A:2889:LYS:N	2:A:2889:LYS:HD2	2.28	0.49
2:B:1561:VAL:HG12	2:B:1562:ILE:HG23	1.95	0.49
2:B:2626:LEU:HD22	2:B:2640:PRO:HB3	1.94	0.49
2:B:4901:ILE:HG13	2:B:4913:ARG:NH2	2.28	0.49
2:C:2178:MET:CE	2:C:2210:VAL:HG11	2.38	0.49
2:C:4150:LEU:HB3	2:C:4160:LEU:HD21	1.94	0.49
2:B:3545:THR:HG22	2:B:3547:GLU:H	1.78	0.49
2:D:1141:ARG:HD3	2:C:3477:LYS:HB3	1.95	0.49
2:D:1299:GLN:OE1	2:D:1299:GLN:O	2.30	0.49
2:C:1561:VAL:HG12	2:C:1562:ILE:HG23	1.95	0.49
2:C:2889:LYS:N	2:C:2889:LYS:HD2	2.28	0.49
2:C:3107:VAL:HG12	2:C:3175:LEU:HD22	1.94	0.49
2:C:4071:ILE:HG21	2:C:4097:MET:HE1	1.94	0.49
2:A:1299:GLN:OE1	2:A:1299:GLN:O	2.30	0.48
2:D:3528:THR:HG23	2:D:3573:MET:HE3	1.92	0.48
2:C:1299:GLN:OE1	2:C:1299:GLN:O	2.30	0.48
2:A:1434:TYR:HB2	2:A:1572:ILE:HG21	1.94	0.48
2:B:368:ARG:HE	2:B:368:ARG:N	2.11	0.48
2:B:2209:GLU:HA	2:B:2209:GLU:OE2	2.14	0.48
2:B:3296:LEU:HB2	2:B:3297:PRO:HD3	1.94	0.48
2:D:2285:GLU:HG2	2:D:3858:MET:HG2	1.94	0.48
2:C:368:ARG:HE	2:C:368:ARG:N	2.11	0.48
2:A:2209:GLU:HA	2:A:2209:GLU:OE2	2.14	0.48
2:A:3296:LEU:HB2	2:A:3297:PRO:HD3	1.94	0.48
2:A:3350:ARG:HG3	2:A:3351:PRO:HD2	1.96	0.48
2:A:3545:THR:HG22	2:A:3547:GLU:H	1.78	0.48
2:A:4901:ILE:HG13	2:A:4913:ARG:NH2	2.28	0.48
2:B:826:ILE:HG22	2:B:827:LYS:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1482:ASN:CG	2:B:1482:ASN:O	2.57	0.48
2:B:2301:TYR:HB3	2:B:2331:TYR:CZ	2.49	0.48
2:C:619:ASP:O	2:C:623:GLU:HG3	2.12	0.48
2:C:2209:GLU:HA	2:C:2209:GLU:OE2	2.13	0.48
2:C:3326:ASN:O	2:C:3329:ILE:HG22	2.13	0.48
2:C:3606:LEU:O	2:C:3606:LEU:HD23	2.14	0.48
2:A:368:ARG:HE	2:A:368:ARG:N	2.11	0.48
2:A:1046:LEU:HD22	2:A:1053:ILE:HG13	1.96	0.48
2:D:972:LEU:HD22	2:D:1045:THR:HA	1.96	0.48
2:D:3545:THR:HG22	2:D:3547:GLU:H	1.78	0.48
2:C:2902:HIS:HB3	2:C:2905:LEU:HD23	1.95	0.48
2:C:3316:LEU:HD11	2:C:3346:VAL:HG23	1.93	0.48
2:A:972:LEU:HD22	2:A:1045:THR:HA	1.96	0.48
2:B:211:GLU:OE1	2:B:211:GLU:HA	2.14	0.48
2:B:924:MET:SD	2:B:924:MET:N	2.86	0.48
2:B:1046:LEU:HD22	2:B:1053:ILE:HG13	1.96	0.48
2:B:1869:GLU:HA	2:B:1869:GLU:OE1	2.14	0.48
2:D:2209:GLU:HA	2:D:2209:GLU:OE2	2.14	0.48
2:D:2889:LYS:N	2:D:2889:LYS:HD2	2.28	0.48
2:D:3350:ARG:HG3	2:D:3351:PRO:HD2	1.96	0.48
2:D:4071:ILE:HG21	2:D:4097:MET:HE1	1.94	0.48
2:D:4722:ARG:HB2	2:D:4722:ARG:CZ	2.44	0.48
2:C:972:LEU:HD22	2:C:1045:THR:HA	1.95	0.48
2:A:2593:ARG:NH1	2:A:2593:ARG:HB2	2.28	0.48
2:B:3326:ASN:O	2:B:3329:ILE:HG22	2.13	0.48
2:D:368:ARG:HE	2:D:368:ARG:N	2.11	0.48
2:D:1046:LEU:HD22	2:D:1053:ILE:HG13	1.96	0.48
2:D:1426:ILE:HD12	2:D:1426:ILE:N	2.29	0.48
2:D:2490:MET:CE	2:D:2495:VAL:HG12	2.43	0.48
2:D:3107:VAL:HG12	2:D:3175:LEU:HD22	1.94	0.48
2:D:3606:LEU:O	2:D:3606:LEU:HD23	2.14	0.48
2:C:2301:TYR:HB3	2:C:2331:TYR:CZ	2.49	0.48
2:A:4722:ARG:HB2	2:A:4722:ARG:CZ	2.44	0.48
2:B:1426:ILE:HD12	2:B:1426:ILE:N	2.29	0.48
2:B:4071:ILE:HG21	2:B:4097:MET:HE1	1.94	0.48
2:D:924:MET:N	2:D:924:MET:SD	2.86	0.48
2:D:1869:GLU:OE1	2:D:1869:GLU:HA	2.14	0.48
7:D:5305:PCW:H483	7:C:5305:PCW:H461	1.95	0.48
2:C:1426:ILE:N	2:C:1426:ILE:HD12	2.29	0.48
2:C:4722:ARG:CZ	2:C:4722:ARG:HB2	2.44	0.48
2:B:972:LEU:HD22	2:B:1045:THR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:908:VAL:HG13	2:D:912:SER:HB2	1.96	0.48
2:D:2754:PHE:HE2	2:D:2813:LEU:HD21	1.79	0.48
2:C:211:GLU:HA	2:C:211:GLU:OE1	2.14	0.48
2:A:1758:ARG:HD2	2:A:1758:ARG:N	2.29	0.48
2:B:2889:LYS:HD2	2:B:2889:LYS:N	2.28	0.48
2:B:3405:LEU:HD13	2:B:3510:ILE:CD1	2.44	0.48
2:B:4722:ARG:CZ	2:B:4722:ARG:HB2	2.44	0.48
7:B:5305:PCW:H461	7:C:5306:PCW:H483	1.96	0.48
2:D:3532:LEU:HD21	2:D:3560:GLN:HA	1.96	0.48
2:C:1869:GLU:OE1	2:C:1869:GLU:HA	2.14	0.48
2:C:3532:LEU:HD21	2:C:3560:GLN:HA	1.96	0.48
2:A:908:VAL:HG13	2:A:912:SER:HB2	1.96	0.48
2:A:1426:ILE:HD12	2:A:1426:ILE:N	2.29	0.48
7:A:5305:PCW:H461	7:B:5306:PCW:H483	1.96	0.48
2:B:2026:ASP:OD1	2:B:2027:ILE:N	2.47	0.48
2:B:2801:ASP:O	2:B:2804:ILE:HG22	2.14	0.48
2:B:3858:MET:HE1	2:B:3868:ARG:HG2	1.96	0.48
2:D:211:GLU:OE1	2:D:211:GLU:HA	2.14	0.48
2:D:3326:ASN:O	2:D:3329:ILE:HG22	2.13	0.48
2:C:2026:ASP:OD1	2:C:2027:ILE:N	2.47	0.48
2:C:2490:MET:CE	2:C:2495:VAL:HG12	2.44	0.48
2:C:2754:PHE:HE2	2:C:2813:LEU:HD21	1.79	0.48
2:A:924:MET:N	2:A:924:MET:SD	2.86	0.47
2:A:2301:TYR:HB3	2:A:2331:TYR:CZ	2.49	0.47
2:C:1758:ARG:N	2:C:1758:ARG:HD2	2.29	0.47
2:C:2801:ASP:O	2:C:2804:ILE:HG22	2.14	0.47
2:A:1482:ASN:O	2:A:1482:ASN:CG	2.57	0.47
2:A:1561:VAL:HG12	2:A:1562:ILE:HG23	1.95	0.47
2:A:2801:ASP:O	2:A:2804:ILE:HG22	2.14	0.47
2:B:3350:ARG:HG3	2:B:3351:PRO:HD2	1.95	0.47
2:D:2301:TYR:HB3	2:D:2331:TYR:CZ	2.49	0.47
2:A:1869:GLU:OE1	2:A:1869:GLU:HA	2.14	0.47
2:A:2754:PHE:HE2	2:A:2813:LEU:HD21	1.79	0.47
2:A:3405:LEU:HD13	2:A:3510:ILE:CD1	2.44	0.47
2:A:3532:LEU:HD21	2:A:3560:GLN:HA	1.96	0.47
2:D:3066:ASN:O	2:D:3070:ILE:HD12	2.15	0.47
2:D:3405:LEU:HD13	2:D:3510:ILE:CD1	2.44	0.47
2:D:4901:ILE:HG13	2:D:4913:ARG:NH2	2.28	0.47
2:C:3350:ARG:HG3	2:C:3351:PRO:HD2	1.96	0.47
2:C:3405:LEU:HD13	2:C:3510:ILE:CD1	2.44	0.47
2:C:4911:LEU:HA	2:C:4914:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:211:GLU:OE1	2:A:211:GLU:HA	2.14	0.47
2:B:3532:LEU:HD21	2:B:3560:GLN:HA	1.96	0.47
2:C:908:VAL:HG13	2:C:912:SER:HB2	1.96	0.47
2:C:1482:ASN:O	2:C:1482:ASN:CG	2.57	0.47
2:C:1791:VAL:O	2:C:1792:ALA:HB3	2.14	0.47
2:C:2876:GLU:OE1	2:C:2920:ARG:HG3	2.14	0.47
2:A:950:LEU:HD22	2:A:970:LEU:HD21	1.96	0.47
2:A:2920:ARG:O	2:A:2924:GLN:HG2	2.15	0.47
2:A:3066:ASN:O	2:A:3070:ILE:HD12	2.14	0.47
2:A:3606:LEU:O	2:A:3606:LEU:HD23	2.14	0.47
2:B:3477:LYS:HB3	2:C:1141:ARG:HD3	1.95	0.47
2:B:3528:THR:HG23	2:B:3573:MET:HE2	1.97	0.47
2:B:4911:LEU:HA	2:B:4914:VAL:HG22	1.97	0.47
2:D:2876:GLU:OE1	2:D:2920:ARG:HG3	2.14	0.47
2:C:924:MET:N	2:C:924:MET:SD	2.86	0.47
2:C:1046:LEU:HD22	2:C:1053:ILE:HG13	1.96	0.47
2:C:2518:LEU:HD21	2:C:2569:PHE:CE1	2.50	0.47
2:A:3459:VAL:HG11	2:A:3503:TYR:CD1	2.50	0.47
2:B:3606:LEU:HD23	2:B:3606:LEU:O	2.14	0.47
2:D:568:LEU:HD12	2:D:602:VAL:HG13	1.97	0.47
2:D:924:MET:O	2:D:928:THR:HG23	2.15	0.47
2:D:950:LEU:HD22	2:D:970:LEU:HD21	1.97	0.47
2:D:2801:ASP:O	2:D:2804:ILE:HG22	2.14	0.47
2:D:3540:TYR:CE1	2:D:3549:VAL:HG21	2.50	0.47
2:C:3066:ASN:O	2:C:3070:ILE:HD12	2.15	0.47
2:A:1280:GLN:O	2:A:1281:ASN:CG	2.58	0.47
2:A:1791:VAL:O	2:A:1792:ALA:HB3	2.14	0.47
2:A:2668:SER:O	2:A:2669:GLU:HB3	2.15	0.47
2:A:3326:ASN:O	2:A:3329:ILE:HG22	2.13	0.47
2:A:3732:SER:O	2:A:3735:LEU:HD23	2.15	0.47
2:A:3858:MET:HE1	2:A:3868:ARG:HG2	1.96	0.47
2:A:4911:LEU:HA	2:A:4914:VAL:HG22	1.97	0.47
2:B:872:GLU:HG2	2:B:922:LEU:HD21	1.97	0.47
2:B:924:MET:O	2:B:928:THR:HG23	2.15	0.47
2:B:961:MET:HE1	2:B:967:PRO:HD2	1.97	0.47
2:B:1079:LYS:HA	2:B:1189:LEU:HD11	1.96	0.47
2:B:1791:VAL:O	2:B:1792:ALA:HB3	2.14	0.47
2:B:1996:ARG:HG2	2:B:1996:ARG:HH11	1.79	0.47
2:B:2668:SER:O	2:B:2669:GLU:HB3	2.15	0.47
2:B:3459:VAL:HG11	2:B:3503:TYR:CD1	2.50	0.47
2:B:3539:ARG:HD3	2:B:3552:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1482:ASN:CG	2:D:1482:ASN:O	2.57	0.47
2:D:1561:VAL:HG12	2:D:1562:ILE:HG23	1.95	0.47
2:D:1758:ARG:HD2	2:D:1758:ARG:N	2.29	0.47
2:D:2026:ASP:OD1	2:D:2027:ILE:N	2.47	0.47
2:D:2724:GLU:HA	2:D:2724:GLU:OE2	2.14	0.47
2:C:421:PHE:HE2	2:C:436:LEU:HD11	1.80	0.47
2:C:2668:SER:O	2:C:2669:GLU:HB3	2.15	0.47
2:C:2715:VAL:HG13	2:C:2953:LYS:HB3	1.97	0.47
2:C:3540:TYR:CE1	2:C:3549:VAL:HG21	2.50	0.47
2:C:4091:LYS:HE3	2:C:4095:LYS:HZ3	1.80	0.47
2:A:2819:TRP:HB3	2:A:2821:TRP:CE2	2.50	0.47
2:A:3346:VAL:HG11	2:A:3414:ARG:HB3	1.97	0.47
2:A:3433:GLU:O	2:A:3437:MET:HG3	2.15	0.47
2:B:2724:GLU:HA	2:B:2724:GLU:OE2	2.14	0.47
2:B:2876:GLU:OE1	2:B:2920:ARG:HG3	2.14	0.47
2:B:2920:ARG:O	2:B:2924:GLN:HG2	2.14	0.47
2:B:3066:ASN:O	2:B:3070:ILE:HD12	2.14	0.47
2:B:3540:TYR:CE1	2:B:3549:VAL:HG21	2.50	0.47
2:D:2600:ARG:O	2:D:2604:GLU:HG3	2.15	0.47
2:D:4911:LEU:HA	2:D:4914:VAL:HG22	1.97	0.47
2:C:819:GLU:OE1	2:C:819:GLU:HA	2.15	0.47
2:C:3528:THR:HG23	2:C:3573:MET:HE2	1.97	0.47
2:A:2724:GLU:HA	2:A:2724:GLU:OE2	2.14	0.47
2:A:2876:GLU:OE1	2:A:2920:ARG:HG3	2.14	0.47
2:B:2464:ASP:C	2:B:2464:ASP:OD1	2.57	0.47
2:B:2518:LEU:HD21	2:B:2569:PHE:CE1	2.50	0.47
2:B:2819:TRP:HB3	2:B:2821:TRP:CE2	2.50	0.47
2:D:1280:GLN:O	2:D:1281:ASN:CG	2.58	0.47
2:D:2668:SER:O	2:D:2669:GLU:HB3	2.15	0.47
2:D:4971:THR:HG23	2:D:4972:PRO:HD2	1.97	0.47
2:C:924:MET:O	2:C:928:THR:HG23	2.15	0.47
2:C:961:MET:HE1	2:C:967:PRO:HD2	1.97	0.47
2:C:2724:GLU:OE2	2:C:2724:GLU:HA	2.14	0.47
2:C:3858:MET:HE1	2:C:3868:ARG:HG2	1.96	0.47
2:C:4564:PHE:C	2:C:4564:PHE:CD1	2.93	0.47
2:C:4971:THR:HG23	2:C:4972:PRO:HD2	1.97	0.47
1:E:14:ARG:HG3	1:E:15:THR:HG23	1.97	0.47
2:A:872:GLU:HG2	2:A:922:LEU:HD21	1.97	0.47
2:A:961:MET:HE1	2:A:967:PRO:HD2	1.97	0.47
2:A:1141:ARG:HD3	2:D:3477:LYS:HB3	1.97	0.47
2:A:2026:ASP:OD1	2:A:2027:ILE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3539:ARG:HD3	2:A:3552:PHE:CE1	2.50	0.47
2:B:1758:ARG:N	2:B:1758:ARG:HD2	2.29	0.47
2:B:2715:VAL:HG13	2:B:2953:LYS:HB3	1.97	0.47
2:B:2791:LEU:HD13	2:B:2792:ARG:H	1.80	0.47
2:B:4971:THR:HG23	2:B:4972:PRO:HD2	1.97	0.47
2:D:575:LEU:HD22	2:D:609:CYS:HB2	1.97	0.47
2:D:2920:ARG:O	2:D:2924:GLN:HG2	2.14	0.47
2:D:3346:VAL:HG11	2:D:3414:ARG:HB3	1.97	0.47
2:D:3539:ARG:HD3	2:D:3552:PHE:CE1	2.50	0.47
2:C:568:LEU:HD12	2:C:602:VAL:HG13	1.97	0.47
2:C:1996:ARG:HG2	2:C:1996:ARG:HH11	1.79	0.47
2:C:2464:ASP:C	2:C:2464:ASP:OD1	2.57	0.47
2:C:2752:ASP:O	2:C:2755:ILE:HG12	2.15	0.47
2:C:3039:ILE:HD11	2:C:3071:LEU:HD23	1.97	0.47
2:A:504:ALA:HB2	2:A:512:ALA:HB2	1.97	0.46
2:A:575:LEU:HD22	2:A:609:CYS:HB2	1.97	0.46
2:A:1043:VAL:O	2:A:1047:LEU:HD23	2.15	0.46
2:A:1996:ARG:HG2	2:A:1996:ARG:HH11	1.79	0.46
2:A:3214:ASN:HB2	2:A:3304:CYS:SG	2.56	0.46
2:A:4063:ASP:O	2:A:4067:LYS:HG3	2.15	0.46
2:B:3732:SER:O	2:B:3735:LEU:HD23	2.15	0.46
2:B:4091:LYS:HE3	2:B:4095:LYS:HZ3	1.79	0.46
2:D:3039:ILE:HD11	2:D:3071:LEU:HD23	1.97	0.46
2:C:2791:LEU:HD13	2:C:2792:ARG:H	1.81	0.46
2:C:3459:VAL:HG11	2:C:3503:TYR:CD1	2.50	0.46
2:C:3732:SER:O	2:C:3735:LEU:HD23	2.15	0.46
2:A:1079:LYS:HA	2:A:1189:LEU:HD11	1.96	0.46
2:A:3540:TYR:CE1	2:A:3549:VAL:HG21	2.50	0.46
2:A:4678:ALA:HB1	2:A:4720:VAL:HG21	1.97	0.46
2:D:244:LEU:HD23	2:D:300:VAL:HG12	1.98	0.46
2:D:932:LEU:HD22	2:D:988:LEU:HD11	1.98	0.46
2:D:2752:ASP:O	2:D:2755:ILE:HG12	2.15	0.46
2:D:3400:VAL:HG23	2:D:3403:ARG:NH2	2.30	0.46
2:D:3433:GLU:O	2:D:3437:MET:HG3	2.15	0.46
2:C:575:LEU:HD22	2:C:609:CYS:HB2	1.97	0.46
2:C:1280:GLN:O	2:C:1281:ASN:CG	2.58	0.46
2:A:4971:THR:HG23	2:A:4972:PRO:HD2	1.97	0.46
2:B:504:ALA:HB2	2:B:512:ALA:HB2	1.97	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB2	1.97	0.46
2:B:819:GLU:OE1	2:B:819:GLU:HA	2.15	0.46
2:B:2752:ASP:O	2:B:2755:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3433:GLU:O	2:B:3437:MET:HG3	2.15	0.46
2:B:4963:ILE:HD13	2:B:5030:LYS:HE3	1.98	0.46
2:D:421:PHE:HE2	2:D:436:LEU:HD11	1.80	0.46
2:D:866:HIS:HB2	2:D:941:MET:HE3	1.97	0.46
2:D:1043:VAL:O	2:D:1047:LEU:HD23	2.15	0.46
2:D:1791:VAL:O	2:D:1792:ALA:HB3	2.14	0.46
2:D:2791:LEU:HD13	2:D:2792:ARG:H	1.80	0.46
2:D:4063:ASP:O	2:D:4067:LYS:HG3	2.15	0.46
2:D:4244:GLU:OE1	2:D:4668:LEU:HD22	2.15	0.46
2:D:4564:PHE:CD1	2:D:4564:PHE:C	2.93	0.46
2:C:932:LEU:HD22	2:C:988:LEU:HD11	1.97	0.46
2:C:950:LEU:HD22	2:C:970:LEU:HD21	1.96	0.46
2:C:1870:VAL:HG22	2:C:2090:LYS:HD3	1.97	0.46
2:C:3539:ARG:HD3	2:C:3552:PHE:CE1	2.50	0.46
2:C:4678:ALA:HB1	2:C:4720:VAL:HG21	1.97	0.46
2:A:819:GLU:OE1	2:A:819:GLU:HA	2.15	0.46
2:A:2752:ASP:O	2:A:2755:ILE:HG12	2.15	0.46
2:A:2791:LEU:HD13	2:A:2792:ARG:H	1.80	0.46
2:A:3400:VAL:HG23	2:A:3403:ARG:NH2	2.30	0.46
2:B:568:LEU:HD12	2:B:602:VAL:HG13	1.97	0.46
2:B:908:VAL:HG13	2:B:912:SER:HB2	1.96	0.46
2:B:2490:MET:CE	2:B:2495:VAL:HG12	2.44	0.46
2:D:1123:VAL:HG23	2:D:1132:TRP:HB2	1.97	0.46
2:D:2715:VAL:HG13	2:D:2953:LYS:HB3	1.97	0.46
2:D:3858:MET:HE1	2:D:3868:ARG:HG2	1.96	0.46
2:C:3400:VAL:HG23	2:C:3403:ARG:NH2	2.30	0.46
2:C:4097:MET:HE2	2:C:4103:PHE:CD2	2.51	0.46
2:C:4963:ILE:HD13	2:C:5030:LYS:HE3	1.98	0.46
1:H:14:ARG:HG3	1:H:15:THR:HG23	1.97	0.46
2:A:924:MET:O	2:A:928:THR:HG23	2.15	0.46
2:A:2464:ASP:C	2:A:2464:ASP:OD1	2.57	0.46
2:A:2600:ARG:O	2:A:2604:GLU:HG3	2.15	0.46
2:A:3039:ILE:HD11	2:A:3071:LEU:HD23	1.97	0.46
2:B:421:PHE:HE2	2:B:436:LEU:HD11	1.80	0.46
2:B:1280:GLN:O	2:B:1281:ASN:CG	2.58	0.46
2:B:1870:VAL:HG22	2:B:2090:LYS:HD3	1.97	0.46
2:B:4244:GLU:OE1	2:B:4668:LEU:HD22	2.15	0.46
2:B:4564:PHE:CD1	2:B:4564:PHE:C	2.93	0.46
2:D:819:GLU:OE1	2:D:819:GLU:HA	2.15	0.46
2:D:2464:ASP:C	2:D:2464:ASP:OD1	2.57	0.46
2:D:3459:VAL:HG11	2:D:3503:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3433:GLU:O	2:C:3437:MET:HG3	2.15	0.46
2:A:1870:VAL:HG22	2:A:2090:LYS:HD3	1.97	0.46
2:A:2715:VAL:HG13	2:A:2953:LYS:HB3	1.97	0.46
2:B:856:VAL:HG12	2:B:991:ASN:OD1	2.16	0.46
2:B:3916:ILE:HD12	2:B:3916:ILE:N	2.31	0.46
2:D:504:ALA:HB2	2:D:512:ALA:HB2	1.97	0.46
2:D:856:VAL:HG12	2:D:991:ASN:OD1	2.16	0.46
2:D:1079:LYS:HA	2:D:1189:LEU:HD11	1.96	0.46
2:D:3214:ASN:HB2	2:D:3304:CYS:SG	2.56	0.46
2:C:866:HIS:HB2	2:C:941:MET:HE3	1.97	0.46
2:C:872:GLU:HG2	2:C:922:LEU:HD21	1.97	0.46
2:C:2920:ARG:O	2:C:2924:GLN:HG2	2.14	0.46
2:C:4244:GLU:OE1	2:C:4668:LEU:HD22	2.15	0.46
2:A:844:ARG:H	2:A:844:ARG:HD2	1.81	0.46
2:A:2490:MET:CE	2:A:2495:VAL:HG12	2.44	0.46
2:A:4244:GLU:OE1	2:A:4668:LEU:HD22	2.15	0.46
2:A:4564:PHE:CD1	2:A:4564:PHE:C	2.93	0.46
2:B:1043:VAL:O	2:B:1047:LEU:HD23	2.15	0.46
2:B:3346:VAL:HG11	2:B:3414:ARG:HB3	1.97	0.46
2:D:961:MET:HE1	2:D:967:PRO:HD2	1.97	0.46
2:D:1810:LYS:O	2:D:1814:MET:HG3	2.16	0.46
2:D:1996:ARG:HG2	2:D:1996:ARG:HH11	1.79	0.46
2:D:3732:SER:O	2:D:3735:LEU:HD23	2.15	0.46
2:C:1079:LYS:HA	2:C:1189:LEU:HD11	1.96	0.46
2:C:2600:ARG:O	2:C:2604:GLU:HG3	2.15	0.46
2:C:3591:LYS:O	2:C:3595:ARG:HG2	2.16	0.46
1:F:14:ARG:HG3	1:F:15:THR:HG23	1.98	0.46
2:A:244:LEU:HD23	2:A:300:VAL:HG12	1.98	0.46
2:A:3916:ILE:N	2:A:3916:ILE:HD12	2.31	0.46
2:B:950:LEU:HD22	2:B:970:LEU:HD21	1.96	0.46
2:B:3400:VAL:HG23	2:B:3403:ARG:NH2	2.30	0.46
2:D:574:VAL:HA	2:D:577:ILE:HG12	1.98	0.46
2:D:1483:VAL:O	2:D:1483:VAL:HG23	2.16	0.46
2:C:504:ALA:HB2	2:C:512:ALA:HB2	1.97	0.46
2:C:3346:VAL:HG11	2:C:3414:ARG:HB3	1.97	0.46
2:A:421:PHE:HE2	2:A:436:LEU:HD11	1.80	0.46
2:A:2178:MET:CE	2:A:2210:VAL:HG11	2.38	0.46
2:A:2746:ILE:O	2:A:2746:ILE:CD1	2.63	0.46
2:A:3003:LEU:HB2	2:A:3004:PRO:HD3	1.97	0.46
2:A:3061:ALA:O	2:A:3062:PRO:C	2.59	0.46
2:A:4091:LYS:HE3	2:A:4095:LYS:HZ3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:988:LEU:HB3	2:B:1039:LEU:HD12	1.98	0.46
2:B:2759:ALA:HB1	2:B:2806:ARG:HA	1.98	0.46
2:D:4097:MET:HE2	2:D:4103:PHE:CD2	2.51	0.46
2:A:568:LEU:HD12	2:A:602:VAL:HG13	1.97	0.46
2:A:2419:GLY:O	2:A:2423:MET:HG3	2.16	0.46
2:A:2518:LEU:HD21	2:A:2569:PHE:CE1	2.50	0.46
2:A:4206:GLU:HA	2:A:4206:GLU:OE2	2.16	0.46
2:B:1812:LEU:HD21	2:B:1862:ILE:HG13	1.98	0.46
2:B:2419:GLY:O	2:B:2423:MET:HG3	2.16	0.46
2:B:3214:ASN:HB2	2:B:3304:CYS:SG	2.56	0.46
2:B:4063:ASP:O	2:B:4067:LYS:HG3	2.15	0.46
2:D:418:LEU:HD23	2:D:421:PHE:CZ	2.51	0.46
2:D:872:GLU:HG2	2:D:922:LEU:HD21	1.97	0.46
2:D:2819:TRP:HB3	2:D:2821:TRP:CE2	2.50	0.46
2:C:213:TYR:HA	2:C:339:ILE:O	2.16	0.46
2:C:1810:LYS:O	2:C:1814:MET:HG3	2.16	0.46
2:C:2819:TRP:HB3	2:C:2821:TRP:CE2	2.50	0.46
2:C:3036:LYS:O	2:C:3039:ILE:HG22	2.16	0.46
2:C:4063:ASP:O	2:C:4067:LYS:HG3	2.15	0.46
2:A:574:VAL:HA	2:A:577:ILE:HG12	1.98	0.45
2:A:1810:LYS:O	2:A:1814:MET:HG3	2.16	0.45
2:A:3061:ALA:O	2:A:3064:VAL:HG12	2.16	0.45
2:A:3591:LYS:O	2:A:3595:ARG:HG2	2.16	0.45
2:A:4091:LYS:HG3	2:A:4092:ASP:N	2.32	0.45
2:B:2470:ILE:HG22	2:B:2525:GLY:HA3	1.98	0.45
2:B:3061:ALA:O	2:B:3064:VAL:HG12	2.16	0.45
2:B:3070:ILE:HD12	2:B:3070:ILE:N	2.31	0.45
2:B:4206:GLU:HA	2:B:4206:GLU:OE2	2.16	0.45
2:D:988:LEU:HB3	2:D:1039:LEU:HD12	1.98	0.45
2:D:1870:VAL:HG22	2:D:2090:LYS:HD3	1.97	0.45
2:D:2419:GLY:O	2:D:2423:MET:HG3	2.16	0.45
2:D:2518:LEU:HD21	2:D:2569:PHE:CE1	2.50	0.45
2:C:856:VAL:HG12	2:C:991:ASN:OD1	2.16	0.45
2:C:2419:GLY:O	2:C:2423:MET:HG3	2.16	0.45
2:C:3061:ALA:O	2:C:3064:VAL:HG12	2.16	0.45
2:C:4091:LYS:HG3	2:C:4092:ASP:N	2.32	0.45
2:A:866:HIS:HB2	2:A:941:MET:HE3	1.97	0.45
2:A:988:LEU:HB3	2:A:1039:LEU:HD12	1.98	0.45
2:B:1123:VAL:HG23	2:B:1132:TRP:HB2	1.97	0.45
2:B:1483:VAL:HG23	2:B:1483:VAL:O	2.16	0.45
2:B:2600:ARG:O	2:B:2604:GLU:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3039:ILE:HD11	2:B:3071:LEU:HD23	1.97	0.45
2:B:3547:GLU:O	2:B:3551:GLU:HG2	2.17	0.45
2:B:4678:ALA:HB1	2:B:4720:VAL:HG21	1.97	0.45
2:D:509:GLU:O	2:D:513:GLU:HG2	2.16	0.45
2:D:719:LEU:HD12	2:D:737:LEU:HD13	1.98	0.45
2:D:862:VAL:O	2:D:863:LEU:C	2.59	0.45
2:D:3036:LYS:O	2:D:3039:ILE:HG22	2.16	0.45
2:D:4678:ALA:HB1	2:D:4720:VAL:HG21	1.97	0.45
2:C:844:ARG:H	2:C:844:ARG:HD2	1.81	0.45
1:G:14:ARG:HG3	1:G:15:THR:HG23	1.97	0.45
2:A:862:VAL:O	2:A:863:LEU:C	2.59	0.45
2:A:867:LEU:HA	2:A:870:ILE:HD11	1.99	0.45
2:A:1812:LEU:HD21	2:A:1862:ILE:HG13	1.98	0.45
2:A:2759:ALA:HB1	2:A:2806:ARG:HA	1.98	0.45
2:A:4097:MET:HE2	2:A:4103:PHE:CD2	2.51	0.45
2:B:213:TYR:HA	2:B:339:ILE:O	2.16	0.45
2:B:844:ARG:H	2:B:844:ARG:HD2	1.81	0.45
2:B:866:HIS:HB2	2:B:941:MET:HE3	1.97	0.45
2:D:3003:LEU:HB2	2:D:3004:PRO:HD3	1.97	0.45
2:D:3413:ILE:HG13	2:D:3513:THR:HG22	1.98	0.45
2:D:3547:GLU:O	2:D:3551:GLU:HG2	2.17	0.45
2:D:4091:LYS:HG3	2:D:4092:ASP:N	2.32	0.45
2:D:4640:GLU:HB3	2:D:4641:PRO:HD3	1.98	0.45
2:C:1043:VAL:O	2:C:1047:LEU:HD23	2.15	0.45
2:C:3518:LEU:HD12	2:C:3522:LEU:HD23	1.98	0.45
2:A:1123:VAL:HG23	2:A:1132:TRP:HB2	1.98	0.45
2:A:1733:GLU:HG2	2:A:2201:LEU:HD23	1.99	0.45
2:A:2470:ILE:HG22	2:A:2525:GLY:HA3	1.98	0.45
2:B:891:TRP:HA	2:B:902:ARG:HB3	1.99	0.45
2:B:4016:LEU:O	2:B:4020:GLN:HG3	2.17	0.45
2:B:4640:GLU:HB3	2:B:4641:PRO:HD3	1.98	0.45
2:D:3916:ILE:N	2:D:3916:ILE:HD12	2.31	0.45
2:C:867:LEU:HA	2:C:870:ILE:HD11	1.99	0.45
2:A:856:VAL:HG12	2:A:991:ASN:OD1	2.16	0.45
2:A:891:TRP:HA	2:A:902:ARG:HB3	1.99	0.45
2:A:2284:ASN:HB3	2:A:3856:LEU:HD11	1.98	0.45
2:A:4963:ILE:HD13	2:A:5030:LYS:HE3	1.98	0.45
2:B:867:LEU:HA	2:B:870:ILE:HD11	1.99	0.45
2:B:2775:TRP:CG	2:B:2786:LYS:HZ1	2.34	0.45
2:B:4097:MET:HE2	2:B:4103:PHE:CD2	2.51	0.45
2:D:213:TYR:HA	2:D:339:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2464:ASP:OD1	2:D:2465:ASP:N	2.50	0.45
2:D:4206:GLU:HA	2:D:4206:GLU:OE2	2.16	0.45
2:C:3214:ASN:HB2	2:C:3304:CYS:SG	2.55	0.45
2:A:932:LEU:HD22	2:A:988:LEU:HD11	1.98	0.45
2:A:2858:GLN:HB2	2:A:2859:PRO:HD3	1.98	0.45
2:A:3518:LEU:HD12	2:A:3522:LEU:HD23	1.98	0.45
2:A:3704:HIS:O	2:A:3708:THR:HG23	2.17	0.45
2:A:4016:LEU:O	2:A:4020:GLN:HG3	2.17	0.45
2:B:509:GLU:O	2:B:513:GLU:HG2	2.16	0.45
2:B:574:VAL:HA	2:B:577:ILE:HG12	1.98	0.45
2:B:1810:LYS:O	2:B:1814:MET:HG3	2.16	0.45
2:B:2472:LEU:HD13	2:B:2473:PRO:HD2	1.99	0.45
2:B:3413:ILE:HG13	2:B:3513:THR:HG22	1.98	0.45
2:D:2178:MET:CE	2:D:2210:VAL:HG11	2.38	0.45
2:D:3545:THR:O	2:D:3549:VAL:HG23	2.17	0.45
2:D:4963:ILE:HD13	2:D:5030:LYS:HE3	1.98	0.45
2:C:418:LEU:HD23	2:C:421:PHE:CZ	2.52	0.45
2:C:504:ALA:HB2	2:C:512:ALA:CB	2.47	0.45
2:C:509:GLU:O	2:C:513:GLU:HG2	2.16	0.45
2:C:1123:VAL:HG23	2:C:1132:TRP:HB2	1.97	0.45
2:C:3003:LEU:HB2	2:C:3004:PRO:HD3	1.97	0.45
2:C:3916:ILE:N	2:C:3916:ILE:HD12	2.31	0.45
2:C:4206:GLU:HA	2:C:4206:GLU:OE2	2.16	0.45
2:A:280:LEU:C	2:A:280:LEU:HD12	2.42	0.45
2:A:719:LEU:HD12	2:A:737:LEU:HD13	1.98	0.45
2:A:875:ALA:O	2:A:879:HIS:CD2	2.70	0.45
2:A:2791:LEU:HD13	2:A:2792:ARG:N	2.32	0.45
2:A:3036:LYS:O	2:A:3039:ILE:HG22	2.16	0.45
2:A:3070:ILE:HD12	2:A:3070:ILE:N	2.31	0.45
2:A:3521:GLY:O	2:A:3524:MET:HG2	2.17	0.45
2:B:244:LEU:HD23	2:B:300:VAL:HG12	1.98	0.45
2:B:280:LEU:HD12	2:B:280:LEU:C	2.42	0.45
2:B:862:VAL:O	2:B:863:LEU:C	2.59	0.45
2:B:1733:GLU:HG2	2:B:2201:LEU:HD23	1.99	0.45
2:B:2515:GLN:O	2:B:2519:LEU:HD23	2.17	0.45
2:B:3545:THR:O	2:B:3549:VAL:HG23	2.17	0.45
2:D:928:THR:O	2:D:932:LEU:HD23	2.17	0.45
2:D:2515:GLN:O	2:D:2519:LEU:HD23	2.17	0.45
2:D:2624:ARG:HH22	2:D:2912:THR:HG22	1.82	0.45
2:D:4016:LEU:O	2:D:4020:GLN:HG3	2.17	0.45
2:C:1483:VAL:HG23	2:C:1483:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2624:ARG:HH22	2:C:2912:THR:HG22	1.82	0.45
2:A:2031:LEU:HD11	2:A:3657:TYR:CE2	2.52	0.45
2:A:3413:ILE:HG13	2:A:3513:THR:HG22	1.98	0.45
2:B:937:CYS:SG	2:B:1053:ILE:HG23	2.57	0.45
2:B:2390:PRO:O	2:B:2391:ALA:HB3	2.17	0.45
2:B:2464:ASP:OD1	2:B:2465:ASP:N	2.50	0.45
2:B:3003:LEU:HB2	2:B:3004:PRO:HD3	1.97	0.45
2:B:3518:LEU:HD12	2:B:3522:LEU:HD23	1.98	0.45
2:D:504:ALA:HB2	2:D:512:ALA:CB	2.47	0.45
2:D:2791:LEU:HD13	2:D:2792:ARG:N	2.32	0.45
2:D:3682:GLU:CD	2:D:3682:GLU:N	2.75	0.45
2:D:3704:HIS:O	2:D:3708:THR:HG23	2.17	0.45
2:C:244:LEU:HD23	2:C:300:VAL:HG12	1.98	0.45
2:C:3545:THR:O	2:C:3549:VAL:HG23	2.17	0.45
2:C:4567:LEU:HD11	2:C:4816:ILE:HG22	1.99	0.45
2:A:2624:ARG:HH22	2:A:2912:THR:HG22	1.82	0.45
2:A:3545:THR:O	2:A:3549:VAL:HG23	2.17	0.45
2:A:4567:LEU:HD11	2:A:4816:ILE:HG22	1.99	0.45
2:B:2624:ARG:HH22	2:B:2912:THR:HG22	1.82	0.45
2:B:2816:MET:CE	2:B:2823:ILE:HD12	2.47	0.45
2:B:3591:LYS:O	2:B:3595:ARG:HG2	2.16	0.45
2:D:280:LEU:C	2:D:280:LEU:HD12	2.42	0.45
2:D:844:ARG:H	2:D:844:ARG:HD2	1.81	0.45
2:D:1812:LEU:HD21	2:D:1862:ILE:HG13	1.98	0.45
2:D:2205:GLU:O	2:D:2209:GLU:HG2	2.17	0.45
2:D:2759:ALA:HB1	2:D:2806:ARG:HA	1.98	0.45
2:C:891:TRP:HA	2:C:902:ARG:HB3	1.99	0.45
2:C:937:CYS:SG	2:C:1053:ILE:HG23	2.57	0.45
2:C:988:LEU:HB3	2:C:1039:LEU:HD12	1.98	0.45
2:C:2761:TYR:O	2:C:2765:LYS:HG2	2.17	0.45
2:A:928:THR:O	2:A:932:LEU:HD23	2.17	0.45
2:A:937:CYS:SG	2:A:1053:ILE:HG23	2.57	0.45
2:A:2660:GLY:HA3	2:A:2666:VAL:HG12	1.99	0.45
2:A:2816:MET:CE	2:A:2823:ILE:HD12	2.47	0.45
2:A:3682:GLU:CD	2:A:3682:GLU:N	2.75	0.45
2:B:504:ALA:HB2	2:B:512:ALA:CB	2.47	0.45
2:B:719:LEU:HD12	2:B:737:LEU:HD13	1.98	0.45
2:B:932:LEU:HD22	2:B:988:LEU:HD11	1.98	0.45
2:B:2031:LEU:HD11	2:B:3657:TYR:CE2	2.52	0.45
2:B:3521:GLY:O	2:B:3524:MET:HG2	2.17	0.45
2:B:4091:LYS:HG3	2:B:4092:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:867:LEU:HA	2:D:870:ILE:HD11	1.99	0.45
2:D:937:CYS:SG	2:D:1053:ILE:HG23	2.57	0.45
2:D:2031:LEU:HD11	2:D:3657:TYR:CE2	2.52	0.45
2:D:3162:GLN:NE2	2:D:3203:VAL:HG21	2.33	0.45
2:D:4547:GLN:OE1	2:D:4547:GLN:HA	2.17	0.45
2:C:107:ILE:CG2	2:C:150:MET:HE2	2.47	0.45
2:C:862:VAL:O	2:C:863:LEU:C	2.59	0.45
2:C:1812:LEU:HD21	2:C:1862:ILE:HG13	1.98	0.45
2:C:2284:ASN:HB3	2:C:3856:LEU:HD11	1.98	0.45
2:C:2858:GLN:HB2	2:C:2859:PRO:HD3	1.99	0.45
2:A:213:TYR:HA	2:A:339:ILE:O	2.16	0.44
2:A:3987:ASP:OD1	2:B:162:LYS:HE3	2.17	0.44
2:B:293:LEU:HD13	2:B:378:LEU:HD12	1.99	0.44
2:B:875:ALA:O	2:B:879:HIS:CD2	2.70	0.44
2:B:2746:ILE:O	2:B:2746:ILE:CD1	2.63	0.44
2:B:2791:LEU:HD13	2:B:2792:ARG:N	2.32	0.44
2:B:2957:PHE:CD1	2:B:2957:PHE:C	2.95	0.44
2:D:1733:GLU:HG2	2:D:2201:LEU:HD23	1.99	0.44
2:D:3521:GLY:O	2:D:3524:MET:HG2	2.17	0.44
2:D:3591:LYS:O	2:D:3595:ARG:HG2	2.16	0.44
2:C:293:LEU:HD13	2:C:378:LEU:HD12	1.99	0.44
2:C:2472:LEU:HD13	2:C:2473:PRO:HD2	1.99	0.44
2:C:3413:ILE:HG13	2:C:3513:THR:HG22	1.98	0.44
2:C:3521:GLY:O	2:C:3524:MET:HG2	2.17	0.44
2:C:3547:GLU:O	2:C:3551:GLU:HG2	2.17	0.44
2:A:418:LEU:HD23	2:A:421:PHE:CZ	2.52	0.44
2:A:509:GLU:O	2:A:513:GLU:HG2	2.16	0.44
2:A:2761:TYR:O	2:A:2765:LYS:HG2	2.17	0.44
2:A:3350:ARG:NH1	2:A:3350:ARG:HB2	2.32	0.44
2:A:4640:GLU:HB3	2:A:4641:PRO:HD3	1.98	0.44
2:B:368:ARG:HE	2:B:368:ARG:CA	2.31	0.44
2:B:2205:GLU:O	2:B:2209:GLU:HG2	2.17	0.44
2:B:2284:ASN:HB3	2:B:3856:LEU:HD11	1.98	0.44
2:B:2481:LYS:O	2:B:2481:LYS:CG	2.66	0.44
2:B:2536:LEU:HD23	2:B:2547:ALA:HB2	1.99	0.44
2:B:3036:LYS:O	2:B:3039:ILE:HG22	2.16	0.44
2:B:3350:ARG:NH1	2:B:3350:ARG:HB2	2.32	0.44
2:D:2816:MET:CE	2:D:2823:ILE:HD12	2.47	0.44
2:D:2957:PHE:CD1	2:D:2957:PHE:C	2.96	0.44
2:C:280:LEU:C	2:C:280:LEU:HD12	2.42	0.44
2:C:719:LEU:HD12	2:C:737:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:875:ALA:O	2:C:879:HIS:CD2	2.70	0.44
2:C:928:THR:O	2:C:932:LEU:HD23	2.17	0.44
2:C:2390:PRO:O	2:C:2391:ALA:HB3	2.17	0.44
2:C:2470:ILE:HG22	2:C:2525:GLY:HA3	1.98	0.44
2:C:2660:GLY:HA3	2:C:2666:VAL:HG12	1.99	0.44
2:C:3704:HIS:O	2:C:3708:THR:HG23	2.17	0.44
2:C:4640:GLU:HB3	2:C:4641:PRO:HD3	1.98	0.44
2:A:3170:CYS:HB3	2:A:3240:CYS:HB3	1.81	0.44
2:A:3547:GLU:O	2:A:3551:GLU:HG2	2.17	0.44
2:A:3971:GLY:N	2:A:3972:PRO:HA	2.32	0.44
2:A:4955:GLU:HA	2:A:4955:GLU:OE2	2.18	0.44
2:D:162:LYS:HE3	2:C:3987:ASP:OD1	2.18	0.44
2:D:2284:ASN:HB3	2:D:3856:LEU:HD11	1.98	0.44
2:D:2663:ASN:O	2:D:2663:ASN:ND2	2.49	0.44
2:D:3528:THR:HG23	2:D:3573:MET:HE2	1.97	0.44
2:C:2759:ALA:HB1	2:C:2806:ARG:HA	1.98	0.44
2:C:3006:ILE:HG21	2:C:3067:CYS:SG	2.58	0.44
2:C:3070:ILE:HD12	2:C:3070:ILE:N	2.32	0.44
2:C:3162:GLN:NE2	2:C:3203:VAL:HG21	2.32	0.44
2:C:4955:GLU:OE2	2:C:4955:GLU:HA	2.18	0.44
2:A:977:LEU:HD11	2:A:981:GLN:HB3	1.99	0.44
2:A:2481:LYS:O	2:A:2481:LYS:CG	2.65	0.44
2:A:3219:TYR:HE1	2:A:3239:MET:HE3	1.83	0.44
2:B:107:ILE:CG2	2:B:150:MET:HE2	2.47	0.44
2:B:418:LEU:HD23	2:B:421:PHE:CZ	2.52	0.44
2:B:928:THR:O	2:B:932:LEU:HD23	2.17	0.44
2:D:875:ALA:O	2:D:879:HIS:CD2	2.70	0.44
2:D:2660:GLY:HA3	2:D:2666:VAL:HG12	2.00	0.44
2:D:2761:TYR:O	2:D:2765:LYS:HG2	2.17	0.44
2:D:3006:ILE:HG21	2:D:3067:CYS:SG	2.58	0.44
2:D:3070:ILE:HD12	2:D:3070:ILE:N	2.31	0.44
2:D:3350:ARG:NH1	2:D:3350:ARG:HB2	2.32	0.44
2:D:3518:LEU:HD12	2:D:3522:LEU:HD23	1.98	0.44
2:C:2464:ASP:OD1	2:C:2465:ASP:N	2.50	0.44
2:C:2515:GLN:O	2:C:2519:LEU:HD23	2.17	0.44
2:C:3359:ILE:HB	2:C:3360:PRO:HD3	2.00	0.44
2:A:107:ILE:CG2	2:A:150:MET:HE2	2.47	0.44
2:A:2464:ASP:OD1	2:A:2465:ASP:N	2.50	0.44
2:A:2515:GLN:O	2:A:2519:LEU:HD23	2.17	0.44
2:A:2536:LEU:HD23	2:A:2547:ALA:HA	2.00	0.44
2:A:2957:PHE:CD1	2:A:2957:PHE:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2536:LEU:HD23	2:B:2547:ALA:HA	2.00	0.44
2:B:2660:GLY:HA3	2:B:2666:VAL:HG12	2.00	0.44
2:B:2858:GLN:HB2	2:B:2859:PRO:HD3	1.98	0.44
2:B:2951:ILE:HD13	2:B:2951:ILE:N	2.33	0.44
2:B:3162:GLN:NE2	2:B:3203:VAL:HG21	2.32	0.44
2:B:3359:ILE:HB	2:B:3360:PRO:HD3	2.00	0.44
2:B:4081:VAL:HG21	2:B:4125:PHE:CE2	2.53	0.44
2:D:293:LEU:HD13	2:D:378:LEU:HD12	1.99	0.44
2:D:977:LEU:HD11	2:D:981:GLN:HB3	1.99	0.44
2:D:1046:LEU:C	2:D:1046:LEU:CD2	2.91	0.44
2:D:2858:GLN:HB2	2:D:2859:PRO:HD3	1.99	0.44
2:D:3219:TYR:HE1	2:D:3239:MET:HE3	1.83	0.44
2:C:574:VAL:HA	2:C:577:ILE:HG12	1.98	0.44
2:C:729:PRO:O	2:C:1476:MET:HE3	2.18	0.44
2:C:1733:GLU:HG2	2:C:2201:LEU:HD23	1.99	0.44
2:C:4016:LEU:O	2:C:4020:GLN:HG3	2.17	0.44
2:A:945:LYS:HD2	2:A:945:LYS:O	2.18	0.44
2:A:2390:PRO:O	2:A:2391:ALA:HB3	2.17	0.44
2:A:2628:PHE:CE1	2:A:2735:PHE:HB2	2.53	0.44
2:A:3477:LYS:HB3	2:B:1141:ARG:HD3	1.99	0.44
2:B:1478:ASP:O	2:B:1479:GLU:C	2.61	0.44
2:B:3046:LEU:O	2:B:3050:VAL:HG12	2.18	0.44
2:B:3219:TYR:HE1	2:B:3239:MET:HE3	1.83	0.44
2:B:3733:CYS:SG	2:B:3770:LEU:HD12	2.58	0.44
2:D:2470:ILE:HG22	2:D:2525:GLY:HA3	1.98	0.44
2:D:3061:ALA:O	2:D:3064:VAL:HG12	2.16	0.44
2:C:421:PHE:CE2	2:C:436:LEU:HD11	2.53	0.44
2:C:2746:ILE:O	2:C:2746:ILE:CD1	2.63	0.44
2:C:3046:LEU:HD11	2:C:3064:VAL:CG2	2.48	0.44
2:A:293:LEU:HD13	2:A:378:LEU:HD12	1.99	0.44
2:A:1469:VAL:HG13	2:A:1492:CYS:HB3	2.00	0.44
2:A:3528:THR:HG23	2:A:3573:MET:HE2	1.97	0.44
2:B:3006:ILE:HG21	2:B:3067:CYS:SG	2.58	0.44
2:B:4547:GLN:OE1	2:B:4547:GLN:HA	2.17	0.44
2:B:4567:LEU:HD11	2:B:4816:ILE:HG22	1.99	0.44
2:D:107:ILE:CG2	2:D:150:MET:HE2	2.47	0.44
2:D:3971:GLY:N	2:D:3972:PRO:HA	2.32	0.44
2:C:368:ARG:HE	2:C:368:ARG:CA	2.31	0.44
2:C:1469:VAL:HG13	2:C:1492:CYS:HB3	2.00	0.44
2:C:1477:GLY:HA2	2:C:1484:HIS:H	1.83	0.44
2:C:1478:ASP:O	2:C:1479:GLU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2536:LEU:HD23	2:C:2547:ALA:HB2	1.99	0.44
2:C:2775:TRP:CG	2:C:2786:LYS:HZ1	2.36	0.44
2:C:2791:LEU:HD13	2:C:2792:ARG:N	2.32	0.44
2:C:3346:VAL:HG11	2:C:3414:ARG:HB2	2.00	0.44
2:C:3350:ARG:HB2	2:C:3350:ARG:NH1	2.32	0.44
2:C:3749:VAL:O	2:C:3749:VAL:HG22	2.18	0.44
2:A:3006:ILE:HG21	2:A:3067:CYS:SG	2.58	0.44
2:B:1820:ARG:NH1	2:B:1820:ARG:HB3	2.33	0.44
2:B:2686:LEU:HD11	2:B:2699:ALA:HB3	2.00	0.44
2:B:2761:TYR:O	2:B:2765:LYS:HG2	2.17	0.44
2:B:3704:HIS:O	2:B:3708:THR:HG23	2.17	0.44
2:D:891:TRP:HA	2:D:902:ARG:HB3	1.99	0.44
2:D:2522:LEU:HD23	2:D:2578:MET:SD	2.58	0.44
2:D:3046:LEU:O	2:D:3050:VAL:HG12	2.18	0.44
2:D:4567:LEU:HD11	2:D:4816:ILE:HG22	1.99	0.44
2:C:958:THR:C	2:C:960:MET:HE2	2.43	0.44
2:C:2481:LYS:O	2:C:2481:LYS:CG	2.65	0.44
2:C:2536:LEU:HD23	2:C:2547:ALA:HA	2.00	0.44
2:C:2957:PHE:C	2:C:2957:PHE:CD1	2.96	0.44
2:C:3046:LEU:O	2:C:3050:VAL:HG12	2.18	0.44
2:C:3219:TYR:HE1	2:C:3239:MET:HE3	1.83	0.44
2:C:3682:GLU:CD	2:C:3682:GLU:N	2.75	0.44
2:A:2522:LEU:HD23	2:A:2578:MET:SD	2.58	0.44
2:A:4081:VAL:HG21	2:A:4125:PHE:CE2	2.53	0.44
2:B:2522:LEU:HD23	2:B:2578:MET:SD	2.58	0.44
2:B:2628:PHE:CE1	2:B:2735:PHE:HB2	2.53	0.44
2:B:2754:PHE:HE2	2:B:2813:LEU:HD21	1.79	0.44
2:B:3046:LEU:HD11	2:B:3064:VAL:CG2	2.48	0.44
2:B:3169:LEU:HG	2:B:3194:LEU:HD11	2.00	0.44
2:B:3682:GLU:CD	2:B:3682:GLU:N	2.75	0.44
2:D:421:PHE:CE2	2:D:436:LEU:HD11	2.53	0.44
2:D:729:PRO:O	2:D:1476:MET:HE3	2.18	0.44
2:D:1820:ARG:HB3	2:D:1820:ARG:NH1	2.33	0.44
2:D:2536:LEU:HD23	2:D:2547:ALA:HB2	1.99	0.44
2:D:3359:ILE:HB	2:D:3360:PRO:HD3	2.00	0.44
2:D:4125:PHE:CD1	2:D:4126:GLU:N	2.86	0.44
2:C:2031:LEU:HD11	2:C:3657:TYR:CE2	2.52	0.44
2:C:2686:LEU:HD11	2:C:2699:ALA:HB3	2.00	0.44
2:C:4543:GLU:O	2:C:4546:VAL:HG12	2.18	0.44
2:C:4802:GLY:HA2	2:C:4808:PHE:HB2	2.00	0.44
2:A:1477:GLY:HA2	2:A:1484:HIS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1820:ARG:HB3	2:A:1820:ARG:NH1	2.33	0.43
2:A:2024:PRO:HG2	2:A:2027:ILE:HG12	2.00	0.43
2:A:2536:LEU:HD23	2:A:2547:ALA:HB2	1.99	0.43
2:A:3162:GLN:NE2	2:A:3203:VAL:HG21	2.32	0.43
2:B:945:LYS:O	2:B:945:LYS:HD2	2.18	0.43
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.00	0.43
2:B:4955:GLU:HA	2:B:4955:GLU:OE2	2.18	0.43
2:D:2624:ARG:HD3	2:D:2906:VAL:HG11	2.00	0.43
2:D:3061:ALA:O	2:D:3062:PRO:C	2.59	0.43
2:D:3749:VAL:O	2:D:3749:VAL:HG22	2.18	0.43
2:C:654:GLU:OE1	2:C:654:GLU:HA	2.18	0.43
2:C:2417:HIS:CG	2:C:2492:ALA:HB2	2.53	0.43
2:C:2816:MET:CE	2:C:2823:ILE:HD12	2.47	0.43
2:C:3971:GLY:N	2:C:3972:PRO:HA	2.33	0.43
2:C:4125:PHE:CD1	2:C:4126:GLU:N	2.86	0.43
2:A:504:ALA:HB2	2:A:512:ALA:CB	2.47	0.43
2:A:2472:LEU:HD13	2:A:2473:PRO:HD2	1.99	0.43
2:A:2951:ILE:HD13	2:A:2951:ILE:N	2.33	0.43
2:A:4125:PHE:CD1	2:A:4126:GLU:N	2.86	0.43
2:B:421:PHE:CE2	2:B:436:LEU:HD11	2.53	0.43
2:B:925:SER:O	2:B:929:LEU:HG	2.18	0.43
2:B:958:THR:C	2:B:960:MET:HE2	2.43	0.43
2:B:2692:ASP:OD2	2:B:2692:ASP:C	2.61	0.43
2:B:2874:MET:HE3	2:B:2937:VAL:CG2	2.48	0.43
2:B:3346:VAL:HG11	2:B:3414:ARG:HB2	2.00	0.43
2:B:4543:GLU:O	2:B:4546:VAL:HG12	2.18	0.43
2:D:368:ARG:HE	2:D:368:ARG:CA	2.31	0.43
2:D:3169:LEU:HG	2:D:3194:LEU:HD11	2.00	0.43
2:D:3733:CYS:SG	2:D:3770:LEU:HD12	2.58	0.43
2:D:4543:GLU:O	2:D:4546:VAL:HG12	2.18	0.43
2:A:421:PHE:CE2	2:A:436:LEU:HD11	2.53	0.43
2:A:681:HIS:C	2:A:681:HIS:CD2	2.96	0.43
2:A:2624:ARG:HD3	2:A:2906:VAL:HG11	2.00	0.43
2:A:2823:ILE:HD11	2:A:2930:LEU:HD13	2.01	0.43
2:A:3359:ILE:HB	2:A:3360:PRO:HD3	2.00	0.43
2:B:654:GLU:OE1	2:B:654:GLU:HA	2.18	0.43
2:B:729:PRO:O	2:B:1476:MET:HE3	2.18	0.43
2:D:945:LYS:O	2:D:945:LYS:HD2	2.18	0.43
2:D:2823:ILE:HD11	2:D:2930:LEU:HD13	2.01	0.43
2:C:309:THR:O	2:C:309:THR:CG2	2.66	0.43
2:C:866:HIS:CB	2:C:941:MET:HE3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3061:ALA:O	2:C:3062:PRO:C	2.59	0.43
2:C:3733:CYS:SG	2:C:3770:LEU:HD12	2.58	0.43
2:C:4547:GLN:OE1	2:C:4547:GLN:HA	2.17	0.43
2:A:309:THR:O	2:A:309:THR:CG2	2.66	0.43
2:A:654:GLU:OE1	2:A:654:GLU:HA	2.18	0.43
2:A:1483:VAL:O	2:A:1483:VAL:HG23	2.16	0.43
2:A:2205:GLU:O	2:A:2209:GLU:HG2	2.17	0.43
2:A:3046:LEU:O	2:A:3050:VAL:HG12	2.18	0.43
2:A:4093:PHE:O	2:A:4097:MET:HG2	2.19	0.43
2:A:4547:GLN:OE1	2:A:4547:GLN:HA	2.17	0.43
2:B:866:HIS:CB	2:B:941:MET:HE3	2.49	0.43
2:B:1013:ILE:HB	2:B:1014:PRO:HD3	2.00	0.43
2:B:2024:PRO:HG2	2:B:2027:ILE:HG12	2.00	0.43
2:B:2417:HIS:CG	2:B:2492:ALA:HB2	2.53	0.43
2:D:309:THR:O	2:D:309:THR:CG2	2.66	0.43
2:D:865:PRO:HA	2:D:868:GLU:HG3	2.00	0.43
2:D:866:HIS:CB	2:D:941:MET:HE3	2.49	0.43
2:D:1477:GLY:HA2	2:D:1484:HIS:H	1.83	0.43
2:D:2390:PRO:O	2:D:2391:ALA:HB3	2.17	0.43
2:D:2417:HIS:CG	2:D:2492:ALA:HB2	2.53	0.43
2:D:2472:LEU:HD13	2:D:2473:PRO:HD2	1.99	0.43
2:D:2481:LYS:O	2:D:2481:LYS:CG	2.66	0.43
2:D:2536:LEU:HD23	2:D:2547:ALA:HA	2.00	0.43
2:D:2692:ASP:C	2:D:2692:ASP:OD2	2.61	0.43
2:D:3518:LEU:CD1	2:D:3522:LEU:HD23	2.49	0.43
2:C:925:SER:O	2:C:929:LEU:HG	2.18	0.43
2:C:2205:GLU:O	2:C:2209:GLU:HG2	2.17	0.43
2:C:2522:LEU:HD23	2:C:2578:MET:SD	2.58	0.43
2:C:2628:PHE:CE1	2:C:2735:PHE:HB2	2.53	0.43
2:C:2874:MET:HE3	2:C:2937:VAL:CG2	2.48	0.43
2:C:4071:ILE:HD13	2:C:4097:MET:HE1	2.01	0.43
2:A:368:ARG:HE	2:A:368:ARG:CA	2.31	0.43
2:A:866:HIS:CB	2:A:941:MET:HE3	2.49	0.43
2:A:3066:ASN:O	2:A:3070:ILE:CD1	2.67	0.43
2:A:3145:GLN:O	2:A:3149:GLN:HG3	2.18	0.43
2:A:3169:LEU:HG	2:A:3194:LEU:HD11	2.00	0.43
2:A:3518:LEU:CD1	2:A:3522:LEU:HD23	2.49	0.43
2:A:4071:ILE:HD13	2:A:4097:MET:HE1	2.01	0.43
2:A:4802:GLY:HA2	2:A:4808:PHE:HB2	2.00	0.43
2:B:3256:LEU:HD12	2:B:3266:MET:SD	2.59	0.43
2:B:3971:GLY:N	2:B:3972:PRO:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2874:MET:HE3	2:D:2937:VAL:CG2	2.48	0.43
2:D:2951:ILE:HD13	2:D:2951:ILE:N	2.33	0.43
2:D:3066:ASN:O	2:D:3070:ILE:CD1	2.67	0.43
2:D:4081:VAL:HG21	2:D:4125:PHE:CE2	2.53	0.43
2:C:2692:ASP:C	2:C:2692:ASP:OD2	2.61	0.43
2:C:3169:LEU:HG	2:C:3194:LEU:HD11	2.00	0.43
2:A:729:PRO:O	2:A:1476:MET:HE3	2.18	0.43
2:B:3061:ALA:O	2:B:3062:PRO:C	2.59	0.43
2:B:3749:VAL:HG22	2:B:3749:VAL:O	2.18	0.43
2:B:4071:ILE:HD13	2:B:4097:MET:HE1	2.01	0.43
2:D:958:THR:C	2:D:960:MET:HE2	2.43	0.43
2:D:1013:ILE:HB	2:D:1014:PRO:HD3	2.00	0.43
2:D:2024:PRO:HG2	2:D:2027:ILE:HG12	2.00	0.43
2:C:945:LYS:HD2	2:C:945:LYS:O	2.18	0.43
2:C:1820:ARG:HB3	2:C:1820:ARG:NH1	2.33	0.43
2:C:2951:ILE:HD13	2:C:2951:ILE:N	2.33	0.43
2:A:865:PRO:HA	2:A:868:GLU:HG3	2.00	0.43
2:A:2417:HIS:CG	2:A:2492:ALA:HB2	2.53	0.43
2:A:3501:ASP:OD1	2:A:3501:ASP:C	2.62	0.43
2:A:4821:LYS:CD	2:A:4821:LYS:H	2.32	0.43
2:B:2624:ARG:HD3	2:B:2906:VAL:HG11	2.00	0.43
2:B:3987:ASP:OD1	2:C:162:LYS:HE3	2.18	0.43
2:B:4767:TRP:CZ3	2:B:4768:LEU:HD22	2.54	0.43
2:D:3046:LEU:HD11	2:D:3064:VAL:CG2	2.48	0.43
2:D:4767:TRP:CZ3	2:D:4768:LEU:HD22	2.54	0.43
2:C:977:LEU:HD11	2:C:981:GLN:HB3	1.99	0.43
2:C:2024:PRO:HG2	2:C:2027:ILE:HG12	2.00	0.43
2:A:2001:PRO:O	2:A:2005:GLN:HG3	2.19	0.43
2:A:3046:LEU:HD11	2:A:3064:VAL:CG2	2.48	0.43
2:A:3294:PRO:HB2	2:A:3297:PRO:HD2	2.01	0.43
2:A:3733:CYS:SG	2:A:3770:LEU:HD12	2.58	0.43
2:A:3749:VAL:O	2:A:3749:VAL:HG22	2.18	0.43
2:B:977:LEU:HD11	2:B:981:GLN:HB3	1.99	0.43
2:B:3248:ARG:O	2:B:3252:ASP:OD2	2.37	0.43
2:B:3518:LEU:CD1	2:B:3522:LEU:HD23	2.49	0.43
2:B:4125:PHE:CD1	2:B:4126:GLU:N	2.86	0.43
2:D:2628:PHE:CE1	2:D:2735:PHE:HB2	2.53	0.43
2:D:3248:ARG:O	2:D:3252:ASP:OD2	2.37	0.43
2:D:3501:ASP:OD1	2:D:3501:ASP:C	2.62	0.43
2:D:4955:GLU:HA	2:D:4955:GLU:OE2	2.18	0.43
2:C:2624:ARG:HD3	2:C:2906:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:925:SER:O	2:A:929:LEU:HG	2.18	0.43
2:A:1115:LEU:HD12	2:A:1193:SER:HB3	2.01	0.43
2:A:2977:LEU:O	2:A:2981:VAL:HG23	2.19	0.43
2:B:1477:GLY:HA2	2:B:1484:HIS:H	1.83	0.43
2:B:2875:ALA:HB2	2:B:2927:LEU:HD23	2.00	0.43
2:B:4696:ASP:O	2:B:4696:ASP:OD2	2.37	0.43
2:D:4071:ILE:HD13	2:D:4097:MET:HE1	2.01	0.43
2:C:2977:LEU:O	2:C:2981:VAL:HG23	2.19	0.43
2:C:3066:ASN:O	2:C:3070:ILE:CD1	2.67	0.43
2:C:3294:PRO:HB2	2:C:3297:PRO:HD2	2.01	0.43
2:A:82:LEU:HD13	2:A:144:GLU:HG2	2.01	0.43
2:A:2874:MET:HE3	2:A:2937:VAL:CG2	2.48	0.43
2:A:3256:LEU:HD12	2:A:3266:MET:SD	2.59	0.43
2:B:309:THR:O	2:B:309:THR:CG2	2.66	0.43
2:D:1478:ASP:O	2:D:1479:GLU:C	2.61	0.43
2:D:2686:LEU:HD11	2:D:2699:ALA:HB3	2.00	0.43
2:D:4093:PHE:O	2:D:4097:MET:HG2	2.19	0.43
2:C:681:HIS:CD2	2:C:681:HIS:C	2.96	0.43
2:C:752:VAL:HB	2:C:753:PRO:C	2.44	0.43
2:C:3145:GLN:O	2:C:3149:GLN:HG3	2.18	0.43
2:C:4081:VAL:HG21	2:C:4125:PHE:CE2	2.53	0.43
2:A:722:TRP:CZ2	2:A:727:ALA:HB2	2.54	0.42
2:A:958:THR:C	2:A:960:MET:HE2	2.43	0.42
2:A:1465:ASP:OD2	2:A:1465:ASP:C	2.62	0.42
2:A:3276:MET:HE2	2:A:3276:MET:HB3	1.97	0.42
2:B:2872:GLN:O	2:B:2876:GLU:OE2	2.37	0.42
2:D:244:LEU:HD22	2:D:375:LYS:HE2	2.01	0.42
2:D:681:HIS:CD2	2:D:681:HIS:C	2.96	0.42
2:D:925:SER:O	2:D:929:LEU:HG	2.18	0.42
2:D:1469:VAL:HG13	2:D:1492:CYS:HB3	2.00	0.42
2:D:2686:LEU:HD13	2:D:3001:ILE:HG13	2.01	0.42
2:D:2746:ILE:O	2:D:2746:ILE:CD1	2.63	0.42
2:D:2977:LEU:O	2:D:2981:VAL:HG23	2.19	0.42
2:D:3145:GLN:O	2:D:3149:GLN:HG3	2.18	0.42
2:C:3170:CYS:HB3	2:C:3240:CYS:HB3	1.81	0.42
2:C:3518:LEU:CD1	2:C:3522:LEU:HD23	2.49	0.42
1:E:8:ILE:HA	2:A:719:LEU:HD11	2.01	0.42
2:A:1013:ILE:HB	2:A:1014:PRO:HD3	2.00	0.42
2:A:2692:ASP:C	2:A:2692:ASP:OD2	2.61	0.42
2:A:4767:TRP:CZ3	2:A:4768:LEU:HD22	2.54	0.42
2:B:82:LEU:HD13	2:B:144:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:VAL:HB	2:B:753:PRO:C	2.44	0.42
2:B:1469:VAL:HG13	2:B:1492:CYS:HB3	2.00	0.42
2:B:2469:ILE:HG21	2:B:2502:MET:HG3	2.01	0.42
2:B:2823:ILE:HD11	2:B:2930:LEU:HD13	2.00	0.42
2:B:3145:GLN:O	2:B:3149:GLN:HG3	2.18	0.42
2:D:654:GLU:OE1	2:D:654:GLU:HA	2.18	0.42
2:D:2755:ILE:HG13	2:D:2810:LYS:HE3	2.01	0.42
2:D:3666:ASP:OD2	2:D:3666:ASP:N	2.53	0.42
2:C:865:PRO:HA	2:C:868:GLU:HG3	2.00	0.42
2:C:3050:VAL:HG11	2:C:3068:LEU:HD11	2.01	0.42
2:C:4172:GLU:HA	2:C:4172:GLU:OE2	2.20	0.42
2:A:873:LYS:HG2	2:A:1049:TYR:OH	2.19	0.42
2:A:2253:HIS:O	2:A:2254:LEU:C	2.63	0.42
2:A:2686:LEU:HD11	2:A:2699:ALA:HB3	2.00	0.42
2:A:4885:PHE:CE1	2:A:4889:VAL:HG21	2.55	0.42
2:A:4951:LYS:O	2:A:4955:GLU:HG2	2.19	0.42
2:B:681:HIS:CD2	2:B:681:HIS:C	2.96	0.42
2:B:865:PRO:HA	2:B:868:GLU:HG3	2.00	0.42
2:B:873:LYS:HG2	2:B:1049:TYR:OH	2.20	0.42
2:B:2977:LEU:O	2:B:2981:VAL:HG23	2.19	0.42
2:B:4093:PHE:O	2:B:4097:MET:HG2	2.19	0.42
2:B:4576:ILE:HG21	2:B:4643:LEU:HB2	2.02	0.42
2:B:4885:PHE:CE1	2:B:4889:VAL:HG21	2.55	0.42
2:B:4951:LYS:O	2:B:4955:GLU:HG2	2.19	0.42
2:D:752:VAL:HB	2:D:753:PRO:C	2.44	0.42
2:D:3294:PRO:HB2	2:D:3297:PRO:HD2	2.01	0.42
2:D:4576:ILE:HG21	2:D:4643:LEU:HB2	2.02	0.42
2:D:4802:GLY:HA2	2:D:4808:PHE:HB2	2.00	0.42
2:C:82:LEU:HD13	2:C:144:GLU:HG2	2.01	0.42
2:C:565:TYR:CZ	2:C:569:ILE:HD11	2.55	0.42
2:A:2225:PHE:N	2:A:2226:PRO:CD	2.83	0.42
2:A:2767:ALA:HB2	2:A:2791:LEU:HD11	2.02	0.42
2:A:4543:GLU:O	2:A:4546:VAL:HG12	2.18	0.42
2:B:974:HIS:ND1	2:B:975:VAL:HG23	2.35	0.42
2:B:1115:LEU:HD13	2:B:1123:VAL:HG11	2.02	0.42
2:B:2253:HIS:O	2:B:2254:LEU:C	2.63	0.42
2:B:2686:LEU:HD13	2:B:3001:ILE:HG13	2.01	0.42
2:B:3294:PRO:HB2	2:B:3297:PRO:HD2	2.01	0.42
2:B:3501:ASP:OD1	2:B:3501:ASP:C	2.62	0.42
2:D:565:TYR:CZ	2:D:569:ILE:HD11	2.55	0.42
2:D:2875:ALA:HB2	2:D:2927:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3256:LEU:HD12	2:D:3266:MET:SD	2.59	0.42
2:C:873:LYS:HG2	2:C:1049:TYR:OH	2.20	0.42
2:C:974:HIS:ND1	2:C:975:VAL:HG23	2.35	0.42
2:C:1115:LEU:HD13	2:C:1123:VAL:HG11	2.02	0.42
2:C:3666:ASP:OD2	2:C:3666:ASP:N	2.53	0.42
2:C:4767:TRP:CZ3	2:C:4768:LEU:HD22	2.54	0.42
2:A:752:VAL:HB	2:A:753:PRO:C	2.44	0.42
2:A:974:HIS:ND1	2:A:975:VAL:HG23	2.35	0.42
2:A:1996:ARG:NE	2:A:1996:ARG:HA	2.34	0.42
2:A:2254:LEU:CD1	2:A:2276:ALA:HB1	2.50	0.42
2:A:4696:ASP:O	2:A:4696:ASP:OD2	2.37	0.42
7:A:5307:PCW:H212	7:A:5307:PCW:H262	2.02	0.42
2:B:2001:PRO:O	2:B:2005:GLN:HG3	2.19	0.42
2:B:3066:ASN:O	2:B:3070:ILE:CD1	2.67	0.42
2:B:4217:PHE:O	2:B:4221:VAL:HG22	2.20	0.42
2:B:4818:MET:N	2:B:4818:MET:SD	2.92	0.42
2:D:873:LYS:HG2	2:D:1049:TYR:OH	2.20	0.42
2:D:955:LEU:HD12	2:D:966:LYS:HG3	2.02	0.42
2:D:974:HIS:ND1	2:D:975:VAL:HG23	2.35	0.42
2:D:2001:PRO:O	2:D:2005:GLN:HG3	2.19	0.42
2:D:3371:LYS:HD2	2:D:3371:LYS:N	2.35	0.42
2:C:244:LEU:HD22	2:C:375:LYS:HE2	2.01	0.42
2:C:648:ILE:HG23	2:C:814:ALA:HB3	2.02	0.42
2:C:1115:LEU:HD12	2:C:1193:SER:HB3	2.01	0.42
2:C:2001:PRO:O	2:C:2005:GLN:HG3	2.19	0.42
2:C:2225:PHE:N	2:C:2226:PRO:CD	2.83	0.42
2:C:2823:ILE:HD11	2:C:2930:LEU:HD13	2.01	0.42
2:C:3371:LYS:N	2:C:3371:LYS:HD2	2.35	0.42
2:C:4093:PHE:O	2:C:4097:MET:HG2	2.19	0.42
2:C:4217:PHE:O	2:C:4221:VAL:HG22	2.20	0.42
2:B:421:PHE:CD1	2:B:421:PHE:C	2.98	0.42
2:B:722:TRP:CZ2	2:B:727:ALA:HB2	2.54	0.42
2:B:1996:ARG:HA	2:B:1996:ARG:NE	2.34	0.42
2:B:2267:MET:HE2	2:B:2267:MET:HB3	1.96	0.42
2:B:3374:ALA:O	2:B:3377:GLU:HG2	2.19	0.42
2:B:4693:GLY:O	2:B:4694:ASP:HB3	2.20	0.42
2:D:121:LEU:HD11	2:D:136:GLY:HA3	2.02	0.42
2:D:4818:MET:N	2:D:4818:MET:SD	2.92	0.42
2:D:4821:LYS:CD	2:D:4821:LYS:H	2.32	0.42
2:C:1013:ILE:HB	2:C:1014:PRO:HD3	2.00	0.42
2:C:2767:ALA:HB2	2:C:2791:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:244:LEU:HD22	2:A:375:LYS:HE2	2.01	0.42
2:A:2469:ILE:HG21	2:A:2502:MET:HG3	2.01	0.42
2:A:2875:ALA:HB2	2:A:2927:LEU:HD23	2.00	0.42
2:A:3266:MET:HG3	2:A:3266:MET:O	2.20	0.42
2:A:3374:ALA:O	2:A:3377:GLU:HG2	2.19	0.42
2:A:4172:GLU:HA	2:A:4172:GLU:OE2	2.19	0.42
2:A:4576:ILE:HG21	2:A:4643:LEU:HB2	2.02	0.42
7:A:5305:PCW:H262	7:A:5305:PCW:H212	2.02	0.42
2:B:3050:VAL:HG11	2:B:3068:LEU:HD11	2.01	0.42
2:D:722:TRP:CZ2	2:D:727:ALA:HB2	2.54	0.42
2:D:842:PRO:O	2:D:1196:PRO:HA	2.19	0.42
2:D:2254:LEU:CD1	2:D:2276:ALA:HB1	2.50	0.42
2:D:2751:LEU:O	2:D:2752:ASP:C	2.63	0.42
2:D:4172:GLU:HA	2:D:4172:GLU:OE2	2.19	0.42
2:C:121:LEU:HD11	2:C:136:GLY:HA3	2.02	0.42
2:C:2875:ALA:HB2	2:C:2927:LEU:HD23	2.00	0.42
2:C:3256:LEU:HD12	2:C:3266:MET:SD	2.59	0.42
2:C:4696:ASP:O	2:C:4696:ASP:OD2	2.37	0.42
2:A:421:PHE:CD1	2:A:421:PHE:C	2.98	0.42
2:A:1925:GLY:O	2:A:1929:MET:HG3	2.20	0.42
2:A:4217:PHE:O	2:A:4221:VAL:HG22	2.20	0.42
2:A:4818:MET:N	2:A:4818:MET:SD	2.92	0.42
2:B:121:LEU:HD11	2:B:136:GLY:HA3	2.02	0.42
2:B:1115:LEU:HD12	2:B:1193:SER:HB3	2.00	0.42
2:B:1981:MET:SD	2:B:1981:MET:C	3.03	0.42
2:B:2663:ASN:O	2:B:2663:ASN:ND2	2.49	0.42
2:B:4821:LYS:CD	2:B:4821:LYS:H	2.32	0.42
2:D:3374:ALA:O	2:D:3377:GLU:HG2	2.19	0.42
2:C:4951:LYS:O	2:C:4955:GLU:HG2	2.19	0.42
7:C:5305:PCW:H212	7:C:5305:PCW:H262	2.02	0.42
2:A:1115:LEU:HD13	2:A:1123:VAL:HG11	2.02	0.42
2:A:2751:LEU:O	2:A:2752:ASP:C	2.63	0.42
2:B:1472:VAL:HG22	2:B:1473:THR:N	2.35	0.42
2:C:722:TRP:CZ2	2:C:727:ALA:HB2	2.54	0.42
2:C:879:HIS:NE2	2:C:921:ASN:HB2	2.35	0.42
2:C:960:MET:HG2	2:C:966:LYS:HD2	2.02	0.42
2:C:1046:LEU:C	2:C:1046:LEU:CD2	2.91	0.42
2:C:1981:MET:C	2:C:1981:MET:SD	3.03	0.42
2:C:1996:ARG:NE	2:C:1996:ARG:HA	2.34	0.42
2:C:3226:GLU:O	2:C:3227:ARG:HG2	2.20	0.42
2:C:3374:ALA:O	2:C:3377:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3501:ASP:C	2:C:3501:ASP:OD1	2.62	0.42
2:C:4576:ILE:HG21	2:C:4643:LEU:HB2	2.02	0.42
2:C:4818:MET:SD	2:C:4818:MET:N	2.92	0.42
2:C:4885:PHE:CE1	2:C:4889:VAL:HG21	2.55	0.42
2:A:960:MET:HG2	2:A:966:LYS:HD2	2.02	0.42
2:A:2686:LEU:HD13	2:A:3001:ILE:HG13	2.01	0.42
2:A:3227:ARG:NE	2:A:3232:LEU:HD21	2.35	0.42
2:B:3226:GLU:O	2:B:3227:ARG:HG2	2.20	0.42
2:B:3227:ARG:NE	2:B:3232:LEU:HD21	2.35	0.42
2:D:1472:VAL:HG22	2:D:1473:THR:N	2.35	0.42
2:D:4026:MET:HE2	2:D:4026:MET:HB3	1.99	0.42
2:C:1465:ASP:OD2	2:C:1465:ASP:C	2.62	0.42
2:C:1925:GLY:O	2:C:1929:MET:HG3	2.20	0.42
2:C:2686:LEU:HD13	2:C:3001:ILE:HG13	2.01	0.42
2:C:3582:ARG:H	2:C:3582:ARG:HG2	1.67	0.42
1:H:24:VAL:HG13	1:H:48:LYS:HG2	2.02	0.42
2:A:3576:TYR:O	2:A:3582:ARG:HG3	2.21	0.41
2:B:1925:GLY:O	2:B:1929:MET:HG3	2.20	0.41
2:D:648:ILE:HG23	2:D:814:ALA:HB3	2.02	0.41
2:D:960:MET:HG2	2:D:966:LYS:HD2	2.02	0.41
2:D:1115:LEU:HD12	2:D:1193:SER:HB3	2.01	0.41
2:D:2872:GLN:O	2:D:2876:GLU:OE2	2.37	0.41
2:D:3226:GLU:O	2:D:3227:ARG:HG2	2.20	0.41
2:D:4693:GLY:O	2:D:4694:ASP:HB3	2.20	0.41
2:D:4885:PHE:CE1	2:D:4889:VAL:HG21	2.55	0.41
2:C:955:LEU:HD12	2:C:966:LYS:HG3	2.02	0.41
2:C:2572:THR:HB	2:C:2579:VAL:HG21	2.02	0.41
2:C:2755:ILE:HG13	2:C:2810:LYS:HE3	2.01	0.41
2:C:2872:GLN:O	2:C:2876:GLU:OE2	2.37	0.41
2:A:121:LEU:HD11	2:A:136:GLY:HA3	2.02	0.41
2:A:565:TYR:CZ	2:A:569:ILE:HD11	2.55	0.41
2:A:626:LEU:N	2:A:627:PRO:HD2	2.36	0.41
2:A:879:HIS:NE2	2:A:921:ASN:HB2	2.35	0.41
2:A:3405:LEU:HD13	2:A:3510:ILE:HD11	2.02	0.41
2:A:3788:GLY:HA3	2:A:3834:ALA:HB3	2.02	0.41
2:B:960:MET:HG2	2:B:966:LYS:HD2	2.02	0.41
2:D:1996:ARG:NE	2:D:1996:ARG:HA	2.34	0.41
2:D:3276:MET:HE2	2:D:3276:MET:HB3	1.97	0.41
2:D:3576:TYR:O	2:D:3582:ARG:HG3	2.21	0.41
2:C:842:PRO:O	2:C:1196:PRO:HA	2.19	0.41
2:C:862:VAL:O	2:C:862:VAL:CG1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:VAL:HG13	1:G:48:LYS:HG2	2.02	0.41
2:A:1981:MET:SD	2:A:1981:MET:C	3.03	0.41
2:A:2663:ASN:O	2:A:2663:ASN:ND2	2.49	0.41
2:A:2968:ASP:OD2	2:A:2968:ASP:C	2.63	0.41
2:A:3248:ARG:O	2:A:3252:ASP:OD2	2.37	0.41
2:A:3321:ARG:HA	2:A:3324:VAL:HG12	2.03	0.41
2:A:4693:GLY:O	2:A:4694:ASP:HB3	2.20	0.41
2:B:244:LEU:HD22	2:B:375:LYS:HE2	2.01	0.41
2:B:565:TYR:CZ	2:B:569:ILE:HD11	2.55	0.41
2:B:3453:ARG:HH11	2:B:3453:ARG:HG3	1.86	0.41
2:D:870:ILE:C	2:D:870:ILE:CD1	2.94	0.41
2:D:1694:LEU:HB3	2:D:1715:LEU:HD12	2.02	0.41
2:D:1981:MET:SD	2:D:1981:MET:C	3.03	0.41
2:D:2267:MET:HE2	2:D:2267:MET:HB3	1.96	0.41
2:D:3061:ALA:HB3	2:D:3062:PRO:CD	2.50	0.41
2:D:4039:MET:SD	2:D:4043:GLN:OE1	2.79	0.41
2:D:4951:LYS:O	2:D:4955:GLU:HG2	2.19	0.41
2:C:626:LEU:N	2:C:627:PRO:HD2	2.36	0.41
2:C:4693:GLY:O	2:C:4694:ASP:HB3	2.20	0.41
2:A:1478:ASP:O	2:A:1479:GLU:C	2.61	0.41
2:A:2755:ILE:HG13	2:A:2810:LYS:HE3	2.02	0.41
2:A:3061:ALA:HB3	2:A:3062:PRO:CD	2.50	0.41
2:A:3666:ASP:OD2	2:A:3666:ASP:N	2.53	0.41
2:B:648:ILE:HG23	2:B:814:ALA:HB3	2.02	0.41
2:B:907:LEU:O	2:B:961:MET:HE2	2.21	0.41
2:B:2369[B]:ARG:HA	2:B:2369[B]:ARG:HD3	1.86	0.41
2:B:2755:ILE:HG13	2:B:2810:LYS:HE3	2.01	0.41
2:B:3266:MET:O	2:B:3266:MET:HG3	2.20	0.41
2:B:3321:ARG:HA	2:B:3324:VAL:HG12	2.03	0.41
2:B:4172:GLU:HA	2:B:4172:GLU:OE2	2.19	0.41
2:D:82:LEU:HD13	2:D:144:GLU:HG2	2.01	0.41
2:D:1115:LEU:HD13	2:D:1123:VAL:HG11	2.02	0.41
2:D:1925:GLY:O	2:D:1929:MET:HG3	2.20	0.41
2:D:2253:HIS:O	2:D:2254:LEU:C	2.63	0.41
2:D:2639:MET:HE3	2:D:2639:MET:HB3	1.99	0.41
2:D:4696:ASP:O	2:D:4696:ASP:OD2	2.37	0.41
2:C:1472:VAL:HG22	2:C:1473:THR:N	2.35	0.41
2:C:3227:ARG:NE	2:C:3232:LEU:HD21	2.35	0.41
2:C:3248:ARG:O	2:C:3252:ASP:OD2	2.37	0.41
2:C:3252:ASP:O	2:C:3256:LEU:HD23	2.21	0.41
2:C:3321:ARG:HA	2:C:3324:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2582:MET:O	2:A:2586:VAL:HG23	2.21	0.41
2:A:2865:VAL:HG21	2:A:2928:LYS:NZ	2.36	0.41
2:B:879:HIS:NE2	2:B:921:ASN:HB2	2.35	0.41
2:B:1465:ASP:OD2	2:B:1465:ASP:C	2.62	0.41
2:B:2225:PHE:N	2:B:2226:PRO:CD	2.83	0.41
2:D:3227:ARG:NE	2:D:3232:LEU:HD21	2.35	0.41
2:D:3266:MET:O	2:D:3266:MET:HG3	2.20	0.41
2:D:3945:GLU:OE1	2:D:3945:GLU:N	2.54	0.41
2:C:1812:LEU:HD11	2:C:1858:ASP:HB3	2.03	0.41
2:C:2254:LEU:CD1	2:C:2276:ALA:HB1	2.50	0.41
2:C:2469:ILE:HG21	2:C:2502:MET:HG3	2.01	0.41
2:C:4821:LYS:H	2:C:4821:LYS:CD	2.32	0.41
1:E:26:HIS:HD2	1:E:105:LEU:HD11	1.85	0.41
2:A:648:ILE:HG23	2:A:814:ALA:HB3	2.02	0.41
2:A:2414:ASN:O	2:A:2414:ASN:CG	2.63	0.41
2:A:3039:ILE:HD11	2:A:3071:LEU:CD2	2.51	0.41
2:A:3076:ASP:OD1	2:A:3076:ASP:C	2.64	0.41
2:A:4064:MET:HE1	2:A:4110:PHE:CD2	2.56	0.41
2:B:987:ARG:HH11	2:B:987:ARG:HG3	1.86	0.41
2:B:2254:LEU:CD1	2:B:2276:ALA:HB1	2.50	0.41
2:B:3576:TYR:O	2:B:3582:ARG:HG3	2.21	0.41
2:B:3666:ASP:OD2	2:B:3666:ASP:N	2.53	0.41
7:B:5305:PCW:H212	7:B:5305:PCW:H262	2.02	0.41
2:D:1465:ASP:OD2	2:D:1465:ASP:C	2.62	0.41
2:D:1812:LEU:HD11	2:D:1858:ASP:HB3	2.03	0.41
2:D:2225:PHE:N	2:D:2226:PRO:CD	2.83	0.41
2:D:3050:VAL:HG11	2:D:3068:LEU:HD11	2.01	0.41
2:D:4064:MET:HE1	2:D:4110:PHE:CD2	2.56	0.41
2:D:4658:ILE:HD12	2:D:4796:MET:HG3	2.02	0.41
2:C:421:PHE:CD1	2:C:421:PHE:C	2.98	0.41
2:C:2253:HIS:O	2:C:2254:LEU:C	2.63	0.41
2:C:2663:ASN:O	2:C:2663:ASN:ND2	2.49	0.41
2:C:3276:MET:HE2	2:C:3276:MET:HB3	1.97	0.41
2:C:3405:LEU:HD13	2:C:3510:ILE:HD11	2.02	0.41
2:C:3788:GLY:HA3	2:C:3834:ALA:HB3	2.02	0.41
2:C:4039:MET:SD	2:C:4043:GLN:OE1	2.78	0.41
2:A:887:ILE:HG23	2:A:959:TYR:CE2	2.56	0.41
2:A:907:LEU:O	2:A:961:MET:HE2	2.21	0.41
2:A:955:LEU:HD12	2:A:966:LYS:HG3	2.02	0.41
2:A:1472:VAL:HG22	2:A:1473:THR:N	2.35	0.41
2:A:2872:GLN:O	2:A:2876:GLU:OE2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3050:VAL:HG11	2:A:3068:LEU:HD11	2.01	0.41
2:A:4543:GLU:O	2:A:4547:GLN:HG2	2.21	0.41
2:A:4839:MET:HG3	2:D:4822:THR:HG21	2.03	0.41
2:B:842:PRO:O	2:B:1196:PRO:HA	2.19	0.41
2:B:2185:ILE:HG21	2:B:2203:MET:HE1	2.03	0.41
2:B:2767:ALA:HB2	2:B:2791:LEU:HD11	2.02	0.41
2:B:2906:VAL:CG1	2:B:2907:PRO:HD2	2.48	0.41
2:B:3137:LEU:HB2	2:B:3138:PRO:HD3	2.03	0.41
2:B:4543:GLU:O	2:B:4547:GLN:HG2	2.21	0.41
2:D:421:PHE:CD1	2:D:421:PHE:C	2.98	0.41
2:D:2536:LEU:HD23	2:D:2547:ALA:CB	2.51	0.41
2:D:3568:SER:HA	2:D:3571:TRP:CD1	2.56	0.41
2:C:870:ILE:C	2:C:870:ILE:CD1	2.94	0.41
2:C:887:ILE:HG23	2:C:959:TYR:CE2	2.56	0.41
2:C:928:THR:O	2:C:932:LEU:CD2	2.69	0.41
2:C:1694:LEU:HB3	2:C:1715:LEU:HD12	2.03	0.41
2:C:2185:ILE:HG21	2:C:2203:MET:HE1	2.03	0.41
2:C:2518:LEU:O	2:C:2521:VAL:HG12	2.21	0.41
2:C:3266:MET:HG3	2:C:3266:MET:O	2.20	0.41
2:A:870:ILE:C	2:A:870:ILE:CD1	2.94	0.41
2:A:990:GLU:HA	2:A:1024:TYR:CD2	2.56	0.41
2:A:4039:MET:SD	2:A:4043:GLN:OE1	2.79	0.41
2:B:516:LYS:O	2:B:519:VAL:HG22	2.21	0.41
2:B:928:THR:O	2:B:932:LEU:CD2	2.69	0.41
2:B:2968:ASP:OD2	2:B:2968:ASP:C	2.63	0.41
2:B:3039:ILE:HD11	2:B:3071:LEU:CD2	2.51	0.41
2:B:3114:LYS:HA	2:B:3114:LYS:HE3	2.03	0.41
2:D:879:HIS:NE2	2:D:921:ASN:HB2	2.35	0.41
2:D:1051:TYR:N	2:D:1051:TYR:CD1	2.89	0.41
2:D:1069:TRP:HB3	2:D:1603:VAL:CG2	2.51	0.41
2:D:3434:LEU:CD2	2:D:3517:MET:SD	3.09	0.41
2:D:3788:GLY:HA3	2:D:3834:ALA:HB3	2.02	0.41
2:C:2968:ASP:OD2	2:C:2968:ASP:C	2.63	0.41
2:C:4543:GLU:O	2:C:4547:GLN:HG2	2.21	0.41
2:C:4658:ILE:HD12	2:C:4796:MET:HG3	2.02	0.41
1:E:24:VAL:HG13	1:E:48:LYS:HG2	2.02	0.41
2:A:759:ILE:O	2:A:759:ILE:HG23	2.21	0.41
2:A:842:PRO:O	2:A:1196:PRO:HA	2.19	0.41
2:A:1069:TRP:HB3	2:A:1603:VAL:CG2	2.51	0.41
2:A:1812:LEU:HD11	2:A:1858:ASP:HB3	2.02	0.41
2:A:2123:LEU:O	2:A:2127:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2185:ILE:HG21	2:A:2203:MET:HE1	2.03	0.41
2:A:2518:LEU:O	2:A:2521:VAL:HG12	2.21	0.41
2:A:3162:GLN:NE2	2:A:3218:VAL:HG23	2.36	0.41
2:A:3226:GLU:O	2:A:3227:ARG:HG2	2.20	0.41
2:A:3768:SER:HA	2:A:3771:HIS:CD2	2.56	0.41
2:B:626:LEU:N	2:B:627:PRO:HD2	2.35	0.41
2:B:821:LEU:HD23	2:B:822:ARG:H	1.86	0.41
2:B:1069:TRP:HB3	2:B:1603:VAL:CG2	2.51	0.41
2:B:2165:LEU:HD23	2:B:2165:LEU:HA	1.97	0.41
2:B:2639:MET:HB3	2:B:2640:PRO:HD3	2.02	0.41
2:B:2679:PHE:HB2	2:B:2706:ILE:HG21	2.03	0.41
2:B:2742:THR:O	2:B:2742:THR:HG22	2.21	0.41
2:B:2865:VAL:HG21	2:B:2928:LYS:NZ	2.36	0.41
2:B:2971:GLN:O	2:B:2974:ILE:HG22	2.21	0.41
2:B:3106:MET:SD	2:B:3110:LEU:CD2	3.09	0.41
2:B:3252:ASP:O	2:B:3256:LEU:HD23	2.21	0.41
2:B:3405:LEU:HD13	2:B:3510:ILE:HD11	2.02	0.41
2:B:3768:SER:HA	2:B:3771:HIS:CD2	2.56	0.41
2:B:3788:GLY:HA3	2:B:3834:ALA:HB3	2.02	0.41
2:B:4064:MET:HE1	2:B:4110:PHE:CD2	2.56	0.41
2:D:76:ARG:HG2	2:D:76:ARG:HH11	1.86	0.41
2:D:260:TRP:CE3	2:D:282:ILE:HG22	2.56	0.41
2:D:516:LYS:O	2:D:519:VAL:HG22	2.21	0.41
2:D:626:LEU:N	2:D:627:PRO:HD2	2.36	0.41
2:D:1500:PHE:CD1	2:D:1531:ALA:HB2	2.56	0.41
2:D:2185:ILE:HG21	2:D:2203:MET:HE1	2.03	0.41
2:D:2469:ILE:HG21	2:D:2502:MET:HG3	2.01	0.41
2:D:2572:THR:HB	2:D:2579:VAL:HG21	2.02	0.41
2:D:2700:MET:HB3	2:D:2701:PRO:HD3	2.03	0.41
2:D:2767:ALA:HB2	2:D:2791:LEU:HD11	2.02	0.41
2:D:2971:GLN:O	2:D:2974:ILE:HG22	2.21	0.41
2:D:3039:ILE:HD11	2:D:3071:LEU:CD2	2.51	0.41
2:D:3114:LYS:HA	2:D:3114:LYS:HE3	2.03	0.41
2:D:3227:ARG:HE	2:D:3232:LEU:HD21	1.86	0.41
2:D:3252:ASP:O	2:D:3256:LEU:HD23	2.21	0.41
2:D:3321:ARG:HA	2:D:3324:VAL:HG12	2.03	0.41
2:D:3399:SER:HA	2:D:3454:GLU:OE1	2.21	0.41
2:D:4217:PHE:O	2:D:4221:VAL:HG22	2.20	0.41
2:C:260:TRP:CE3	2:C:282:ILE:HG22	2.56	0.41
2:C:516:LYS:O	2:C:519:VAL:HG22	2.21	0.41
2:C:821:LEU:HD23	2:C:822:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:907:LEU:O	2:C:961:MET:HE2	2.21	0.41
2:C:919:ASN:OD1	2:C:919:ASN:C	2.64	0.41
2:C:1069:TRP:HB3	2:C:1603:VAL:CG2	2.51	0.41
2:C:1500:PHE:CD1	2:C:1531:ALA:HB2	2.56	0.41
2:C:2414:ASN:O	2:C:2414:ASN:CG	2.63	0.41
2:C:2582:MET:O	2:C:2586:VAL:HG23	2.21	0.41
2:C:3039:ILE:HD11	2:C:3071:LEU:CD2	2.51	0.41
2:C:3453:ARG:HG3	2:C:3453:ARG:HH11	1.86	0.41
2:C:3568:SER:HA	2:C:3571:TRP:CD1	2.56	0.41
2:C:3576:TYR:O	2:C:3582:ARG:HG3	2.21	0.41
2:A:862:VAL:O	2:A:862:VAL:CG1	2.68	0.41
2:A:891:TRP:CE3	2:A:904:HIS:HB2	2.56	0.41
2:A:1500:PHE:CD1	2:A:1531:ALA:HB2	2.56	0.41
2:A:2821:TRP:CZ3	2:A:2874:MET:HG3	2.56	0.41
2:A:3137:LEU:HB2	2:A:3138:PRO:HD3	2.03	0.41
2:A:3227:ARG:HE	2:A:3232:LEU:HD21	1.86	0.41
2:A:3399:SER:HA	2:A:3454:GLU:OE1	2.21	0.41
2:A:3453:ARG:HH11	2:A:3453:ARG:HG3	1.86	0.41
2:A:3568:SER:HA	2:A:3571:TRP:CD1	2.56	0.41
2:B:76:ARG:HH11	2:B:76:ARG:HG2	1.86	0.41
2:B:759:ILE:HG23	2:B:759:ILE:O	2.21	0.41
2:B:870:ILE:C	2:B:870:ILE:CD1	2.94	0.41
2:B:955:LEU:HD12	2:B:966:LYS:HG3	2.02	0.41
2:B:3434:LEU:CD2	2:B:3517:MET:SD	3.09	0.41
2:B:3945:GLU:N	2:B:3945:GLU:OE1	2.54	0.41
2:B:4039:MET:SD	2:B:4043:GLN:OE1	2.78	0.41
2:D:759:ILE:HG23	2:D:759:ILE:O	2.21	0.41
2:D:887:ILE:HG23	2:D:959:TYR:CE2	2.56	0.41
2:D:928:THR:O	2:D:932:LEU:CD2	2.69	0.41
2:D:2123:LEU:O	2:D:2127:GLN:HG2	2.21	0.41
2:D:2865:VAL:HG21	2:D:2928:LYS:NZ	2.36	0.41
2:D:3162:GLN:NE2	2:D:3218:VAL:HG23	2.36	0.41
2:D:3596:VAL:O	2:D:3600:SER:OG	2.36	0.41
2:C:2865:VAL:HG21	2:C:2928:LYS:NZ	2.36	0.41
2:C:3434:LEU:CD2	2:C:3517:MET:SD	3.09	0.41
2:A:102:LEU:HD22	2:A:160:GLY:O	2.22	0.40
2:A:1051:TYR:N	2:A:1051:TYR:CD1	2.89	0.40
2:A:2178:MET:HE2	2:A:2178:MET:HB2	1.99	0.40
2:A:2369[B]:ARG:HD3	2:A:2369[B]:ARG:HA	1.86	0.40
2:A:2572:THR:HB	2:A:2579:VAL:HG21	2.02	0.40
2:A:2874:MET:HE3	2:A:2937:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:TRP:CE3	2:B:282:ILE:HG22	2.56	0.40
2:B:932:LEU:CD2	2:B:988:LEU:HD11	2.51	0.40
2:B:1500:PHE:CD1	2:B:1531:ALA:HB2	2.56	0.40
2:D:102:LEU:HD22	2:D:160:GLY:O	2.21	0.40
2:D:2371:GLU:OE2	2:D:2371:GLU:N	2.54	0.40
2:D:2518:LEU:O	2:D:2521:VAL:HG12	2.21	0.40
2:D:2757:LYS:HD2	2:D:2830:GLU:HG2	2.03	0.40
2:D:3453:ARG:HG3	2:D:3453:ARG:HH11	1.86	0.40
2:C:76:ARG:HG2	2:C:76:ARG:HH11	1.86	0.40
2:C:891:TRP:CE3	2:C:904:HIS:HB2	2.56	0.40
2:C:987:ARG:HG3	2:C:987:ARG:HH11	1.86	0.40
2:C:1020:ARG:HH11	2:C:1020:ARG:HG2	1.86	0.40
2:C:2679:PHE:HB2	2:C:2706:ILE:HG21	2.03	0.40
2:C:2751:LEU:O	2:C:2752:ASP:C	2.63	0.40
2:C:3076:ASP:C	2:C:3076:ASP:OD1	2.64	0.40
2:C:4026:MET:HE2	2:C:4026:MET:HB3	1.99	0.40
1:F:24:VAL:HG13	1:F:48:LYS:HG2	2.02	0.40
2:A:260:TRP:CE3	2:A:282:ILE:HG22	2.56	0.40
2:A:442:ILE:HD11	2:A:514:SER:HB3	2.03	0.40
2:A:2700:MET:HB3	2:A:2701:PRO:HD3	2.03	0.40
2:A:3434:LEU:CD2	2:A:3517:MET:SD	3.09	0.40
2:B:2123:LEU:O	2:B:2127:GLN:HG2	2.21	0.40
2:B:2757:LYS:HD2	2:B:2830:GLU:HG2	2.03	0.40
2:B:3399:SER:HA	2:B:3454:GLU:OE1	2.21	0.40
2:B:3771:HIS:ND1	2:B:3771:HIS:C	2.79	0.40
2:D:932:LEU:CD2	2:D:988:LEU:HD11	2.51	0.40
2:D:987:ARG:HH11	2:D:987:ARG:HG3	1.86	0.40
2:D:3106:MET:SD	2:D:3110:LEU:CD2	3.09	0.40
2:D:3768:SER:HA	2:D:3771:HIS:CD2	2.56	0.40
2:D:4543:GLU:O	2:D:4547:GLN:HG2	2.21	0.40
2:C:69:LEU:HD23	2:C:109:LEU:CD2	2.52	0.40
2:C:1051:TYR:N	2:C:1051:TYR:CD1	2.89	0.40
2:C:2639:MET:HB3	2:C:2640:PRO:HD3	2.03	0.40
2:C:3184:GLU:C	2:C:3184:GLU:CD	2.90	0.40
2:C:3210:LEU:HD12	2:C:3210:LEU:N	2.37	0.40
2:C:3399:SER:HA	2:C:3454:GLU:OE1	2.21	0.40
2:C:4064:MET:HE1	2:C:4110:PHE:CD2	2.56	0.40
7:C:5305:PCW:H241	7:C:5305:PCW:H271	1.94	0.40
1:F:26:HIS:HD2	1:F:105:LEU:HD11	1.85	0.40
2:A:367:LEU:HD23	2:A:367:LEU:HA	1.99	0.40
2:A:516:LYS:O	2:A:519:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:919:ASN:OD1	2:A:919:ASN:C	2.64	0.40
2:A:932:LEU:CD2	2:A:988:LEU:HD11	2.51	0.40
2:A:983:THR:O	2:A:987:ARG:HG2	2.22	0.40
2:A:2355:ARG:O	2:A:2358:ILE:HG12	2.22	0.40
2:A:3184:GLU:C	2:A:3184:GLU:CD	2.90	0.40
2:A:3371:LYS:N	2:A:3371:LYS:HD2	2.35	0.40
2:B:919:ASN:OD1	2:B:919:ASN:C	2.64	0.40
2:B:990:GLU:HA	2:B:1024:TYR:CD2	2.56	0.40
2:B:2518:LEU:O	2:B:2521:VAL:HG12	2.21	0.40
2:B:2572:THR:HB	2:B:2579:VAL:HG21	2.02	0.40
2:B:2751:LEU:O	2:B:2752:ASP:C	2.63	0.40
2:D:69:LEU:HD23	2:D:109:LEU:HD21	2.03	0.40
2:D:69:LEU:HD23	2:D:109:LEU:CD2	2.51	0.40
2:D:862:VAL:O	2:D:862:VAL:CG1	2.68	0.40
2:D:2368:LEU:HD12	2:D:2368:LEU:N	2.37	0.40
2:D:3170:CYS:HB3	2:D:3240:CYS:HB3	1.81	0.40
2:C:983:THR:O	2:C:987:ARG:HG2	2.22	0.40
2:C:1742:THR:O	2:C:1960:ALA:HB2	2.21	0.40
2:A:928:THR:O	2:A:932:LEU:CD2	2.69	0.40
2:A:1694:LEU:HB3	2:A:1715:LEU:HD12	2.03	0.40
2:A:2368:LEU:HD12	2:A:2368:LEU:N	2.37	0.40
2:A:2577:ILE:HD13	2:A:2577:ILE:N	2.37	0.40
2:A:2742:THR:O	2:A:2742:THR:HG22	2.21	0.40
2:A:2757:LYS:HD2	2:A:2830:GLU:HG2	2.03	0.40
2:B:707:VAL:HG23	2:B:782:SER:HB3	2.03	0.40
2:B:2371:GLU:OE2	2:B:2371:GLU:N	2.54	0.40
2:B:3371:LYS:N	2:B:3371:LYS:HD2	2.35	0.40
2:B:3978:GLN:OE1	2:B:4039:MET:HE1	2.21	0.40
2:D:707:VAL:HG23	2:D:782:SER:HB3	2.04	0.40
2:D:3405:LEU:HD13	2:D:3510:ILE:HD11	2.02	0.40
2:D:3978:GLN:OE1	2:D:4039:MET:HE1	2.21	0.40
2:C:707:VAL:HG23	2:C:782:SER:HB3	2.04	0.40
2:C:932:LEU:CD2	2:C:988:LEU:HD11	2.51	0.40
2:C:2536:LEU:HD23	2:C:2547:ALA:CB	2.51	0.40
2:C:2967:MET:HE1	2:C:2998:PHE:HE2	1.87	0.40
2:C:3114:LYS:HE3	2:C:3114:LYS:HA	2.03	0.40
2:C:3162:GLN:NE2	2:C:3218:VAL:HG23	2.36	0.40
2:C:3978:GLN:OE1	2:C:4039:MET:HE1	2.21	0.40
2:A:69:LEU:HD23	2:A:109:LEU:HD21	2.03	0.40
2:A:3106:MET:SD	2:A:3110:LEU:CD2	3.09	0.40
2:A:3945:GLU:N	2:A:3945:GLU:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4658:ILE:HD12	2:A:4796:MET:HG3	2.02	0.40
2:B:2414:ASN:O	2:B:2414:ASN:CG	2.63	0.40
2:B:2536:LEU:HD23	2:B:2547:ALA:CB	2.51	0.40
2:B:2639:MET:HB3	2:B:2639:MET:HE3	1.99	0.40
2:B:2821:TRP:CZ3	2:B:2874:MET:HG3	2.56	0.40
2:B:3276:MET:HE2	2:B:3276:MET:HB3	1.98	0.40
2:D:76:ARG:O	2:D:80:GLU:HG2	2.22	0.40
2:D:907:LEU:O	2:D:961:MET:HE2	2.21	0.40
2:D:919:ASN:OD1	2:D:919:ASN:C	2.64	0.40
2:D:3137:LEU:HB2	2:D:3138:PRO:HD3	2.03	0.40
2:D:4091:LYS:HE3	2:D:4095:LYS:HZ3	1.85	0.40
2:C:2123:LEU:O	2:C:2127:GLN:HG2	2.21	0.40
2:C:2355:ARG:O	2:C:2358:ILE:HG12	2.22	0.40
2:C:2578:MET:HE3	2:C:2578:MET:HB3	2.01	0.40
2:C:2757:LYS:HD2	2:C:2830:GLU:HG2	2.03	0.40
2:C:3771:HIS:ND1	2:C:3771:HIS:C	2.79	0.40
2:C:4666:VAL:N	2:C:4667:PRO:CD	2.84	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%)	102 (97%)	3 (3%)	0	100	100
1	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	A	4359/5037 (86%)	4263 (98%)	95 (2%)	1 (0%)	100	100
2	B	4359/5037 (86%)	4262 (98%)	96 (2%)	1 (0%)	100	100
2	C	4359/5037 (86%)	4263 (98%)	95 (2%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	4359/5037 (86%)	4262 (98%)	96 (2%)	1 (0%)	100	100
All	All	17856/20580 (87%)	17458 (98%)	394 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3300	ALA
2	B	3300	ALA
2	D	3300	ALA
2	C	3300	ALA

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	A	3814/4253 (90%)	3725 (98%)	89 (2%)	44	73
2	B	3814/4253 (90%)	3725 (98%)	89 (2%)	44	73
2	C	3814/4253 (90%)	3725 (98%)	89 (2%)	44	73
2	D	3814/4253 (90%)	3723 (98%)	91 (2%)	43	72
All	All	15612/17372 (90%)	15254 (98%)	358 (2%)	44	73

All (358) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	25	SER
2	A	73	LEU
2	A	155	LYS
2	A	183	SER

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Mol	Chain	Res	Type
2	A	393	CYS
2	A	578	ILE
2	A	747	CYS
2	A	811	CYS
2	A	882	TRP
2	A	887	ILE
2	A	898	ASP
2	A	908	VAL
2	A	913	LEU
2	A	953	THR
2	A	978	THR
2	A	985	VAL
2	A	1022	VAL
2	A	1037	ASP
2	A	1052	ASN
2	A	1141	ARG
2	A	1479	GLU
2	A	1489	CYS
2	A	1501	VAL
2	A	1783	VAL
2	A	1799	SER
2	A	1937	LEU
2	A	1966	VAL
2	A	2006	ILE
2	A	2010	LEU
2	A	2109	ASP
2	A	2309	SER
2	A	2369[A]	ARG
2	A	2369[B]	ARG
2	A	2374	SER
2	A	2418	LEU
2	A	2481	LYS
2	A	2608	MET
2	A	2659	THR
2	A	2722	LYS
2	A	2746	ILE
2	A	2768	PHE
2	A	2779	GLU
2	A	2791	LEU
2	A	2797	PHE
2	A	2798	SER
2	A	2825	LYS

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Mol	Chain	Res	Type
2	A	2867	LEU
2	A	2872	GLN
2	A	2874	MET
2	A	2880	GLU
2	A	2890	LYS
2	A	2891	LYS
2	A	2897	LYS
2	A	2904	LEU
2	A	2906	VAL
2	A	2916	LYS
2	A	2937	VAL
2	A	2952	GLU
2	A	2973	PHE
2	A	3020	THR
2	A	3110	LEU
2	A	3170	CYS
2	A	3223	SER
2	A	3290	GLU
2	A	3305	THR
2	A	3365	LEU
2	A	3367	LYS
2	A	3498	ARG
2	A	3502	ARG
2	A	3582	ARG
2	A	3686	GLU
2	A	3692	GLU
2	A	3693	LYS
2	A	3734	HIS
2	A	3735	LEU
2	A	3862	ASP
2	A	3865	VAL
2	A	3899	PHE
2	A	4006	ASP
2	A	4018	ASP
2	A	4064	MET
2	A	4198	SER
2	A	4223	ASN
2	A	4546	VAL
2	A	4756	ARG
2	A	4765	LEU
2	A	4771	ILE
2	A	4787	ASN

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Mol	Chain	Res	Type
2	A	4869	GLU
2	B	25	SER
2	B	73	LEU
2	B	155	LYS
2	B	158	SER
2	B	183	SER
2	B	393	CYS
2	B	578	ILE
2	B	747	CYS
2	B	811	CYS
2	B	882	TRP
2	B	887	ILE
2	B	898	ASP
2	B	908	VAL
2	B	913	LEU
2	B	953	THR
2	B	978	THR
2	B	1022	VAL
2	B	1037	ASP
2	B	1052	ASN
2	B	1141	ARG
2	B	1479	GLU
2	B	1489	CYS
2	B	1501	VAL
2	B	1799	SER
2	B	1937	LEU
2	B	1966	VAL
2	B	2006	ILE
2	B	2010	LEU
2	B	2109	ASP
2	B	2309	SER
2	B	2369[A]	ARG
2	B	2369[B]	ARG
2	B	2374	SER
2	B	2418	LEU
2	B	2481	LYS
2	B	2608	MET
2	B	2659	THR
2	B	2722	LYS
2	B	2746	ILE
2	B	2768	PHE
2	B	2779	GLU

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Mol	Chain	Res	Type
2	B	2791	LEU
2	B	2797	PHE
2	B	2798	SER
2	B	2825	LYS
2	B	2867	LEU
2	B	2872	GLN
2	B	2874	MET
2	B	2880	GLU
2	B	2890	LYS
2	B	2891	LYS
2	B	2897	LYS
2	B	2904	LEU
2	B	2906	VAL
2	B	2916	LYS
2	B	2937	VAL
2	B	2952	GLU
2	B	2973	PHE
2	B	3020	THR
2	B	3110	LEU
2	B	3170	CYS
2	B	3223	SER
2	B	3290	GLU
2	B	3305	THR
2	B	3327	LEU
2	B	3365	LEU
2	B	3367	LYS
2	B	3498	ARG
2	B	3502	ARG
2	B	3582	ARG
2	B	3686	GLU
2	B	3692	GLU
2	B	3693	LYS
2	B	3734	HIS
2	B	3735	LEU
2	B	3862	ASP
2	B	3865	VAL
2	B	3899	PHE
2	B	4006	ASP
2	B	4018	ASP
2	B	4064	MET
2	B	4198	SER
2	B	4223	ASN

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Mol	Chain	Res	Type
2	B	4546	VAL
2	B	4756	ARG
2	B	4765	LEU
2	B	4768	LEU
2	B	4787	ASN
2	B	4869	GLU
2	D	25	SER
2	D	73	LEU
2	D	155	LYS
2	D	183	SER
2	D	393	CYS
2	D	578	ILE
2	D	747	CYS
2	D	811	CYS
2	D	845	CYS
2	D	882	TRP
2	D	887	ILE
2	D	898	ASP
2	D	908	VAL
2	D	913	LEU
2	D	953	THR
2	D	978	THR
2	D	985	VAL
2	D	1022	VAL
2	D	1037	ASP
2	D	1052	ASN
2	D	1141	ARG
2	D	1479	GLU
2	D	1489	CYS
2	D	1501	VAL
2	D	1783	VAL
2	D	1799	SER
2	D	1937	LEU
2	D	1966	VAL
2	D	2006	ILE
2	D	2010	LEU
2	D	2109	ASP
2	D	2309	SER
2	D	2369[A]	ARG
2	D	2369[B]	ARG
2	D	2374	SER
2	D	2418	LEU

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Mol	Chain	Res	Type
2	D	2481	LYS
2	D	2608	MET
2	D	2659	THR
2	D	2722	LYS
2	D	2746	ILE
2	D	2768	PHE
2	D	2779	GLU
2	D	2791	LEU
2	D	2797	PHE
2	D	2798	SER
2	D	2825	LYS
2	D	2867	LEU
2	D	2872	GLN
2	D	2874	MET
2	D	2880	GLU
2	D	2890	LYS
2	D	2891	LYS
2	D	2897	LYS
2	D	2904	LEU
2	D	2906	VAL
2	D	2916	LYS
2	D	2937	VAL
2	D	2952	GLU
2	D	2973	PHE
2	D	3020	THR
2	D	3110	LEU
2	D	3170	CYS
2	D	3223	SER
2	D	3290	GLU
2	D	3305	THR
2	D	3365	LEU
2	D	3367	LYS
2	D	3498	ARG
2	D	3502	ARG
2	D	3582	ARG
2	D	3686	GLU
2	D	3692	GLU
2	D	3693	LYS
2	D	3734	HIS
2	D	3735	LEU
2	D	3862	ASP
2	D	3865	VAL

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Mol	Chain	Res	Type
2	D	3899	PHE
2	D	4006	ASP
2	D	4018	ASP
2	D	4064	MET
2	D	4082	THR
2	D	4198	SER
2	D	4223	ASN
2	D	4546	VAL
2	D	4756	ARG
2	D	4765	LEU
2	D	4771	ILE
2	D	4787	ASN
2	D	4869	GLU
2	C	25	SER
2	C	73	LEU
2	C	155	LYS
2	C	158	SER
2	C	183	SER
2	C	393	CYS
2	C	578	ILE
2	C	747	CYS
2	C	811	CYS
2	C	882	TRP
2	C	887	ILE
2	C	898	ASP
2	C	908	VAL
2	C	913	LEU
2	C	953	THR
2	C	978	THR
2	C	985	VAL
2	C	1022	VAL
2	C	1037	ASP
2	C	1052	ASN
2	C	1141	ARG
2	C	1479	GLU
2	C	1489	CYS
2	C	1501	VAL
2	C	1799	SER
2	C	1937	LEU
2	C	1966	VAL
2	C	2006	ILE
2	C	2010	LEU

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Mol	Chain	Res	Type
2	C	2109	ASP
2	C	2309	SER
2	C	2369[A]	ARG
2	C	2369[B]	ARG
2	C	2374	SER
2	C	2418	LEU
2	C	2481	LYS
2	C	2608	MET
2	C	2659	THR
2	C	2722	LYS
2	C	2746	ILE
2	C	2768	PHE
2	C	2779	GLU
2	C	2791	LEU
2	C	2797	PHE
2	C	2798	SER
2	C	2825	LYS
2	C	2867	LEU
2	C	2872	GLN
2	C	2874	MET
2	C	2880	GLU
2	C	2890	LYS
2	C	2891	LYS
2	C	2897	LYS
2	C	2904	LEU
2	C	2906	VAL
2	C	2916	LYS
2	C	2937	VAL
2	C	2952	GLU
2	C	2973	PHE
2	C	3020	THR
2	C	3110	LEU
2	C	3170	CYS
2	C	3223	SER
2	C	3290	GLU
2	C	3305	THR
2	C	3365	LEU
2	C	3367	LYS
2	C	3498	ARG
2	C	3502	ARG
2	C	3582	ARG
2	C	3686	GLU

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Mol	Chain	Res	Type
2	C	3692	GLU
2	C	3693	LYS
2	C	3734	HIS
2	C	3735	LEU
2	C	3862	ASP
2	C	3865	VAL
2	C	3899	PHE
2	C	4006	ASP
2	C	4018	ASP
2	C	4198	SER
2	C	4223	ASN
2	C	4546	VAL
2	C	4756	ARG
2	C	4765	LEU
2	C	4768	LEU
2	C	4771	ILE
2	C	4787	ASN
2	C	4869	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	95	HIS
2	A	113	HIS
2	A	224	HIS
2	A	297	GLN
2	A	479	GLN
2	A	579	GLN
2	A	581	ASN
2	A	923	GLN
2	A	1003	GLN
2	A	1299	GLN
2	A	1300	HIS
2	A	1484	HIS
2	A	1545	ASN
2	A	1559	GLN
2	A	1665	HIS
2	A	1702	HIS
2	A	1719	HIS
2	A	1928	GLN
2	A	1938	GLN
2	A	2858	GLN

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Mol	Chain	Res	Type
2	A	2881	ASN
2	A	2976	HIS
2	A	3162	GLN
2	A	3313	ASN
2	A	3556	ASN
2	A	3560	GLN
2	A	3605	HIS
2	A	3766	GLN
2	A	3869	GLN
2	A	3927	GLN
2	A	3950	ASN
2	A	4700	GLN
2	B	57	ASN
2	B	224	HIS
2	B	297	GLN
2	B	412	ASN
2	B	479	GLN
2	B	579	GLN
2	B	581	ASN
2	B	923	GLN
2	B	1003	GLN
2	B	1299	GLN
2	B	1300	HIS
2	B	1545	ASN
2	B	1559	GLN
2	B	1665	HIS
2	B	1702	HIS
2	B	1928	GLN
2	B	1938	GLN
2	B	2324	ASN
2	B	2858	GLN
2	B	2881	ASN
2	B	2962	GLN
2	B	2976	HIS
2	B	3162	GLN
2	B	3313	ASN
2	B	3560	GLN
2	B	3605	HIS
2	B	3766	GLN
2	B	3869	GLN
2	B	3927	GLN
2	B	3950	ASN

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Mol	Chain	Res	Type
2	D	224	HIS
2	D	479	GLN
2	D	579	GLN
2	D	581	ASN
2	D	923	GLN
2	D	1003	GLN
2	D	1299	GLN
2	D	1300	HIS
2	D	1484	HIS
2	D	1545	ASN
2	D	1559	GLN
2	D	1665	HIS
2	D	1702	HIS
2	D	1928	GLN
2	D	1938	GLN
2	D	2858	GLN
2	D	2881	ASN
2	D	2962	GLN
2	D	2976	HIS
2	D	3162	GLN
2	D	3313	ASN
2	D	3556	ASN
2	D	3560	GLN
2	D	3605	HIS
2	D	3766	GLN
2	D	3869	GLN
2	D	3927	GLN
2	D	3950	ASN
2	D	4700	GLN
2	C	57	ASN
2	C	224	HIS
2	C	297	GLN
2	C	479	GLN
2	C	579	GLN
2	C	581	ASN
2	C	923	GLN
2	C	1003	GLN
2	C	1299	GLN
2	C	1300	HIS
2	C	1484	HIS
2	C	1545	ASN
2	C	1665	HIS

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Mol	Chain	Res	Type
2	C	1702	HIS
2	C	1928	GLN
2	C	1938	GLN
2	C	2324	ASN
2	C	2856	ASN
2	C	2858	GLN
2	C	2881	ASN
2	C	2962	GLN
2	C	2976	HIS
2	C	3162	GLN
2	C	3313	ASN
2	C	3556	ASN
2	C	3560	GLN
2	C	3605	HIS
2	C	3766	GLN
2	C	3927	GLN
2	C	3950	ASN
2	C	4700	GLN
1	F	95	HIS
1	G	95	HIS
1	H	95	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	D	5301	-	32,33,33	0.31	0	48,52,52	0.70	0
3	ATP	C	5301	-	32,33,33	0.31	0	48,52,52	0.70	0
6	CFF	B	5304	-	15,15,15	0.51	0	23,23,23	0.55	0
7	PCW	D	5305	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
7	PCW	A	5306	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
3	ATP	A	5301	-	32,33,33	0.31	0	48,52,52	0.70	0
6	CFF	C	5304	-	15,15,15	0.52	0	23,23,23	0.53	0
7	PCW	A	5307	-	53,53,53	0.50	0	59,61,61	0.48	0
7	PCW	C	5305	-	53,53,53	0.50	0	59,61,61	0.49	0
3	ATP	B	5301	-	32,33,33	0.31	0	48,52,52	0.70	0
7	PCW	A	5305	-	53,53,53	0.50	0	59,61,61	0.48	0
7	PCW	C	5306	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
7	PCW	B	5306	-	53,53,53	0.50	0	59,61,61	0.49	1 (1%)
6	CFF	D	5304	-	15,15,15	0.51	0	23,23,23	0.54	0
6	CFF	A	5304	-	15,15,15	0.51	0	23,23,23	0.54	0
7	PCW	B	5305	-	53,53,53	0.50	0	59,61,61	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	5301	-	-	5/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	5/22/38/38	0/3/3/3
6	CFF	B	5304	-	-	-	0/2/2/2
7	PCW	D	5305	-	-	32/57/57/57	-
7	PCW	A	5306	-	-	32/57/57/57	-
3	ATP	A	5301	-	-	5/22/38/38	0/3/3/3
7	PCW	A	5307	-	-	32/57/57/57	-
7	PCW	C	5305	-	-	32/57/57/57	-
6	CFF	C	5304	-	-	-	0/2/2/2
3	ATP	B	5301	-	-	5/22/38/38	0/3/3/3
7	PCW	A	5305	-	-	32/57/57/57	-
7	PCW	C	5306	-	-	32/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	B	5306	-	-	32/57/57/57	-
6	CFF	D	5304	-	-	-	0/2/2/2
6	CFF	A	5304	-	-	-	0/2/2/2
7	PCW	B	5305	-	-	32/57/57/57	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	5306	PCW	C3-C2-C1	2.03	116.53	111.78
7	C	5306	PCW	C3-C2-C1	2.03	116.51	111.78
7	A	5306	PCW	C3-C2-C1	2.02	116.49	111.78
7	D	5305	PCW	C3-C2-C1	2.01	116.48	111.78

There are no chirality outliers.

All (276) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5305	PCW	O4P-C4-C5-N
7	A	5305	PCW	C1-O3P-P-O2P
7	A	5305	PCW	C4-O4P-P-O2P
7	A	5305	PCW	C4-O4P-P-O3P
7	A	5306	PCW	C32-C31-O2-C2
7	A	5306	PCW	C4-O4P-P-O1P
7	A	5306	PCW	C4-O4P-P-O2P
7	A	5306	PCW	C4-O4P-P-O3P
7	A	5307	PCW	O4P-C4-C5-N
7	A	5307	PCW	C1-O3P-P-O2P
7	A	5307	PCW	C4-O4P-P-O2P
7	A	5307	PCW	C4-O4P-P-O3P
7	B	5305	PCW	O4P-C4-C5-N
7	B	5305	PCW	C1-O3P-P-O2P
7	B	5305	PCW	C4-O4P-P-O2P
7	B	5305	PCW	C4-O4P-P-O3P
7	B	5306	PCW	C32-C31-O2-C2
7	B	5306	PCW	C4-O4P-P-O1P
7	B	5306	PCW	C4-O4P-P-O2P
7	B	5306	PCW	C4-O4P-P-O3P
7	D	5305	PCW	C32-C31-O2-C2
7	D	5305	PCW	C4-O4P-P-O1P
7	D	5305	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
7	D	5305	PCW	C4-O4P-P-O3P
7	C	5305	PCW	O4P-C4-C5-N
7	C	5305	PCW	C1-O3P-P-O2P
7	C	5305	PCW	C4-O4P-P-O2P
7	C	5305	PCW	C4-O4P-P-O3P
7	C	5306	PCW	C32-C31-O2-C2
7	C	5306	PCW	C4-O4P-P-O1P
7	C	5306	PCW	C4-O4P-P-O2P
7	C	5306	PCW	C4-O4P-P-O3P
7	A	5306	PCW	O31-C31-O2-C2
7	B	5306	PCW	O31-C31-O2-C2
7	D	5305	PCW	O31-C31-O2-C2
7	C	5306	PCW	O31-C31-O2-C2
7	A	5305	PCW	C11-C12-C13-C14
7	A	5306	PCW	C11-C12-C13-C14
7	A	5307	PCW	C11-C12-C13-C14
7	B	5305	PCW	C11-C12-C13-C14
7	B	5306	PCW	C11-C12-C13-C14
7	D	5305	PCW	C11-C12-C13-C14
7	C	5305	PCW	C11-C12-C13-C14
7	C	5306	PCW	C11-C12-C13-C14
7	A	5306	PCW	C12-C11-O3-C3
7	B	5306	PCW	C12-C11-O3-C3
7	D	5305	PCW	C12-C11-O3-C3
7	C	5306	PCW	C12-C11-O3-C3
7	A	5305	PCW	C24-C25-C26-C27
7	A	5307	PCW	C24-C25-C26-C27
7	B	5305	PCW	C24-C25-C26-C27
7	C	5305	PCW	C24-C25-C26-C27
7	B	5305	PCW	C31-C32-C33-C34
7	A	5305	PCW	C31-C32-C33-C34
7	A	5307	PCW	C31-C32-C33-C34
7	C	5305	PCW	C31-C32-C33-C34
7	A	5305	PCW	C40-C41-C42-C43
7	A	5307	PCW	C40-C41-C42-C43
7	B	5305	PCW	C40-C41-C42-C43
7	C	5305	PCW	C40-C41-C42-C43
7	A	5306	PCW	O11-C11-O3-C3
7	D	5305	PCW	O11-C11-O3-C3
7	C	5306	PCW	O11-C11-O3-C3
7	B	5306	PCW	O11-C11-O3-C3
7	A	5305	PCW	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
7	A	5306	PCW	C13-C14-C15-C16
7	A	5307	PCW	C13-C14-C15-C16
7	B	5305	PCW	C13-C14-C15-C16
7	B	5306	PCW	C13-C14-C15-C16
7	D	5305	PCW	C13-C14-C15-C16
7	C	5305	PCW	C13-C14-C15-C16
7	C	5306	PCW	C13-C14-C15-C16
7	A	5305	PCW	C21-C22-C23-C24
7	A	5307	PCW	C21-C22-C23-C24
7	B	5305	PCW	C21-C22-C23-C24
7	C	5305	PCW	C21-C22-C23-C24
7	A	5306	PCW	C44-C45-C46-C47
7	A	5307	PCW	C34-C35-C36-C37
7	B	5305	PCW	C34-C35-C36-C37
7	B	5306	PCW	C44-C45-C46-C47
7	D	5305	PCW	C44-C45-C46-C47
7	C	5305	PCW	C34-C35-C36-C37
7	C	5306	PCW	C44-C45-C46-C47
7	A	5305	PCW	C34-C35-C36-C37
7	A	5306	PCW	C42-C43-C44-C45
7	B	5306	PCW	C42-C43-C44-C45
7	D	5305	PCW	C42-C43-C44-C45
7	C	5306	PCW	C42-C43-C44-C45
7	A	5305	PCW	C32-C31-O2-C2
7	A	5307	PCW	C32-C31-O2-C2
7	B	5305	PCW	C32-C31-O2-C2
7	C	5305	PCW	C32-C31-O2-C2
7	A	5305	PCW	O31-C31-O2-C2
7	A	5307	PCW	O31-C31-O2-C2
7	B	5305	PCW	O31-C31-O2-C2
7	C	5305	PCW	O31-C31-O2-C2
7	A	5306	PCW	C24-C25-C26-C27
7	B	5306	PCW	C24-C25-C26-C27
7	D	5305	PCW	C24-C25-C26-C27
7	C	5306	PCW	C24-C25-C26-C27
7	C	5306	PCW	C32-C33-C34-C35
7	A	5306	PCW	C32-C33-C34-C35
7	B	5306	PCW	C32-C33-C34-C35
7	D	5305	PCW	C32-C33-C34-C35
7	A	5305	PCW	C16-C17-C18-C19
7	A	5306	PCW	C16-C17-C18-C19
7	A	5307	PCW	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	B	5305	PCW	C16-C17-C18-C19
7	B	5306	PCW	C16-C17-C18-C19
7	D	5305	PCW	C16-C17-C18-C19
7	C	5305	PCW	C16-C17-C18-C19
7	C	5306	PCW	C16-C17-C18-C19
7	A	5306	PCW	C35-C36-C37-C38
7	B	5306	PCW	C35-C36-C37-C38
7	D	5305	PCW	C35-C36-C37-C38
7	C	5306	PCW	C35-C36-C37-C38
7	A	5305	PCW	C19-C20-C21-C22
7	A	5307	PCW	C19-C20-C21-C22
7	B	5305	PCW	C19-C20-C21-C22
7	C	5305	PCW	C19-C20-C21-C22
7	B	5305	PCW	C15-C16-C17-C18
7	A	5305	PCW	C15-C16-C17-C18
7	A	5307	PCW	C15-C16-C17-C18
7	C	5305	PCW	C15-C16-C17-C18
7	D	5305	PCW	C21-C22-C23-C24
7	A	5306	PCW	C21-C22-C23-C24
7	C	5306	PCW	C21-C22-C23-C24
7	B	5306	PCW	C21-C22-C23-C24
7	A	5305	PCW	C43-C44-C45-C46
7	A	5307	PCW	C43-C44-C45-C46
7	B	5305	PCW	C43-C44-C45-C46
7	C	5305	PCW	C43-C44-C45-C46
7	A	5305	PCW	C14-C15-C16-C17
7	B	5305	PCW	C14-C15-C16-C17
7	C	5305	PCW	C14-C15-C16-C17
7	A	5307	PCW	C14-C15-C16-C17
7	A	5305	PCW	O3P-C1-C2-O2
7	A	5307	PCW	O3P-C1-C2-O2
7	B	5305	PCW	O3P-C1-C2-O2
7	C	5305	PCW	O3P-C1-C2-O2
7	A	5306	PCW	C45-C46-C47-C48
7	B	5306	PCW	C45-C46-C47-C48
7	D	5305	PCW	C45-C46-C47-C48
7	C	5306	PCW	C45-C46-C47-C48
7	A	5305	PCW	C12-C11-O3-C3
7	A	5307	PCW	C12-C11-O3-C3
7	B	5305	PCW	C12-C11-O3-C3
7	C	5305	PCW	C12-C11-O3-C3
7	B	5306	PCW	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
7	D	5305	PCW	C23-C24-C25-C26
7	C	5306	PCW	C23-C24-C25-C26
7	A	5306	PCW	C23-C24-C25-C26
7	A	5305	PCW	C25-C26-C27-C28
7	A	5307	PCW	C25-C26-C27-C28
7	B	5305	PCW	C25-C26-C27-C28
7	C	5305	PCW	C25-C26-C27-C28
3	A	5301	ATP	PB-O3B-PG-O1G
3	B	5301	ATP	PB-O3B-PG-O1G
3	D	5301	ATP	PB-O3B-PG-O1G
3	C	5301	ATP	PB-O3B-PG-O1G
7	A	5307	PCW	O11-C11-O3-C3
7	C	5305	PCW	O11-C11-O3-C3
7	A	5306	PCW	O3P-C1-C2-O2
7	B	5306	PCW	O3P-C1-C2-O2
7	D	5305	PCW	O3P-C1-C2-O2
7	C	5306	PCW	O3P-C1-C2-O2
7	A	5305	PCW	O11-C11-O3-C3
7	B	5305	PCW	O11-C11-O3-C3
7	A	5305	PCW	C20-C21-C22-C23
7	A	5307	PCW	C20-C21-C22-C23
7	B	5305	PCW	C20-C21-C22-C23
7	C	5305	PCW	C20-C21-C22-C23
7	A	5305	PCW	C33-C34-C35-C36
7	A	5307	PCW	C33-C34-C35-C36
7	C	5305	PCW	C33-C34-C35-C36
7	B	5305	PCW	C33-C34-C35-C36
7	A	5306	PCW	O4P-C4-C5-N
7	B	5306	PCW	O4P-C4-C5-N
7	D	5305	PCW	O4P-C4-C5-N
7	C	5306	PCW	O4P-C4-C5-N
7	A	5306	PCW	C40-C41-C42-C43
7	B	5306	PCW	C40-C41-C42-C43
7	D	5305	PCW	C40-C41-C42-C43
7	C	5306	PCW	C40-C41-C42-C43
7	A	5305	PCW	C44-C45-C46-C47
7	C	5305	PCW	C44-C45-C46-C47
7	A	5307	PCW	C44-C45-C46-C47
7	B	5305	PCW	C44-C45-C46-C47
7	A	5305	PCW	C1-O3P-P-O1P
7	A	5305	PCW	C1-O3P-P-O4P
7	A	5306	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
7	A	5306	PCW	C1-O3P-P-O2P
7	A	5306	PCW	C1-O3P-P-O4P
7	A	5307	PCW	C1-O3P-P-O1P
7	A	5307	PCW	C1-O3P-P-O4P
7	B	5305	PCW	C1-O3P-P-O1P
7	B	5305	PCW	C1-O3P-P-O4P
7	B	5306	PCW	C1-O3P-P-O1P
7	B	5306	PCW	C1-O3P-P-O2P
7	B	5306	PCW	C1-O3P-P-O4P
7	D	5305	PCW	C1-O3P-P-O1P
7	D	5305	PCW	C1-O3P-P-O2P
7	D	5305	PCW	C1-O3P-P-O4P
7	C	5305	PCW	C1-O3P-P-O1P
7	C	5305	PCW	C1-O3P-P-O4P
7	C	5306	PCW	C1-O3P-P-O1P
7	C	5306	PCW	C1-O3P-P-O2P
7	C	5306	PCW	C1-O3P-P-O4P
7	A	5305	PCW	O3P-C1-C2-C3
7	A	5307	PCW	O3P-C1-C2-C3
7	B	5305	PCW	O3P-C1-C2-C3
7	C	5305	PCW	O3P-C1-C2-C3
3	A	5301	ATP	O4'-C1'-N9-C4
3	B	5301	ATP	O4'-C1'-N9-C4
3	D	5301	ATP	O4'-C1'-N9-C4
3	C	5301	ATP	O4'-C1'-N9-C4
7	D	5305	PCW	C31-C32-C33-C34
7	A	5306	PCW	C31-C32-C33-C34
7	B	5306	PCW	C31-C32-C33-C34
7	C	5306	PCW	C31-C32-C33-C34
7	A	5306	PCW	C39-C40-C41-C42
7	B	5306	PCW	C39-C40-C41-C42
7	D	5305	PCW	C39-C40-C41-C42
7	C	5306	PCW	C39-C40-C41-C42
7	A	5306	PCW	C25-C26-C27-C28
7	B	5306	PCW	C25-C26-C27-C28
7	D	5305	PCW	C25-C26-C27-C28
7	C	5306	PCW	C25-C26-C27-C28
3	A	5301	ATP	O4'-C1'-N9-C8
3	B	5301	ATP	O4'-C1'-N9-C8
3	D	5301	ATP	O4'-C1'-N9-C8
3	C	5301	ATP	O4'-C1'-N9-C8
7	B	5305	PCW	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
7	A	5307	PCW	C23-C24-C25-C26
7	C	5305	PCW	C23-C24-C25-C26
7	A	5305	PCW	C23-C24-C25-C26
7	A	5305	PCW	O2-C2-C3-O3
7	A	5307	PCW	O2-C2-C3-O3
7	B	5305	PCW	O2-C2-C3-O3
7	C	5305	PCW	O2-C2-C3-O3
7	A	5306	PCW	O3P-C1-C2-C3
7	B	5306	PCW	O3P-C1-C2-C3
7	D	5305	PCW	O3P-C1-C2-C3
7	C	5306	PCW	O3P-C1-C2-C3
3	A	5301	ATP	PB-O3B-PG-O2G
3	A	5301	ATP	PB-O3B-PG-O3G
3	B	5301	ATP	PB-O3B-PG-O2G
3	B	5301	ATP	PB-O3B-PG-O3G
3	D	5301	ATP	PB-O3B-PG-O2G
3	D	5301	ATP	PB-O3B-PG-O3G
3	C	5301	ATP	PB-O3B-PG-O2G
3	C	5301	ATP	PB-O3B-PG-O3G
7	A	5305	PCW	C37-C38-C39-C40
7	A	5307	PCW	C37-C38-C39-C40
7	B	5305	PCW	C37-C38-C39-C40
7	C	5305	PCW	C37-C38-C39-C40
7	A	5306	PCW	C20-C21-C22-C23
7	D	5305	PCW	C20-C21-C22-C23
7	C	5306	PCW	C20-C21-C22-C23
7	B	5306	PCW	C20-C21-C22-C23
7	A	5305	PCW	C1-C2-C3-O3
7	A	5307	PCW	C1-C2-C3-O3
7	B	5305	PCW	C1-C2-C3-O3
7	C	5305	PCW	C1-C2-C3-O3
7	A	5306	PCW	O2-C31-C32-C33
7	D	5305	PCW	O2-C31-C32-C33
7	B	5306	PCW	O2-C31-C32-C33
7	C	5306	PCW	O2-C31-C32-C33
7	D	5305	PCW	C2-C3-O3-C11
7	C	5306	PCW	C2-C3-O3-C11
7	A	5306	PCW	C2-C3-O3-C11
7	B	5306	PCW	C2-C3-O3-C11
7	A	5306	PCW	O31-C31-C32-C33
7	B	5306	PCW	O31-C31-C32-C33
7	D	5305	PCW	O31-C31-C32-C33

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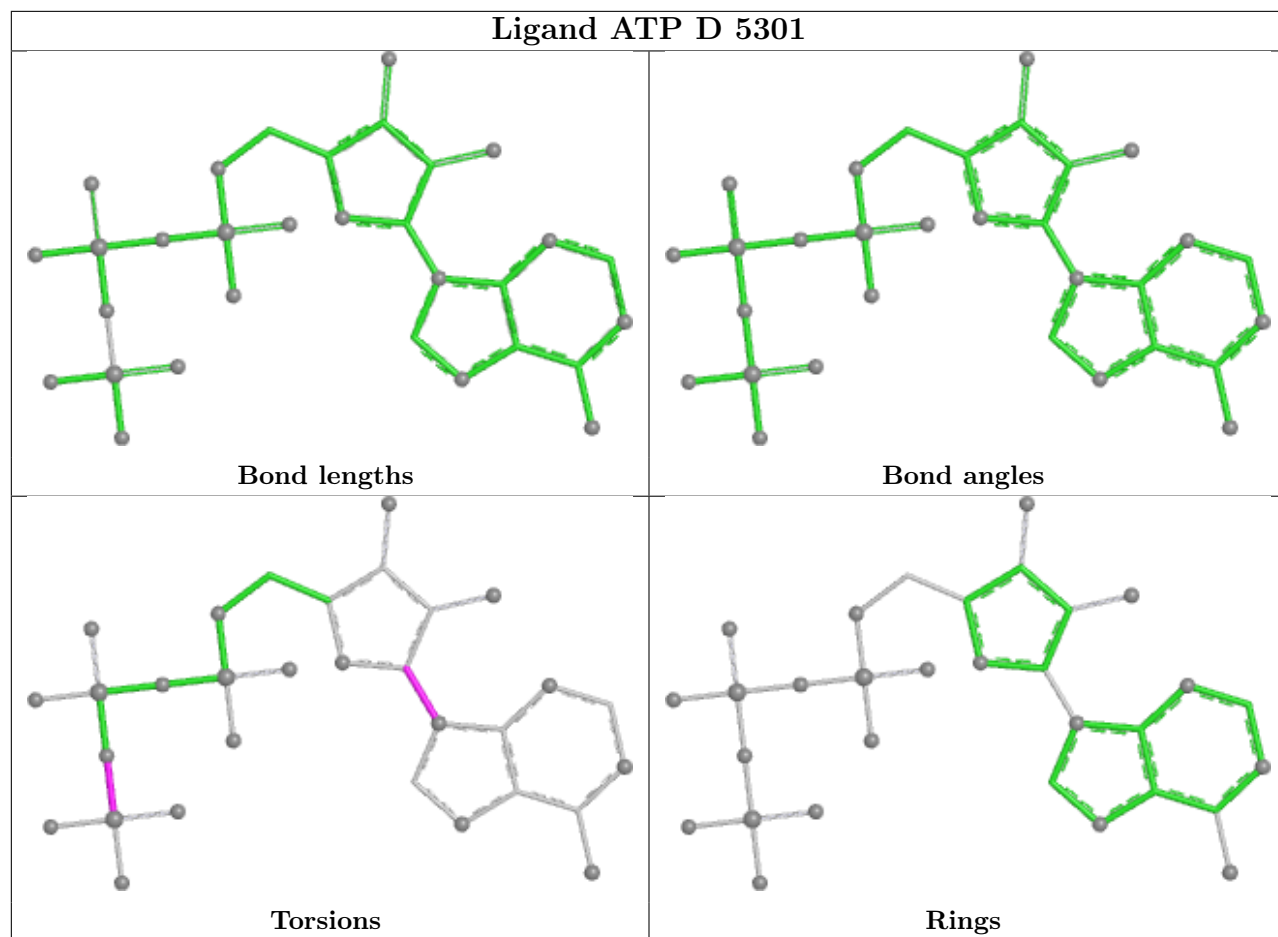
Mol	Chain	Res	Type	Atoms
7	C	5306	PCW	O31-C31-C32-C33

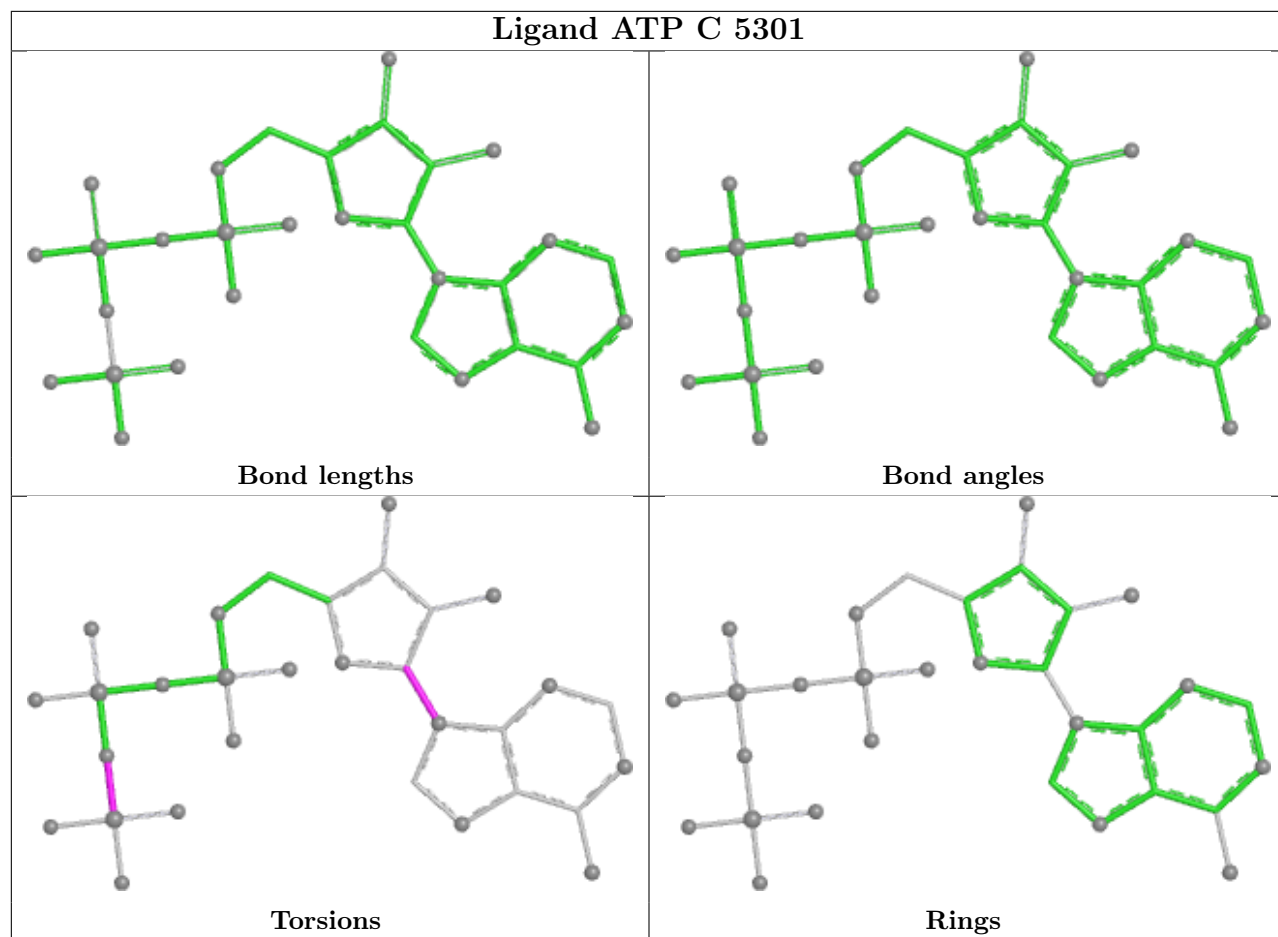
There are no ring outliers.

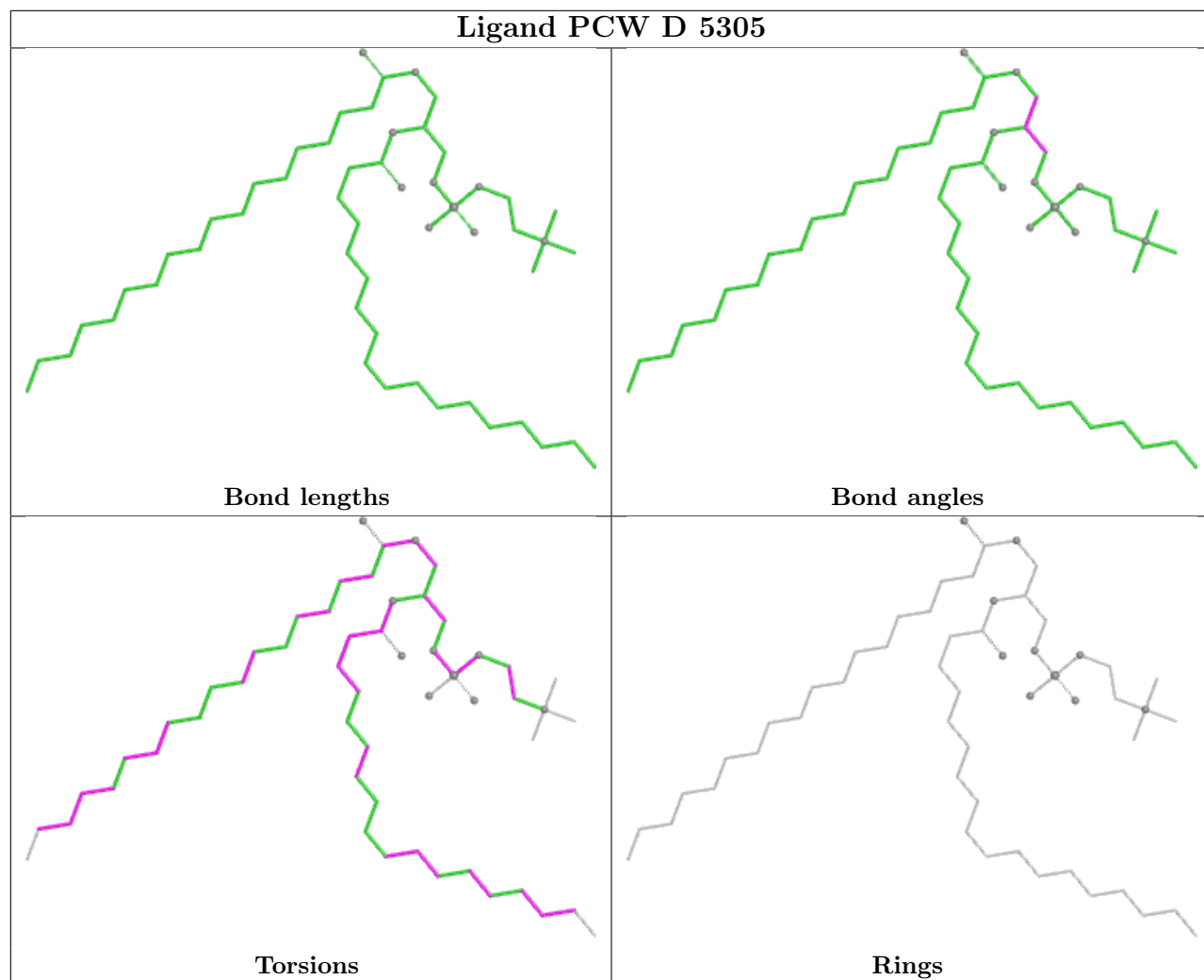
8 monomers are involved in 13 short contacts:

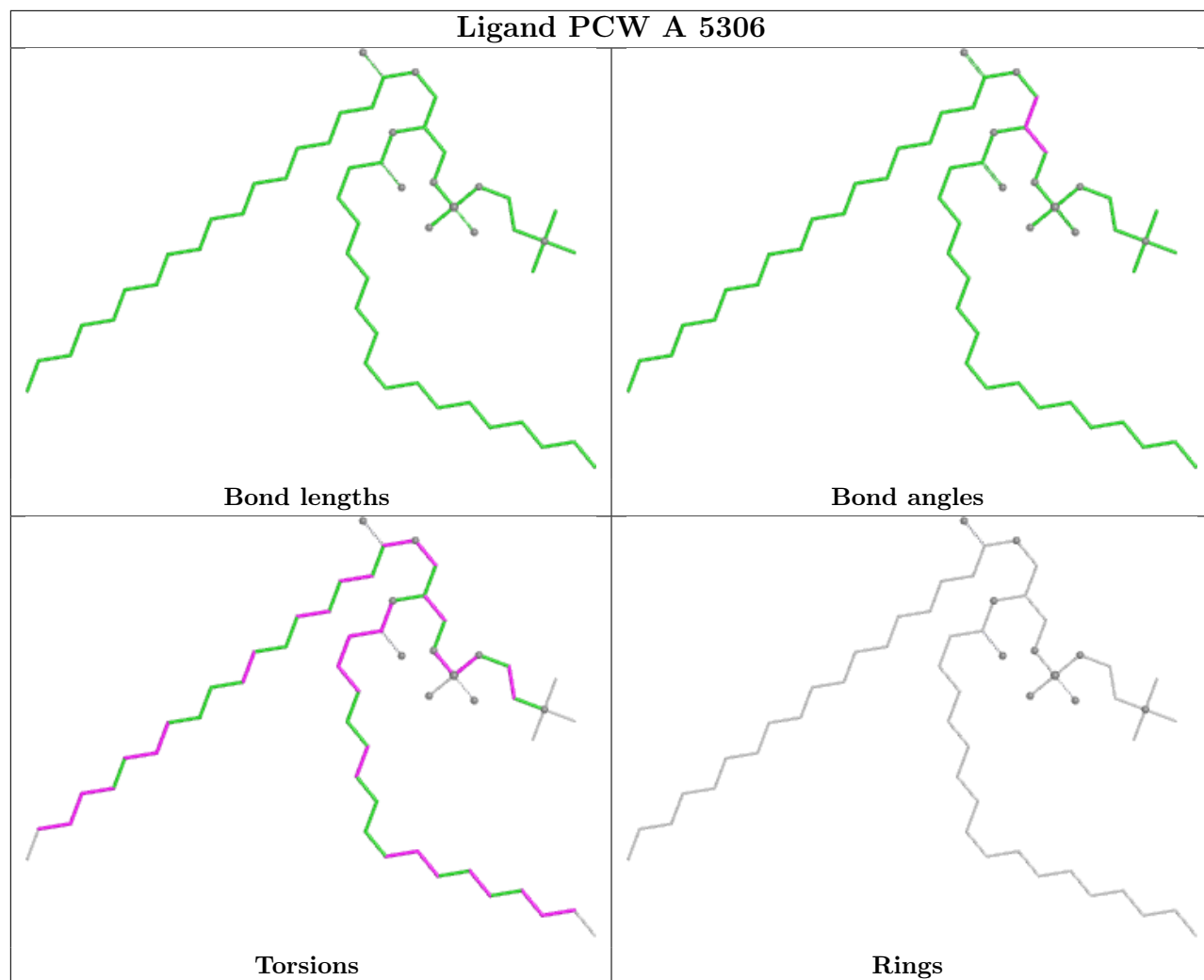
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	5305	PCW	1	0
7	A	5306	PCW	1	0
7	A	5307	PCW	3	0
7	C	5305	PCW	4	0
7	A	5305	PCW	3	0
7	C	5306	PCW	1	0
7	B	5306	PCW	1	0
7	B	5305	PCW	3	0

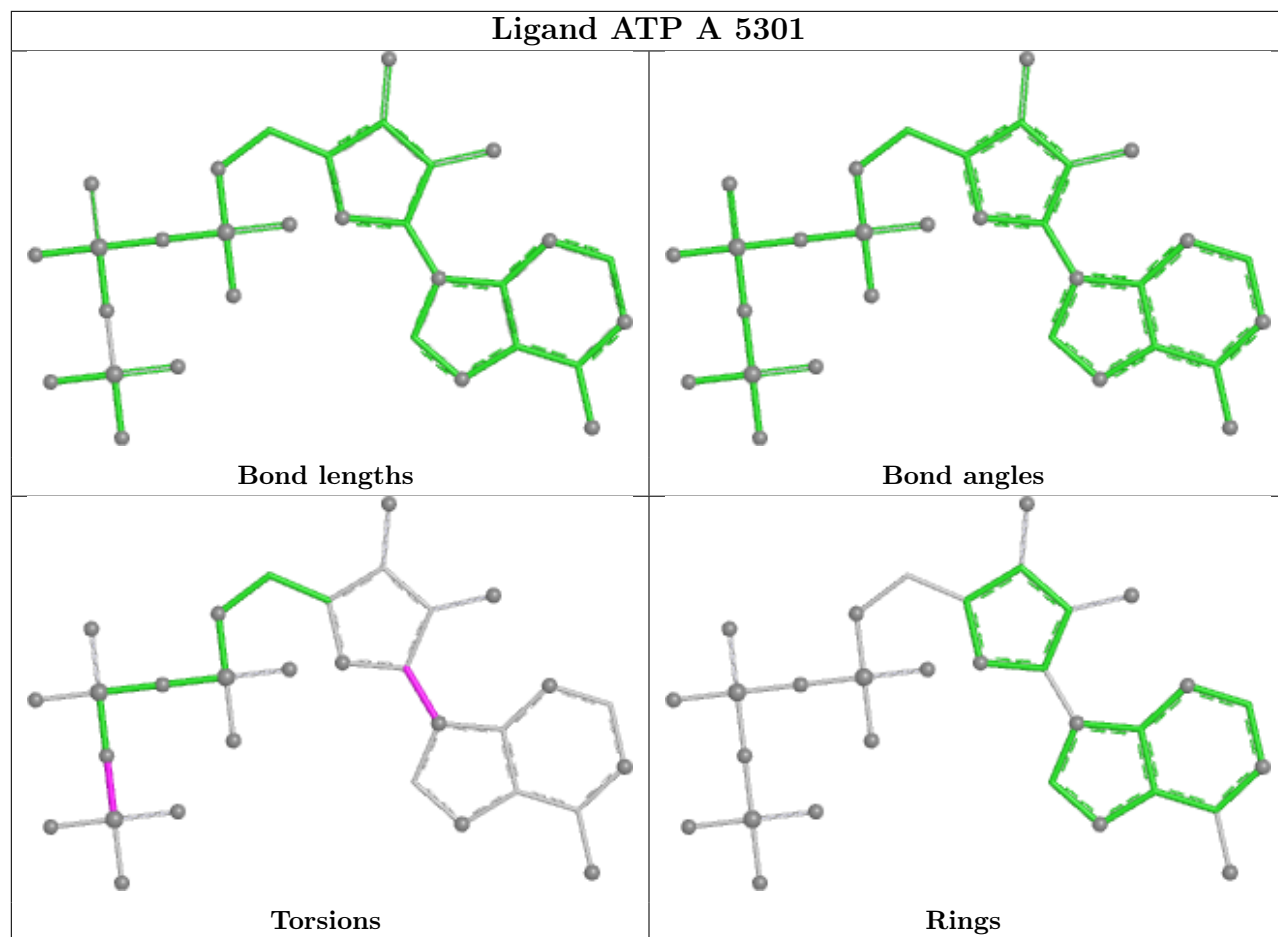
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

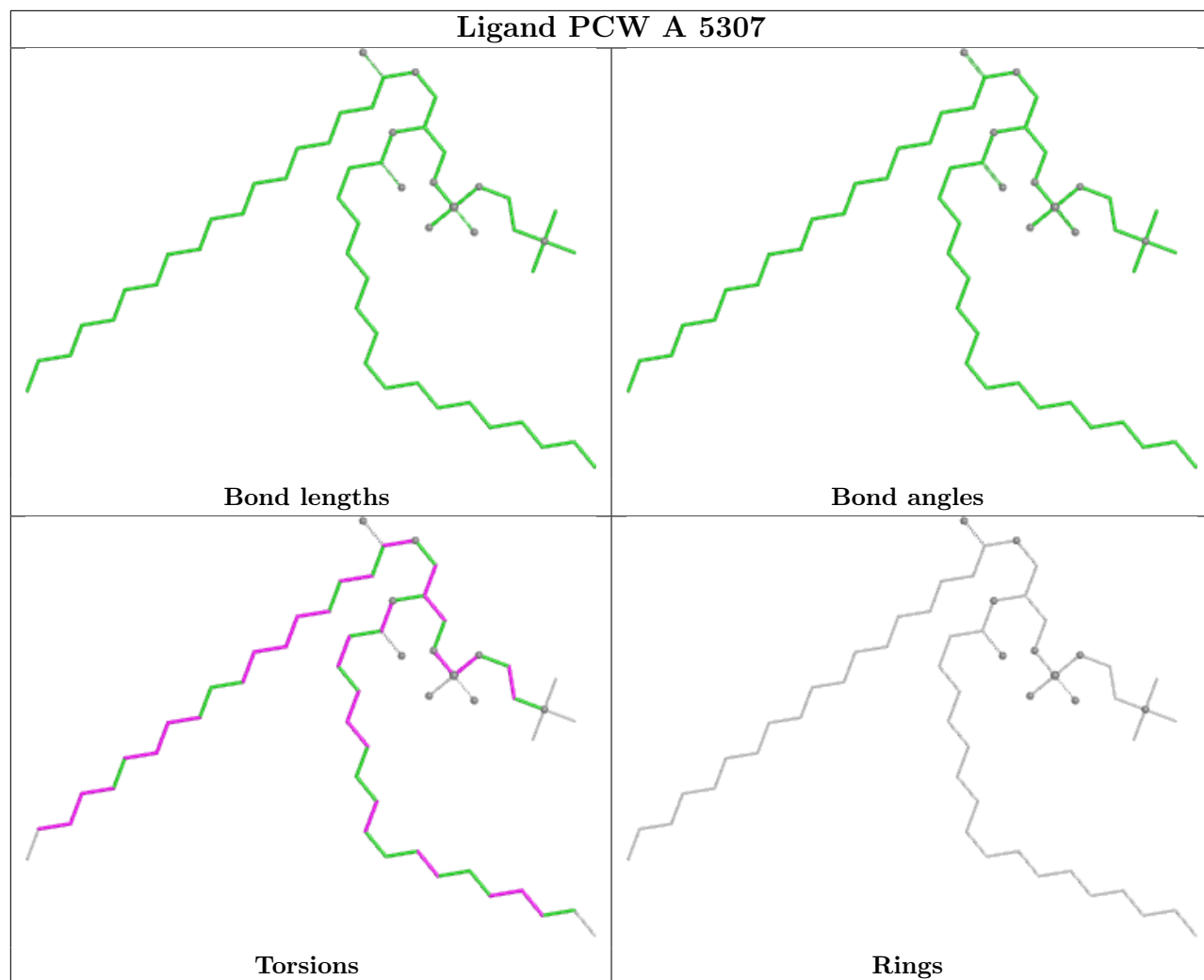


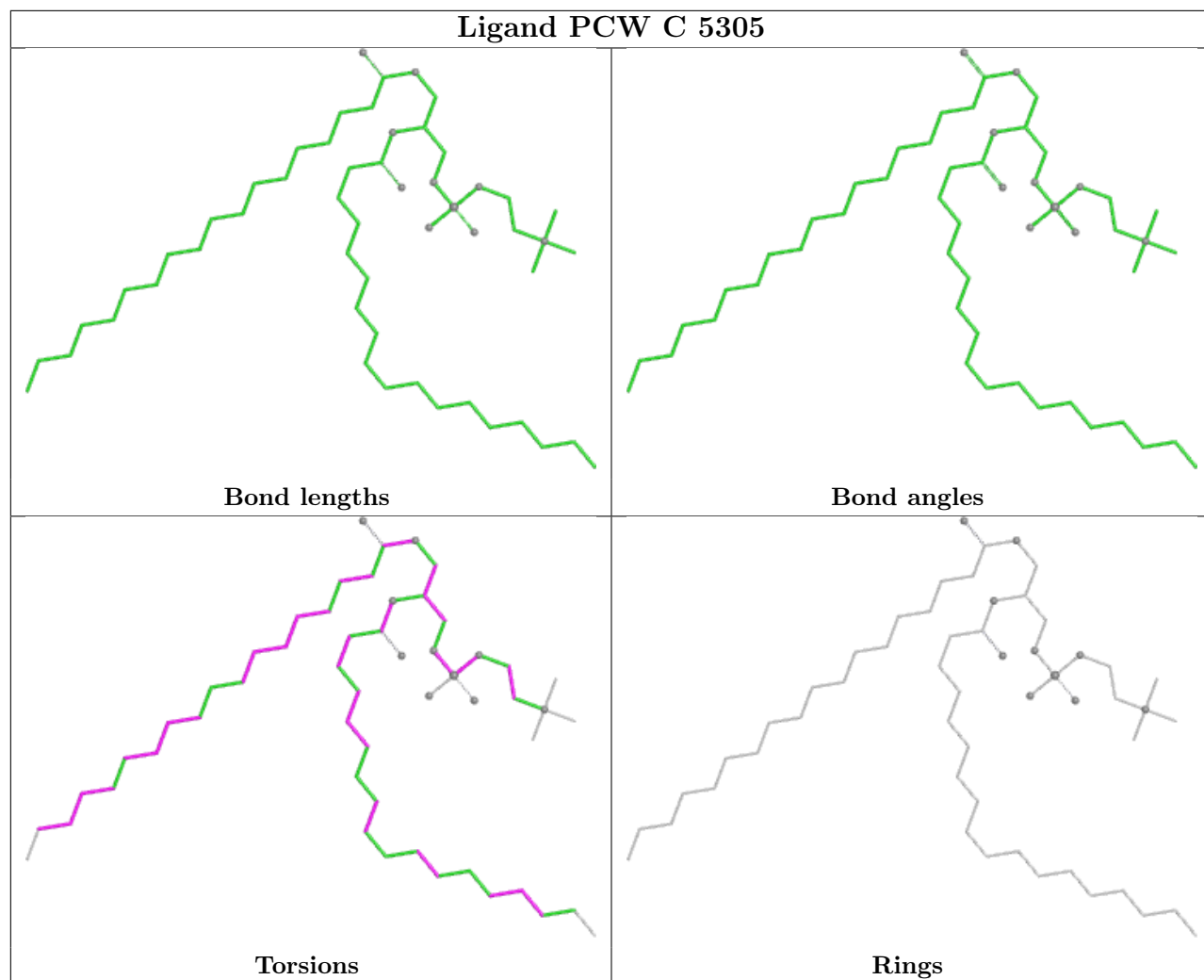


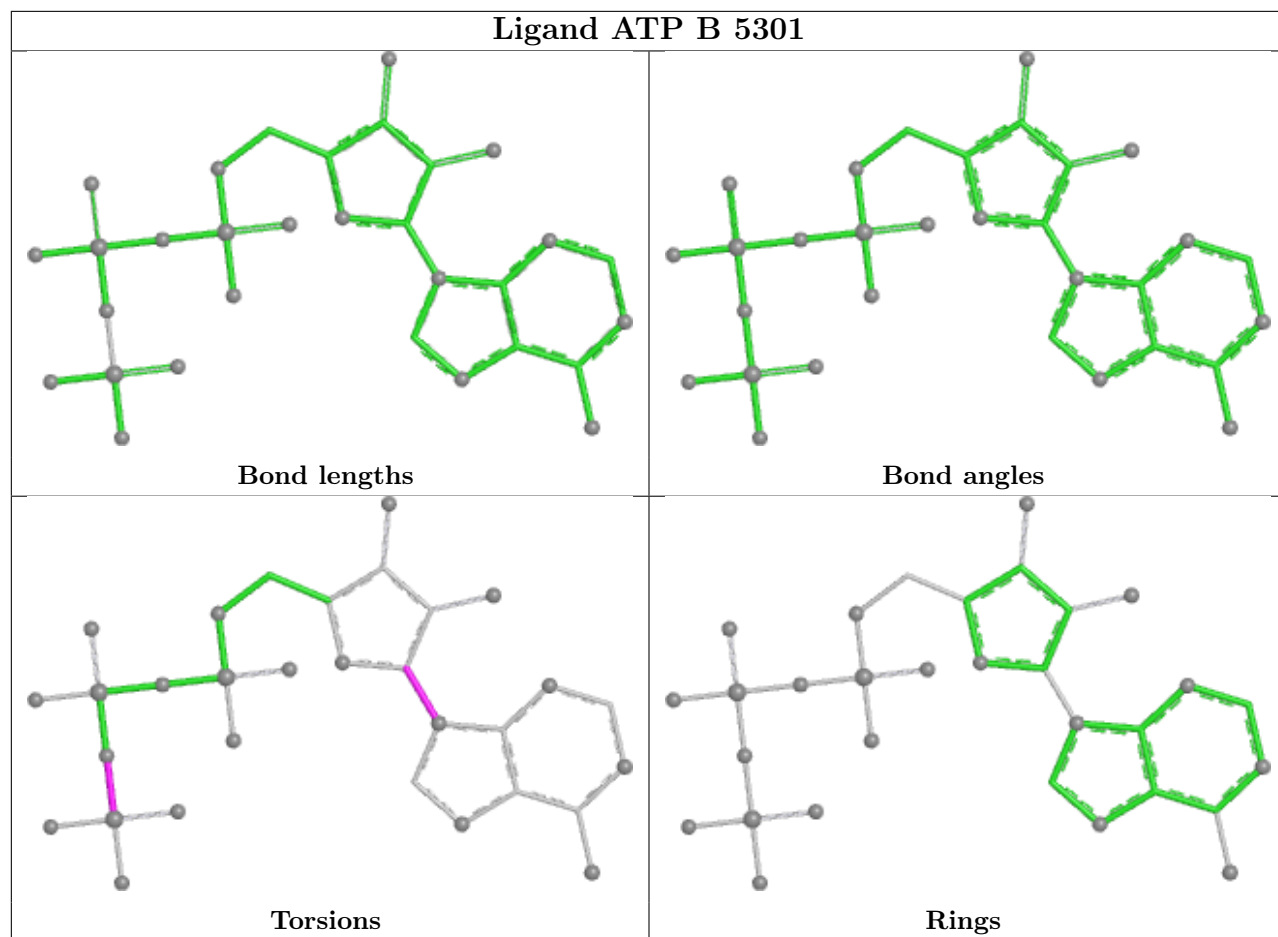


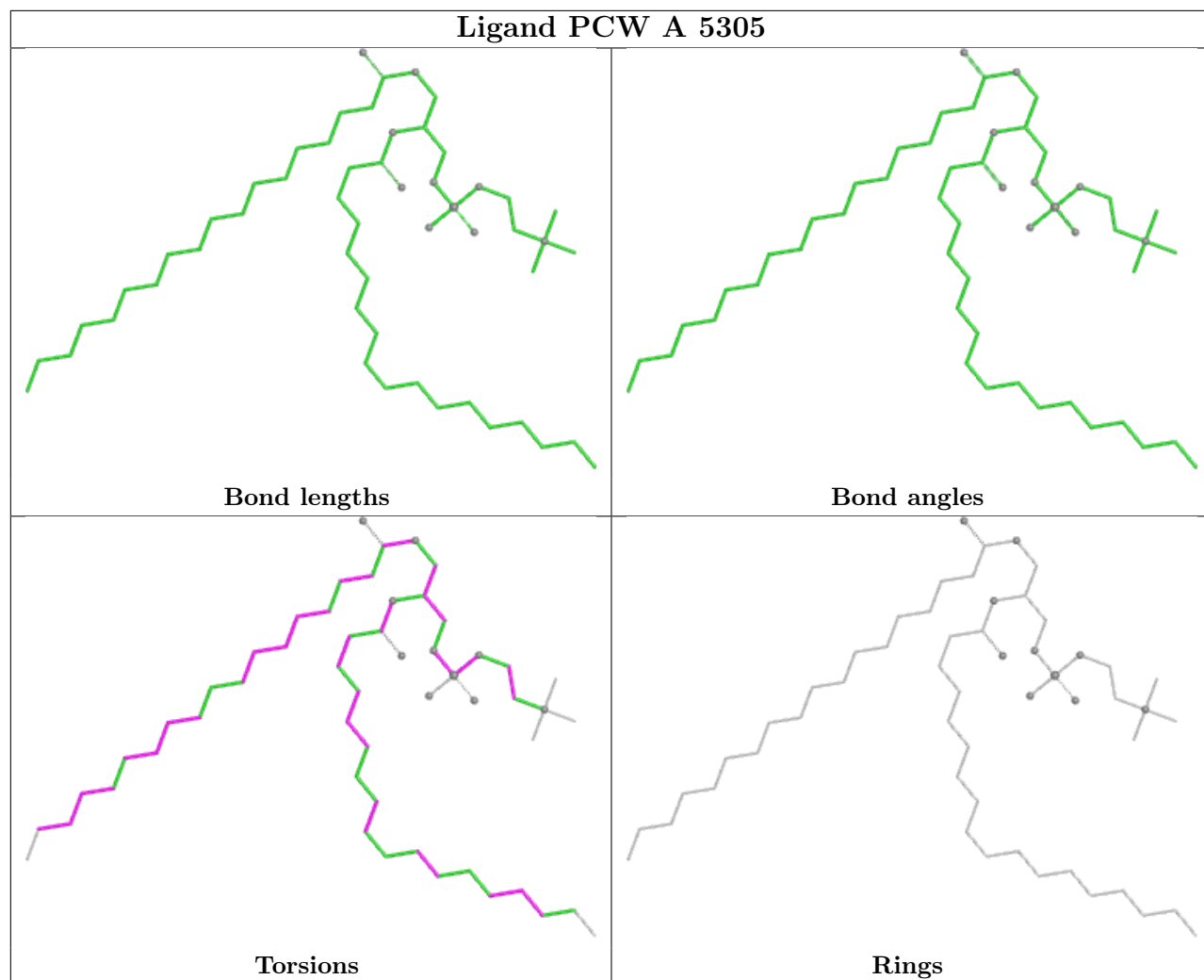


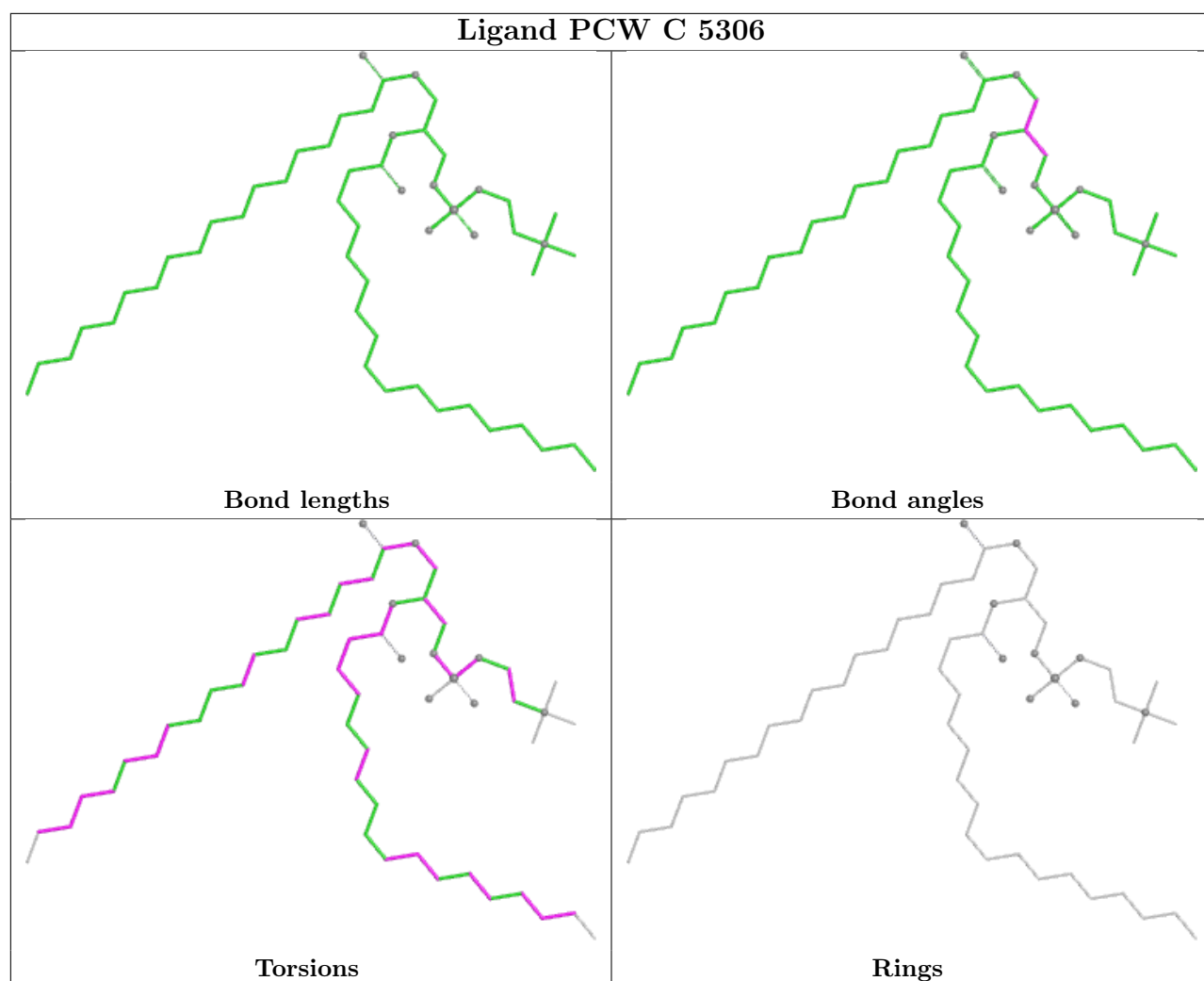


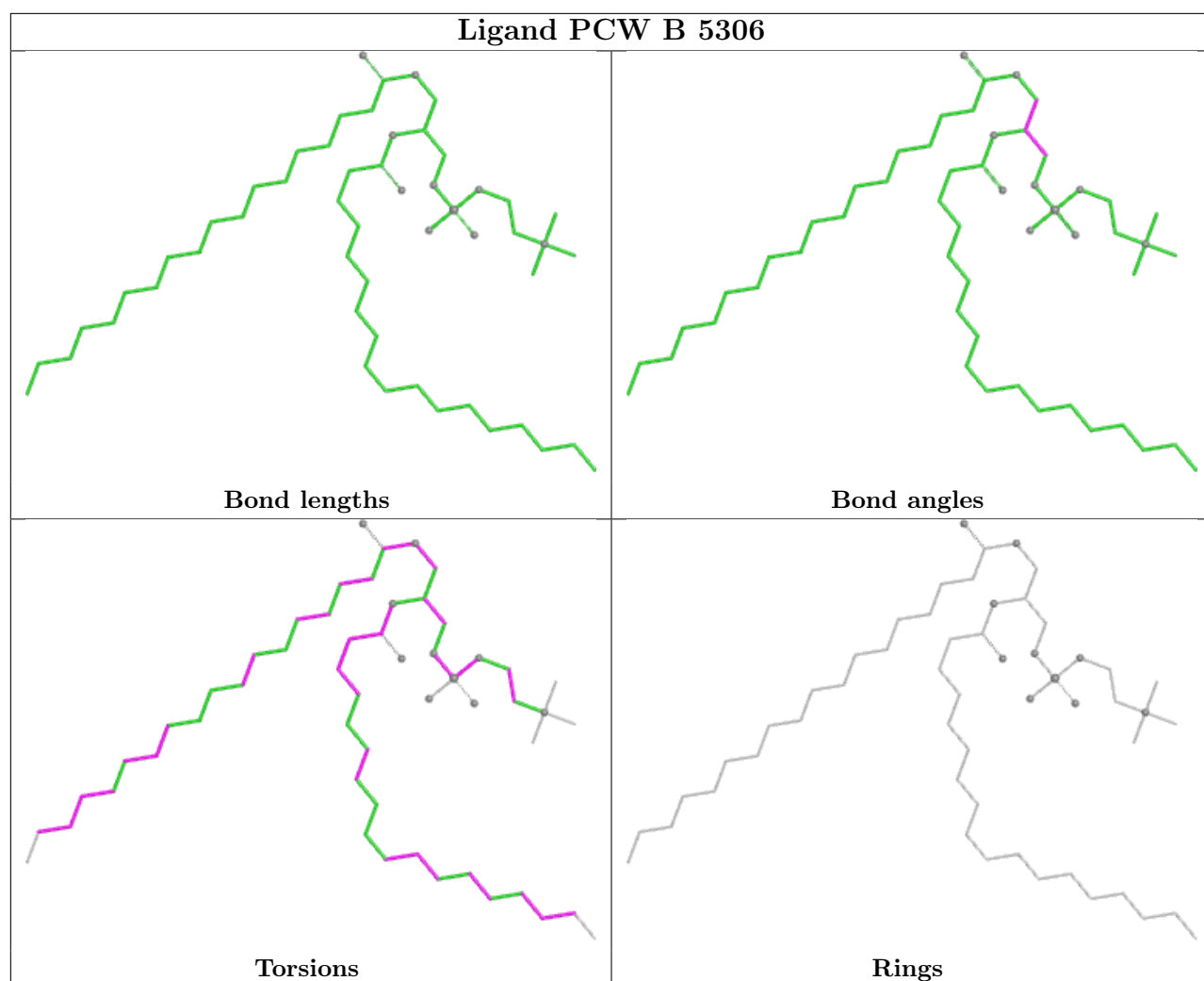


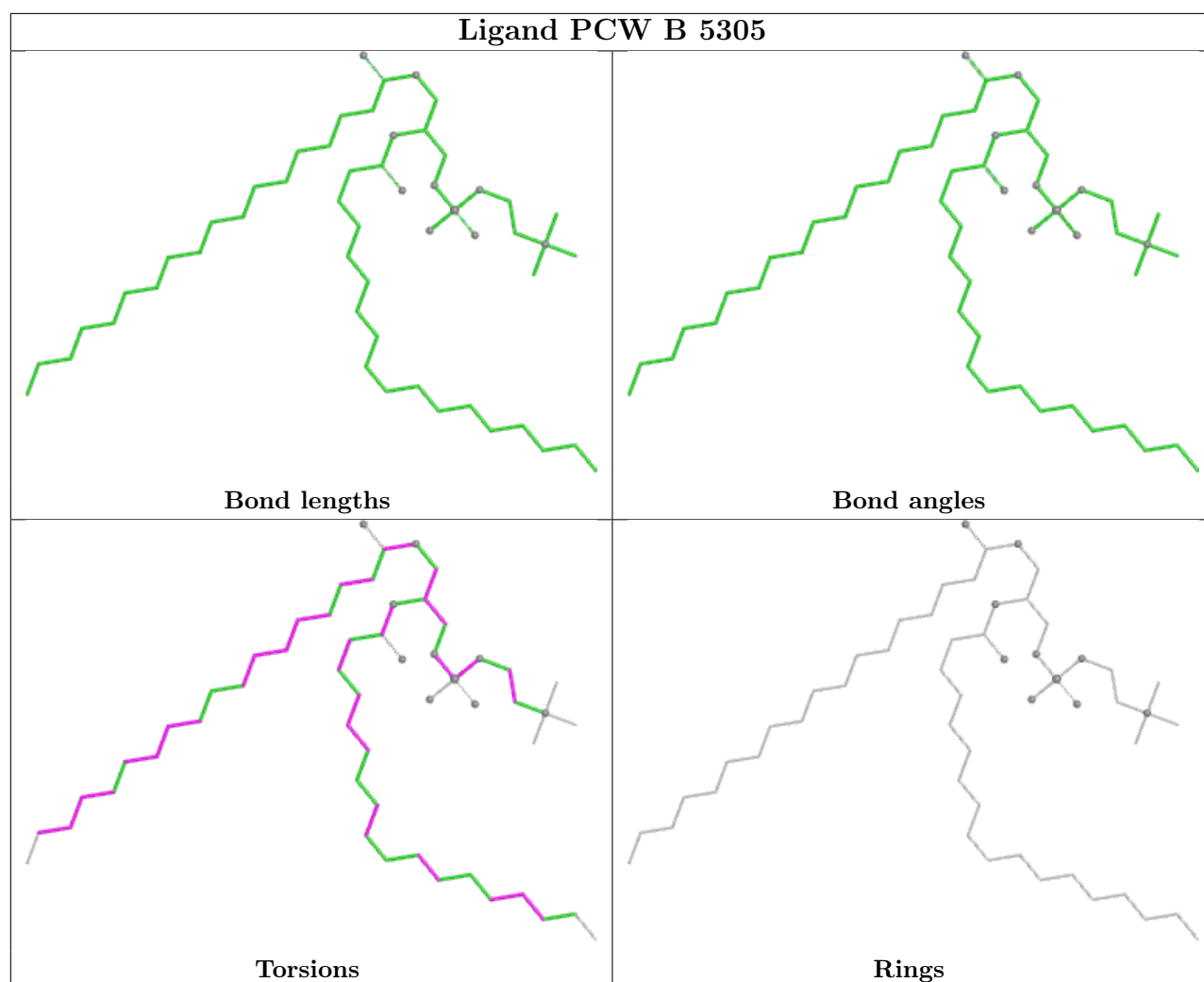












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

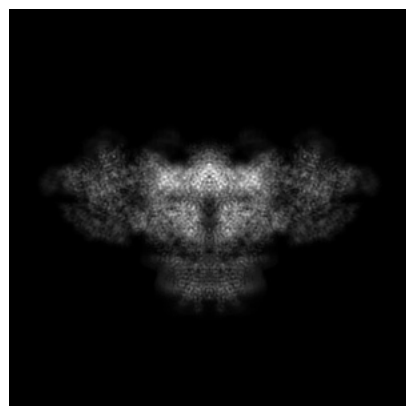
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74471. These allow visual inspection of the internal detail of the map and identification of artifacts.

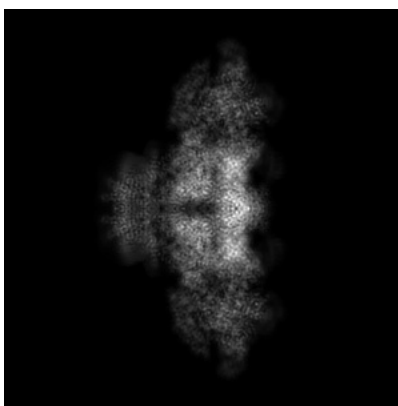
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

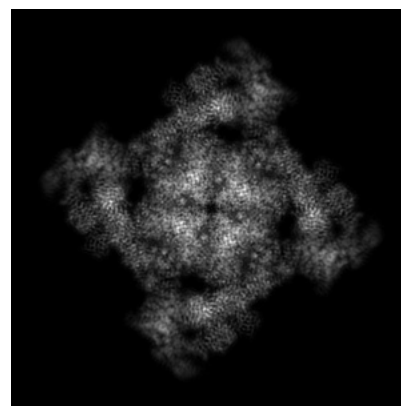
6.1.1 Primary map



X

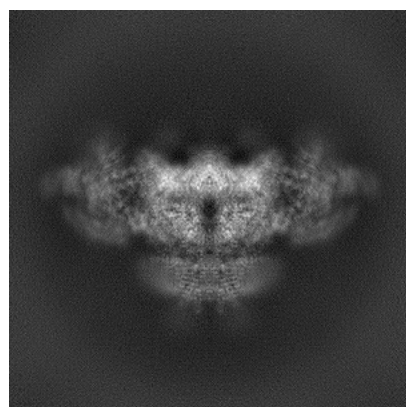


Y

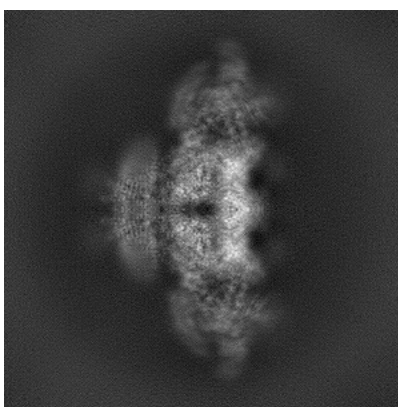


Z

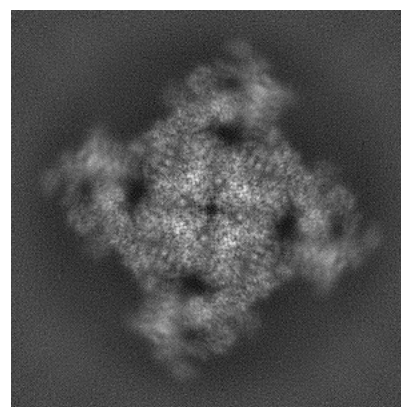
6.1.2 Raw map



X



Y



Z

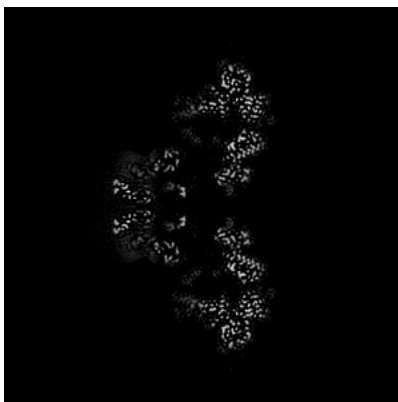
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

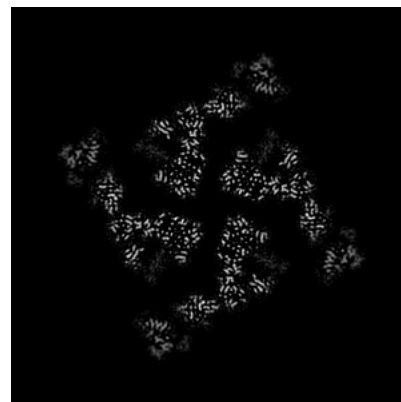
6.2.1 Primary map



X Index: 256

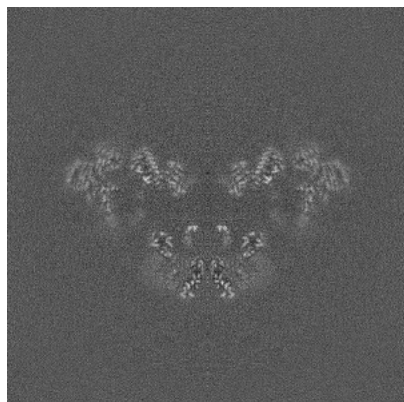


Y Index: 256

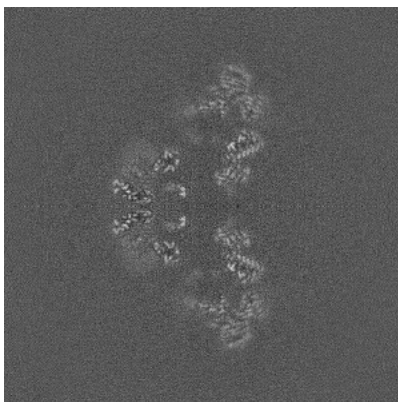


Z Index: 256

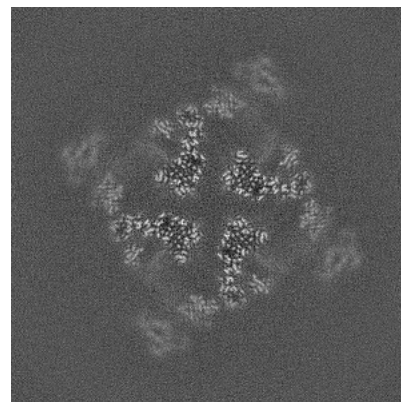
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

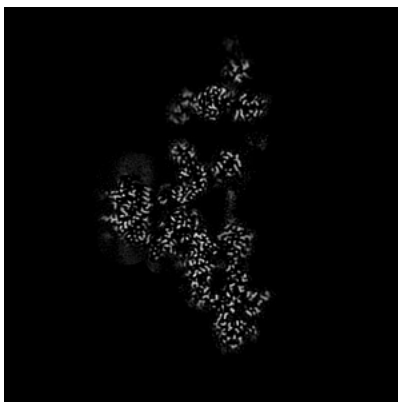
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

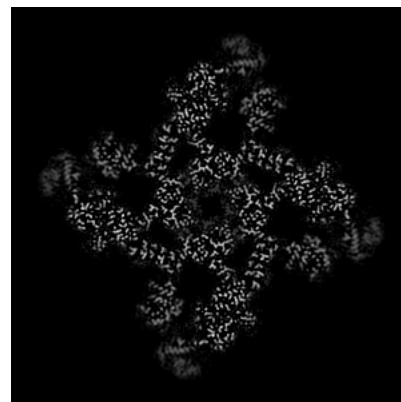
6.3.1 Primary map



X Index: 238

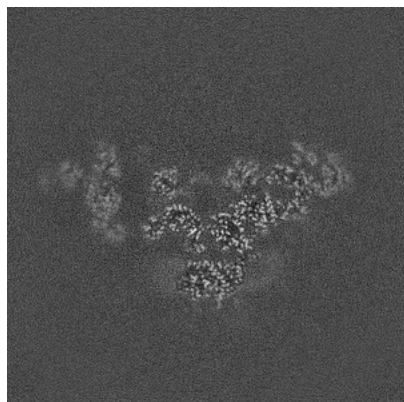


Y Index: 238

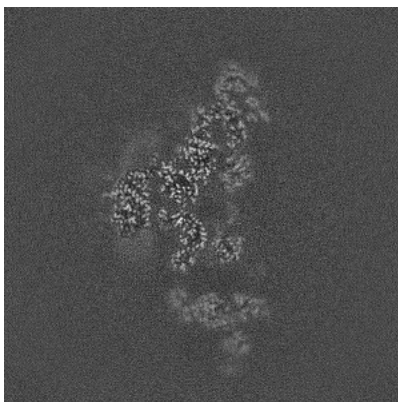


Z Index: 287

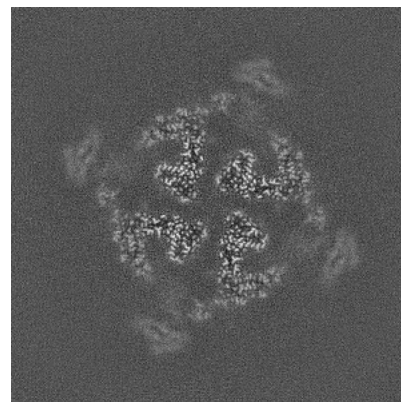
6.3.2 Raw map



X Index: 237



Y Index: 275

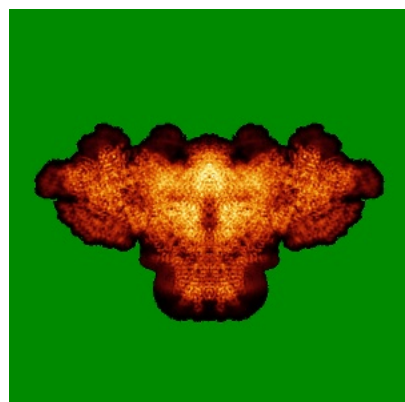


Z Index: 249

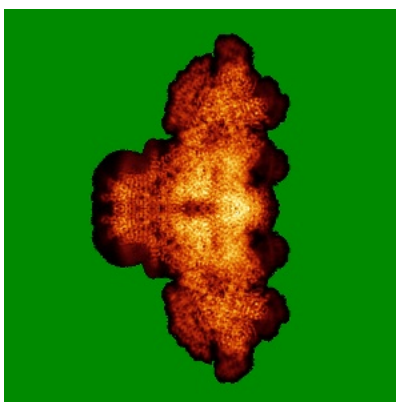
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

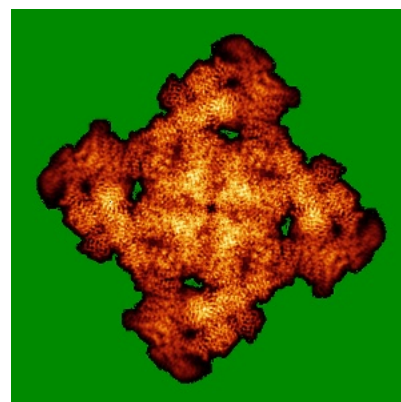
6.4.1 Primary map



X

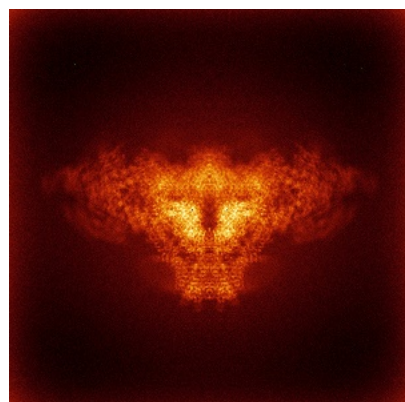


Y

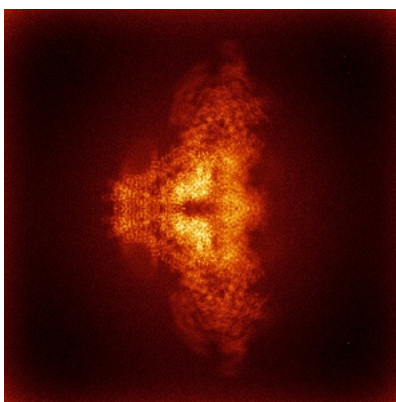


Z

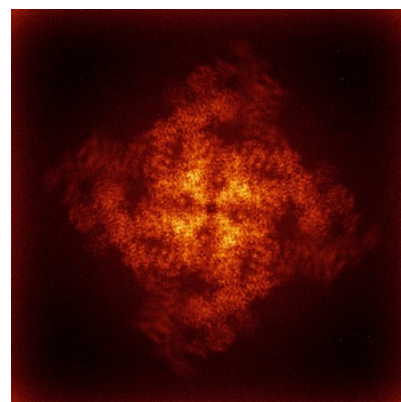
6.4.2 Raw map



X



Y

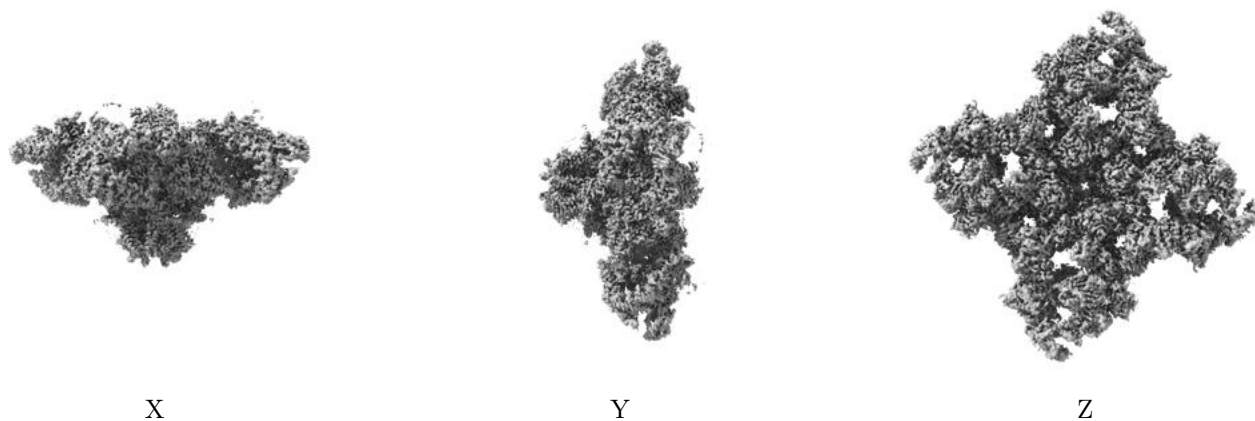


Z

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

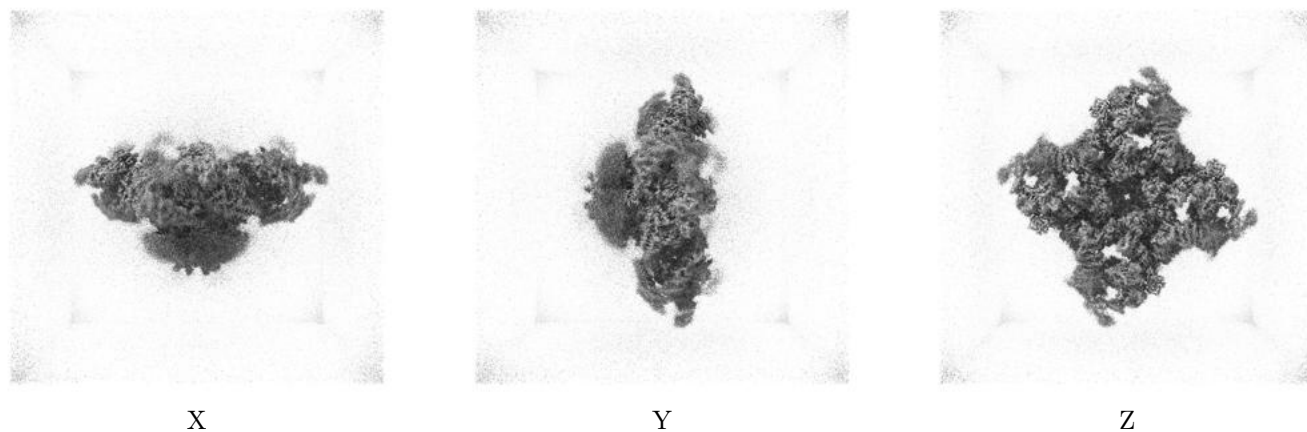
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

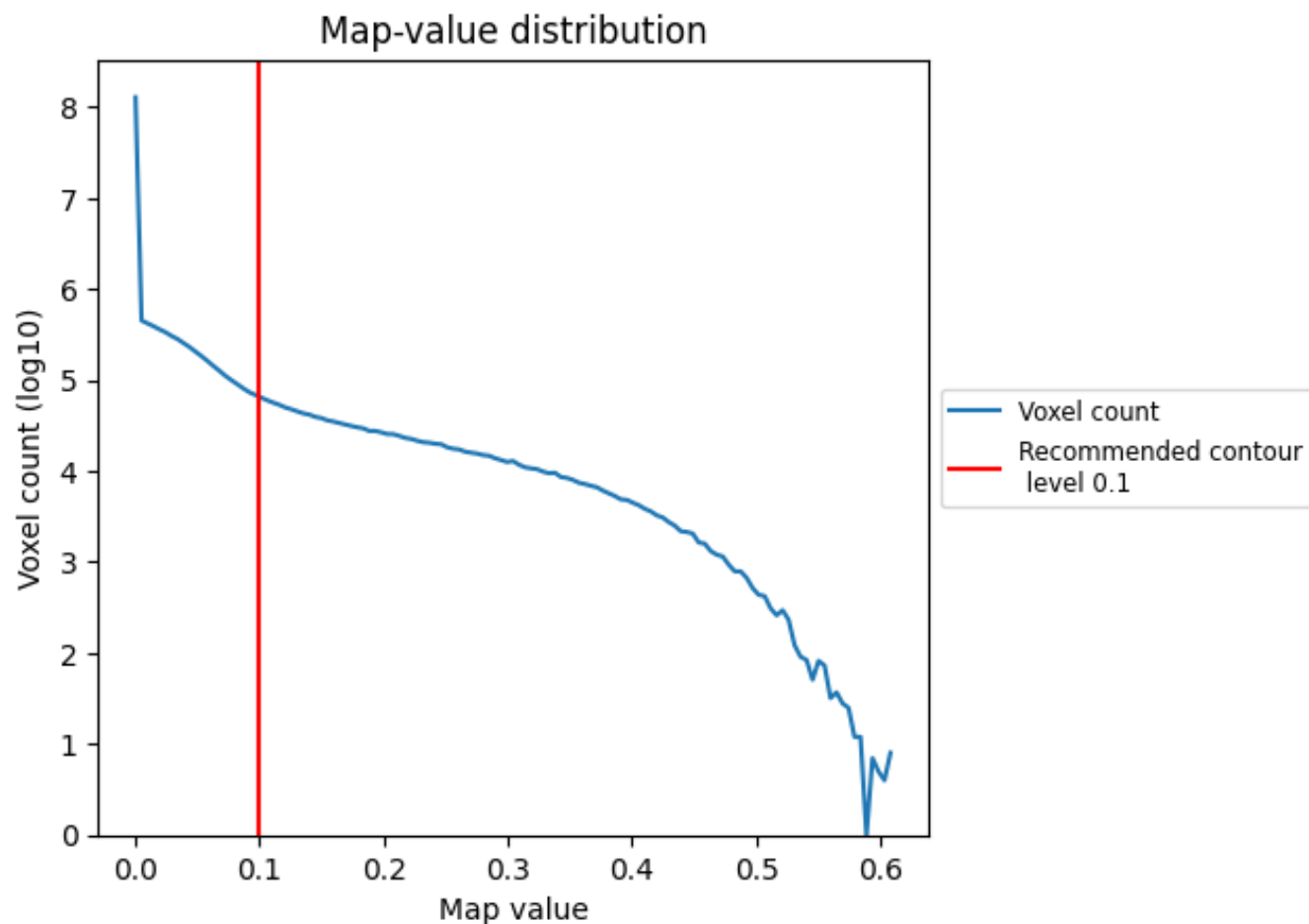
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

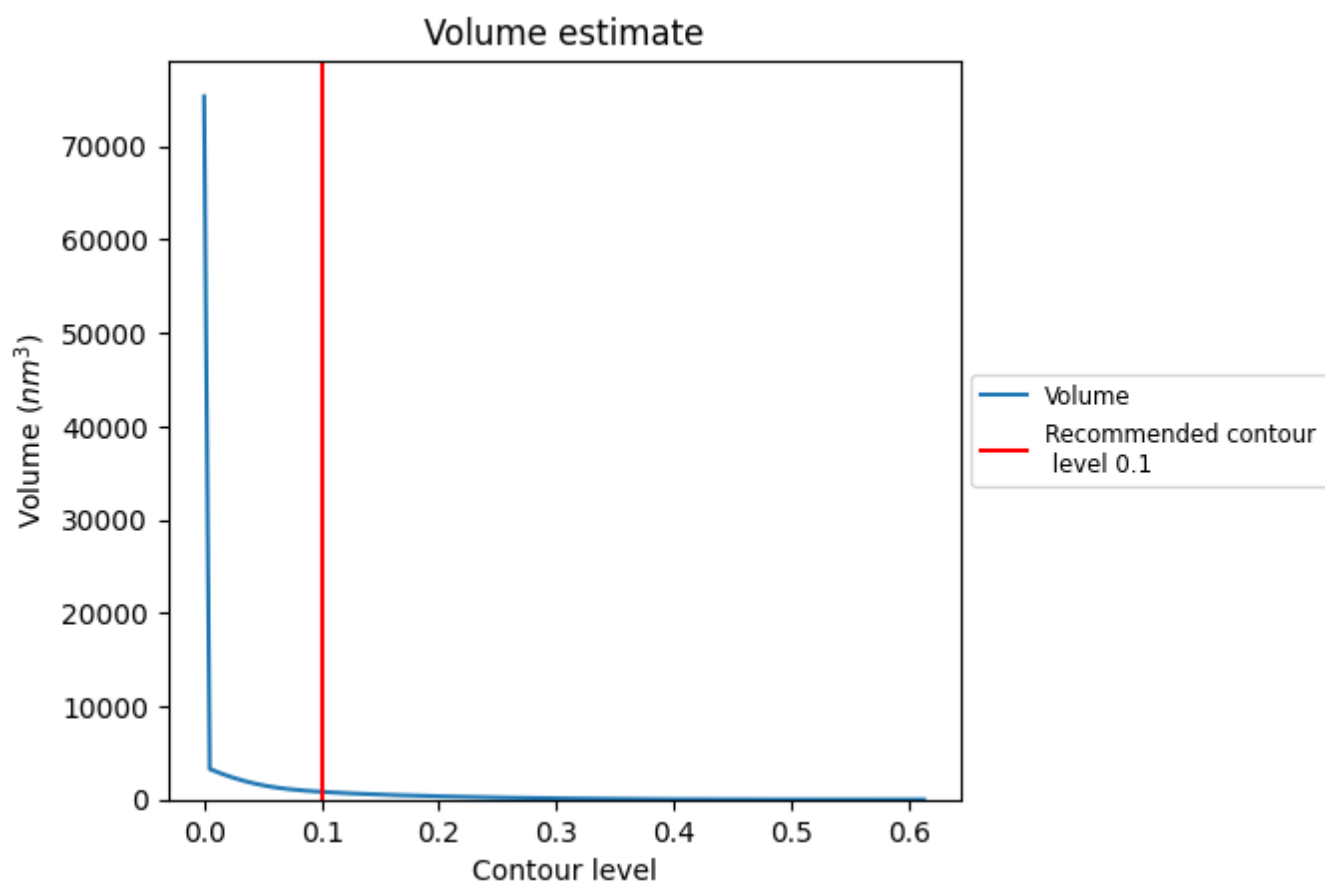
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

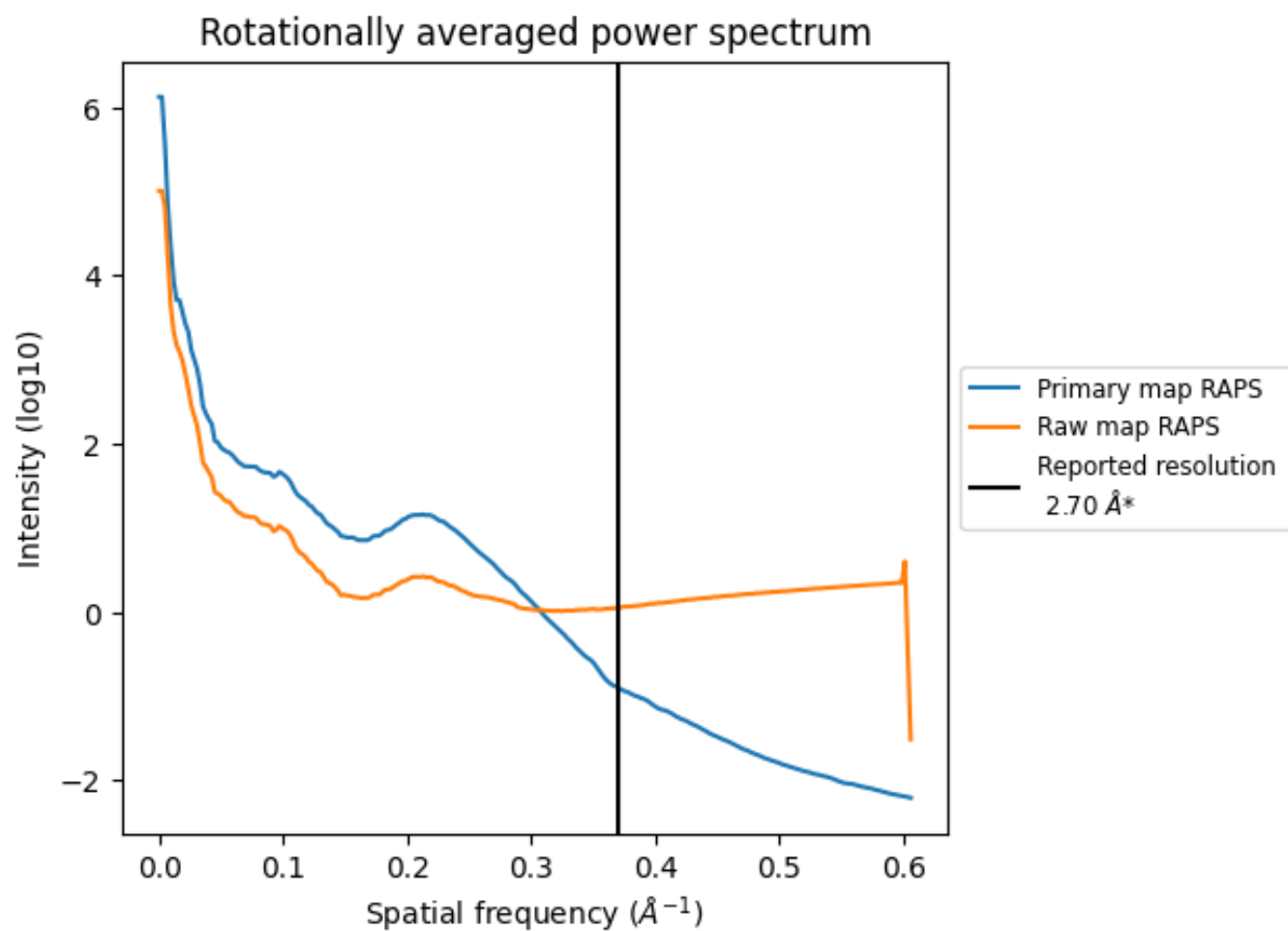
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm^3 ; this corresponds to an approximate mass of 749 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 ⓘ

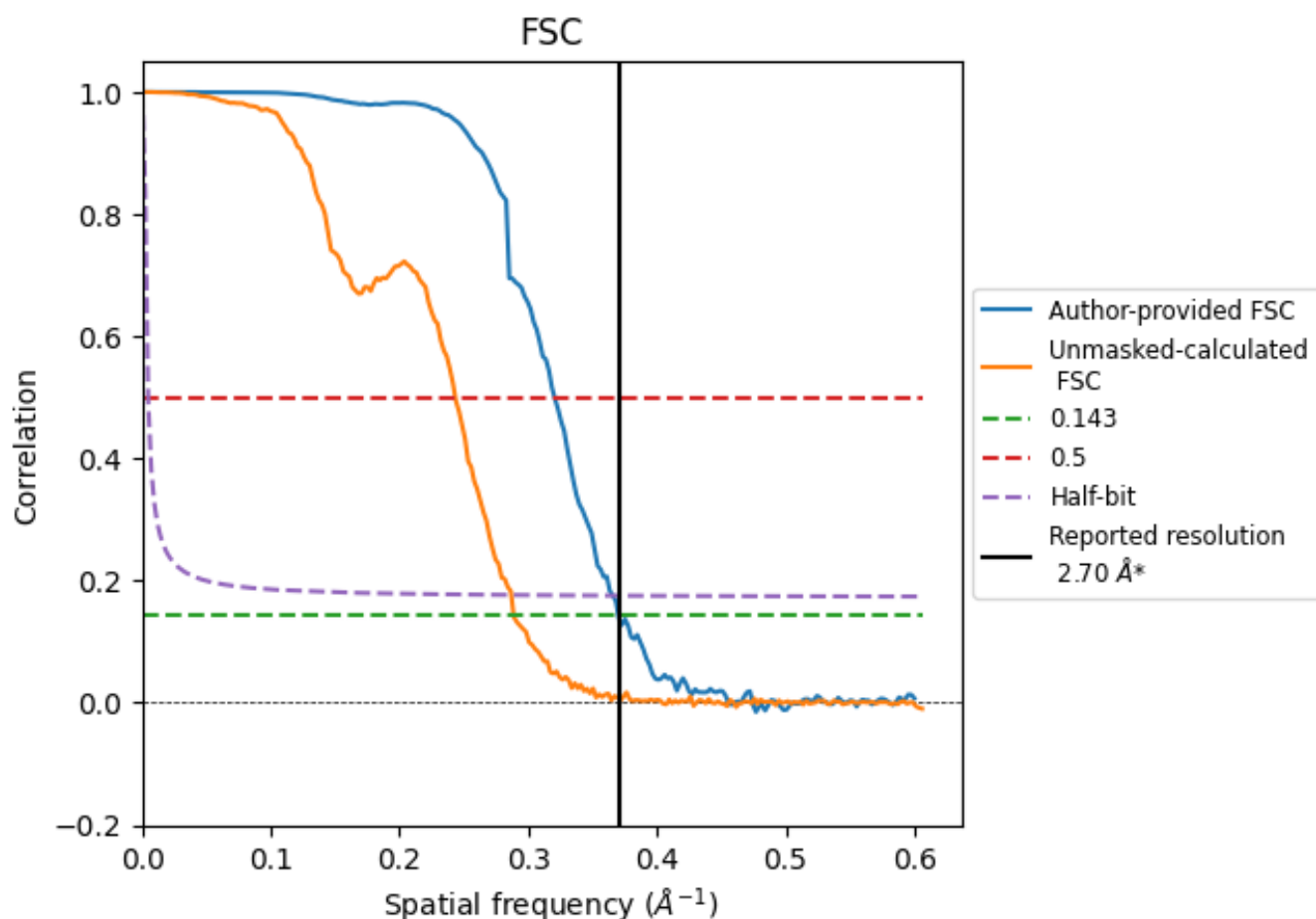


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

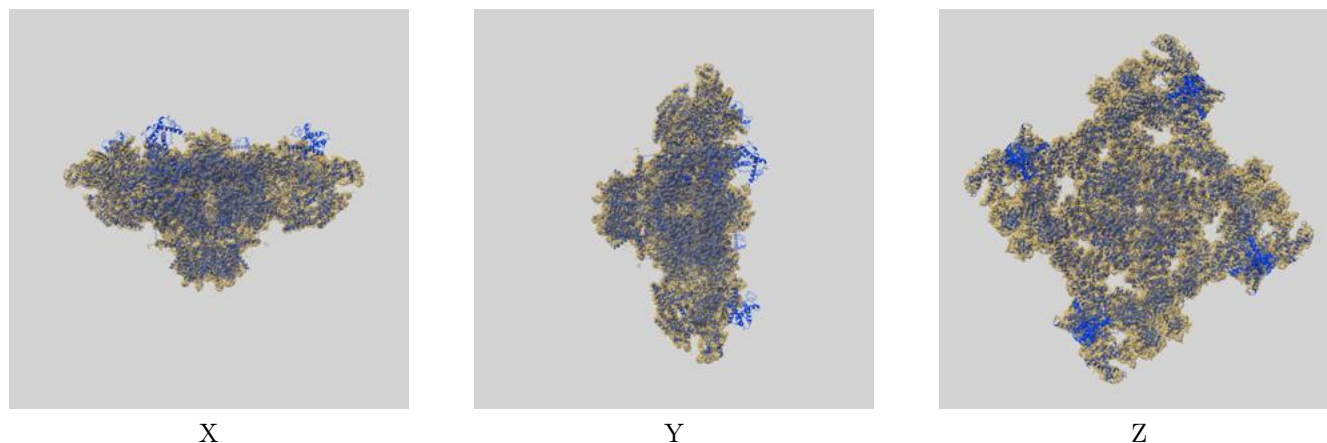
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.12	2.73
Unmasked-calculated*	3.46	4.11	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

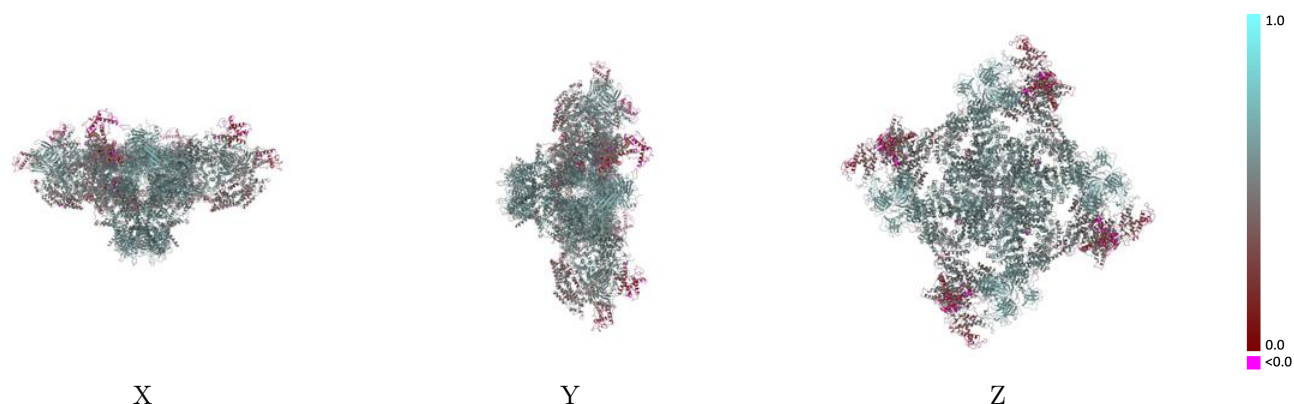
This section contains information regarding the fit between EMDB map EMD-74471 and PDB model 9ZO8. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



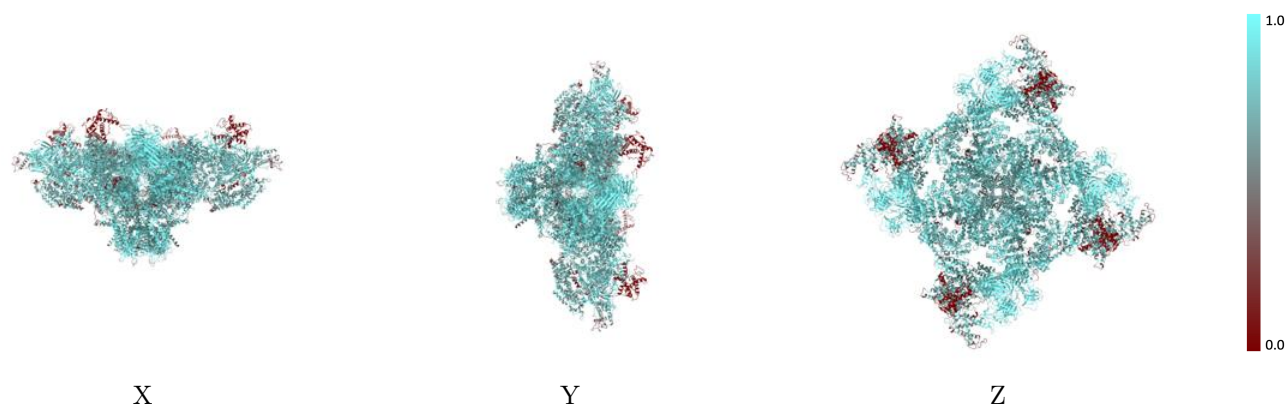
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



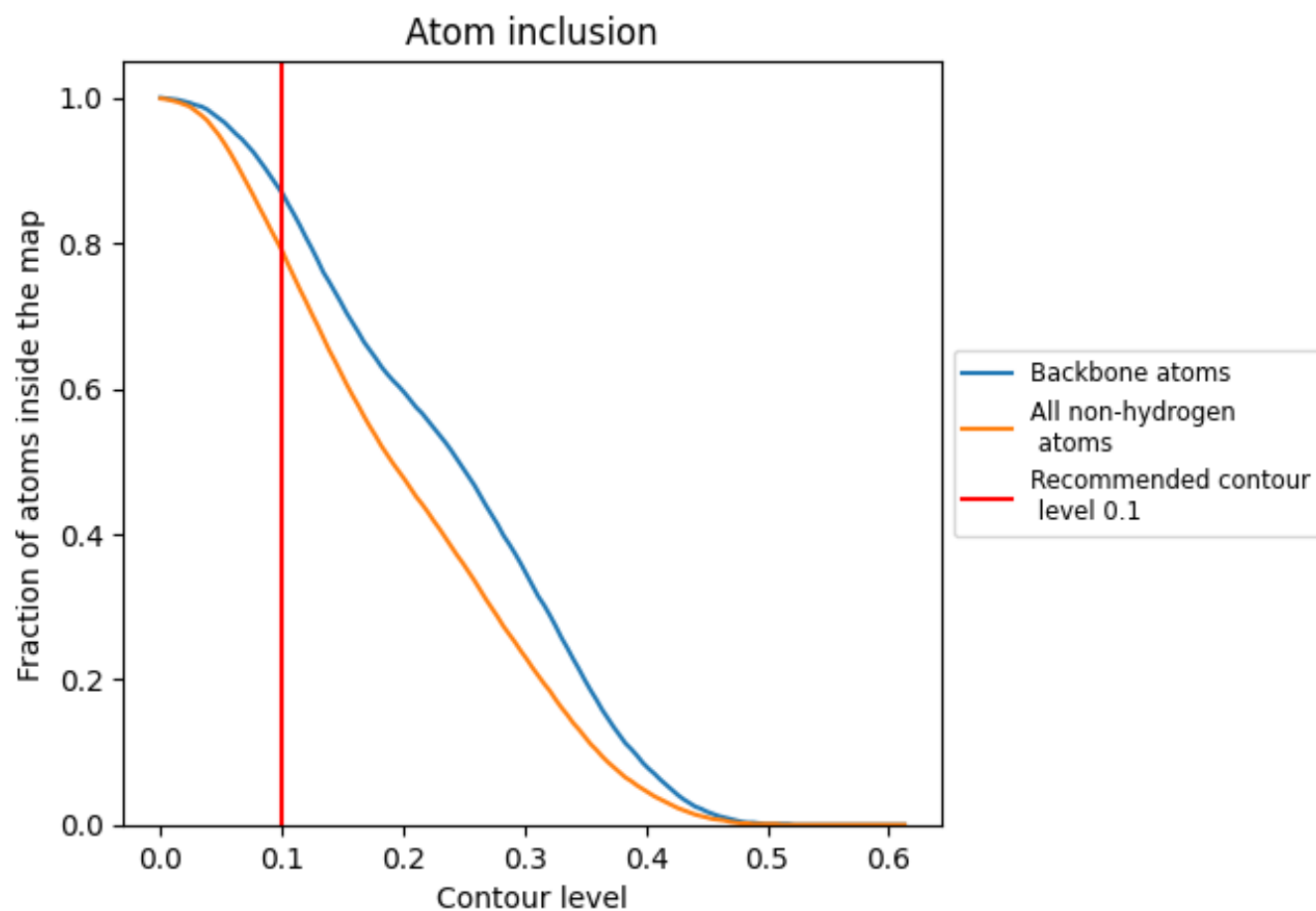
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.5130
A	0.7870	0.5120
B	0.7870	0.5110
C	0.7870	0.5110
D	0.7880	0.5120
E	0.8920	0.5970
F	0.8880	0.5970
G	0.8870	0.5960
H	0.8880	0.5970

1.0

0.0

<0.0