



Full wwPDB EM Validation Report ⓘ

Jul 20, 2026 – 05:00 pm BST

PDB ID : 9S16 / pdb_00009s16
EMDB ID : EMD-54445
Title : Apo-state RyR1 in the native membrane solved by "SPA"
Authors : Mikirtumov, V.
Deposited on : 2025-07-17
Resolution : 3.60 Å(reported)
Based on initial model : 7tzc

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:

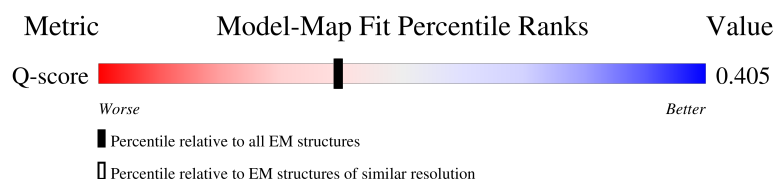
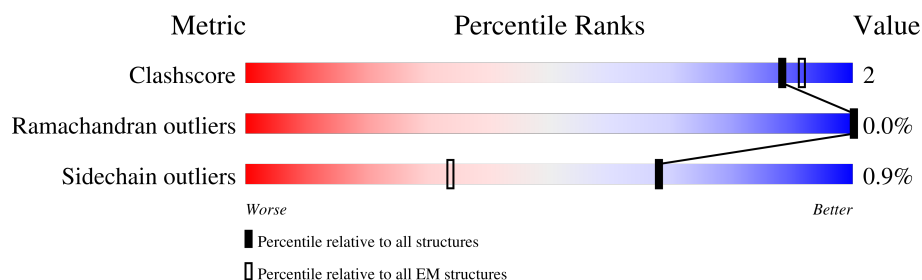
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	25% 81% 6% 13%
1	B	5037	25% 81% 6% 13%
1	C	5037	25% 81% 6% 13%
1	D	5037	25% 81% 6% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	 96%
2	F	108	 96%
2	G	108	 95%
2	H	108	 96%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 287008 atoms, of which 142908 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

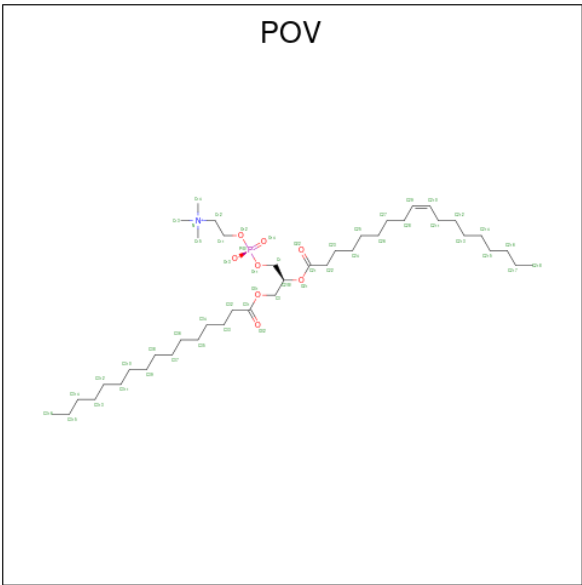
- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

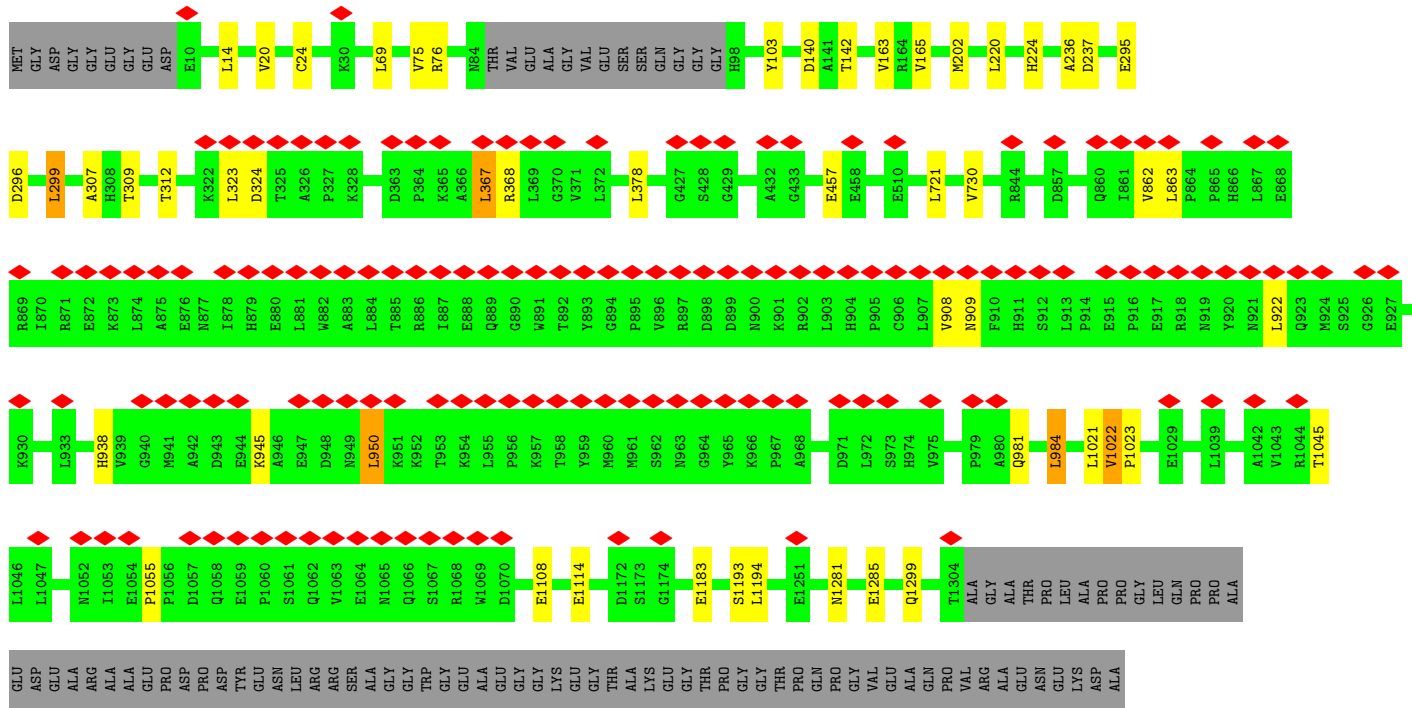
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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	D	1	1	1	0

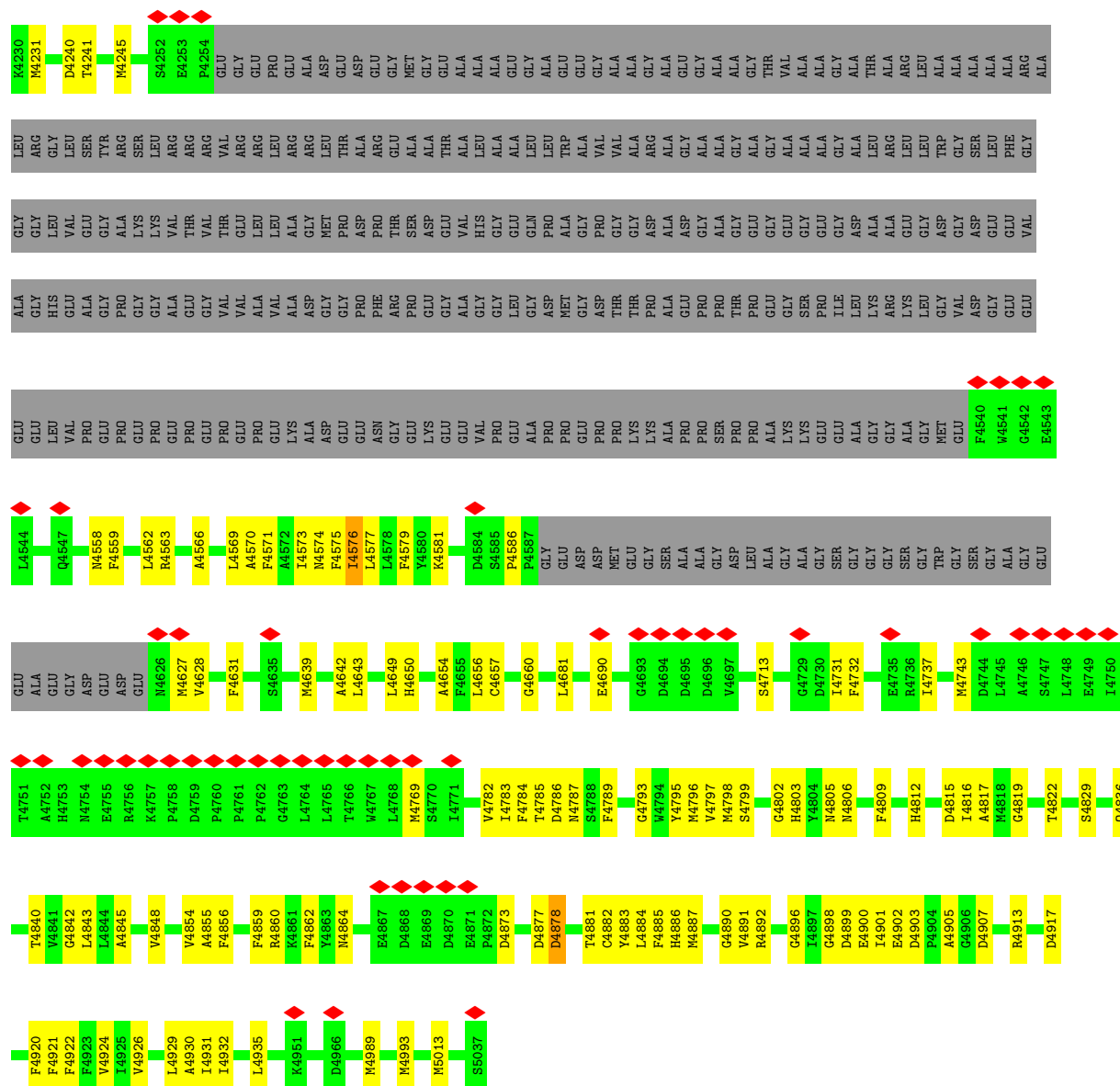




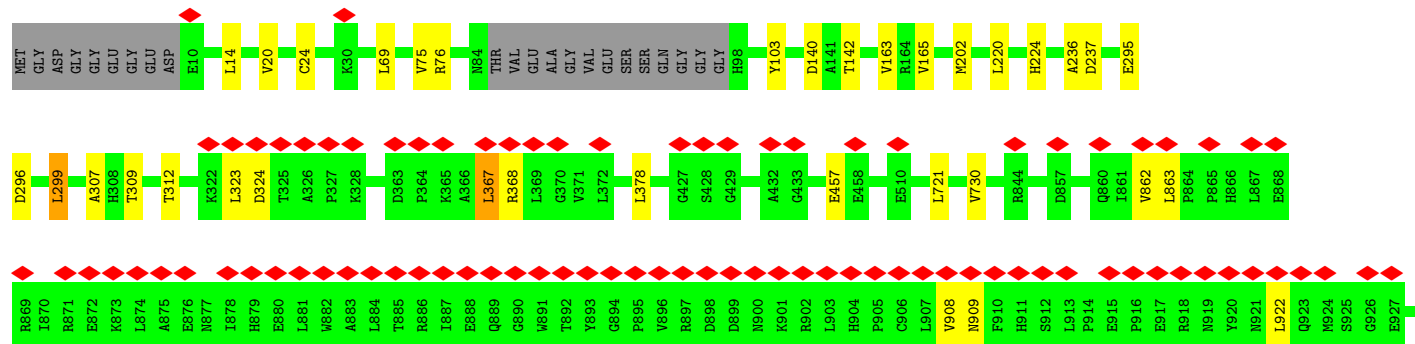
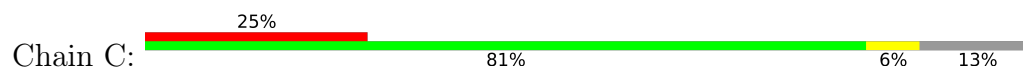


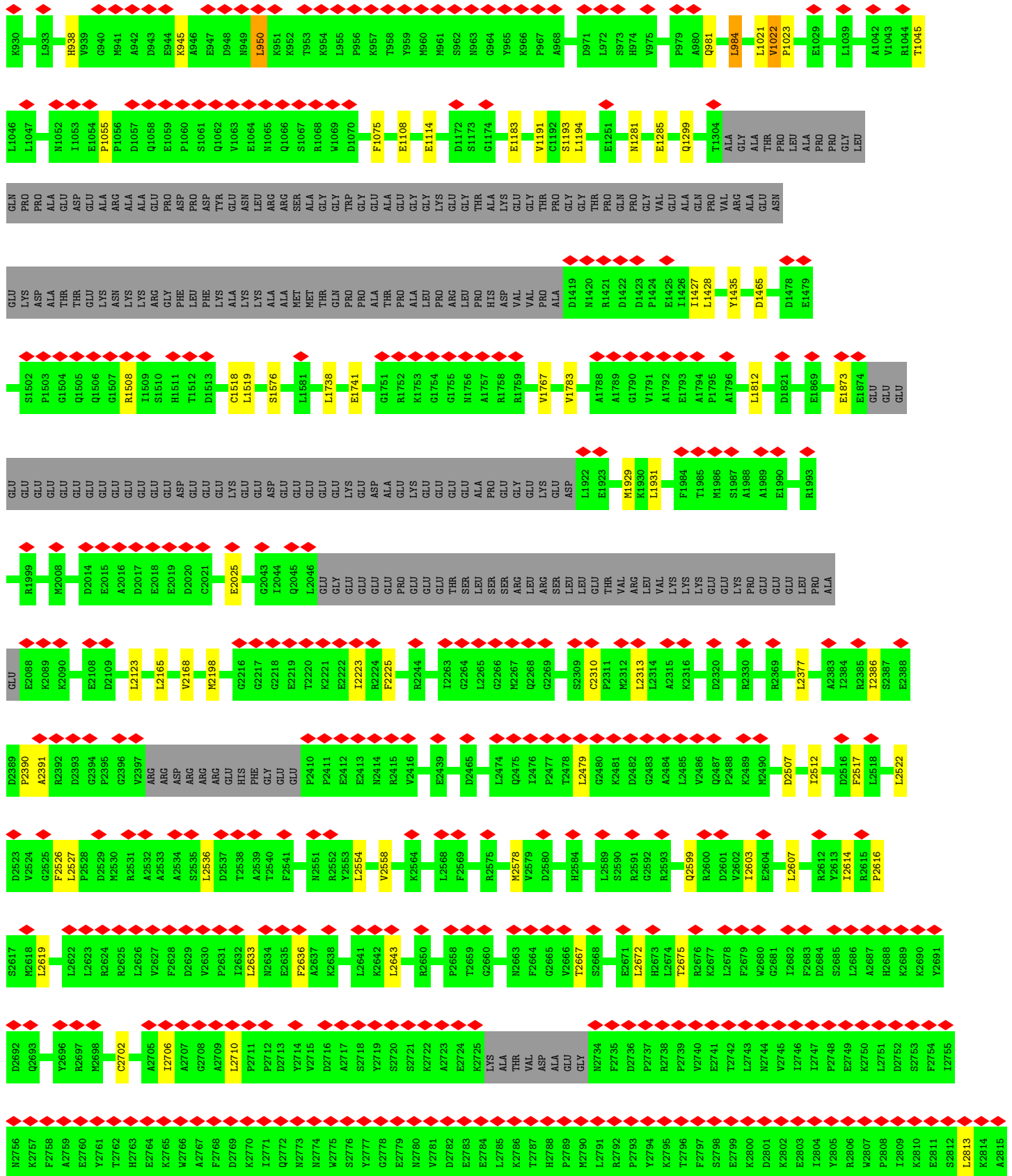




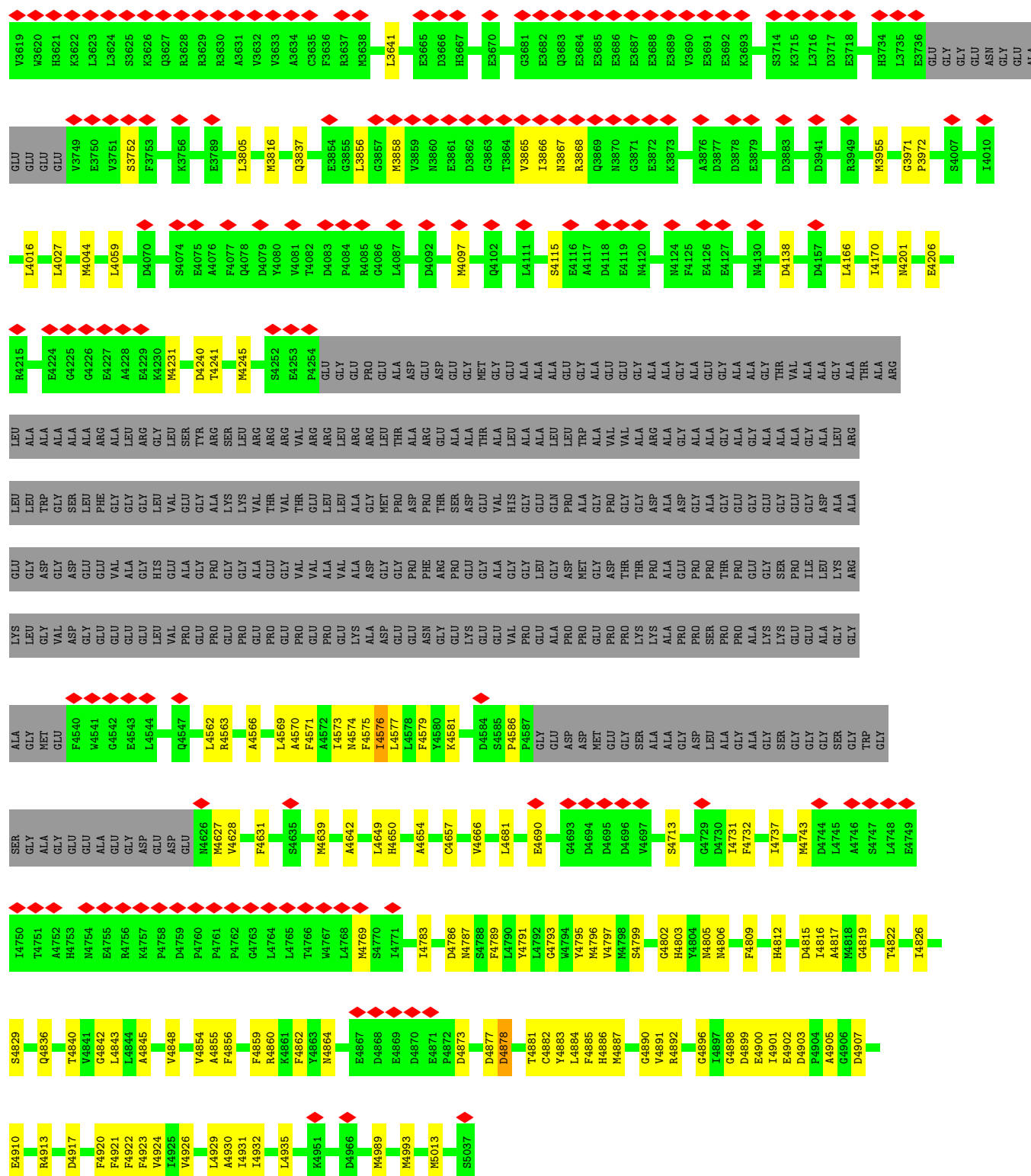


• Molecule 1: Ryanodine receptor 1





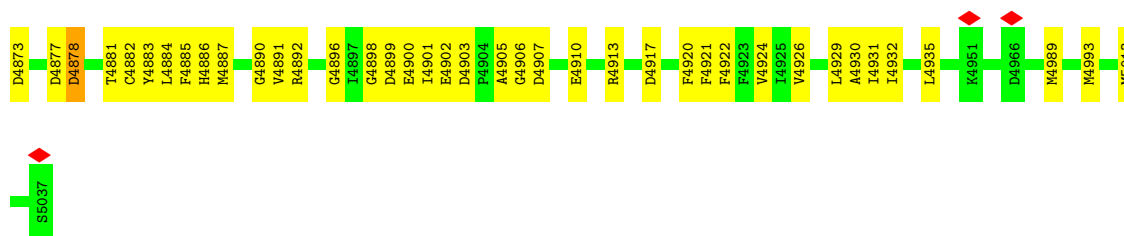






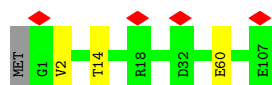
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GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	THR	GLN	ALA	GLN	THR	TVR	ASP	PRO	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	K2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890						
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V4791	L4681	P4587	VAL	GLY	ALA	ALA	L4111	G3855	C3635	A3574	V3511	F3451
C4792	E4690	GLY	GLU	GLY	LEU	GLU	S4115	L3856	F3636		A3512	K3452
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N4801	G4729	GLY	GLY	GLY	ALA	GLU	F4125	G3863	H3667	E3583	P3519	V3459
N4802	D4730	GLY	GLY	GLY	ALA	GLY	E4126	T3864	E3670	E3584	I3520	V3460
N4803	I4731	PRO	PRO	GLY	ALA	ALA	N4130	V3865		D3585	G3521	Q3461
N4804	F4732	PRO	PRO	GLY	THR	THR	E4138	I3866	G3681	A3586	M3524	N3462
N4805	L4733	GLY	GLY	GLY	ALA	VAL	D4139	R3867	E3682	D3587	C3525	E3463
N4806	E4735	GLY	GLY	GLY	GLY	ALA	L4166	R3868	Q3683	D3588		I3464
N4807	R4736	SER	SER	GLY	ALA	ALA	L4170	Q3869	E3684	P3589	T3528	N3465
N4808	I4737	ILE	ILE	GLY	GLY	ALA	T4170	R3870	E3685	E3590	D3529	N3466
N4809	M4743	LYS	LYS	ASP	ASP	ALA	E4206	G3871	E3686	K3591	Q3530	N3467
N4810	D4744	ARG	ARG	ALA	ALA	LEU	N4201	K3872	E3687	T3592	D3531	S3468
N4811	L4745	GLY	GLY	ALA	ALA	LEU	E4215	R3873	E3688	V3593	L3532	F3469
N4812	A4746	LEU	LEU	GLY	GLY	ALA	R4215	D3883	E3689	R3594	I3533	L3470
N4813	E4747	ASP	ASP	GLY	SER	ALA	R4224	G3841	E3691	R3595	M3534	T3471
N4814	L4748	GLY	GLY	GLY	GLY	ALA	E4225	R3849	E3692	V3596	L3535	A3472
N4815	E4749	GLU	GLU	PHE	GLU	ALA	G4226	M3955	K3715	Q3597	A3536	A3473
N4816	I4750	VAL	VAL	GLY	GLY	ALA	G4227	G3971	L3716	V3599	K3537	S3474
N4817	T4751	GLY	GLY	GLY	GLY	ALA	E4228	P3972	D3717	S3600	T3538	K3475
N4818	A4752	HIS	HIS	GLY	LEU	GLY	A4228	S4007		A3601	R3539	S3476
N4819	R4753	GLU	GLU	VAL	VAL	LEU	E4229	L4016	H3734	V3602	Y3540	K3477
N4820	L4754	PRO	PRO	ALA	ALA	LEU	E4230	L4027	L3735	L3603	L3542	N3478
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N4822	R4756	GLY	GLY	LYS	LYS	SER	D4240	M4044	GLU	E3607	D3545	ALA
N4823	L4757	VAL	VAL	VAL	VAL	ARG	T4241	E4050	GLY	Q3608	Y3546	ALA
N4824	F4758	ALA	ALA	THR	THR	ARG	M4245	M4044	GLY	T3609	E3547	GLN
N4825	D4759	GLY	GLY	THR	THR	ARG	S4252	E4075	GLY	E3610	Y3549	SER
N4826	P4760	PRO	PRO	VAL	VAL	VAL	E4253	D4070	GLY	Q3611	R3550	GLY
N4827	L4761	PRO	PRO	VAL	VAL	ALA	P4254	E4075	GLY	Y3612	E3551	SER
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N4830	L4764	ALA	ALA	ASP	ASP	ARG	GLY	E4075	GLY	S3615	F3553	GLU
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N4832	L4766	GLY	GLY	GLY	GLY	THR	ALA	E4075	GLY	K3617	N3555	LYS
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N4837	L4771	LYS	LYS	ASP	ASP	ALA	ASP	R4085	GLY	K3622	Q3560	LYS
N4838	L4772	GLY	GLY	GLY	GLY	GLY	GLY	L4087	GLY	L3623	Q3561	LYS
N4839	L4773	GLY	GLY	GLY	GLY	GLY	GLY	D4092	GLY	L3624	K3562	LYS
N4840	L4774	GLY	GLY	GLY	GLY	GLY	GLY	M4097	GLY	S3625	V3563	LYS
N4841	L4775	GLY	GLY	GLY	GLY	GLY	GLY		GLY	K3626	E3564	LYS
N4842	L4776	GLY	GLY	GLY	GLY	GLY	GLY		GLY	Q3627	G3565	LYS
N4843	L4777	GLY	GLY	GLY	GLY	GLY	GLY		GLY	R3628	T3507	LYS
N4844	L4778	GLY	GLY	GLY	GLY	GLY	GLY		GLY	R3629	S3508	LYS
N4845	L4779	GLY	GLY	GLY	GLY	GLY	GLY		GLY	R3630	L3509	LYS
N4846	L4780	GLY	GLY	GLY	GLY	GLY	GLY		GLY	V3632		LYS
N4847	L4781	GLY	GLY	GLY	GLY	GLY	GLY		GLY	V3633		LYS
N4848	L4782	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4849	L4783	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4850	L4784	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4851	L4785	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4852	L4786	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4853	L4787	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4854	L4788	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4855	L4789	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4856	L4790	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4857	L4791	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4858	L4792	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4859	L4793	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4860	L4794	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4861	L4795	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4862	L4796	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4863	L4797	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4864	L4798	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4865	L4799	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4866	L4800	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4867	L4801	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4868	L4802	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4869	L4803	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4870	L4804	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4871	L4805	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4872	L4806	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4873	L4807	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4874	L4808	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4875	L4809	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4876	L4810	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4877	L4811	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4878	L4812	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4879	L4813	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4880	L4814	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4881	L4815	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4882	L4816	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4883	L4817	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4884	L4818	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4885	L4819	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4886	L4820	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4887	L4821	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4888	L4822	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4889	L4823	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4890	L4824	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4891	L4825	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4892	L4826	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4893	L4827	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4894	L4828	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4895	L4829	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4896	L4830	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4897	L4831	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4898	L4832	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4899	L4833	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4900	L4834	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4901	L4835	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4902	L4836	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4903	L4837	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4904	L4838	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4905	L4839	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4906	L4840	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4907	L4841	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4908	L4842	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4909	L4843	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4910	L4844	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4911	L4845	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4912	L4846	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4913	L4847	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4914	L4848	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4915	L4849	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4916	L4850	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4917	L4851	GLY	GLY	GLY	GLY	GLY	GLY		GLY			LYS
N4918	L4852	GLY	GLY	GLY	GLY	GLY	GLY					



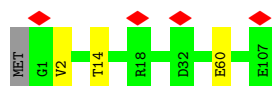
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 96%



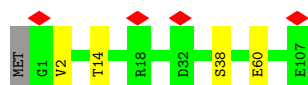
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 96%



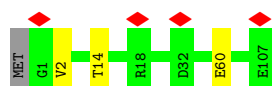
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 95%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	25786	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 ($e^-/\text{\AA}^2$)	60.9	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.271	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.269	Depositor
Recommended contour level	1.12	Depositor
Map size (Å)	409.80002, 409.80002, 409.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366, 1.366, 1.366	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	31/35885 (0.1%)	0.61	175/48603 (0.4%)
1	B	0.51	31/35885 (0.1%)	0.63	185/48603 (0.4%)
1	C	0.50	30/35885 (0.1%)	0.62	174/48603 (0.4%)
1	D	0.50	31/35885 (0.1%)	0.61	173/48603 (0.4%)
2	E	0.13	0/851	0.35	0/1146
2	F	0.14	0/851	0.36	0/1146
2	G	0.13	0/851	0.35	0/1146
2	H	0.13	0/851	0.35	0/1146
All	All	0.50	123/146944 (0.1%)	0.61	707/198996 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4812	HIS	CE1-NE2	-8.87	1.23	1.32
1	A	4812	HIS	CE1-NE2	-8.85	1.23	1.32
1	A	4803	HIS	ND1-CE1	-8.80	1.23	1.32
1	B	4886	HIS	ND1-CE1	-8.79	1.23	1.32
1	D	4886	HIS	ND1-CE1	-8.77	1.23	1.32
1	D	4803	HIS	ND1-CE1	-8.77	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4812	HIS	CE1-NE2	-8.75	1.23	1.32
1	C	4812	HIS	CE1-NE2	-8.75	1.23	1.32
1	B	4803	HIS	ND1-CE1	-8.74	1.23	1.32
1	B	4812	HIS	ND1-CE1	-8.74	1.23	1.32
1	C	4812	HIS	ND1-CE1	-8.74	1.23	1.32
1	A	4886	HIS	ND1-CE1	-8.74	1.23	1.32
1	C	4886	HIS	ND1-CE1	-8.74	1.23	1.32
1	B	4650	HIS	CE1-NE2	-8.74	1.23	1.32
1	C	4650	HIS	CE1-NE2	-8.74	1.23	1.32
1	D	4650	HIS	CE1-NE2	-8.74	1.23	1.32
1	A	4650	HIS	ND1-CE1	-8.73	1.23	1.32
1	C	4650	HIS	ND1-CE1	-8.73	1.23	1.32
1	D	4650	HIS	ND1-CE1	-8.73	1.23	1.32
1	A	4812	HIS	ND1-CE1	-8.72	1.23	1.32
1	D	4812	HIS	ND1-CE1	-8.70	1.23	1.32
1	B	4650	HIS	ND1-CE1	-8.70	1.23	1.32
1	A	4650	HIS	CE1-NE2	-8.64	1.24	1.32
1	C	4803	HIS	ND1-CE1	-8.59	1.24	1.32
1	B	4892	ARG	CZ-NH2	-8.21	1.22	1.33
1	A	4563	ARG	CZ-NH2	-8.16	1.22	1.33
1	B	4563	ARG	CZ-NH2	-8.16	1.22	1.33
1	C	4563	ARG	CZ-NH2	-8.16	1.22	1.33
1	C	4892	ARG	CZ-NH2	-8.16	1.22	1.33
1	A	4892	ARG	CZ-NH2	-8.15	1.22	1.33
1	D	4892	ARG	CZ-NH2	-8.15	1.22	1.33
1	C	4860	ARG	CZ-NH2	-8.10	1.23	1.33
1	D	4563	ARG	CZ-NH2	-8.10	1.23	1.33
1	B	4860	ARG	CZ-NH2	-8.09	1.23	1.33
1	A	4860	ARG	CZ-NH2	-8.07	1.23	1.33
1	D	4860	ARG	CZ-NH2	-8.07	1.23	1.33
1	D	4650	HIS	CD2-NE2	-8.03	1.29	1.37
1	C	4812	HIS	CD2-NE2	-7.99	1.29	1.37
1	B	4650	HIS	CD2-NE2	-7.96	1.29	1.37
1	A	4812	HIS	CD2-NE2	-7.95	1.29	1.37
1	B	4812	HIS	CD2-NE2	-7.95	1.29	1.37
1	D	4812	HIS	CD2-NE2	-7.95	1.29	1.37
1	A	4650	HIS	CD2-NE2	-7.94	1.29	1.37
1	C	4650	HIS	CD2-NE2	-7.90	1.29	1.37
1	D	4570	ALA	CA-CB	-7.01	1.42	1.53
1	A	4817	ALA	CA-CB	-7.00	1.42	1.53
1	B	4817	ALA	CA-CB	-7.00	1.42	1.53
1	C	4570	ALA	CA-CB	-6.99	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4817	ALA	CA-CB	-6.98	1.42	1.53
1	D	4930	ALA	CA-CB	-6.97	1.42	1.53
1	B	4586	PRO	CA-CB	-6.96	1.47	1.53
1	C	4930	ALA	CA-CB	-6.95	1.42	1.53
1	B	4566	ALA	CA-CB	-6.94	1.42	1.53
1	B	4930	ALA	CA-CB	-6.94	1.42	1.53
1	A	4570	ALA	CA-CB	-6.94	1.42	1.53
1	A	4586	PRO	CA-CB	-6.94	1.47	1.53
1	A	4855	ALA	CA-CB	-6.94	1.42	1.53
1	B	4570	ALA	CA-CB	-6.94	1.42	1.53
1	C	4586	PRO	CA-CB	-6.94	1.47	1.53
1	D	4817	ALA	CA-CB	-6.94	1.42	1.53
1	D	4845	ALA	CA-CB	-6.92	1.42	1.53
1	C	4654	ALA	CA-CB	-6.92	1.42	1.53
1	A	4930	ALA	CA-CB	-6.89	1.42	1.53
1	A	4845	ALA	CA-CB	-6.88	1.42	1.53
1	A	4654	ALA	CA-CB	-6.88	1.42	1.53
1	B	4654	ALA	CA-CB	-6.88	1.42	1.53
1	D	4654	ALA	CA-CB	-6.87	1.42	1.53
1	C	4855	ALA	CA-CB	-6.86	1.42	1.53
1	D	4855	ALA	CA-CB	-6.86	1.42	1.53
1	A	4905	ALA	CA-CB	-6.84	1.42	1.53
1	B	4905	ALA	CA-CB	-6.84	1.42	1.53
1	B	4845	ALA	CA-CB	-6.84	1.42	1.53
1	C	4845	ALA	CA-CB	-6.84	1.42	1.53
1	D	4586	PRO	CA-CB	-6.82	1.47	1.53
1	D	4905	ALA	CA-CB	-6.80	1.42	1.53
1	B	4855	ALA	CA-CB	-6.80	1.42	1.53
1	C	4905	ALA	CA-CB	-6.80	1.42	1.53
1	A	4892	ARG	CZ-NH1	-6.64	1.23	1.32
1	D	4892	ARG	CZ-NH1	-6.62	1.23	1.32
1	D	4563	ARG	CZ-NH1	-6.61	1.23	1.32
1	A	4563	ARG	CZ-NH1	-6.60	1.23	1.32
1	B	4563	ARG	CZ-NH1	-6.60	1.23	1.32
1	C	4563	ARG	CZ-NH1	-6.60	1.23	1.32
1	C	4892	ARG	CZ-NH1	-6.58	1.23	1.32
1	B	4892	ARG	CZ-NH1	-6.56	1.23	1.32
1	B	4860	ARG	CZ-NH1	-6.56	1.23	1.32
1	C	4860	ARG	CZ-NH1	-6.56	1.23	1.32
1	A	4860	ARG	CZ-NH1	-6.54	1.23	1.32
1	D	4860	ARG	CZ-NH1	-6.54	1.23	1.32
1	A	4819	GLY	N-CA	-6.06	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4819	GLY	N-CA	-6.06	1.38	1.45
1	B	4802	GLY	N-CA	-6.06	1.38	1.45
1	C	4802	GLY	N-CA	-6.03	1.38	1.45
1	B	4793	GLY	N-CA	-6.03	1.38	1.45
1	A	4802	GLY	N-CA	-6.02	1.38	1.45
1	D	4802	GLY	N-CA	-6.02	1.38	1.45
1	C	4793	GLY	N-CA	-6.02	1.38	1.45
1	C	4819	GLY	N-CA	-6.01	1.38	1.45
1	D	4842	GLY	N-CA	-5.99	1.38	1.45
1	D	4819	GLY	N-CA	-5.97	1.38	1.45
1	A	4793	GLY	N-CA	-5.97	1.38	1.45
1	A	4842	GLY	N-CA	-5.95	1.38	1.45
1	B	4842	GLY	N-CA	-5.95	1.38	1.45
1	C	4842	GLY	N-CA	-5.93	1.38	1.45
1	D	4793	GLY	N-CA	-5.92	1.38	1.45
1	C	4898	GLY	N-CA	-5.63	1.38	1.45
1	B	4898	GLY	N-CA	-5.58	1.38	1.45
1	A	4898	GLY	N-CA	-5.54	1.38	1.45
1	D	4898	GLY	N-CA	-5.54	1.38	1.45
1	D	4892	ARG	CD-NE	-5.37	1.38	1.46
1	B	4860	ARG	CD-NE	-5.35	1.38	1.46
1	C	4860	ARG	CD-NE	-5.35	1.38	1.46
1	D	4860	ARG	CD-NE	-5.33	1.38	1.46
1	A	4892	ARG	CD-NE	-5.30	1.38	1.46
1	B	4892	ARG	CD-NE	-5.30	1.38	1.46
1	C	4892	ARG	CD-NE	-5.30	1.38	1.46
1	A	4563	ARG	CD-NE	-5.30	1.38	1.46
1	A	4860	ARG	CD-NE	-5.28	1.38	1.46
1	C	4563	ARG	CD-NE	-5.24	1.39	1.46
1	B	4563	ARG	CD-NE	-5.17	1.39	1.46
1	D	4563	ARG	CD-NE	-5.17	1.39	1.46
1	D	4906	GLY	N-CA	-5.02	1.38	1.45
1	A	4906	GLY	N-CA	-5.01	1.38	1.45

All (707) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4784	PHE	CA-CB-CG	7.70	121.50	113.80
1	B	4922	PHE	CA-CB-CG	7.64	121.44	113.80
1	D	4922	PHE	CA-CB-CG	7.63	121.44	113.80
1	A	4922	PHE	CA-CB-CG	7.62	121.42	113.80
1	C	4922	PHE	CA-CB-CG	7.62	121.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4877	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	4877	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	4877	ASP	CA-CB-CG	7.45	120.05	112.60
1	D	4877	ASP	CA-CB-CG	7.37	119.97	112.60
1	D	4571	PHE	CA-CB-CG	7.36	121.16	113.80
1	A	4571	PHE	CA-CB-CG	7.34	121.14	113.80
1	B	4571	PHE	CA-CB-CG	7.34	121.14	113.80
1	C	4571	PHE	CA-CB-CG	7.34	121.14	113.80
1	B	4899	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	4899	ASP	CA-CB-CG	7.23	119.83	112.60
1	C	4899	ASP	CA-CB-CG	7.22	119.82	112.60
1	D	4899	ASP	CA-CB-CG	7.21	119.81	112.60
1	C	4917	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	4917	ASP	CA-CB-CG	7.15	119.75	112.60
1	B	4917	ASP	CA-CB-CG	7.15	119.75	112.60
1	C	4574	ASN	CA-CB-CG	7.15	119.75	112.60
1	D	4917	ASP	CA-CB-CG	7.14	119.74	112.60
1	A	4574	ASN	CA-CB-CG	7.13	119.73	112.60
1	B	4886	HIS	CA-CB-CG	7.13	120.93	113.80
1	A	4886	HIS	CA-CB-CG	7.12	120.92	113.80
1	D	4886	HIS	CA-CB-CG	7.12	120.92	113.80
1	C	4886	HIS	CA-CB-CG	7.12	120.92	113.80
1	D	4574	ASN	CA-CB-CG	7.07	119.67	112.60
1	B	4574	ASN	CA-CB-CG	7.07	119.67	112.60
1	B	4809	PHE	CA-CB-CG	7.06	120.86	113.80
1	C	4809	PHE	CA-CB-CG	7.04	120.84	113.80
1	A	4809	PHE	CA-CB-CG	7.03	120.83	113.80
1	D	4809	PHE	CA-CB-CG	6.97	120.77	113.80
1	B	4920	PHE	CA-CB-CG	6.93	120.73	113.80
1	B	4907	ASP	CA-CB-CG	6.92	119.53	112.60
1	D	4920	PHE	CA-CB-CG	6.92	120.72	113.80
1	A	4920	PHE	CA-CB-CG	6.91	120.71	113.80
1	C	4920	PHE	CA-CB-CG	6.91	120.71	113.80
1	C	4903	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	4907	ASP	CA-CB-CG	6.88	119.48	112.60
1	C	4907	ASP	CA-CB-CG	6.88	119.48	112.60
1	D	4907	ASP	CA-CB-CG	6.87	119.47	112.60
1	D	4903	ASP	CA-CB-CG	6.84	119.44	112.60
1	D	4579	PHE	CA-CB-CG	6.84	120.64	113.80
1	C	4815	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	4579	PHE	CA-CB-CG	6.82	120.62	113.80
1	A	4903	ASP	CA-CB-CG	6.81	119.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4579	PHE	CA-CB-CG	6.80	120.60	113.80
1	C	4579	PHE	CA-CB-CG	6.80	120.60	113.80
1	A	4815	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	4903	ASP	CA-CB-CG	6.77	119.37	112.60
1	B	4815	ASP	CA-CB-CG	6.77	119.37	112.60
1	C	4862	PHE	CA-CB-CG	6.76	120.56	113.80
1	B	4864	ASN	CA-CB-CG	6.76	119.36	112.60
1	C	4864	ASN	CA-CB-CG	6.75	119.35	112.60
1	D	4885	PHE	CA-CB-CG	6.75	120.55	113.80
1	A	4862	PHE	CA-CB-CG	6.75	120.55	113.80
1	D	4862	PHE	CA-CB-CG	6.75	120.55	113.80
1	B	4885	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	4885	PHE	CA-CB-CG	6.73	120.53	113.80
1	C	4885	PHE	CA-CB-CG	6.73	120.53	113.80
1	D	4815	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	4862	PHE	CA-CB-CG	6.73	120.53	113.80
1	A	4864	ASN	CA-CB-CG	6.72	119.32	112.60
1	D	4864	ASN	CA-CB-CG	6.72	119.32	112.60
1	B	4650	HIS	CA-CB-CG	6.66	120.45	113.80
1	A	4650	HIS	CA-CB-CG	6.65	120.45	113.80
1	B	4786	ASP	CA-CB-CG	6.63	119.23	112.60
1	D	4803	HIS	CA-CB-CG	6.63	120.43	113.80
1	D	4650	HIS	CA-CB-CG	6.63	120.43	113.80
1	B	4803	HIS	CA-CB-CG	6.59	120.39	113.80
1	C	4803	HIS	CA-CB-CG	6.59	120.39	113.80
1	C	4650	HIS	CA-CB-CG	6.59	120.39	113.80
1	A	4803	HIS	CA-CB-CG	6.55	120.36	113.80
1	A	4806	ASN	CA-CB-CG	6.54	119.14	112.60
1	D	4806	ASN	CA-CB-CG	6.50	119.10	112.60
1	D	4812	HIS	CA-CB-CG	6.47	120.27	113.80
1	B	4806	ASN	CA-CB-CG	6.46	119.06	112.60
1	C	4806	ASN	CA-CB-CG	6.46	119.06	112.60
1	C	4812	HIS	CA-CB-CG	6.46	120.26	113.80
1	A	4812	HIS	CA-CB-CG	6.45	120.25	113.80
1	B	4812	HIS	CA-CB-CG	6.43	120.23	113.80
1	C	4923	PHE	CA-C-N	6.39	128.67	120.88
1	C	4923	PHE	C-N-CA	6.39	128.67	120.88
1	C	4789	PHE	CA-CB-CG	6.37	120.17	113.80
1	D	4789	PHE	CA-CB-CG	6.36	120.16	113.80
1	B	4789	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	4789	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	4575	PHE	CA-CB-CG	6.29	120.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4575	PHE	CA-CB-CG	6.24	120.04	113.80
1	C	4575	PHE	CA-CB-CG	6.23	120.03	113.80
1	B	4575	PHE	CA-CB-CG	6.22	120.02	113.80
1	B	4856	PHE	CA-CB-CG	6.21	120.01	113.80
1	D	4787	ASN	CA-CB-CG	6.18	118.78	112.60
1	B	4787	ASN	CA-CB-CG	6.17	118.77	112.60
1	C	4787	ASN	CA-CB-CG	6.17	118.77	112.60
1	C	4856	PHE	CA-CB-CG	6.16	119.96	113.80
1	D	4819	GLY	CA-C-N	6.16	131.12	123.12
1	D	4819	GLY	C-N-CA	6.16	131.12	123.12
1	D	4856	PHE	CA-CB-CG	6.15	119.95	113.80
1	B	4819	GLY	CA-C-N	6.15	131.12	123.12
1	B	4819	GLY	C-N-CA	6.15	131.12	123.12
1	A	4856	PHE	CA-CB-CG	6.14	119.94	113.80
1	A	4787	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	4819	GLY	CA-C-N	6.11	131.07	123.12
1	A	4819	GLY	C-N-CA	6.11	131.07	123.12
1	C	4819	GLY	CA-C-N	6.11	131.07	123.12
1	C	4819	GLY	C-N-CA	6.11	131.07	123.12
1	B	4921	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	4921	PHE	CA-CB-CG	6.00	119.80	113.80
1	C	4921	PHE	CA-CB-CG	6.00	119.80	113.80
1	D	4581	LYS	CA-C-N	5.98	130.98	123.14
1	D	4581	LYS	C-N-CA	5.98	130.98	123.14
1	D	4921	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	4581	LYS	CA-C-N	5.97	130.96	123.14
1	A	4581	LYS	C-N-CA	5.97	130.96	123.14
1	C	4581	LYS	CA-C-N	5.96	130.94	123.14
1	C	4581	LYS	C-N-CA	5.96	130.94	123.14
1	B	4581	LYS	CA-C-N	5.93	130.91	123.14
1	B	4581	LYS	C-N-CA	5.93	130.91	123.14
1	B	4559	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	4873	ASP	CA-C-N	5.77	129.75	121.50
1	A	4873	ASP	C-N-CA	5.77	129.75	121.50
1	C	4873	ASP	CA-C-N	5.75	129.73	121.50
1	C	4873	ASP	C-N-CA	5.75	129.73	121.50
1	A	4829	SER	CA-C-N	5.75	127.80	120.56
1	A	4829	SER	C-N-CA	5.75	127.80	120.56
1	B	4829	SER	CA-C-N	5.75	127.80	120.56
1	B	4829	SER	C-N-CA	5.75	127.80	120.56
1	C	4829	SER	CA-C-N	5.75	127.80	120.56
1	C	4829	SER	C-N-CA	5.75	127.80	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4873	ASP	CA-C-N	5.74	129.71	121.50
1	D	4873	ASP	C-N-CA	5.74	129.71	121.50
1	D	4859	PHE	CA-CB-CG	5.74	119.54	113.80
1	D	4892	ARG	CD-NE-CZ	5.74	132.43	124.40
1	B	4873	ASP	CA-C-N	5.73	129.70	121.50
1	B	4873	ASP	C-N-CA	5.73	129.70	121.50
1	A	4892	ARG	CD-NE-CZ	5.73	132.42	124.40
1	D	4829	SER	CA-C-N	5.73	127.78	120.56
1	D	4829	SER	C-N-CA	5.73	127.78	120.56
1	C	4892	ARG	CD-NE-CZ	5.71	132.40	124.40
1	A	4563	ARG	CD-NE-CZ	5.70	132.37	124.40
1	A	4926	VAL	CA-C-N	5.70	127.67	120.72
1	A	4926	VAL	C-N-CA	5.70	127.67	120.72
1	B	4892	ARG	CD-NE-CZ	5.70	132.37	124.40
1	A	4878	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	4859	PHE	CA-CB-CG	5.68	119.48	113.80
1	D	4878	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	4859	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	4878	ASP	CA-CB-CG	5.67	118.27	112.60
1	C	4563	ARG	CD-NE-CZ	5.66	132.32	124.40
1	B	4563	ARG	CD-NE-CZ	5.65	132.31	124.40
1	D	4563	ARG	CD-NE-CZ	5.65	132.31	124.40
1	D	4926	VAL	CA-C-N	5.65	127.61	120.72
1	D	4926	VAL	C-N-CA	5.65	127.61	120.72
1	A	4854	VAL	CA-C-N	5.65	127.78	120.44
1	A	4854	VAL	C-N-CA	5.65	127.78	120.44
1	B	4926	VAL	CA-C-N	5.64	127.61	120.72
1	B	4926	VAL	C-N-CA	5.64	127.61	120.72
1	C	4926	VAL	CA-C-N	5.64	127.61	120.72
1	C	4926	VAL	C-N-CA	5.64	127.61	120.72
1	B	4859	PHE	CA-CB-CG	5.64	119.44	113.80
1	C	4878	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	4924	VAL	CA-C-N	5.59	127.72	120.56
1	B	4924	VAL	C-N-CA	5.59	127.72	120.56
1	C	4627	MET	CA-C-N	5.59	130.18	121.85
1	C	4627	MET	C-N-CA	5.59	130.18	121.85
1	B	4627	MET	CA-C-N	5.58	130.17	121.85
1	B	4627	MET	C-N-CA	5.58	130.17	121.85
1	A	4924	VAL	CA-C-N	5.58	127.70	120.56
1	A	4924	VAL	C-N-CA	5.58	127.70	120.56
1	C	4924	VAL	CA-C-N	5.57	127.69	120.56
1	C	4924	VAL	C-N-CA	5.57	127.69	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4917	ASP	CA-C-N	5.56	127.56	120.56
1	C	4917	ASP	C-N-CA	5.56	127.56	120.56
1	D	4924	VAL	CA-C-N	5.56	127.67	120.56
1	D	4924	VAL	C-N-CA	5.56	127.67	120.56
1	D	4627	MET	CA-C-N	5.55	130.13	121.85
1	D	4627	MET	C-N-CA	5.55	130.13	121.85
1	B	4917	ASP	CA-C-N	5.55	127.55	120.56
1	B	4917	ASP	C-N-CA	5.55	127.55	120.56
1	A	4917	ASP	CA-C-N	5.55	127.55	120.56
1	A	4917	ASP	C-N-CA	5.55	127.55	120.56
1	A	4627	MET	CA-C-N	5.54	130.11	121.85
1	A	4627	MET	C-N-CA	5.54	130.11	121.85
1	D	4917	ASP	CA-C-N	5.53	127.52	120.56
1	D	4917	ASP	C-N-CA	5.53	127.52	120.56
1	C	4845	ALA	CA-C-N	5.52	127.52	120.56
1	C	4845	ALA	C-N-CA	5.52	127.52	120.56
1	D	4845	ALA	CA-C-N	5.52	127.52	120.56
1	D	4845	ALA	C-N-CA	5.52	127.52	120.56
1	D	4854	VAL	CA-C-N	5.51	127.94	120.44
1	D	4854	VAL	C-N-CA	5.51	127.94	120.44
1	B	4845	ALA	CA-C-N	5.50	127.48	120.56
1	B	4845	ALA	C-N-CA	5.50	127.48	120.56
1	B	4782	VAL	CA-C-N	5.49	127.48	120.56
1	B	4782	VAL	C-N-CA	5.49	127.48	120.56
1	C	4900	GLU	CA-C-N	5.49	128.81	120.13
1	C	4900	GLU	C-N-CA	5.49	128.81	120.13
1	B	4854	VAL	CA-C-N	5.48	127.90	120.44
1	B	4854	VAL	C-N-CA	5.48	127.90	120.44
1	A	4920	PHE	CA-C-N	5.48	127.57	120.44
1	A	4920	PHE	C-N-CA	5.48	127.57	120.44
1	B	4920	PHE	CA-C-N	5.48	127.57	120.44
1	B	4920	PHE	C-N-CA	5.48	127.57	120.44
1	A	4845	ALA	CA-C-N	5.47	127.45	120.56
1	A	4845	ALA	C-N-CA	5.47	127.45	120.56
1	B	4877	ASP	CA-C-N	5.47	131.14	122.94
1	B	4877	ASP	C-N-CA	5.47	131.14	122.94
1	D	4877	ASP	CA-C-N	5.47	131.14	122.94
1	D	4877	ASP	C-N-CA	5.47	131.14	122.94
1	D	4900	GLU	CA-C-N	5.46	128.76	120.13
1	D	4900	GLU	C-N-CA	5.46	128.76	120.13
1	C	4877	ASP	CA-C-N	5.46	131.13	122.94
1	C	4877	ASP	C-N-CA	5.46	131.13	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4900	GLU	CA-C-N	5.46	128.75	120.13
1	B	4900	GLU	C-N-CA	5.46	128.75	120.13
1	A	4900	GLU	CA-C-N	5.46	128.75	120.13
1	A	4900	GLU	C-N-CA	5.46	128.75	120.13
1	A	4901	ILE	CA-C-N	5.46	128.99	120.75
1	A	4901	ILE	C-N-CA	5.46	128.99	120.75
1	B	4901	ILE	CA-C-N	5.46	128.99	120.75
1	B	4901	ILE	C-N-CA	5.46	128.99	120.75
1	C	4920	PHE	CA-C-N	5.45	127.53	120.44
1	C	4920	PHE	C-N-CA	5.45	127.53	120.44
1	A	4877	ASP	CA-C-N	5.45	131.12	122.94
1	A	4877	ASP	C-N-CA	5.45	131.12	122.94
1	C	4901	ILE	CA-C-N	5.44	128.97	120.75
1	C	4901	ILE	C-N-CA	5.44	128.97	120.75
1	B	4932	ILE	N-CA-CB	5.44	116.55	110.51
1	D	4920	PHE	CA-C-N	5.44	127.51	120.44
1	D	4920	PHE	C-N-CA	5.44	127.51	120.44
1	D	4901	ILE	CA-C-N	5.43	128.94	120.75
1	D	4901	ILE	C-N-CA	5.43	128.94	120.75
1	C	4930	ALA	CA-C-N	5.40	127.36	120.56
1	C	4930	ALA	C-N-CA	5.40	127.36	120.56
1	B	4886	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	C	4887	MET	CA-C-N	5.39	129.20	121.71
1	C	4887	MET	C-N-CA	5.39	129.20	121.71
1	A	4887	MET	CA-C-N	5.39	129.20	121.71
1	A	4887	MET	C-N-CA	5.39	129.20	121.71
1	D	4886	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	D	4887	MET	CA-C-N	5.39	129.20	121.71
1	D	4887	MET	C-N-CA	5.39	129.20	121.71
1	C	4932	ILE	N-CA-CB	5.38	116.49	110.51
1	A	4930	ALA	CA-C-N	5.38	127.34	120.56
1	A	4930	ALA	C-N-CA	5.38	127.34	120.56
1	D	4840	THR	CA-C-N	5.38	127.34	120.56
1	D	4840	THR	C-N-CA	5.38	127.34	120.56
1	D	4930	ALA	CA-C-N	5.38	127.34	120.56
1	D	4930	ALA	C-N-CA	5.38	127.34	120.56
1	D	4803	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	A	4886	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
1	B	4930	ALA	CA-C-N	5.37	127.32	120.56
1	B	4930	ALA	C-N-CA	5.37	127.32	120.56
1	B	4803	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	B	4887	MET	CA-C-N	5.36	129.16	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4887	MET	C-N-CA	5.36	129.16	121.71
1	C	4886	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	D	4935	LEU	CA-C-N	5.36	127.31	120.56
1	D	4935	LEU	C-N-CA	5.36	127.31	120.56
1	A	4803	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
1	C	4890	GLY	CA-C-N	5.35	127.41	120.56
1	C	4890	GLY	C-N-CA	5.35	127.41	120.56
1	C	4935	LEU	CA-C-N	5.35	127.30	120.56
1	C	4935	LEU	C-N-CA	5.35	127.30	120.56
1	A	4931	ILE	CA-C-N	5.35	127.30	120.56
1	A	4931	ILE	C-N-CA	5.35	127.30	120.56
1	B	4935	LEU	CA-C-N	5.34	127.29	120.56
1	B	4935	LEU	C-N-CA	5.34	127.29	120.56
1	D	4931	ILE	CA-C-N	5.34	127.29	120.56
1	D	4931	ILE	C-N-CA	5.34	127.29	120.56
1	D	4657	CYS	CA-C-N	5.34	127.29	120.56
1	D	4657	CYS	C-N-CA	5.34	127.29	120.56
1	B	4796	MET	CA-C-N	5.33	127.28	120.56
1	B	4796	MET	C-N-CA	5.33	127.28	120.56
1	B	4890	GLY	CA-C-N	5.33	127.38	120.56
1	B	4890	GLY	C-N-CA	5.33	127.38	120.56
1	C	4854	VAL	CA-C-N	5.33	127.69	120.44
1	C	4854	VAL	C-N-CA	5.33	127.69	120.44
1	B	4657	CYS	CA-C-N	5.33	127.28	120.56
1	B	4657	CYS	C-N-CA	5.33	127.28	120.56
1	C	4803	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
1	B	4840	THR	CA-C-N	5.32	127.27	120.56
1	B	4840	THR	C-N-CA	5.32	127.27	120.56
1	A	4840	THR	CA-C-N	5.32	127.26	120.56
1	A	4840	THR	C-N-CA	5.32	127.26	120.56
1	C	4840	THR	CA-C-N	5.32	127.26	120.56
1	C	4840	THR	C-N-CA	5.32	127.26	120.56
1	A	4657	CYS	CA-C-N	5.32	127.26	120.56
1	A	4657	CYS	C-N-CA	5.32	127.26	120.56
1	A	4890	GLY	CA-C-N	5.31	127.36	120.56
1	A	4890	GLY	C-N-CA	5.31	127.36	120.56
1	D	4896	GLY	CA-C-N	5.31	127.73	120.46
1	D	4896	GLY	C-N-CA	5.31	127.73	120.46
1	C	4826	ILE	CA-C-N	5.30	127.39	120.28
1	C	4826	ILE	C-N-CA	5.30	127.39	120.28
1	C	4884	LEU	CA-C-N	5.30	127.33	120.44
1	C	4884	LEU	C-N-CA	5.30	127.33	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4890	GLY	CA-C-N	5.30	127.34	120.56
1	D	4890	GLY	C-N-CA	5.30	127.34	120.56
1	C	4796	MET	CA-C-N	5.30	127.23	120.56
1	C	4796	MET	C-N-CA	5.30	127.23	120.56
1	C	4657	CYS	CA-C-N	5.29	127.23	120.56
1	C	4657	CYS	C-N-CA	5.29	127.23	120.56
1	A	4795	TYR	CA-C-N	5.29	127.64	120.44
1	A	4795	TYR	C-N-CA	5.29	127.64	120.44
1	A	4805	ASN	CA-C-N	5.29	129.15	120.63
1	A	4805	ASN	C-N-CA	5.29	129.15	120.63
1	B	4886	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	A	4896	GLY	CA-C-N	5.29	127.71	120.46
1	A	4896	GLY	C-N-CA	5.29	127.71	120.46
1	B	4896	GLY	CA-C-N	5.29	127.71	120.46
1	B	4896	GLY	C-N-CA	5.29	127.71	120.46
1	A	4935	LEU	CA-C-N	5.29	127.22	120.56
1	A	4935	LEU	C-N-CA	5.29	127.22	120.56
1	B	4812	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	C	4812	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	D	4796	MET	CA-C-N	5.29	127.22	120.56
1	D	4796	MET	C-N-CA	5.29	127.22	120.56
1	D	4886	HIS	ND1-CG-CD2	-5.28	100.83	106.10
1	A	4796	MET	CA-C-N	5.27	127.20	120.56
1	A	4796	MET	C-N-CA	5.27	127.20	120.56
1	B	4795	TYR	CA-C-N	5.27	127.60	120.44
1	B	4795	TYR	C-N-CA	5.27	127.60	120.44
1	C	4795	TYR	CA-C-N	5.27	127.61	120.44
1	C	4795	TYR	C-N-CA	5.27	127.61	120.44
1	C	4896	GLY	CA-C-N	5.27	127.68	120.46
1	C	4896	GLY	C-N-CA	5.27	127.68	120.46
1	D	4795	TYR	CA-C-N	5.27	127.60	120.44
1	D	4795	TYR	C-N-CA	5.27	127.60	120.44
1	B	4884	LEU	CA-C-N	5.26	127.28	120.44
1	B	4884	LEU	C-N-CA	5.26	127.28	120.44
1	B	4805	ASN	CA-C-N	5.26	129.09	120.63
1	B	4805	ASN	C-N-CA	5.26	129.09	120.63
1	B	4886	HIS	CG-CD2-NE2	5.26	112.46	107.20
1	B	4907	ASP	CA-C-N	5.26	127.32	120.28
1	B	4907	ASP	C-N-CA	5.26	127.32	120.28
1	B	4803	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	D	4884	LEU	CA-C-N	5.25	127.27	120.44
1	D	4884	LEU	C-N-CA	5.25	127.27	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4884	LEU	CA-C-N	5.25	127.27	120.44
1	A	4884	LEU	C-N-CA	5.25	127.27	120.44
1	D	4812	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	B	4650	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	D	4803	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	A	4803	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	C	4805	ASN	CA-C-N	5.24	129.07	120.63
1	C	4805	ASN	C-N-CA	5.24	129.07	120.63
1	C	4886	HIS	ND1-CG-CD2	-5.24	100.86	106.10
1	C	4628	VAL	CA-C-N	5.24	130.80	122.94
1	C	4628	VAL	C-N-CA	5.24	130.80	122.94
1	C	4789	PHE	N-CA-CB	5.24	117.60	110.01
1	A	4843	LEU	CA-C-N	5.23	127.29	120.28
1	A	4843	LEU	C-N-CA	5.23	127.29	120.28
1	D	4650	HIS	ND1-CG-CD2	-5.23	100.87	106.10
1	A	4789	PHE	N-CA-CB	5.23	117.59	110.01
1	A	4812	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	D	4628	VAL	CA-C-N	5.22	130.78	122.94
1	D	4628	VAL	C-N-CA	5.22	130.78	122.94
1	D	4886	HIS	CG-CD2-NE2	5.22	112.42	107.20
1	D	4789	PHE	N-CA-CB	5.22	117.58	110.01
1	A	4650	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	A	4886	HIS	CG-CD2-NE2	5.22	112.42	107.20
1	B	4856	PHE	N-CA-CB	5.22	117.58	110.01
1	C	4650	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	A	4886	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	B	4843	LEU	CA-C-N	5.22	127.28	120.28
1	B	4843	LEU	C-N-CA	5.22	127.28	120.28
1	C	4791	TYR	N-CA-CB	5.22	117.58	110.01
1	C	4843	LEU	CA-C-N	5.22	127.28	120.28
1	C	4843	LEU	C-N-CA	5.22	127.28	120.28
1	D	4791	TYR	N-CA-CB	5.21	117.57	110.01
1	D	4843	LEU	CA-C-N	5.21	127.27	120.28
1	D	4843	LEU	C-N-CA	5.21	127.27	120.28
1	A	4791	TYR	N-CA-CB	5.21	117.57	110.01
1	A	4907	ASP	CA-C-N	5.21	127.27	120.28
1	A	4907	ASP	C-N-CA	5.21	127.27	120.28
1	C	4907	ASP	CA-C-N	5.21	127.27	120.28
1	C	4907	ASP	C-N-CA	5.21	127.27	120.28
1	A	4842	GLY	CA-C-N	5.21	127.26	120.28
1	A	4842	GLY	C-N-CA	5.21	127.26	120.28
1	B	4789	PHE	N-CA-CB	5.21	117.57	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4907	ASP	CA-C-N	5.21	127.26	120.28
1	D	4907	ASP	C-N-CA	5.21	127.26	120.28
1	C	4803	HIS	ND1-CG-CD2	-5.21	100.89	106.10
1	D	4805	ASN	CA-C-N	5.21	129.02	120.63
1	D	4805	ASN	C-N-CA	5.21	129.02	120.63
1	A	4628	VAL	CA-C-N	5.21	130.75	122.94
1	A	4628	VAL	C-N-CA	5.21	130.75	122.94
1	B	4628	VAL	CA-C-N	5.20	130.74	122.94
1	B	4628	VAL	C-N-CA	5.20	130.74	122.94
1	B	4931	ILE	CA-C-N	5.20	127.31	120.60
1	B	4931	ILE	C-N-CA	5.20	127.31	120.60
1	B	4803	HIS	CG-CD2-NE2	5.20	112.40	107.20
1	C	4886	HIS	CG-CD2-NE2	5.20	112.40	107.20
1	B	4558	ASN	CA-C-N	5.20	127.19	120.44
1	B	4558	ASN	C-N-CA	5.20	127.19	120.44
1	C	4631	PHE	CA-C-N	5.20	128.25	120.87
1	C	4631	PHE	C-N-CA	5.20	128.25	120.87
1	A	4881	THR	CA-C-N	5.19	127.19	120.44
1	A	4881	THR	C-N-CA	5.19	127.19	120.44
1	B	4882	CYS	CA-C-N	5.19	127.19	120.44
1	B	4882	CYS	C-N-CA	5.19	127.19	120.44
1	C	4842	GLY	CA-C-N	5.19	127.24	120.28
1	C	4842	GLY	C-N-CA	5.19	127.24	120.28
1	C	4803	HIS	CG-CD2-NE2	5.19	112.39	107.20
1	C	4931	ILE	CA-C-N	5.19	127.29	120.60
1	C	4931	ILE	C-N-CA	5.19	127.29	120.60
1	A	4642	ALA	CA-C-N	5.19	127.18	120.44
1	A	4642	ALA	C-N-CA	5.19	127.18	120.44
1	D	4881	THR	CA-C-N	5.19	127.19	120.44
1	D	4881	THR	C-N-CA	5.19	127.19	120.44
1	B	4842	GLY	CA-C-N	5.19	127.23	120.28
1	B	4842	GLY	C-N-CA	5.19	127.23	120.28
1	A	4856	PHE	N-CA-CB	5.18	117.53	110.01
1	C	4883	TYR	CA-C-N	5.18	127.23	120.28
1	C	4883	TYR	C-N-CA	5.18	127.23	120.28
1	A	4803	HIS	CG-CD2-NE2	5.18	112.38	107.20
1	C	4569	LEU	CA-C-N	5.18	127.18	120.44
1	C	4569	LEU	C-N-CA	5.18	127.18	120.44
1	D	4803	HIS	CG-CD2-NE2	5.18	112.38	107.20
1	A	4883	TYR	CA-C-N	5.18	127.22	120.28
1	A	4883	TYR	C-N-CA	5.18	127.22	120.28
1	D	4786	ASP	CA-C-N	5.18	127.17	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4786	ASP	C-N-CA	5.18	127.17	120.44
1	B	4881	THR	CA-C-N	5.18	127.17	120.44
1	B	4881	THR	C-N-CA	5.18	127.17	120.44
1	D	4842	GLY	CA-C-N	5.18	127.22	120.28
1	D	4842	GLY	C-N-CA	5.18	127.22	120.28
1	B	4569	LEU	CA-C-N	5.18	127.17	120.44
1	B	4569	LEU	C-N-CA	5.18	127.17	120.44
1	D	4569	LEU	CA-C-N	5.18	127.17	120.44
1	D	4569	LEU	C-N-CA	5.18	127.17	120.44
1	A	4882	CYS	CA-C-N	5.17	127.16	120.44
1	A	4882	CYS	C-N-CA	5.17	127.16	120.44
1	B	4631	PHE	CA-C-N	5.17	128.21	120.87
1	B	4631	PHE	C-N-CA	5.17	128.21	120.87
1	B	4786	ASP	N-CA-CB	5.17	117.55	109.85
1	B	4836	GLN	CA-C-N	5.17	127.16	120.44
1	B	4836	GLN	C-N-CA	5.17	127.16	120.44
1	A	4799	SER	CA-C-N	5.16	127.15	120.44
1	A	4799	SER	C-N-CA	5.16	127.15	120.44
1	C	4882	CYS	CA-C-N	5.16	127.15	120.44
1	C	4882	CYS	C-N-CA	5.16	127.15	120.44
1	D	4883	TYR	CA-C-N	5.16	127.20	120.28
1	D	4883	TYR	C-N-CA	5.16	127.20	120.28
1	D	4631	PHE	CA-C-N	5.16	128.20	120.87
1	D	4631	PHE	C-N-CA	5.16	128.20	120.87
1	B	4575	PHE	CA-C-N	5.16	127.53	120.46
1	B	4575	PHE	C-N-CA	5.16	127.53	120.46
1	C	4575	PHE	CA-C-N	5.16	127.53	120.46
1	C	4575	PHE	C-N-CA	5.16	127.53	120.46
1	D	4575	PHE	CA-C-N	5.16	127.53	120.46
1	D	4575	PHE	C-N-CA	5.16	127.53	120.46
1	A	4631	PHE	CA-C-N	5.16	128.19	120.87
1	A	4631	PHE	C-N-CA	5.16	128.19	120.87
1	B	4797	VAL	N-CA-CB	5.16	116.58	110.55
1	B	4929	LEU	CA-C-N	5.15	127.19	120.28
1	B	4929	LEU	C-N-CA	5.15	127.19	120.28
1	D	4882	CYS	CA-C-N	5.15	127.14	120.44
1	D	4882	CYS	C-N-CA	5.15	127.14	120.44
1	B	4883	TYR	CA-C-N	5.15	127.18	120.28
1	B	4883	TYR	C-N-CA	5.15	127.18	120.28
1	A	4836	GLN	CA-C-N	5.15	127.13	120.44
1	A	4836	GLN	C-N-CA	5.15	127.13	120.44
1	C	4786	ASP	CA-C-N	5.15	127.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4786	ASP	C-N-CA	5.15	127.13	120.44
1	A	4569	LEU	CA-C-N	5.14	127.13	120.44
1	A	4569	LEU	C-N-CA	5.14	127.13	120.44
1	A	4575	PHE	CA-C-N	5.14	127.51	120.46
1	A	4575	PHE	C-N-CA	5.14	127.51	120.46
1	C	4881	THR	CA-C-N	5.14	127.13	120.44
1	C	4881	THR	C-N-CA	5.14	127.13	120.44
1	D	4929	LEU	CA-C-N	5.14	127.17	120.28
1	D	4929	LEU	C-N-CA	5.14	127.17	120.28
1	A	4786	ASP	CA-C-N	5.14	127.12	120.44
1	A	4786	ASP	C-N-CA	5.14	127.12	120.44
1	A	4848	VAL	CA-C-N	5.14	127.17	120.28
1	A	4848	VAL	C-N-CA	5.14	127.17	120.28
1	A	4902	GLU	N-CA-CB	5.14	117.59	110.04
1	B	4799	SER	CA-C-N	5.14	127.12	120.44
1	B	4799	SER	C-N-CA	5.14	127.12	120.44
1	B	4902	GLU	N-CA-CB	5.14	117.59	110.04
1	B	4642	ALA	CA-C-N	5.14	127.12	120.44
1	B	4642	ALA	C-N-CA	5.14	127.12	120.44
1	C	4650	HIS	CA-C-N	5.14	127.12	120.44
1	C	4650	HIS	C-N-CA	5.14	127.12	120.44
1	C	4836	GLN	CA-C-N	5.14	127.12	120.44
1	C	4836	GLN	C-N-CA	5.14	127.12	120.44
1	B	4786	ASP	CA-C-N	5.14	127.12	120.44
1	B	4786	ASP	C-N-CA	5.14	127.12	120.44
1	B	4566	ALA	CA-C-N	5.13	127.16	120.28
1	B	4566	ALA	C-N-CA	5.13	127.16	120.28
1	C	4902	GLU	N-CA-CB	5.13	117.59	110.04
1	C	4929	LEU	CA-C-N	5.13	127.16	120.28
1	C	4929	LEU	C-N-CA	5.13	127.16	120.28
1	D	4836	GLN	CA-C-N	5.13	127.11	120.44
1	D	4836	GLN	C-N-CA	5.13	127.11	120.44
1	A	4932	ILE	N-CA-CB	5.13	116.55	110.55
1	D	4932	ILE	N-CA-CB	5.13	116.55	110.55
1	C	4649	LEU	CA-C-N	5.13	127.11	120.44
1	C	4649	LEU	C-N-CA	5.13	127.11	120.44
1	A	4575	PHE	N-CA-CB	5.13	117.44	110.01
1	C	4848	VAL	CA-C-N	5.12	127.15	120.28
1	C	4848	VAL	C-N-CA	5.12	127.15	120.28
1	D	4650	HIS	CA-C-N	5.12	127.10	120.44
1	D	4650	HIS	C-N-CA	5.12	127.10	120.44
1	A	4929	LEU	CA-C-N	5.12	127.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4929	LEU	C-N-CA	5.12	127.15	120.28
1	B	4848	VAL	CA-C-N	5.12	127.14	120.28
1	B	4848	VAL	C-N-CA	5.12	127.14	120.28
1	C	4797	VAL	N-CA-CB	5.12	116.54	110.55
1	D	4642	ALA	CA-C-N	5.12	127.10	120.44
1	D	4642	ALA	C-N-CA	5.12	127.10	120.44
1	D	4797	VAL	N-CA-CB	5.12	116.54	110.55
1	D	4902	GLU	N-CA-CB	5.12	117.56	110.04
1	B	4660	GLY	CA-C-N	5.12	127.14	120.28
1	B	4660	GLY	C-N-CA	5.12	127.14	120.28
1	C	4799	SER	CA-C-N	5.12	127.09	120.44
1	C	4799	SER	C-N-CA	5.12	127.09	120.44
1	D	4799	SER	CA-C-N	5.12	127.09	120.44
1	D	4799	SER	C-N-CA	5.12	127.09	120.44
1	A	4650	HIS	CA-C-N	5.11	127.09	120.44
1	A	4650	HIS	C-N-CA	5.11	127.09	120.44
1	B	4650	HIS	CA-C-N	5.11	127.09	120.44
1	B	4650	HIS	C-N-CA	5.11	127.09	120.44
1	B	4650	HIS	N-CA-CB	5.11	117.42	110.01
1	D	4566	ALA	CA-C-N	5.11	127.13	120.28
1	D	4566	ALA	C-N-CA	5.11	127.13	120.28
1	D	4848	VAL	CA-C-N	5.11	127.13	120.28
1	D	4848	VAL	C-N-CA	5.11	127.13	120.28
1	B	4577	LEU	CA-C-N	5.11	127.64	120.28
1	B	4577	LEU	C-N-CA	5.11	127.64	120.28
1	A	4566	ALA	CA-C-N	5.11	127.12	120.28
1	A	4566	ALA	C-N-CA	5.11	127.12	120.28
1	C	4650	HIS	N-CA-CB	5.11	117.41	110.01
1	A	4650	HIS	N-CA-CB	5.10	117.41	110.01
1	B	4575	PHE	N-CA-CB	5.10	117.41	110.01
1	C	4642	ALA	CA-C-N	5.10	127.07	120.44
1	C	4642	ALA	C-N-CA	5.10	127.07	120.44
1	B	4783	ILE	CA-C-N	5.10	127.62	120.28
1	B	4783	ILE	C-N-CA	5.10	127.62	120.28
1	A	4562	LEU	CA-C-N	5.10	127.07	120.44
1	A	4562	LEU	C-N-CA	5.10	127.07	120.44
1	C	4575	PHE	N-CA-CB	5.10	117.40	110.01
1	C	4924	VAL	N-CA-CB	5.10	116.76	110.64
1	D	4812	HIS	CA-C-N	5.10	128.06	120.31
1	D	4812	HIS	C-N-CA	5.10	128.06	120.31
1	A	4649	LEU	CA-C-N	5.09	127.06	120.44
1	A	4649	LEU	C-N-CA	5.09	127.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4577	LEU	CA-C-N	5.09	127.61	120.28
1	A	4577	LEU	C-N-CA	5.09	127.61	120.28
1	A	4812	HIS	CA-C-N	5.09	128.05	120.31
1	A	4812	HIS	C-N-CA	5.09	128.05	120.31
1	B	4649	LEU	CA-C-N	5.09	127.06	120.44
1	B	4649	LEU	C-N-CA	5.09	127.06	120.44
1	B	4812	HIS	CA-C-N	5.09	128.05	120.31
1	B	4812	HIS	C-N-CA	5.09	128.05	120.31
1	C	4812	HIS	CA-C-N	5.09	128.05	120.31
1	C	4812	HIS	C-N-CA	5.09	128.05	120.31
1	C	4816	ILE	CA-C-N	5.09	127.06	120.44
1	C	4816	ILE	C-N-CA	5.09	127.06	120.44
1	C	4822	THR	CA-C-N	5.09	127.10	120.28
1	C	4822	THR	C-N-CA	5.09	127.10	120.28
1	D	4816	ILE	CA-C-N	5.09	127.06	120.44
1	D	4816	ILE	C-N-CA	5.09	127.06	120.44
1	A	4797	VAL	N-CA-CB	5.09	116.50	110.55
1	A	4822	THR	CA-C-N	5.09	127.10	120.28
1	A	4822	THR	C-N-CA	5.09	127.10	120.28
1	B	4789	PHE	CA-C-N	5.09	127.06	120.44
1	B	4789	PHE	C-N-CA	5.09	127.06	120.44
1	C	4855	ALA	CA-C-N	5.09	127.10	120.28
1	C	4855	ALA	C-N-CA	5.09	127.10	120.28
1	A	4789	PHE	CA-C-N	5.09	127.09	120.28
1	A	4789	PHE	C-N-CA	5.09	127.09	120.28
1	A	4855	ALA	CA-C-N	5.09	127.05	120.44
1	A	4855	ALA	C-N-CA	5.09	127.05	120.44
1	D	4575	PHE	N-CA-CB	5.09	117.38	110.01
1	B	4787	ASN	CA-C-N	5.08	127.05	120.44
1	B	4787	ASN	C-N-CA	5.08	127.05	120.44
1	C	4566	ALA	CA-C-N	5.08	127.09	120.28
1	C	4566	ALA	C-N-CA	5.08	127.09	120.28
1	D	4577	LEU	CA-C-N	5.08	127.60	120.28
1	D	4577	LEU	C-N-CA	5.08	127.60	120.28
1	B	4656	LEU	CA-C-N	5.08	127.05	120.44
1	B	4656	LEU	C-N-CA	5.08	127.05	120.44
1	A	4910	GLU	CA-C-N	5.08	127.50	120.29
1	A	4910	GLU	C-N-CA	5.08	127.50	120.29
1	C	4856	PHE	N-CA-CB	5.08	117.59	110.12
1	B	4573	ILE	CA-C-N	5.08	127.08	120.28
1	B	4573	ILE	C-N-CA	5.08	127.08	120.28
1	D	4573	ILE	CA-C-N	5.08	127.08	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4573	ILE	C-N-CA	5.08	127.08	120.28
1	A	4816	ILE	CA-C-N	5.07	127.03	120.44
1	A	4816	ILE	C-N-CA	5.07	127.03	120.44
1	B	4816	ILE	CA-C-N	5.07	127.03	120.44
1	B	4816	ILE	C-N-CA	5.07	127.03	120.44
1	D	4649	LEU	CA-C-N	5.07	127.04	120.44
1	D	4649	LEU	C-N-CA	5.07	127.04	120.44
1	D	4822	THR	CA-C-N	5.07	127.08	120.28
1	D	4822	THR	C-N-CA	5.07	127.08	120.28
1	B	4891	VAL	CA-C-N	5.07	127.58	120.28
1	B	4891	VAL	C-N-CA	5.07	127.58	120.28
1	A	4787	ASN	CA-C-N	5.07	127.03	120.44
1	A	4787	ASN	C-N-CA	5.07	127.03	120.44
1	B	4562	LEU	CA-C-N	5.07	127.03	120.44
1	B	4562	LEU	C-N-CA	5.07	127.03	120.44
1	D	4562	LEU	CA-C-N	5.07	127.03	120.44
1	D	4562	LEU	C-N-CA	5.07	127.03	120.44
1	D	4650	HIS	N-CA-CB	5.07	117.36	110.01
1	D	4855	ALA	CA-C-N	5.07	127.08	120.28
1	D	4855	ALA	C-N-CA	5.07	127.08	120.28
1	B	4855	ALA	CA-C-N	5.07	127.03	120.44
1	B	4855	ALA	C-N-CA	5.07	127.03	120.44
1	C	4570	ALA	CA-C-N	5.07	127.03	120.44
1	C	4570	ALA	C-N-CA	5.07	127.03	120.44
1	A	4643	LEU	N-CA-CB	5.07	117.36	110.01
1	C	4577	LEU	CA-C-N	5.06	127.57	120.28
1	C	4577	LEU	C-N-CA	5.06	127.57	120.28
1	C	4573	ILE	CA-C-N	5.06	127.06	120.28
1	C	4573	ILE	C-N-CA	5.06	127.06	120.28
1	D	4898	GLY	CA-C-N	5.06	127.02	120.44
1	D	4898	GLY	C-N-CA	5.06	127.02	120.44
1	A	4570	ALA	CA-C-N	5.06	127.02	120.44
1	A	4570	ALA	C-N-CA	5.06	127.02	120.44
1	D	4856	PHE	N-CA-CB	5.06	117.56	110.12
1	B	4822	THR	CA-C-N	5.06	127.06	120.28
1	B	4822	THR	C-N-CA	5.06	127.06	120.28
1	C	4898	GLY	CA-C-N	5.06	127.02	120.44
1	C	4898	GLY	C-N-CA	5.06	127.02	120.44
1	C	4576	ILE	CA-C-N	5.06	127.56	120.28
1	C	4576	ILE	C-N-CA	5.06	127.56	120.28
1	D	4787	ASN	N-CA-CB	5.06	117.34	110.01
1	D	4789	PHE	CA-C-N	5.06	127.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4789	PHE	C-N-CA	5.06	127.06	120.28
1	C	4789	PHE	CA-C-N	5.05	127.05	120.28
1	C	4789	PHE	C-N-CA	5.05	127.05	120.28
1	A	4573	ILE	CA-C-N	5.05	127.05	120.28
1	A	4573	ILE	C-N-CA	5.05	127.05	120.28
1	B	4576	ILE	CA-C-N	5.05	127.55	120.28
1	B	4576	ILE	C-N-CA	5.05	127.55	120.28
1	A	4576	ILE	CA-C-N	5.05	127.55	120.28
1	A	4576	ILE	C-N-CA	5.05	127.55	120.28
1	A	4898	GLY	CA-C-N	5.05	127.00	120.44
1	A	4898	GLY	C-N-CA	5.05	127.00	120.44
1	A	4891	VAL	CA-C-N	5.04	127.54	120.28
1	A	4891	VAL	C-N-CA	5.04	127.54	120.28
1	A	4931	ILE	N-CA-CB	5.04	116.45	110.55
1	C	4787	ASN	N-CA-CB	5.04	117.32	110.01
1	A	4802	GLY	CA-C-N	5.04	127.03	120.28
1	A	4802	GLY	C-N-CA	5.04	127.03	120.28
1	B	4559	PHE	N-CA-CB	5.04	117.31	110.01
1	C	4562	LEU	CA-C-N	5.04	126.99	120.44
1	C	4562	LEU	C-N-CA	5.04	126.99	120.44
1	D	4787	ASN	CA-C-N	5.04	126.99	120.44
1	D	4787	ASN	C-N-CA	5.04	126.99	120.44
1	D	4791	TYR	CA-C-N	5.04	127.03	120.28
1	D	4791	TYR	C-N-CA	5.04	127.03	120.28
1	A	4883	TYR	N-CA-CB	5.03	117.31	110.01
1	B	4799	SER	N-CA-CB	5.03	117.37	110.07
1	C	4891	VAL	CA-C-N	5.03	127.52	120.28
1	C	4891	VAL	C-N-CA	5.03	127.52	120.28
1	C	4931	ILE	N-CA-CB	5.03	116.44	110.55
1	D	4576	ILE	CA-C-N	5.03	127.52	120.28
1	D	4576	ILE	C-N-CA	5.03	127.52	120.28
1	B	4883	TYR	N-CA-CB	5.03	117.30	110.01
1	B	4898	GLY	CA-C-N	5.03	126.97	120.44
1	B	4898	GLY	C-N-CA	5.03	126.97	120.44
1	D	4883	TYR	N-CA-CB	5.03	117.30	110.01
1	A	4791	TYR	CA-C-N	5.03	127.01	120.28
1	A	4791	TYR	C-N-CA	5.03	127.01	120.28
1	B	4643	LEU	N-CA-CB	5.03	117.30	110.01
1	B	4787	ASN	N-CA-CB	5.03	117.30	110.01
1	C	4787	ASN	CA-C-N	5.03	126.97	120.44
1	C	4787	ASN	C-N-CA	5.03	126.97	120.44
1	D	4570	ALA	CA-C-N	5.03	126.97	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4570	ALA	C-N-CA	5.03	126.97	120.44
1	D	4891	VAL	CA-C-N	5.03	127.52	120.28
1	D	4891	VAL	C-N-CA	5.03	127.52	120.28
1	D	4931	ILE	N-CA-CB	5.03	116.43	110.55
1	B	4785	THR	CA-C-N	5.02	127.98	120.95
1	B	4785	THR	C-N-CA	5.02	127.98	120.95
1	A	4574	ASN	CA-C-N	5.02	126.97	120.44
1	A	4574	ASN	C-N-CA	5.02	126.97	120.44
1	B	4574	ASN	CA-C-N	5.02	126.97	120.44
1	B	4574	ASN	C-N-CA	5.02	126.97	120.44
1	C	4910	GLU	CA-C-N	5.02	127.42	120.29
1	C	4910	GLU	C-N-CA	5.02	127.42	120.29
1	D	4802	GLY	CA-C-N	5.02	127.01	120.28
1	D	4802	GLY	C-N-CA	5.02	127.01	120.28
1	B	4798	MET	CA-C-N	5.02	127.27	120.44
1	B	4798	MET	C-N-CA	5.02	127.27	120.44
1	A	4787	ASN	N-CA-CB	5.02	117.29	110.01
1	C	4802	GLY	CA-C-N	5.02	127.01	120.28
1	C	4802	GLY	C-N-CA	5.02	127.01	120.28
1	B	4570	ALA	CA-C-N	5.02	126.96	120.44
1	B	4570	ALA	C-N-CA	5.02	126.96	120.44
1	C	4791	TYR	CA-C-N	5.02	127.00	120.28
1	C	4791	TYR	C-N-CA	5.02	127.00	120.28
1	D	4910	GLU	CA-C-N	5.02	127.41	120.29
1	D	4910	GLU	C-N-CA	5.02	127.41	120.29
1	A	4658	ILE	N-CA-CB	5.01	116.41	110.55
1	D	4658	ILE	N-CA-CB	5.01	116.41	110.55
1	A	4849	TYR	N-CA-CB	5.01	117.48	110.12
1	D	4643	LEU	N-CA-CB	5.01	117.27	110.01
1	D	4799	SER	N-CA-CB	5.00	117.32	110.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4913	ARG	Sidechain
1	B	4913	ARG	Sidechain
1	C	4913	ARG	Sidechain
1	D	4913	ARG	Sidechain

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	A	35088	34734	34715	135	0
1	B	35088	34734	34715	135	0
1	C	35088	34734	34715	135	0
1	D	35088	34734	34715	140	0
2	E	832	829	831	1	0
2	F	832	829	831	1	0
2	G	832	829	831	1	0
2	H	832	829	831	1	0
3	A	104	164	164	0	0
3	B	104	164	164	0	0
3	C	104	164	164	0	0
3	D	104	164	164	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
All	All	144100	142908	142840	549	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 2.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:MET:HE2	1:B:3534:MET:HA	1.61	0.82
1:A:3534:MET:HE2	1:A:3534:MET:HA	1.61	0.82
1:C:3534:MET:HA	1:C:3534:MET:HE2	1.61	0.80
1:D:3534:MET:HE2	1:D:3534:MET:HA	1.61	0.80
1:C:4059:LEU:HD22	1:C:4170:ILE:HD13	1.70	0.74
1:A:4059:LEU:HD22	1:A:4170:ILE:HD13	1.70	0.73
1:D:4059:LEU:HD22	1:D:4170:ILE:HD13	1.70	0.73
1:B:4059:LEU:HD22	1:B:4170:ILE:HD13	1.70	0.72
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.71	0.72
1:A:2536:LEU:O	1:A:2536:LEU:HD23	1.89	0.72
1:C:1022:VAL:HG22	1:C:1023:PRO:HD2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2536:LEU:O	1:C:2536:LEU:HD23	1.89	0.72
1:D:2536:LEU:HD23	1:D:2536:LEU:O	1.89	0.71
1:B:2536:LEU:HD23	1:B:2536:LEU:O	1.89	0.71
1:D:1022:VAL:HG22	1:D:1023:PRO:HD2	1.71	0.71
1:B:1022:VAL:HG22	1:B:1023:PRO:HD2	1.71	0.70
1:B:2614:ILE:HG23	1:B:2619:LEU:HD11	1.78	0.66
1:C:2614:ILE:HG23	1:C:2619:LEU:HD11	1.79	0.65
1:D:2614:ILE:HG23	1:D:2619:LEU:HD11	1.79	0.64
1:D:20:VAL:HG21	1:D:202:MET:CE	2.28	0.64
1:C:20:VAL:HG21	1:C:202:MET:CE	2.28	0.64
1:A:20:VAL:HG21	1:A:202:MET:CE	2.28	0.64
1:A:2614:ILE:HG23	1:A:2619:LEU:HD11	1.79	0.63
1:B:20:VAL:HG21	1:B:202:MET:CE	2.28	0.63
1:D:20:VAL:HG21	1:D:202:MET:HE2	1.80	0.63
1:A:20:VAL:HG21	1:A:202:MET:HE2	1.80	0.62
1:B:20:VAL:HG21	1:B:202:MET:HE2	1.80	0.62
1:C:3002:LEU:O	1:C:3006:ILE:HD12	2.00	0.62
1:C:20:VAL:HG21	1:C:202:MET:HE2	1.80	0.62
1:D:3002:LEU:O	1:D:3006:ILE:HD12	2.00	0.62
1:B:3002:LEU:O	1:B:3006:ILE:HD12	2.00	0.62
1:A:14:LEU:HD21	1:A:165:VAL:HG22	1.82	0.61
1:C:2526:PHE:HE1	1:C:2558:VAL:HG22	1.66	0.61
1:B:14:LEU:HD21	1:B:165:VAL:HG22	1.82	0.61
1:B:2633:LEU:O	1:B:2633:LEU:HD23	2.01	0.61
1:C:2198:MET:N	1:C:2198:MET:HE2	2.15	0.61
1:D:2526:PHE:HE1	1:D:2558:VAL:HG22	1.66	0.61
1:A:2198:MET:N	1:A:2198:MET:HE2	2.15	0.61
1:A:3002:LEU:O	1:A:3006:ILE:HD12	2.00	0.60
1:B:2526:PHE:HE1	1:B:2558:VAL:HG22	1.66	0.60
1:B:2198:MET:HE2	1:B:2198:MET:N	2.15	0.60
1:C:14:LEU:HD21	1:C:165:VAL:HG22	1.82	0.60
1:D:14:LEU:HD21	1:D:165:VAL:HG22	1.82	0.60
1:D:2198:MET:HE2	1:D:2198:MET:N	2.15	0.60
1:A:2633:LEU:HD23	1:A:2633:LEU:O	2.01	0.60
1:C:2633:LEU:HD23	1:C:2633:LEU:O	2.01	0.60
1:A:2526:PHE:HE1	1:A:2558:VAL:HG22	1.66	0.60
1:D:2633:LEU:HD23	1:D:2633:LEU:O	2.01	0.59
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.85	0.58
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.85	0.58
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.85	0.58
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2616:PRO:HA	1:C:2619:LEU:HD13	1.86	0.58
1:D:2616:PRO:HA	1:D:2619:LEU:HD13	1.86	0.57
1:B:2616:PRO:HA	1:B:2619:LEU:HD13	1.86	0.57
1:A:69:LEU:HD21	1:A:202:MET:HE1	1.87	0.56
1:B:69:LEU:HD21	1:B:202:MET:HE1	1.87	0.56
1:A:2616:PRO:HA	1:A:2619:LEU:HD13	1.86	0.56
1:D:1518:CYS:C	1:D:1519:LEU:HD12	2.31	0.56
1:D:69:LEU:HD21	1:D:202:MET:HE1	1.87	0.55
1:A:1518:CYS:C	1:A:1519:LEU:HD12	2.31	0.55
1:B:1518:CYS:C	1:B:1519:LEU:HD12	2.31	0.55
1:C:1518:CYS:C	1:C:1519:LEU:HD12	2.31	0.55
1:C:69:LEU:HD21	1:C:202:MET:HE1	1.87	0.55
1:C:3865:VAL:HG11	1:C:3868:ARG:HB2	1.90	0.54
1:A:3865:VAL:HG11	1:A:3868:ARG:HB2	1.90	0.54
1:D:3865:VAL:HG11	1:D:3868:ARG:HB2	1.90	0.54
1:A:1299:GLN:OE1	1:A:1299:GLN:N	2.41	0.54
1:C:1299:GLN:OE1	1:C:1299:GLN:N	2.41	0.54
1:D:1299:GLN:N	1:D:1299:GLN:OE1	2.41	0.54
1:B:3865:VAL:HG11	1:B:3868:ARG:HB2	1.90	0.53
1:A:4241:THR:HG21	1:A:4989:MET:HE1	1.90	0.53
1:B:1299:GLN:N	1:B:1299:GLN:OE1	2.41	0.53
1:B:3162:GLN:OE1	1:B:3218:VAL:HG13	2.09	0.53
1:B:4241:THR:HG21	1:B:4989:MET:HE1	1.90	0.53
1:D:3162:GLN:OE1	1:D:3218:VAL:HG13	2.09	0.53
1:A:3162:GLN:OE1	1:A:3218:VAL:HG13	2.09	0.53
1:D:4241:THR:HG21	1:D:4989:MET:HE1	1.90	0.53
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.91	0.52
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	1.91	0.52
1:B:4201:ASN:OD1	1:B:4993:MET:HE1	2.10	0.52
1:C:3162:GLN:OE1	1:C:3218:VAL:HG13	2.09	0.52
1:C:4201:ASN:OD1	1:C:4993:MET:HE1	2.10	0.52
1:A:984:LEU:HD21	1:A:1055:PRO:CB	2.40	0.52
1:B:984:LEU:HD21	1:B:1055:PRO:CB	2.40	0.52
1:D:4201:ASN:OD1	1:D:4993:MET:HE1	2.10	0.52
1:A:4201:ASN:OD1	1:A:4993:MET:HE1	2.10	0.52
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	1.91	0.51
1:D:2554:LEU:HD23	1:D:2558:VAL:HG21	1.92	0.51
1:C:984:LEU:HD21	1:C:1055:PRO:CB	2.40	0.51
1:C:4241:THR:HG21	1:C:4989:MET:HE1	1.90	0.51
1:B:2619:LEU:HD12	1:B:2619:LEU:N	2.26	0.51
1:C:2554:LEU:HD23	1:C:2558:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2479:LEU:HD23	1:A:2479:LEU:H	1.75	0.51
1:D:2578:MET:HA	1:D:2578:MET:HE2	1.93	0.51
1:D:2599:GLN:O	1:D:2603:ILE:HD12	2.11	0.51
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.91	0.51
1:B:2554:LEU:HD23	1:B:2558:VAL:HG21	1.92	0.51
1:B:2599:GLN:O	1:B:2603:ILE:HD12	2.11	0.51
1:D:984:LEU:HD21	1:D:1055:PRO:CB	2.40	0.51
1:D:2479:LEU:H	1:D:2479:LEU:HD23	1.75	0.51
1:A:367:LEU:HD12	1:A:368:ARG:N	2.26	0.51
1:D:4690:GLU:N	1:D:4690:GLU:OE1	2.44	0.51
1:B:4690:GLU:N	1:B:4690:GLU:OE1	2.44	0.50
1:A:2578:MET:HE2	1:A:2578:MET:HA	1.93	0.50
1:B:2578:MET:HA	1:B:2578:MET:HE2	1.93	0.50
1:C:2619:LEU:N	1:C:2619:LEU:HD12	2.26	0.50
1:D:2619:LEU:HD12	1:D:2619:LEU:N	2.26	0.50
1:A:2554:LEU:HD23	1:A:2558:VAL:HG21	1.92	0.50
1:B:908:VAL:HG13	1:B:909:ASN:H	1.77	0.50
1:C:367:LEU:HD12	1:C:368:ARG:N	2.26	0.50
1:A:2599:GLN:O	1:A:2603:ILE:HD12	2.11	0.50
1:B:2479:LEU:H	1:B:2479:LEU:HD23	1.76	0.50
1:C:2479:LEU:HD23	1:C:2479:LEU:H	1.76	0.50
1:C:2599:GLN:O	1:C:2603:ILE:HD12	2.11	0.50
1:C:4690:GLU:OE1	1:C:4690:GLU:N	2.44	0.50
1:D:367:LEU:HD12	1:D:368:ARG:N	2.26	0.50
1:A:2507:ASP:C	1:A:2507:ASP:OD1	2.55	0.50
1:A:2702:CYS:O	1:A:2706:ILE:HG22	2.12	0.50
1:A:4690:GLU:OE1	1:A:4690:GLU:N	2.44	0.50
1:D:140:ASP:OD1	1:D:142:THR:HG22	2.12	0.50
1:A:140:ASP:OD1	1:A:142:THR:HG22	2.12	0.50
1:A:2619:LEU:N	1:A:2619:LEU:HD12	2.26	0.50
1:C:2310:CYS:HB3	1:C:2313:LEU:HD23	1.93	0.50
1:C:2578:MET:HE2	1:C:2578:MET:HA	1.93	0.50
1:D:908:VAL:HG13	1:D:909:ASN:H	1.77	0.50
1:A:2526:PHE:CE1	1:A:2558:VAL:HG13	2.47	0.50
1:D:2526:PHE:CE1	1:D:2558:VAL:HG13	2.47	0.50
1:D:2702:CYS:O	1:D:2706:ILE:HG22	2.11	0.50
1:B:367:LEU:HD12	1:B:368:ARG:N	2.26	0.49
1:C:2507:ASP:C	1:C:2507:ASP:OD1	2.55	0.49
1:B:3106:MET:HE2	1:B:3106:MET:HA	1.94	0.49
1:C:2526:PHE:CE1	1:C:2558:VAL:HG13	2.47	0.49
1:B:2507:ASP:OD1	1:B:2507:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2225:PHE:N	1:D:2225:PHE:CD1	2.80	0.49
1:A:908:VAL:HG13	1:A:909:ASN:H	1.77	0.49
1:B:2310:CYS:HB3	1:B:2313:LEU:HD23	1.93	0.49
1:C:2862:LEU:O	1:C:2865:VAL:HG22	2.12	0.49
1:C:3106:MET:HE2	1:C:3106:MET:HA	1.94	0.49
1:C:3856:LEU:C	1:C:3856:LEU:HD13	2.38	0.49
1:A:2377:LEU:C	1:A:2377:LEU:HD23	2.38	0.49
1:A:2862:LEU:O	1:A:2865:VAL:HG22	2.12	0.49
1:A:3856:LEU:C	1:A:3856:LEU:HD13	2.38	0.49
1:B:2862:LEU:O	1:B:2865:VAL:HG22	2.12	0.49
1:C:908:VAL:HG13	1:C:909:ASN:H	1.77	0.49
1:D:2507:ASP:C	1:D:2507:ASP:OD1	2.55	0.49
1:A:2310:CYS:HB3	1:A:2313:LEU:HD23	1.93	0.49
1:B:2225:PHE:N	1:B:2225:PHE:CD1	2.79	0.49
1:B:2526:PHE:CE1	1:B:2558:VAL:HG13	2.47	0.49
1:B:2702:CYS:O	1:B:2706:ILE:HG22	2.12	0.49
1:B:3858:MET:SD	1:B:3858:MET:C	2.96	0.49
1:C:140:ASP:OD1	1:C:142:THR:HG22	2.12	0.49
1:D:2310:CYS:HB3	1:D:2313:LEU:HD23	1.93	0.49
1:D:2862:LEU:O	1:D:2865:VAL:HG22	2.12	0.49
1:C:2377:LEU:C	1:C:2377:LEU:HD23	2.38	0.49
1:C:3858:MET:SD	1:C:3858:MET:C	2.96	0.49
1:D:3856:LEU:HD13	1:D:3856:LEU:C	2.38	0.49
1:B:140:ASP:OD1	1:B:142:THR:HG22	2.12	0.49
1:B:1281:ASN:C	1:B:1281:ASN:OD1	2.56	0.49
1:D:3858:MET:SD	1:D:3858:MET:C	2.96	0.49
1:A:3858:MET:SD	1:A:3858:MET:C	2.96	0.49
1:B:2911:LEU:O	1:B:2911:LEU:HD12	2.13	0.49
1:B:3856:LEU:HD13	1:B:3856:LEU:C	2.38	0.49
1:C:3006:ILE:HD12	1:C:3006:ILE:H	1.78	0.49
1:A:457:GLU:N	1:A:457:GLU:OE1	2.46	0.48
1:A:2911:LEU:HD12	1:A:2911:LEU:O	2.13	0.48
1:C:1281:ASN:OD1	1:C:1281:ASN:C	2.56	0.48
1:D:2377:LEU:HD23	1:D:2377:LEU:C	2.38	0.48
1:D:3805:LEU:HD11	1:D:3816:MET:HE1	1.95	0.48
1:A:1108:GLU:OE1	1:A:1108:GLU:N	2.47	0.48
1:A:1281:ASN:OD1	1:A:1281:ASN:C	2.56	0.48
1:B:984:LEU:HD21	1:B:1055:PRO:HB3	1.95	0.48
1:B:2377:LEU:C	1:B:2377:LEU:HD23	2.38	0.48
1:C:457:GLU:N	1:C:457:GLU:OE1	2.47	0.48
1:C:2702:CYS:O	1:C:2706:ILE:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ALA:HB1	1:D:312:THR:HG21	1.95	0.48
2:E:60:GLU:N	2:E:60:GLU:OE1	2.46	0.48
1:A:3805:LEU:HD11	1:A:3816:MET:HE1	1.95	0.48
1:C:2911:LEU:HD12	1:C:2911:LEU:O	2.13	0.48
1:D:457:GLU:N	1:D:457:GLU:OE1	2.47	0.48
1:A:3106:MET:HA	1:A:3106:MET:HE2	1.94	0.48
1:B:457:GLU:OE1	1:B:457:GLU:N	2.46	0.48
1:B:1193:SER:C	1:B:1194:LEU:HD12	2.39	0.48
1:B:3006:ILE:HD12	1:B:3006:ILE:H	1.78	0.48
1:C:984:LEU:HD21	1:C:1055:PRO:HB3	1.95	0.48
2:G:60:GLU:N	2:G:60:GLU:OE1	2.46	0.48
1:A:307:ALA:HB1	1:A:312:THR:HG21	1.95	0.48
1:B:1108:GLU:N	1:B:1108:GLU:OE1	2.46	0.48
1:C:3043:PHE:CD2	1:C:3075:LEU:HD11	2.49	0.48
1:A:1193:SER:C	1:A:1194:LEU:HD12	2.39	0.48
1:A:984:LEU:HD21	1:A:1055:PRO:HB3	1.95	0.48
1:A:2607:LEU:O	1:A:2607:LEU:HD23	2.14	0.48
1:C:3971:GLY:N	1:C:3972:PRO:HA	2.29	0.48
1:D:1193:SER:C	1:D:1194:LEU:HD12	2.39	0.48
1:D:1281:ASN:OD1	1:D:1281:ASN:C	2.56	0.48
1:D:3106:MET:HA	1:D:3106:MET:HE2	1.94	0.48
1:A:2225:PHE:CD1	1:A:2225:PHE:N	2.79	0.48
1:A:3867:ASN:O	1:A:3868:ARG:C	2.57	0.48
1:B:2607:LEU:HD23	1:B:2607:LEU:O	2.14	0.48
1:C:2225:PHE:N	1:C:2225:PHE:CD1	2.79	0.48
1:D:3043:PHE:CD2	1:D:3075:LEU:HD11	2.49	0.48
1:B:3043:PHE:CD2	1:B:3075:LEU:HD11	2.49	0.48
1:C:3805:LEU:HD11	1:C:3816:MET:HE1	1.95	0.48
1:A:3971:GLY:N	1:A:3972:PRO:HA	2.29	0.48
1:B:3867:ASN:O	1:B:3868:ARG:C	2.57	0.48
1:B:3971:GLY:N	1:B:3972:PRO:HA	2.29	0.48
1:C:1193:SER:C	1:C:1194:LEU:HD12	2.39	0.48
1:D:2607:LEU:HD23	1:D:2607:LEU:O	2.14	0.48
1:D:3006:ILE:HD12	1:D:3006:ILE:H	1.78	0.48
1:D:3867:ASN:O	1:D:3868:ARG:C	2.57	0.48
2:H:60:GLU:OE1	2:H:60:GLU:N	2.46	0.48
1:A:3131:TYR:OH	1:A:3136:LEU:HD13	2.14	0.47
1:D:2911:LEU:HD12	1:D:2911:LEU:O	2.13	0.47
1:D:984:LEU:HD21	1:D:1055:PRO:HB3	1.95	0.47
2:F:60:GLU:OE1	2:F:60:GLU:N	2.46	0.47
1:D:3971:GLY:N	1:D:3972:PRO:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3006:ILE:HD12	1:A:3006:ILE:H	1.78	0.47
1:A:3273:THR:O	1:A:3277:LEU:HD22	2.15	0.47
1:B:3131:TYR:OH	1:B:3136:LEU:HD13	2.14	0.47
1:C:1108:GLU:OE1	1:C:1108:GLU:N	2.47	0.47
1:B:3805:LEU:HD11	1:B:3816:MET:HE1	1.95	0.47
1:D:4240:ASP:C	1:D:4240:ASP:OD1	2.58	0.47
1:C:307:ALA:HB1	1:C:312:THR:HG21	1.96	0.47
1:A:4240:ASP:C	1:A:4240:ASP:OD1	2.58	0.47
1:B:307:ALA:HB1	1:B:312:THR:HG21	1.96	0.47
1:C:2607:LEU:HD23	1:C:2607:LEU:O	2.14	0.47
1:C:4731:ILE:HG23	1:C:4732:PHE:HD1	1.80	0.47
1:D:1108:GLU:N	1:D:1108:GLU:OE1	2.46	0.47
1:D:3273:THR:O	1:D:3277:LEU:HD22	2.15	0.47
1:B:2522:LEU:HD22	1:B:2527:LEU:HD21	1.97	0.47
1:B:4731:ILE:HG23	1:B:4732:PHE:HD1	1.80	0.47
1:C:4576:ILE:HG23	1:C:4639:MET:HE3	1.97	0.47
1:B:307:ALA:CB	1:B:312:THR:HG21	2.45	0.47
1:B:3518:LEU:HD21	1:B:3603:LEU:HD21	1.96	0.47
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.97	0.47
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.97	0.47
1:C:307:ALA:CB	1:C:312:THR:HG21	2.45	0.47
1:D:3443:ILE:HG22	1:D:3447:LYS:HD3	1.97	0.47
1:D:3518:LEU:HD21	1:D:3603:LEU:HD21	1.96	0.47
1:A:3043:PHE:CD2	1:A:3075:LEU:HD11	2.49	0.46
1:A:3443:ILE:HG22	1:A:3447:LYS:HD3	1.97	0.46
1:C:299:LEU:HD13	1:C:378:LEU:HG	1.97	0.46
1:C:3131:TYR:OH	1:C:3136:LEU:HD13	2.14	0.46
1:D:4731:ILE:HG23	1:D:4732:PHE:HD1	1.80	0.46
1:B:2636:PHE:N	1:B:2636:PHE:CD1	2.82	0.46
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.97	0.46
1:A:3518:LEU:HD21	1:A:3603:LEU:HD21	1.96	0.46
1:A:4576:ILE:HG23	1:A:4639:MET:HE3	1.97	0.46
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.97	0.46
1:C:3518:LEU:HD21	1:C:3603:LEU:HD21	1.96	0.46
1:C:3867:ASN:O	1:C:3868:ARG:C	2.57	0.46
1:D:307:ALA:CB	1:D:312:THR:HG21	2.45	0.46
1:A:307:ALA:CB	1:A:312:THR:HG21	2.45	0.46
1:A:4731:ILE:HG23	1:A:4732:PHE:HD1	1.80	0.46
1:B:4576:ILE:HG23	1:B:4639:MET:HE3	1.97	0.46
1:C:3443:ILE:HG22	1:C:3447:LYS:HD3	1.97	0.46
1:A:2522:LEU:HD22	1:A:2527:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HD13	1:B:378:LEU:HG	1.97	0.46
1:B:3050:VAL:O	1:B:3050:VAL:HG22	2.16	0.46
1:B:3443:ILE:HG22	1:B:3447:LYS:HD3	1.97	0.46
1:C:4240:ASP:OD1	1:C:4240:ASP:C	2.58	0.46
1:A:3955:MET:HE1	1:A:4016:LEU:HA	1.98	0.46
1:C:1285:GLU:N	1:C:1285:GLU:OE1	2.49	0.46
1:D:3131:TYR:OH	1:D:3136:LEU:HD13	2.14	0.46
1:C:3273:THR:O	1:C:3277:LEU:HD22	2.15	0.46
1:D:299:LEU:HD13	1:D:378:LEU:HG	1.97	0.46
1:D:2479:LEU:HD23	1:D:2479:LEU:N	2.31	0.46
1:C:2479:LEU:HD23	1:C:2479:LEU:N	2.31	0.46
1:C:2522:LEU:HD22	1:C:2527:LEU:HD21	1.97	0.46
1:A:2636:PHE:N	1:A:2636:PHE:CD1	2.82	0.46
1:A:4245:MET:CE	1:A:4989:MET:HE2	2.46	0.46
1:B:1741:GLU:OE2	1:B:1767:VAL:HG11	2.16	0.46
1:B:3273:THR:O	1:B:3277:LEU:HD22	2.15	0.46
1:A:3050:VAL:HG22	1:A:3050:VAL:O	2.16	0.46
1:B:2479:LEU:HD23	1:B:2479:LEU:N	2.31	0.46
1:B:3955:MET:HE1	1:B:4016:LEU:HA	1.98	0.46
1:C:3050:VAL:HG22	1:C:3050:VAL:O	2.16	0.46
1:D:3955:MET:HE1	1:D:4016:LEU:HA	1.98	0.46
1:B:1285:GLU:OE1	1:B:1285:GLU:N	2.49	0.45
1:B:4240:ASP:OD1	1:B:4240:ASP:C	2.58	0.45
1:D:1285:GLU:OE1	1:D:1285:GLU:N	2.49	0.45
1:D:2390:PRO:O	1:D:2391:ALA:HB3	2.16	0.45
1:D:4576:ILE:HG23	1:D:4639:MET:HE3	1.97	0.45
1:A:4241:THR:CG2	1:A:4989:MET:HE1	2.47	0.45
1:B:2390:PRO:O	1:B:2391:ALA:HB3	2.16	0.45
1:B:4245:MET:CE	1:B:4989:MET:HE2	2.46	0.45
1:C:2390:PRO:O	1:C:2391:ALA:HB3	2.16	0.45
1:D:4245:MET:CE	1:D:4989:MET:HE2	2.46	0.45
1:B:4241:THR:CG2	1:B:4989:MET:HE1	2.47	0.45
1:C:4245:MET:CE	1:C:4989:MET:HE2	2.46	0.45
1:D:2025:GLU:OE1	1:D:2025:GLU:HA	2.16	0.45
1:D:4241:THR:CG2	1:D:4989:MET:HE1	2.47	0.45
1:C:3955:MET:HE1	1:C:4016:LEU:HA	1.98	0.45
1:D:2636:PHE:CD1	1:D:2636:PHE:N	2.82	0.45
1:A:299:LEU:HD13	1:A:378:LEU:HG	1.97	0.45
1:A:1285:GLU:N	1:A:1285:GLU:OE1	2.49	0.45
1:D:1741:GLU:OE2	1:D:1767:VAL:HG11	2.16	0.45
1:D:2522:LEU:HD22	1:D:2527:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:GLU:OE2	1:A:1767:VAL:HG11	2.16	0.45
1:A:2479:LEU:HD23	1:A:2479:LEU:N	2.31	0.45
1:B:1783:VAL:O	1:B:1783:VAL:HG22	2.16	0.45
1:C:1741:GLU:OE1	1:C:1741:GLU:HA	2.17	0.45
1:D:1783:VAL:O	1:D:1783:VAL:HG22	2.16	0.45
1:C:950:LEU:HD12	1:C:950:LEU:O	2.17	0.45
1:C:1741:GLU:OE2	1:C:1767:VAL:HG11	2.16	0.45
1:D:3508:SER:OG	1:D:3510:ILE:HG22	2.17	0.45
1:C:2819:TRP:O	1:C:2820:GLU:HG3	2.17	0.45
1:D:1741:GLU:OE1	1:D:1741:GLU:HA	2.17	0.45
1:A:2025:GLU:OE1	1:A:2025:GLU:HA	2.16	0.45
1:A:2390:PRO:O	1:A:2391:ALA:HB3	2.16	0.45
1:A:1741:GLU:HA	1:A:1741:GLU:OE1	2.17	0.45
1:B:1741:GLU:OE1	1:B:1741:GLU:HA	2.17	0.44
1:C:4241:THR:CG2	1:C:4989:MET:HE1	2.47	0.44
1:A:950:LEU:HD12	1:A:950:LEU:O	2.17	0.44
1:A:3343:GLN:O	1:A:3346:VAL:HG22	2.18	0.44
1:B:2025:GLU:HA	1:B:2025:GLU:OE1	2.16	0.44
1:C:1783:VAL:HG22	1:C:1783:VAL:O	2.16	0.44
1:D:950:LEU:HD12	1:D:950:LEU:O	2.17	0.44
1:D:3207:GLU:HG2	1:D:3246:LEU:HD22	1.99	0.44
1:A:3207:GLU:HG2	1:A:3246:LEU:HD22	1.99	0.44
1:A:3508:SER:OG	1:A:3510:ILE:HG22	2.17	0.44
1:A:4737:ILE:N	1:A:4737:ILE:HD13	2.33	0.44
1:B:3508:SER:OG	1:B:3510:ILE:HG22	2.17	0.44
1:D:4097:MET:HE2	1:D:4097:MET:N	2.32	0.44
1:C:2636:PHE:N	1:C:2636:PHE:CD1	2.83	0.44
1:C:3343:GLN:O	1:C:3346:VAL:HG22	2.18	0.44
1:C:4097:MET:N	1:C:4097:MET:HE2	2.32	0.44
1:C:3003:LEU:HD12	1:C:3003:LEU:O	2.18	0.44
1:D:3003:LEU:HD12	1:D:3003:LEU:O	2.18	0.44
1:A:3003:LEU:HD12	1:A:3003:LEU:O	2.18	0.44
1:C:2025:GLU:OE1	1:C:2025:GLU:HA	2.16	0.44
1:C:2386:ILE:N	1:C:2386:ILE:HD13	2.33	0.44
1:D:3050:VAL:O	1:D:3050:VAL:HG22	2.16	0.44
1:A:4027:LEU:HD22	1:A:4044:MET:HE2	2.00	0.44
1:B:950:LEU:O	1:B:950:LEU:HD12	2.17	0.44
1:B:4737:ILE:HD13	1:B:4737:ILE:N	2.33	0.44
1:C:3207:GLU:HG2	1:C:3246:LEU:HD22	2.00	0.44
1:D:2819:TRP:O	1:D:2820:GLU:HG3	2.17	0.44
1:B:4027:LEU:HD22	1:B:4044:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2643:LEU:O	1:C:2643:LEU:HD23	2.18	0.44
1:A:2819:TRP:O	1:A:2820:GLU:HG3	2.17	0.44
1:A:4166:LEU:N	1:A:4166:LEU:HD23	2.33	0.44
1:B:4097:MET:HE2	1:B:4097:MET:N	2.32	0.44
1:C:103:TYR:CE1	1:C:163:VAL:HG22	2.53	0.44
1:C:4737:ILE:N	1:C:4737:ILE:HD13	2.33	0.44
1:A:295:GLU:N	1:A:295:GLU:OE1	2.51	0.43
1:A:2643:LEU:HD23	1:A:2643:LEU:O	2.18	0.43
1:B:103:TYR:CE1	1:B:163:VAL:HG22	2.53	0.43
1:B:2517:PHE:CD1	1:B:2517:PHE:C	2.96	0.43
1:B:2819:TRP:O	1:B:2820:GLU:HG3	2.17	0.43
1:B:3343:GLN:O	1:B:3346:VAL:HG22	2.18	0.43
1:C:3508:SER:OG	1:C:3510:ILE:HG22	2.17	0.43
1:A:981:GLN:HA	1:A:984:LEU:HD23	1.99	0.43
1:C:2517:PHE:C	1:C:2517:PHE:CD1	2.96	0.43
1:D:295:GLU:N	1:D:295:GLU:OE1	2.51	0.43
1:D:3343:GLN:O	1:D:3346:VAL:HG22	2.18	0.43
1:D:4737:ILE:HD13	1:D:4737:ILE:N	2.33	0.43
1:A:1783:VAL:HG22	1:A:1783:VAL:O	2.16	0.43
1:A:4231:MET:HE2	1:A:4231:MET:HA	2.00	0.43
1:A:4743:MET:HE2	1:A:4743:MET:HB3	1.96	0.43
1:B:2165:LEU:HA	1:B:2168:VAL:HG12	2.01	0.43
1:B:4231:MET:HE2	1:B:4231:MET:HA	2.01	0.43
1:D:3456:GLN:O	1:D:3460:VAL:HG22	2.19	0.43
1:A:103:TYR:CE1	1:A:163:VAL:HG22	2.53	0.43
1:A:3456:GLN:O	1:A:3460:VAL:HG22	2.19	0.43
1:B:3207:GLU:HG2	1:B:3246:LEU:HD22	1.99	0.43
1:C:3319:ILE:CD1	1:C:3338:LEU:HD21	2.49	0.43
1:D:236:ALA:O	1:D:237:ASP:OD1	2.36	0.43
1:D:4231:MET:HE2	1:D:4231:MET:HA	2.00	0.43
1:A:4097:MET:N	1:A:4097:MET:HE2	2.32	0.43
1:B:2643:LEU:HD23	1:B:2643:LEU:O	2.18	0.43
1:B:3456:GLN:O	1:B:3460:VAL:HG22	2.19	0.43
1:C:236:ALA:O	1:C:237:ASP:OD1	2.36	0.43
1:C:295:GLU:N	1:C:295:GLU:OE1	2.51	0.43
1:D:2386:ILE:HD13	1:D:2386:ILE:N	2.33	0.43
1:A:2165:LEU:HA	1:A:2168:VAL:HG12	2.01	0.43
1:C:3456:GLN:O	1:C:3460:VAL:HG22	2.19	0.43
1:C:4027:LEU:HD22	1:C:4044:MET:HE2	2.00	0.43
1:C:4166:LEU:HD23	1:C:4166:LEU:N	2.33	0.43
1:D:862:VAL:O	1:D:863:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:981:GLN:HA	1:D:984:LEU:HD23	2.00	0.43
1:B:981:GLN:HA	1:B:984:LEU:HD23	2.00	0.43
1:B:3003:LEU:HD12	1:B:3003:LEU:O	2.18	0.43
1:C:3517:MET:O	1:C:3517:MET:HG3	2.19	0.43
1:D:721:LEU:HD12	1:D:730:VAL:HG21	2.01	0.43
1:B:2386:ILE:HD13	1:B:2386:ILE:N	2.33	0.43
1:B:4166:LEU:N	1:B:4166:LEU:HD23	2.33	0.43
1:C:2165:LEU:HA	1:C:2168:VAL:HG12	2.01	0.43
1:D:103:TYR:CE1	1:D:163:VAL:HG22	2.53	0.43
1:D:2643:LEU:HD23	1:D:2643:LEU:O	2.18	0.43
1:D:3319:ILE:CD1	1:D:3338:LEU:HD21	2.49	0.43
1:D:4027:LEU:HD22	1:D:4044:MET:HE2	2.00	0.43
1:A:862:VAL:O	1:A:863:LEU:C	2.62	0.43
1:B:3319:ILE:CD1	1:B:3338:LEU:HD21	2.49	0.43
1:D:4743:MET:HE2	1:D:4743:MET:HB3	1.96	0.43
1:C:981:GLN:HA	1:C:984:LEU:HD23	2.00	0.43
1:C:3612:PRO:O	1:C:3613:TYR:CD2	2.72	0.43
1:D:2165:LEU:HA	1:D:2168:VAL:HG12	2.01	0.43
1:A:721:LEU:HD12	1:A:730:VAL:HG21	2.01	0.42
1:B:3612:PRO:O	1:B:3613:TYR:CD2	2.72	0.42
1:C:309:THR:O	1:C:309:THR:OG1	2.37	0.42
1:D:4166:LEU:N	1:D:4166:LEU:HD23	2.33	0.42
1:B:236:ALA:O	1:B:237:ASP:OD1	2.36	0.42
1:C:862:VAL:O	1:C:863:LEU:C	2.62	0.42
1:A:236:ALA:O	1:A:237:ASP:OD1	2.36	0.42
1:A:2386:ILE:HD13	1:A:2386:ILE:N	2.33	0.42
1:A:3319:ILE:CD1	1:A:3338:LEU:HD21	2.49	0.42
1:A:3612:PRO:O	1:A:3613:TYR:CD2	2.72	0.42
1:B:1427:ILE:HG23	1:B:1428:LEU:HD22	2.01	0.42
1:B:2667:THR:HG21	1:B:2672:LEU:HD21	2.02	0.42
1:C:4231:MET:HA	1:C:4231:MET:HE2	2.01	0.42
1:B:295:GLU:N	1:B:295:GLU:OE1	2.51	0.42
1:B:309:THR:O	1:B:309:THR:OG1	2.37	0.42
1:B:862:VAL:O	1:B:863:LEU:C	2.62	0.42
1:B:3517:MET:HG3	1:B:3517:MET:O	2.19	0.42
1:C:224:HIS:O	1:C:224:HIS:CG	2.72	0.42
1:C:3137:LEU:HD21	1:C:3189:ALA:HB1	2.01	0.42
1:C:3409:TYR:N	1:C:3410:PRO:HD2	2.35	0.42
1:D:2517:PHE:CD1	1:D:2517:PHE:C	2.96	0.42
1:D:3409:TYR:N	1:D:3410:PRO:HD2	2.35	0.42
1:A:2667:THR:HG21	1:A:2672:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3137:LEU:HD21	1:A:3189:ALA:HB1	2.01	0.42
1:C:2667:THR:HG21	1:C:2672:LEU:HD21	2.02	0.42
1:D:2667:THR:HG21	1:D:2672:LEU:HD21	2.02	0.42
1:D:3612:PRO:O	1:D:3613:TYR:CD2	2.72	0.42
1:D:3517:MET:HG3	1:D:3517:MET:O	2.19	0.42
1:C:721:LEU:HD12	1:C:730:VAL:HG21	2.01	0.42
1:C:1427:ILE:HG23	1:C:1428:LEU:HD22	2.02	0.42
1:D:3003:LEU:HB3	1:D:3004:PRO:HD3	2.02	0.42
1:D:3641:LEU:HD12	1:D:3641:LEU:O	2.20	0.42
1:B:3534:MET:HA	1:B:3534:MET:CE	2.42	0.42
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.97	0.42
1:D:3604:TYR:C	1:D:3604:TYR:CD1	2.98	0.42
1:D:4666:VAL:HG13	1:D:4783:ILE:HD11	2.02	0.42
1:A:224:HIS:O	1:A:224:HIS:CG	2.72	0.42
1:A:3604:TYR:CD1	1:A:3604:TYR:C	2.98	0.42
1:C:3955:MET:HE1	1:C:4016:LEU:CA	2.50	0.42
1:D:1873:GLU:N	1:D:1873:GLU:OE1	2.53	0.42
1:A:3003:LEU:HB3	1:A:3004:PRO:HD3	2.02	0.42
1:B:3137:LEU:HD21	1:B:3189:ALA:HB1	2.01	0.42
1:C:3546:ASP:O	1:C:3549:VAL:HG22	2.20	0.42
1:C:4666:VAL:HG13	1:C:4783:ILE:HD11	2.02	0.42
1:D:224:HIS:O	1:D:224:HIS:CG	2.72	0.42
1:A:2633:LEU:O	1:A:2633:LEU:CD2	2.67	0.41
1:A:3865:VAL:HG22	1:A:3866:ILE:H	1.85	0.41
1:A:4666:VAL:HG13	1:A:4783:ILE:HD11	2.02	0.41
1:C:3003:LEU:HB3	1:C:3004:PRO:HD3	2.02	0.41
1:D:3955:MET:HE1	1:D:4016:LEU:CA	2.50	0.41
1:A:3006:ILE:HG23	1:A:3010:PHE:CE1	2.55	0.41
1:A:3517:MET:O	1:A:3517:MET:HG3	2.19	0.41
1:B:224:HIS:O	1:B:224:HIS:CG	2.72	0.41
1:B:3865:VAL:HG22	1:B:3866:ILE:H	1.85	0.41
1:B:3955:MET:HE1	1:B:4016:LEU:CA	2.50	0.41
1:D:3546:ASP:O	1:D:3549:VAL:HG22	2.20	0.41
1:A:2517:PHE:CD1	1:A:2517:PHE:C	2.96	0.41
1:C:1183:GLU:OE1	1:C:1183:GLU:N	2.54	0.41
1:C:3641:LEU:O	1:C:3641:LEU:HD12	2.20	0.41
1:D:323:LEU:O	1:D:324:ASP:C	2.63	0.41
1:B:75:VAL:HG23	1:B:76:ARG:N	2.36	0.41
1:C:1873:GLU:N	1:C:1873:GLU:OE1	2.53	0.41
1:C:2223:ILE:N	1:C:2223:ILE:HD12	2.36	0.41
1:C:2907:PRO:HB2	1:C:2910:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:LEU:HD12	1:B:730:VAL:HG21	2.01	0.41
1:B:3641:LEU:HD12	1:B:3641:LEU:O	2.20	0.41
1:C:75:VAL:HG23	1:C:76:ARG:N	2.36	0.41
1:C:1929:MET:HE3	1:C:1929:MET:HB3	1.96	0.41
1:C:3550:ARG:HH21	1:C:3550:ARG:HG2	1.86	0.41
1:A:1873:GLU:N	1:A:1873:GLU:OE1	2.53	0.41
1:A:3550:ARG:HG2	1:A:3550:ARG:HH21	1.86	0.41
1:B:2907:PRO:HB2	1:B:2910:THR:HG23	2.02	0.41
1:B:3006:ILE:HG23	1:B:3010:PHE:CE1	2.55	0.41
1:D:1183:GLU:N	1:D:1183:GLU:OE1	2.54	0.41
1:D:2526:PHE:CE1	1:D:2558:VAL:HG22	2.52	0.41
1:A:75:VAL:HG23	1:A:76:ARG:N	2.36	0.41
1:B:3409:TYR:N	1:B:3410:PRO:HD2	2.35	0.41
1:B:3856:LEU:HD12	1:B:3858:MET:HB3	2.03	0.41
1:C:3865:VAL:HG22	1:C:3866:ILE:H	1.85	0.41
1:C:4743:MET:HE2	1:C:4743:MET:HB3	1.96	0.41
1:D:1929:MET:HE3	1:D:1929:MET:HB3	1.96	0.41
1:D:2907:PRO:HB2	1:D:2910:THR:HG23	2.02	0.41
1:D:3534:MET:HA	1:D:3534:MET:CE	2.42	0.41
1:A:1427:ILE:HG23	1:A:1428:LEU:HD22	2.01	0.41
1:A:3129:LEU:O	1:A:3133:THR:HG22	2.21	0.41
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.35	0.41
1:A:3546:ASP:O	1:A:3549:VAL:HG22	2.20	0.41
1:B:1508:ARG:HD2	1:B:1508:ARG:N	2.36	0.41
1:B:3604:TYR:CD1	1:B:3604:TYR:C	2.98	0.41
1:C:3604:TYR:CD1	1:C:3604:TYR:C	2.98	0.41
1:D:2223:ILE:HD12	1:D:2223:ILE:N	2.36	0.41
1:A:323:LEU:O	1:A:324:ASP:C	2.63	0.41
1:A:1114:GLU:OE1	1:A:1114:GLU:N	2.54	0.41
1:A:1508:ARG:H	1:A:1508:ARG:HD2	1.86	0.41
1:A:3854:GLU:HA	1:A:3854:GLU:OE1	2.21	0.41
1:B:1873:GLU:OE1	1:B:1873:GLU:N	2.53	0.41
1:B:2517:PHE:HD1	1:B:2517:PHE:O	2.04	0.41
1:B:3003:LEU:HB3	1:B:3004:PRO:HD3	2.02	0.41
1:B:3550:ARG:HG2	1:B:3550:ARG:HH21	1.86	0.41
1:C:323:LEU:O	1:C:324:ASP:C	2.63	0.41
1:C:1114:GLU:OE1	1:C:1114:GLU:N	2.54	0.41
1:C:3856:LEU:HD12	1:C:3858:MET:HB3	2.03	0.41
1:D:3006:ILE:HG23	1:D:3010:PHE:CE1	2.55	0.41
1:D:3137:LEU:HD21	1:D:3189:ALA:HB1	2.01	0.41
1:D:3856:LEU:HD12	1:D:3858:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2517:PHE:HD1	1:A:2517:PHE:O	2.04	0.41
1:A:3856:LEU:HD12	1:A:3858:MET:HB3	2.03	0.41
1:B:3546:ASP:O	1:B:3549:VAL:HG22	2.20	0.41
1:D:1427:ILE:HG23	1:D:1428:LEU:HD22	2.01	0.41
1:D:3550:ARG:HH21	1:D:3550:ARG:HG2	1.86	0.41
1:B:2633:LEU:O	1:B:2633:LEU:CD2	2.67	0.40
1:B:3129:LEU:O	1:B:3133:THR:HG22	2.21	0.40
1:B:3340:VAL:HG23	1:B:3341:PHE:CD1	2.56	0.40
1:B:4743:MET:HE2	1:B:4743:MET:HB3	1.97	0.40
1:D:688:LEU:HD23	1:D:690:GLU:H	1.86	0.40
1:D:1114:GLU:OE1	1:D:1114:GLU:N	2.54	0.40
1:D:2517:PHE:O	1:D:2517:PHE:HD1	2.04	0.40
1:D:3854:GLU:OE1	1:D:3854:GLU:HA	2.21	0.40
1:D:3865:VAL:HG22	1:D:3866:ILE:H	1.85	0.40
1:A:181:HIS:CE1	1:A:196:MET:HE3	2.56	0.40
1:B:1183:GLU:N	1:B:1183:GLU:OE1	2.54	0.40
1:B:3401:LEU:O	1:B:3405:LEU:HD13	2.22	0.40
1:C:3006:ILE:HG23	1:C:3010:PHE:CE1	2.55	0.40
1:C:3837:GLN:CD	1:C:3837:GLN:C	2.90	0.40
1:D:3129:LEU:O	1:D:3133:THR:HG22	2.21	0.40
1:A:1508:ARG:HD2	1:A:1508:ARG:N	2.36	0.40
1:B:323:LEU:O	1:B:324:ASP:C	2.63	0.40
1:C:2517:PHE:HD1	1:C:2517:PHE:O	2.04	0.40
1:C:3129:LEU:O	1:C:3133:THR:HG22	2.21	0.40
1:C:3340:VAL:HG23	1:C:3341:PHE:CD1	2.57	0.40
1:D:75:VAL:HG23	1:D:76:ARG:N	2.36	0.40
1:D:2633:LEU:O	1:D:2633:LEU:CD2	2.68	0.40
1:D:3401:LEU:O	1:D:3405:LEU:HD13	2.22	0.40
1:A:3340:VAL:HG23	1:A:3341:PHE:CD1	2.57	0.40
1:A:3641:LEU:O	1:A:3641:LEU:HD12	2.20	0.40
1:A:3955:MET:HE1	1:A:4016:LEU:CA	2.50	0.40
1:B:908:VAL:HG13	1:B:909:ASN:N	2.37	0.40
1:B:1114:GLU:N	1:B:1114:GLU:OE1	2.54	0.40
1:B:2223:ILE:N	1:B:2223:ILE:HD12	2.36	0.40
1:C:1075:PHE:O	1:C:1191:VAL:HG23	2.21	0.40
1:C:1508:ARG:N	1:C:1508:ARG:HD2	2.36	0.40
1:D:4839:MET:HE2	1:D:4839:MET:HB2	2.01	0.40
1:A:309:THR:O	1:A:309:THR:OG1	2.37	0.40
1:A:1183:GLU:N	1:A:1183:GLU:OE1	2.54	0.40
1:A:2907:PRO:HB2	1:A:2910:THR:HG23	2.02	0.40
1:A:3230:LEU:HD23	1:A:3230:LEU:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3230:LEU:HD23	1:B:3230:LEU:H	1.87	0.40
1:C:2675:THR:OG1	1:C:2710:LEU:HD11	2.22	0.40
1:D:181:HIS:CE1	1:D:196:MET:HE3	2.56	0.40
1:D:864:PRO:HB2	1:D:866:HIS:CE1	2.57	0.40
1:D:1508:ARG:N	1:D:1508:ARG:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4376/5037 (87%)	4237 (97%)	138 (3%)	1 (0%)	100	100
1	B	4376/5037 (87%)	4237 (97%)	138 (3%)	1 (0%)	100	100
1	C	4376/5037 (87%)	4236 (97%)	139 (3%)	1 (0%)	100	100
1	D	4376/5037 (87%)	4237 (97%)	138 (3%)	1 (0%)	100	100
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17924/20580 (87%)	17359 (97%)	561 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3478	MET
1	B	3478	MET
1	C	3478	MET
1	D	3478	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3827/4276 (90%)	3793 (99%)	34 (1%)	70	76
1	B	3827/4276 (90%)	3792 (99%)	35 (1%)	70	76
1	C	3827/4276 (90%)	3792 (99%)	35 (1%)	70	76
1	D	3827/4276 (90%)	3792 (99%)	35 (1%)	70	76
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	65
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	65
2	G	89/90 (99%)	86 (97%)	3 (3%)	32	57
2	H	89/90 (99%)	87 (98%)	2 (2%)	45	65
All	All	15664/17464 (90%)	15516 (99%)	148 (1%)	68	76

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	220	LEU
1	A	296	ASP
1	A	299	LEU
1	A	367	LEU
1	A	922	LEU
1	A	938	HIS
1	A	945	LYS
1	A	950	LEU
1	A	984	LEU
1	A	1021	LEU
1	A	1022	VAL
1	A	1045	THR
1	A	1435	TYR
1	A	1465	ASP
1	A	1576	SER
1	A	1738	LEU
1	A	1812	LEU
1	A	1931	LEU

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Mol	Chain	Res	Type
1	A	2123	LEU
1	A	2512	ILE
1	A	2813	LEU
1	A	3020	THR
1	A	3131	TYR
1	A	3411	LEU
1	A	3752	SER
1	A	4115	SER
1	A	4138	ASP
1	A	4206	GLU
1	A	4681	LEU
1	A	4713	SER
1	A	4769	MET
1	A	4878	ASP
1	A	5013	MET
1	B	24	CYS
1	B	220	LEU
1	B	296	ASP
1	B	299	LEU
1	B	367	LEU
1	B	922	LEU
1	B	938	HIS
1	B	945	LYS
1	B	950	LEU
1	B	984	LEU
1	B	1021	LEU
1	B	1022	VAL
1	B	1045	THR
1	B	1435	TYR
1	B	1465	ASP
1	B	1576	SER
1	B	1738	LEU
1	B	1812	LEU
1	B	1931	LEU
1	B	2123	LEU
1	B	2512	ILE
1	B	2813	LEU
1	B	3020	THR
1	B	3131	TYR
1	B	3381	LEU
1	B	3411	LEU
1	B	3752	SER

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Mol	Chain	Res	Type
1	B	4115	SER
1	B	4138	ASP
1	B	4206	GLU
1	B	4681	LEU
1	B	4713	SER
1	B	4769	MET
1	B	4878	ASP
1	B	5013	MET
1	C	24	CYS
1	C	220	LEU
1	C	296	ASP
1	C	299	LEU
1	C	367	LEU
1	C	922	LEU
1	C	938	HIS
1	C	945	LYS
1	C	950	LEU
1	C	984	LEU
1	C	1021	LEU
1	C	1022	VAL
1	C	1045	THR
1	C	1435	TYR
1	C	1465	ASP
1	C	1576	SER
1	C	1738	LEU
1	C	1812	LEU
1	C	1931	LEU
1	C	2123	LEU
1	C	2512	ILE
1	C	2813	LEU
1	C	3020	THR
1	C	3131	TYR
1	C	3381	LEU
1	C	3411	LEU
1	C	3752	SER
1	C	4115	SER
1	C	4138	ASP
1	C	4206	GLU
1	C	4681	LEU
1	C	4713	SER
1	C	4769	MET
1	C	4878	ASP

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Mol	Chain	Res	Type
1	C	5013	MET
1	D	24	CYS
1	D	220	LEU
1	D	296	ASP
1	D	299	LEU
1	D	367	LEU
1	D	922	LEU
1	D	938	HIS
1	D	945	LYS
1	D	950	LEU
1	D	984	LEU
1	D	1021	LEU
1	D	1022	VAL
1	D	1045	THR
1	D	1435	TYR
1	D	1465	ASP
1	D	1576	SER
1	D	1738	LEU
1	D	1812	LEU
1	D	1931	LEU
1	D	2123	LEU
1	D	2512	ILE
1	D	2813	LEU
1	D	3020	THR
1	D	3131	TYR
1	D	3381	LEU
1	D	3411	LEU
1	D	3752	SER
1	D	4115	SER
1	D	4138	ASP
1	D	4206	GLU
1	D	4681	LEU
1	D	4713	SER
1	D	4769	MET
1	D	4878	ASP
1	D	5013	MET
2	E	2	VAL
2	E	14	THR
2	F	2	VAL
2	F	14	THR
2	G	2	VAL
2	G	14	THR

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Mol	Chain	Res	Type
2	G	38	SER
2	H	2	VAL
2	H	14	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	98	HIS
1	A	181	HIS
1	A	278	GLN
1	A	284	HIS
1	A	297	GLN
1	A	350	HIS
1	A	582	HIS
1	A	1133	HIS
1	A	1590	GLN
1	A	1702	HIS
1	A	1760	HIS
1	A	1775	HIS
1	A	2417	HIS
1	A	2621	HIS
1	A	2773	ASN
1	A	2856	ASN
1	A	2858	GLN
1	A	2892	GLN
1	A	3030	HIS
1	A	3357	HIS
1	A	3651	ASN
1	A	3867	ASN
1	A	3882	GLN
1	A	3927	GLN
1	A	4707	ASN
1	A	4812	HIS
1	A	4833	ASN
1	A	4836	GLN
1	B	32	GLN
1	B	181	HIS
1	B	278	GLN
1	B	284	HIS
1	B	350	HIS
1	B	582	HIS

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Mol	Chain	Res	Type
1	B	1133	HIS
1	B	1590	GLN
1	B	1702	HIS
1	B	1775	HIS
1	B	2417	HIS
1	B	2487	GLN
1	B	2773	ASN
1	B	2856	ASN
1	B	2858	GLN
1	B	2892	GLN
1	B	3030	HIS
1	B	3357	HIS
1	B	3651	ASN
1	B	3867	ASN
1	B	3882	GLN
1	B	3927	GLN
1	B	4707	ASN
1	B	4812	HIS
1	C	32	GLN
1	C	181	HIS
1	C	278	GLN
1	C	284	HIS
1	C	350	HIS
1	C	582	HIS
1	C	797	HIS
1	C	1133	HIS
1	C	1460	HIS
1	C	1590	GLN
1	C	1702	HIS
1	C	1760	HIS
1	C	1775	HIS
1	C	2417	HIS
1	C	2621	HIS
1	C	2773	ASN
1	C	2856	ASN
1	C	2858	GLN
1	C	3030	HIS
1	C	3651	ASN
1	C	3867	ASN
1	C	3882	GLN
1	C	3927	GLN
1	C	4707	ASN

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Mol	Chain	Res	Type
1	C	4812	HIS
1	C	4833	ASN
1	C	4836	GLN
1	D	32	GLN
1	D	98	HIS
1	D	181	HIS
1	D	278	GLN
1	D	284	HIS
1	D	350	HIS
1	D	582	HIS
1	D	797	HIS
1	D	1133	HIS
1	D	1460	HIS
1	D	1590	GLN
1	D	1702	HIS
1	D	1775	HIS
1	D	2417	HIS
1	D	2773	ASN
1	D	2856	ASN
1	D	2858	GLN
1	D	2892	GLN
1	D	3030	HIS
1	D	3651	ASN
1	D	3867	ASN
1	D	3882	GLN
1	D	3927	GLN
1	D	4707	ASN
1	D	4812	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	B	5101	-	51,51,51	0.72	0	57,59,59	0.50	0
3	POV	D	5102	-	51,51,51	0.72	0	57,59,59	0.49	0
3	POV	A	5102	-	51,51,51	0.70	0	57,59,59	0.52	0
3	POV	C	5101	-	51,51,51	0.75	1 (1%)	57,59,59	0.65	1 (1%)
3	POV	C	5102	-	51,51,51	0.71	0	57,59,59	0.50	0
3	POV	A	5101	-	51,51,51	0.74	1 (1%)	57,59,59	0.65	1 (1%)
3	POV	B	5102	-	51,51,51	0.74	0	57,59,59	0.64	2 (3%)
3	POV	D	5101	-	51,51,51	0.73	0	57,59,59	0.71	2 (3%)

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	POV	B	5101	-	-	9/55/55/55	-
3	POV	D	5102	-	-	9/55/55/55	-
3	POV	A	5102	-	-	8/55/55/55	-
3	POV	C	5101	-	-	12/55/55/55	-
3	POV	C	5102	-	-	10/55/55/55	-
3	POV	A	5101	-	-	14/55/55/55	-
3	POV	B	5102	-	-	14/55/55/55	-
3	POV	D	5101	-	-	13/55/55/55	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5101	POV	C3-C2	2.03	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	POV	C3-C2	2.00	1.56	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	POV	C2-O21-C21	3.34	126.02	117.79
3	A	5101	POV	C2-O21-C21	3.10	125.42	117.79
3	C	5101	POV	C2-O21-C21	3.10	125.42	117.79
3	B	5102	POV	C2-O21-C21	3.05	125.29	117.79
3	B	5102	POV	O21-C21-C22	2.18	116.21	111.50
3	D	5101	POV	O21-C21-C22	2.01	115.84	111.50

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5101	POV	C11-O12-P-O11
3	A	5101	POV	C11-O12-P-O14
3	A	5101	POV	C2-C1-O11-P
3	A	5101	POV	C12-C11-O12-P
3	A	5101	POV	C22-C21-O21-C2
3	A	5101	POV	O22-C21-O21-C2
3	A	5102	POV	C11-O12-P-O14
3	B	5101	POV	C11-O12-P-O14
3	B	5102	POV	C11-O12-P-O11
3	B	5102	POV	C11-O12-P-O14
3	B	5102	POV	C2-C1-O11-P
3	B	5102	POV	C12-C11-O12-P
3	B	5102	POV	C22-C21-O21-C2
3	B	5102	POV	O22-C21-O21-C2
3	C	5101	POV	C11-O12-P-O11
3	C	5101	POV	C11-O12-P-O14
3	C	5101	POV	C2-C1-O11-P
3	C	5101	POV	C12-C11-O12-P
3	C	5101	POV	C22-C21-O21-C2
3	C	5101	POV	O22-C21-O21-C2
3	C	5102	POV	C11-O12-P-O14
3	D	5101	POV	C11-O12-P-O11
3	D	5101	POV	C11-O12-P-O14
3	D	5101	POV	O12-C11-C12-N
3	D	5101	POV	C12-C11-O12-P
3	D	5101	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	D	5101	POV	O22-C21-O21-C2
3	D	5102	POV	C11-O12-P-O14
3	D	5101	POV	C2-C1-O11-P
3	B	5101	POV	C11-O12-P-O11
3	D	5102	POV	C11-O12-P-O11
3	B	5101	POV	C31-C32-C33-C34
3	D	5102	POV	C31-C32-C33-C34
3	D	5102	POV	C310-C311-C312-C313
3	C	5102	POV	C31-C32-C33-C34
3	C	5102	POV	C11-O12-P-O11
3	D	5101	POV	C31-C32-C33-C34
3	A	5101	POV	C1-C2-C3-O31
3	C	5101	POV	C1-C2-C3-O31
3	A	5102	POV	C31-C32-C33-C34
3	C	5102	POV	C312-C313-C314-C315
3	B	5102	POV	C1-C2-C3-O31
3	D	5101	POV	C1-C2-C3-O31
3	A	5102	POV	C11-O12-P-O11
3	B	5102	POV	O21-C2-C3-O31
3	D	5102	POV	C311-C312-C313-C314
3	A	5102	POV	C33-C34-C35-C36
3	A	5101	POV	C31-C32-C33-C34
3	B	5102	POV	C21-C22-C23-C24
3	A	5101	POV	C1-O11-P-O13
3	A	5102	POV	C11-O12-P-O13
3	B	5101	POV	C11-O12-P-O13
3	C	5101	POV	C1-O11-P-O13
3	C	5102	POV	C11-O12-P-O13
3	D	5102	POV	C11-O12-P-O13
3	A	5102	POV	C12-C11-O12-P
3	B	5101	POV	C12-C11-O12-P
3	C	5102	POV	C12-C11-O12-P
3	D	5102	POV	C12-C11-O12-P
3	C	5101	POV	C31-C32-C33-C34
3	C	5102	POV	C33-C34-C35-C36
3	A	5101	POV	O12-C11-C12-N
3	B	5102	POV	O12-C11-C12-N
3	C	5101	POV	O12-C11-C12-N
3	A	5101	POV	O21-C2-C3-O31
3	C	5101	POV	O21-C2-C3-O31
3	D	5101	POV	O21-C2-C3-O31
3	B	5102	POV	C34-C35-C36-C37

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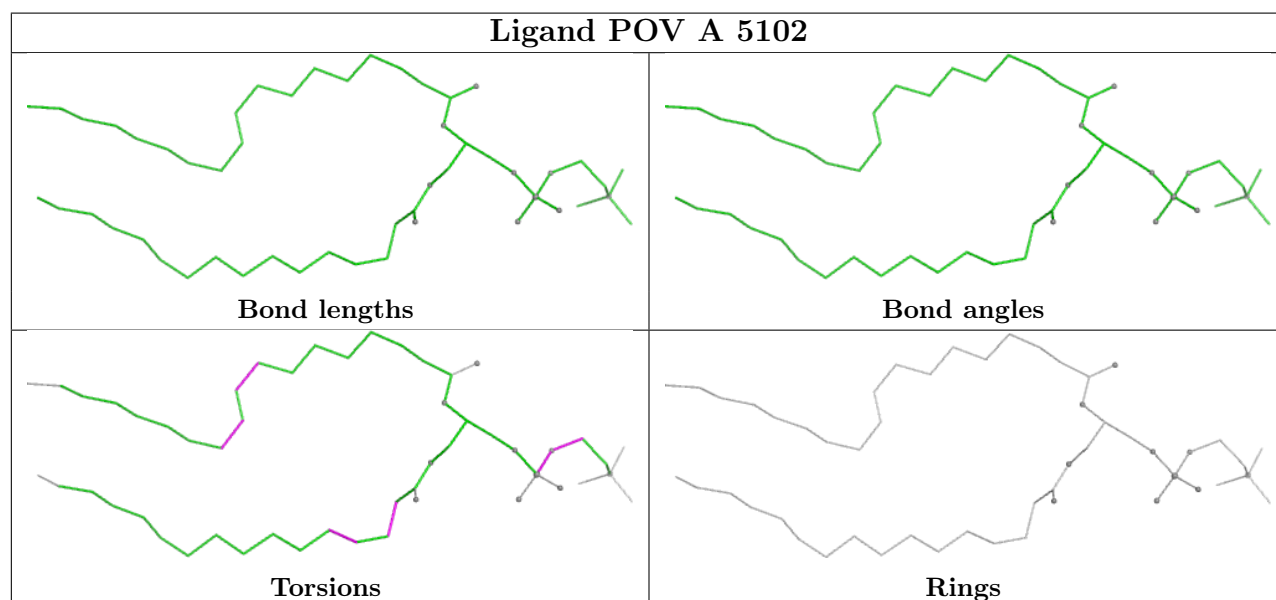
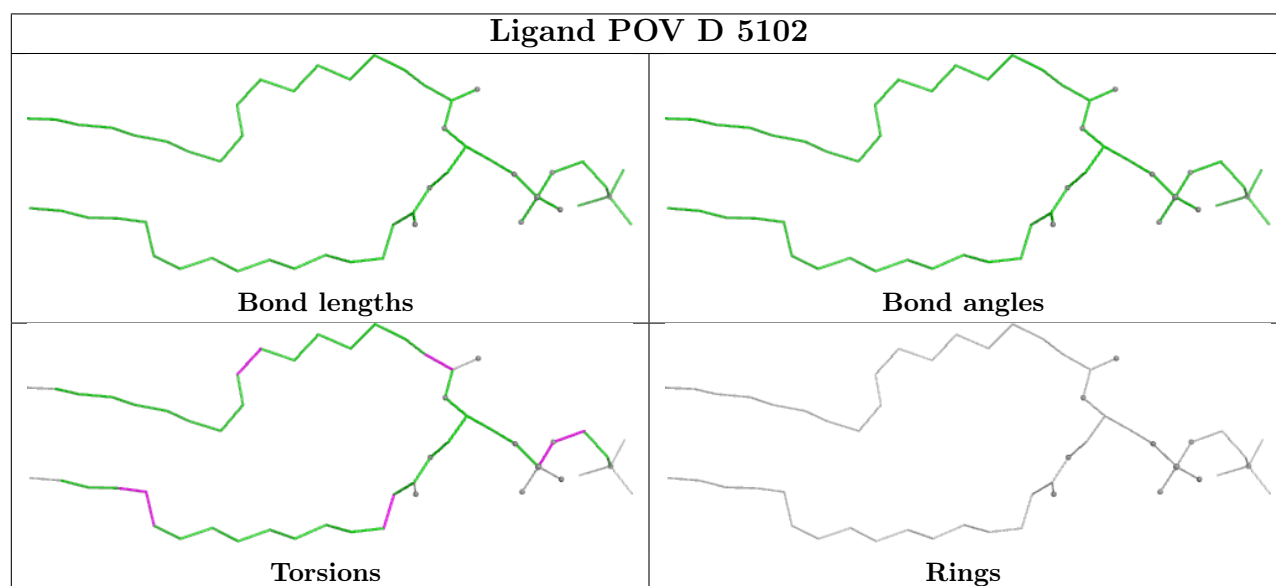
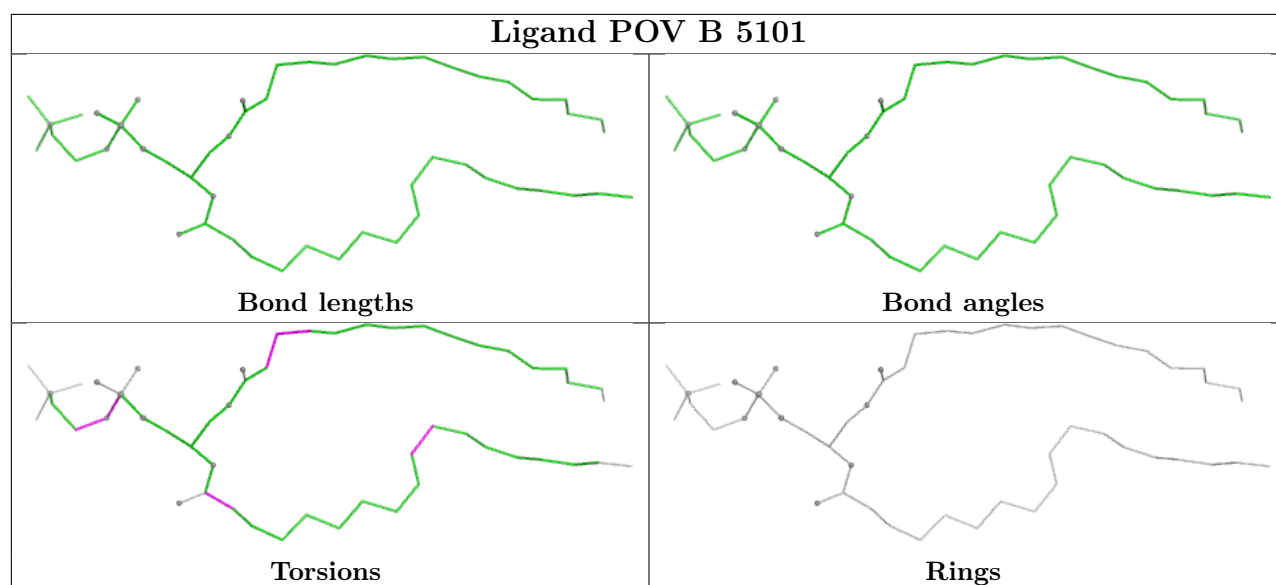
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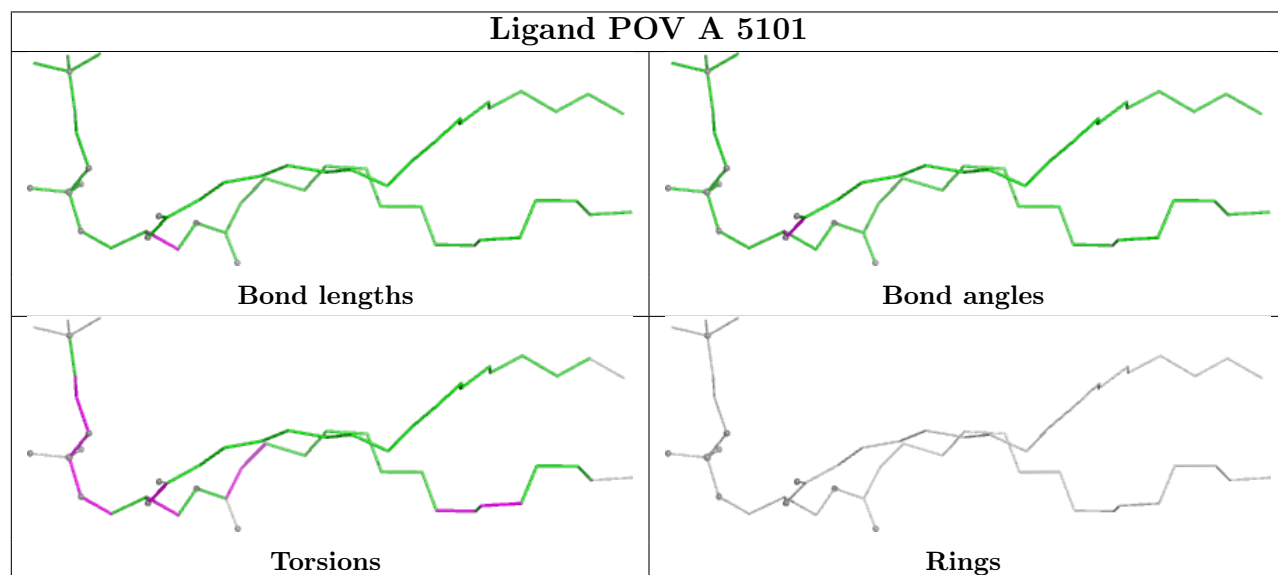
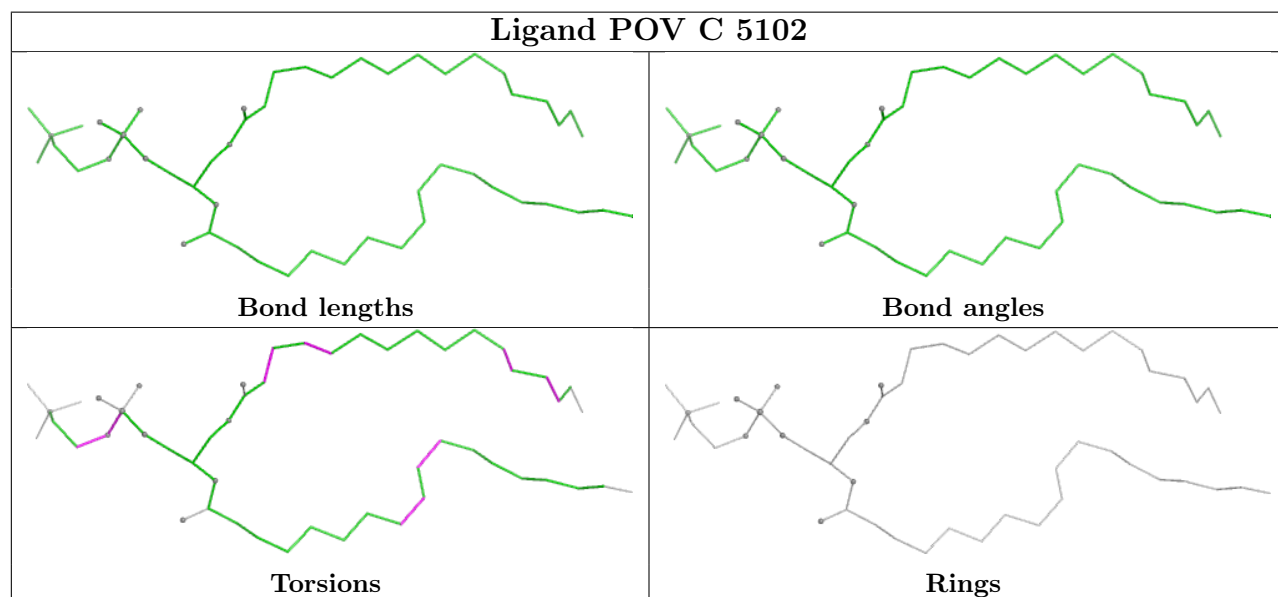
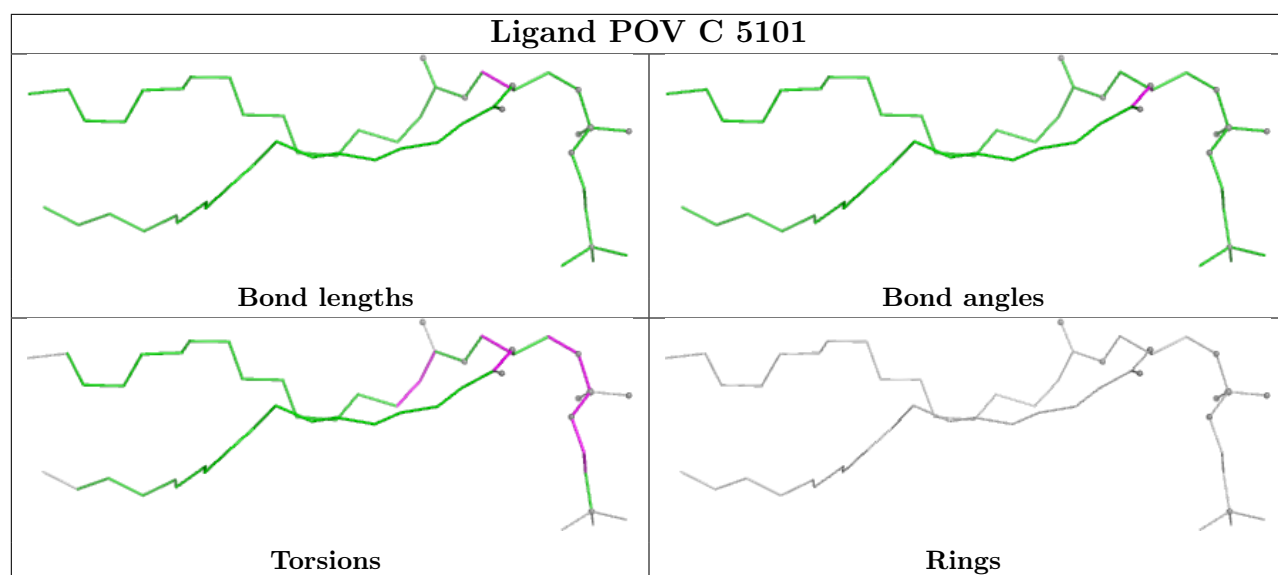
Mol	Chain	Res	Type	Atoms
3	D	5101	POV	C311-C312-C313-C314
3	C	5102	POV	C310-C311-C312-C313
3	D	5101	POV	C35-C36-C37-C38
3	B	5101	POV	C32-C33-C34-C35
3	B	5102	POV	O31-C31-C32-C33
3	A	5101	POV	C310-C311-C312-C313
3	A	5101	POV	C311-C310-C39-C38
3	A	5102	POV	C27-C28-C29-C210
3	C	5102	POV	C27-C28-C29-C210
3	B	5102	POV	O32-C31-C32-C33
3	D	5102	POV	C27-C28-C29-C210
3	C	5101	POV	O31-C31-C32-C33
3	B	5102	POV	C1-O11-P-O13
3	D	5101	POV	C1-O11-P-O13
3	A	5102	POV	C29-C210-C211-C212
3	B	5101	POV	C29-C210-C211-C212
3	C	5102	POV	C29-C210-C211-C212
3	A	5101	POV	O31-C31-C32-C33
3	B	5101	POV	O21-C21-C22-C23
3	D	5102	POV	O21-C21-C22-C23
3	B	5101	POV	O22-C21-C22-C23

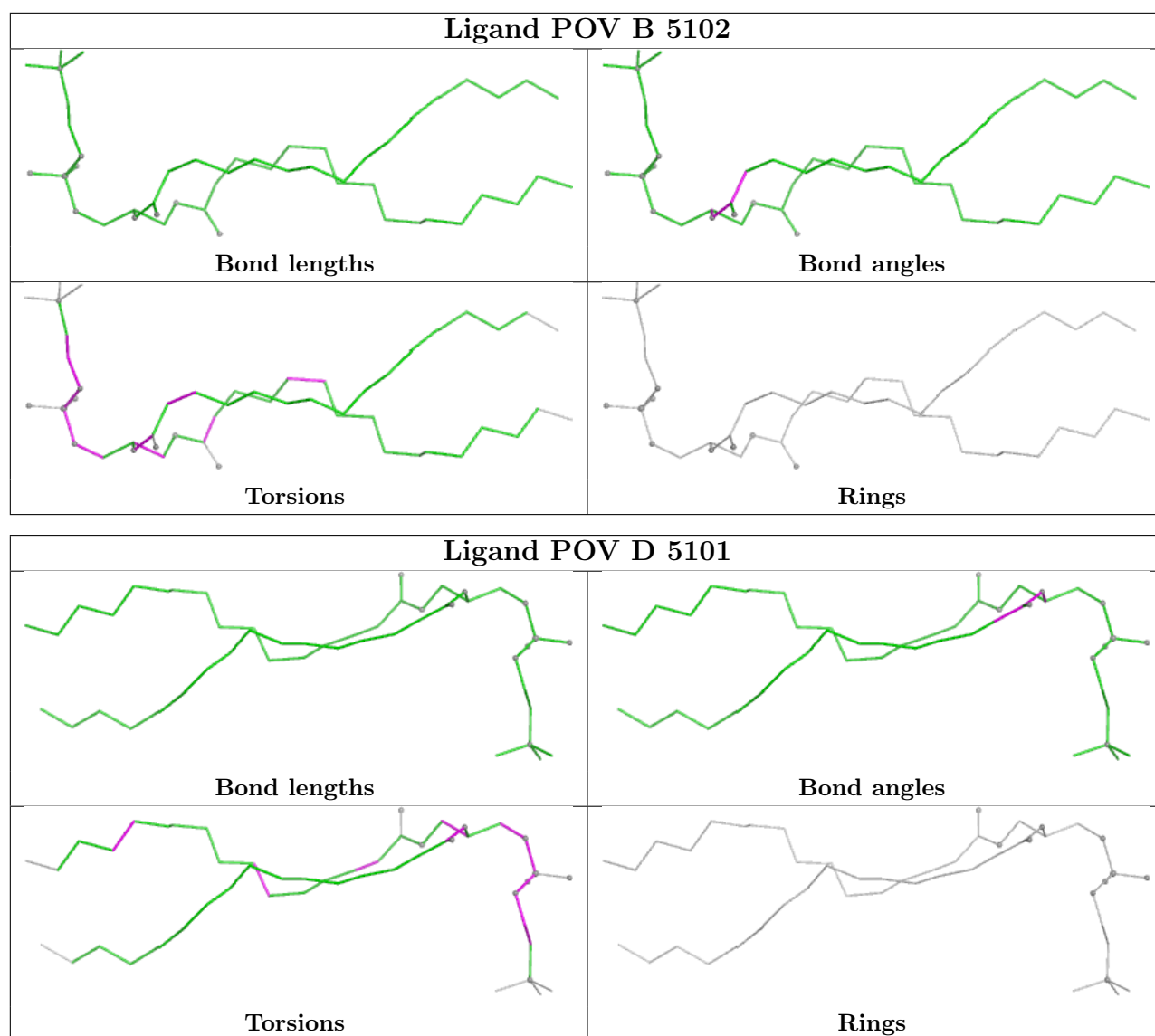
There are no ring outliers.

No monomer is involved in short contacts.

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.

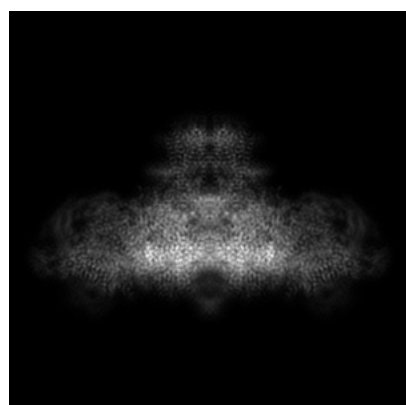
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54445. These allow visual inspection of the internal detail of the map and identification of artifacts.

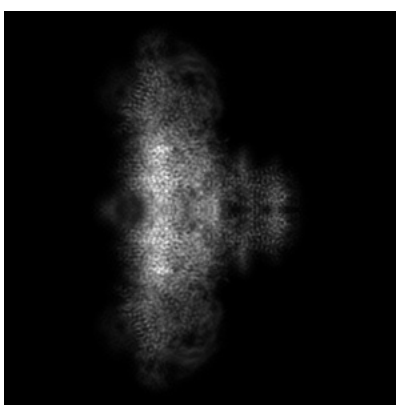
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

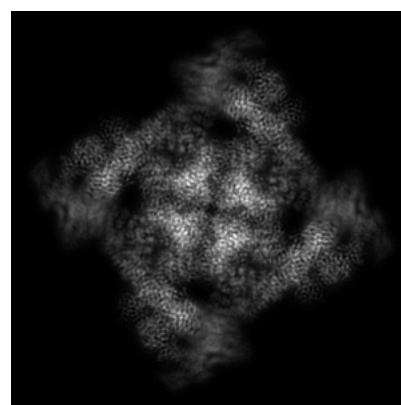
6.1.1 Primary map



X



Y



Z

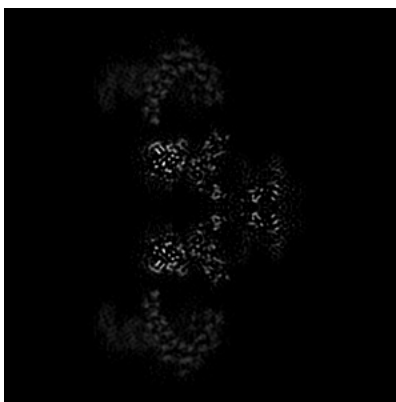
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

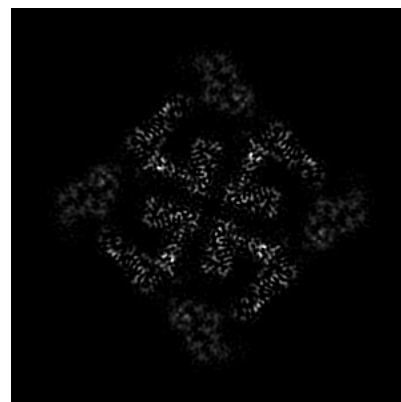
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

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: 173



Y Index: 127

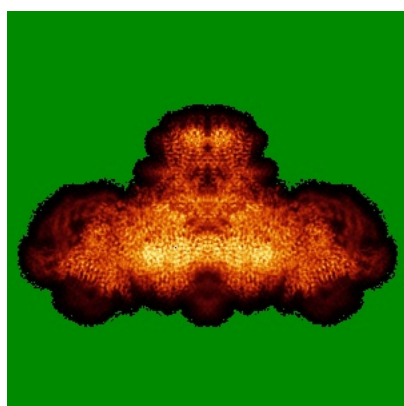


Z Index: 118

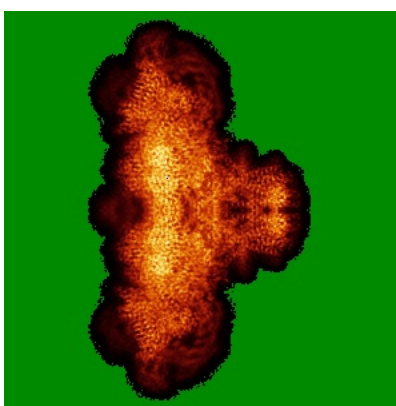
The images above show the largest variance slices of the map in three orthogonal directions.

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

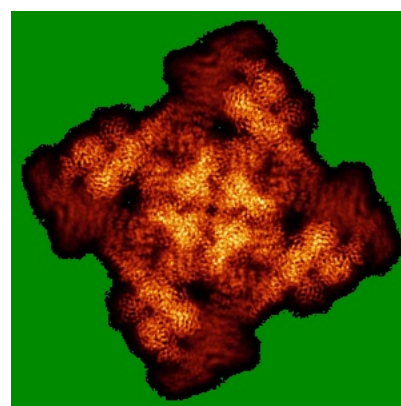
6.4.1 Primary map



X



Y

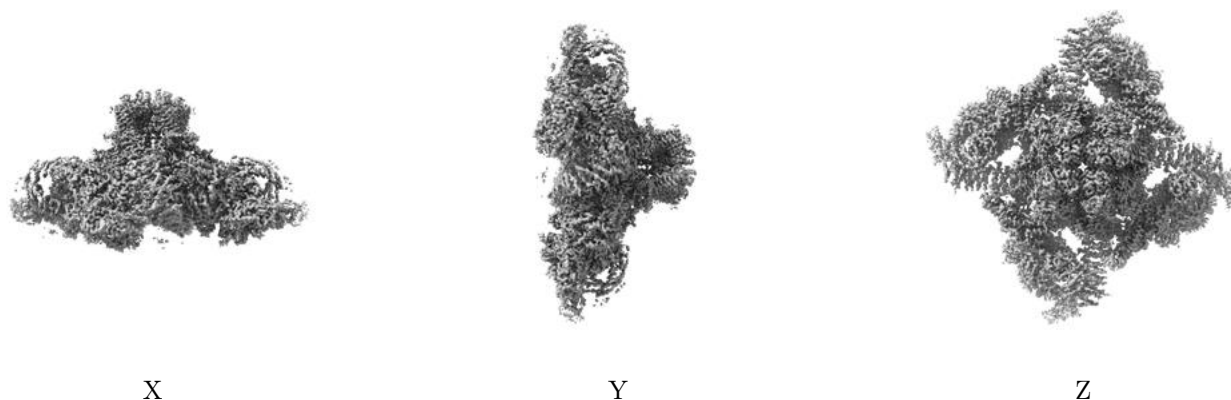


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

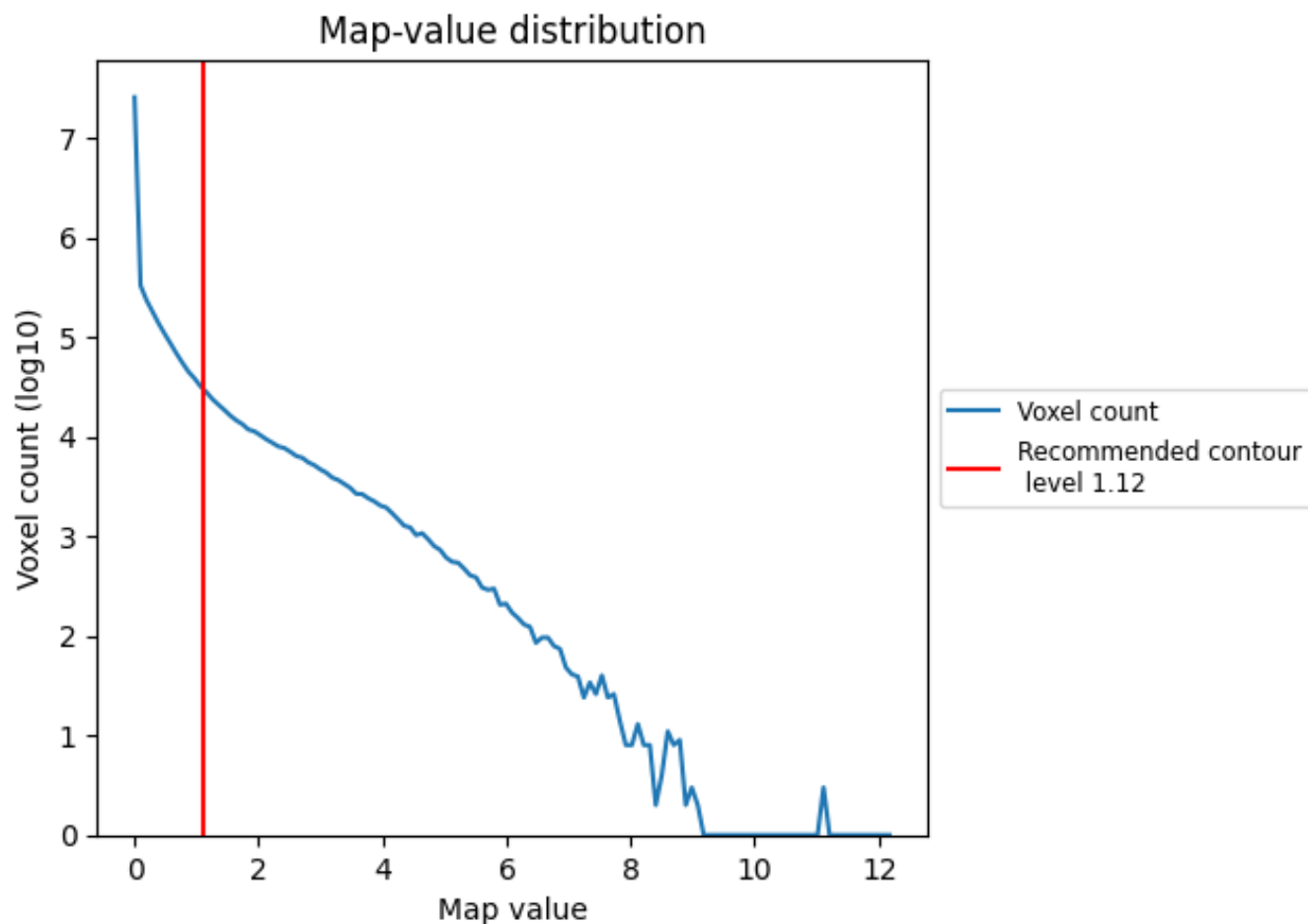
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

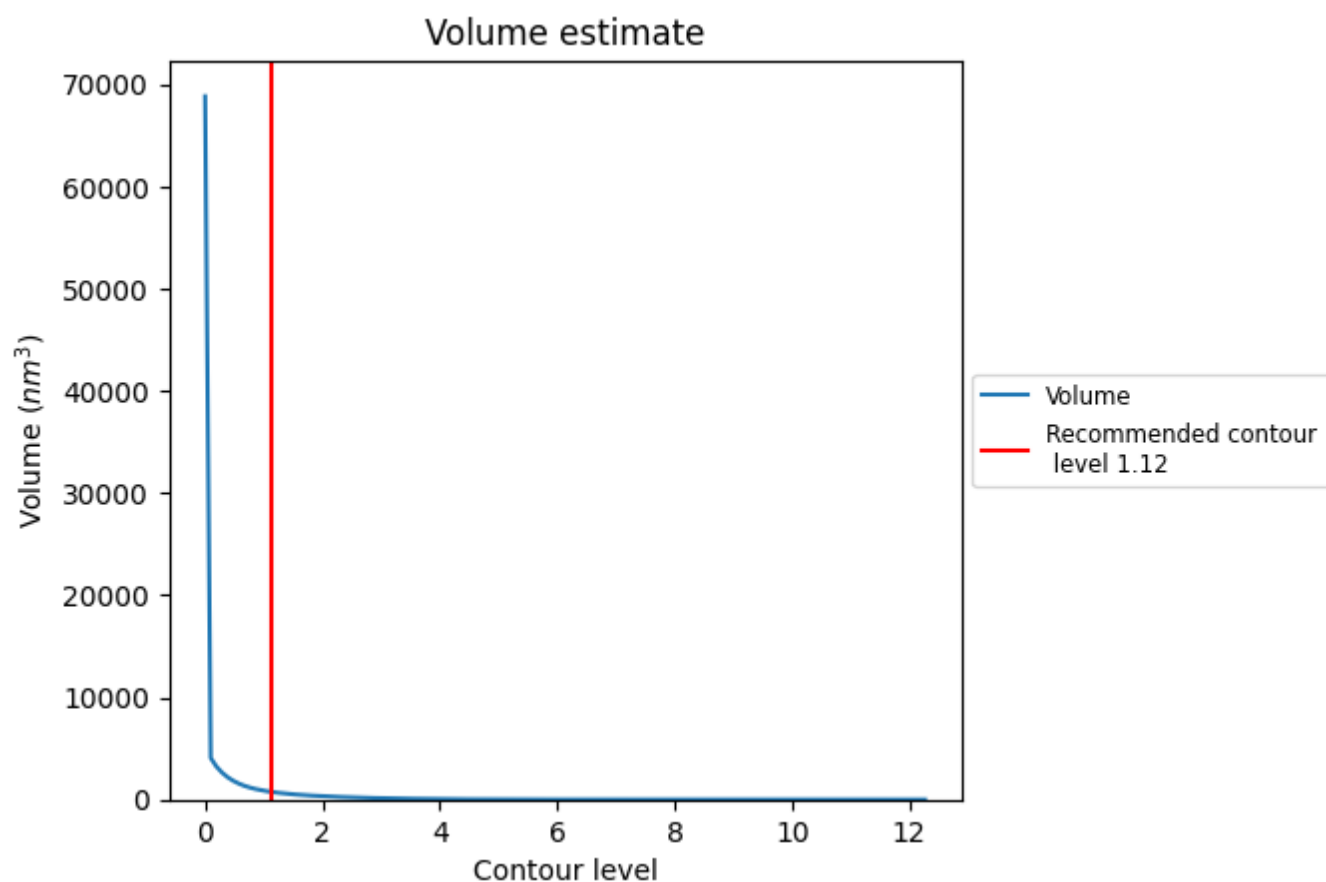
This section contains the results of statistical analysis of the map.

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.

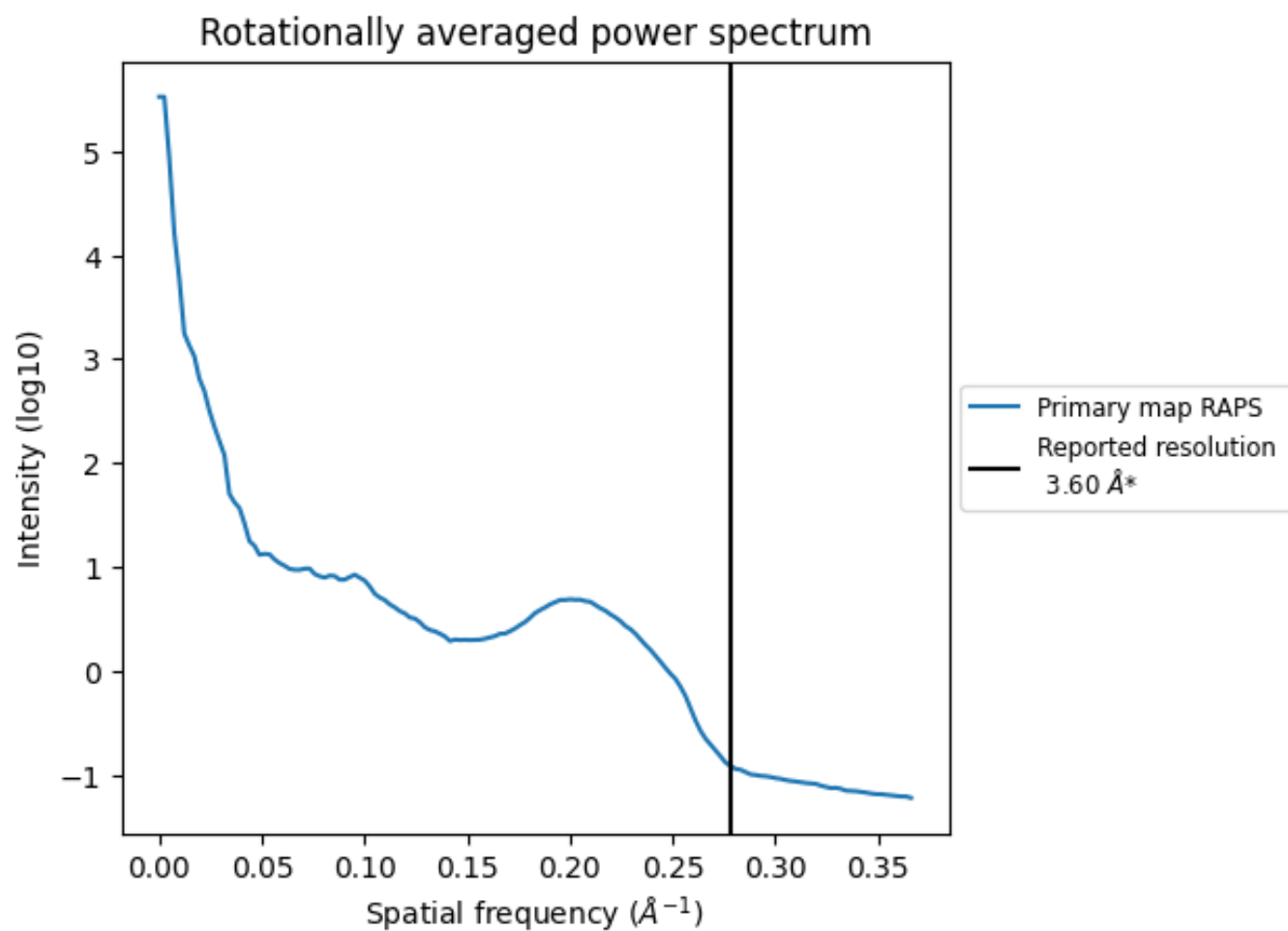
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 759 nm³; this corresponds to an approximate mass of 686 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 0.278 Å⁻¹

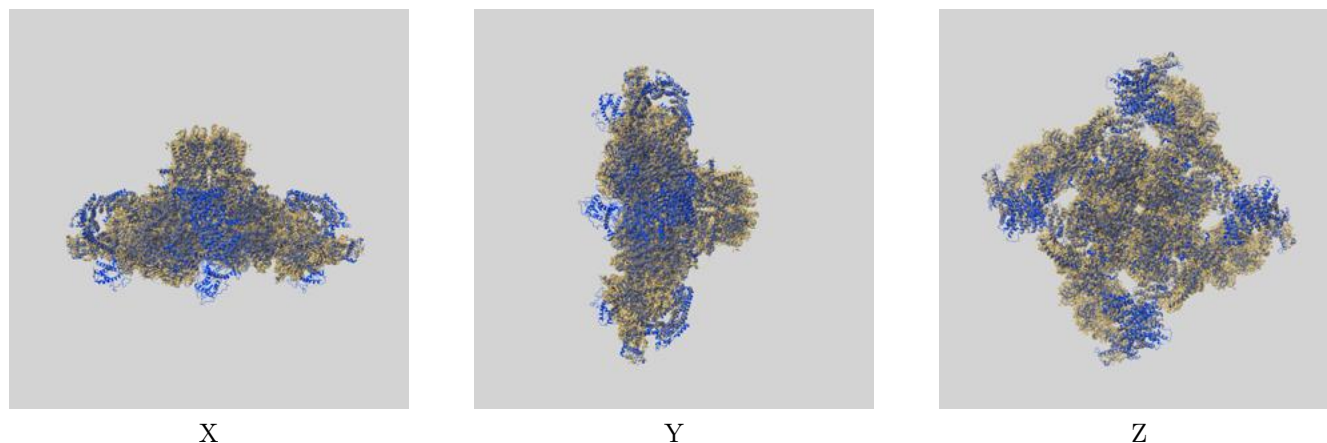
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

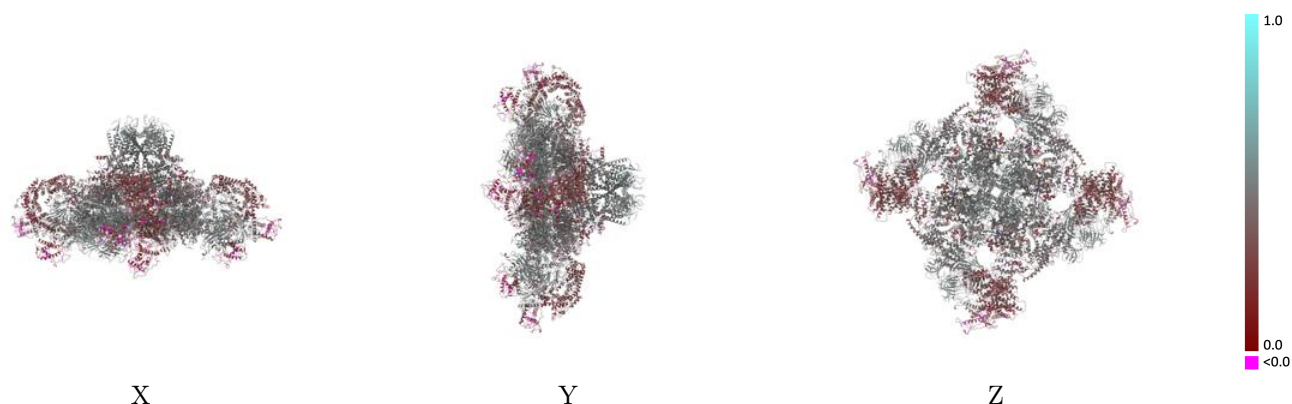
This section contains information regarding the fit between EMDB map EMD-54445 and PDB model 9S16. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



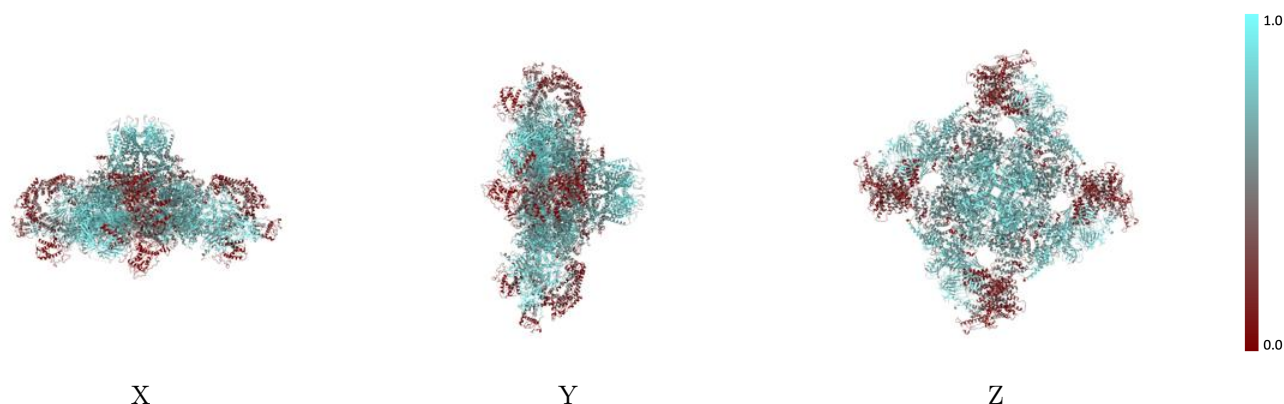
The images above show the 3D surface view of the map at the recommended contour level 1.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



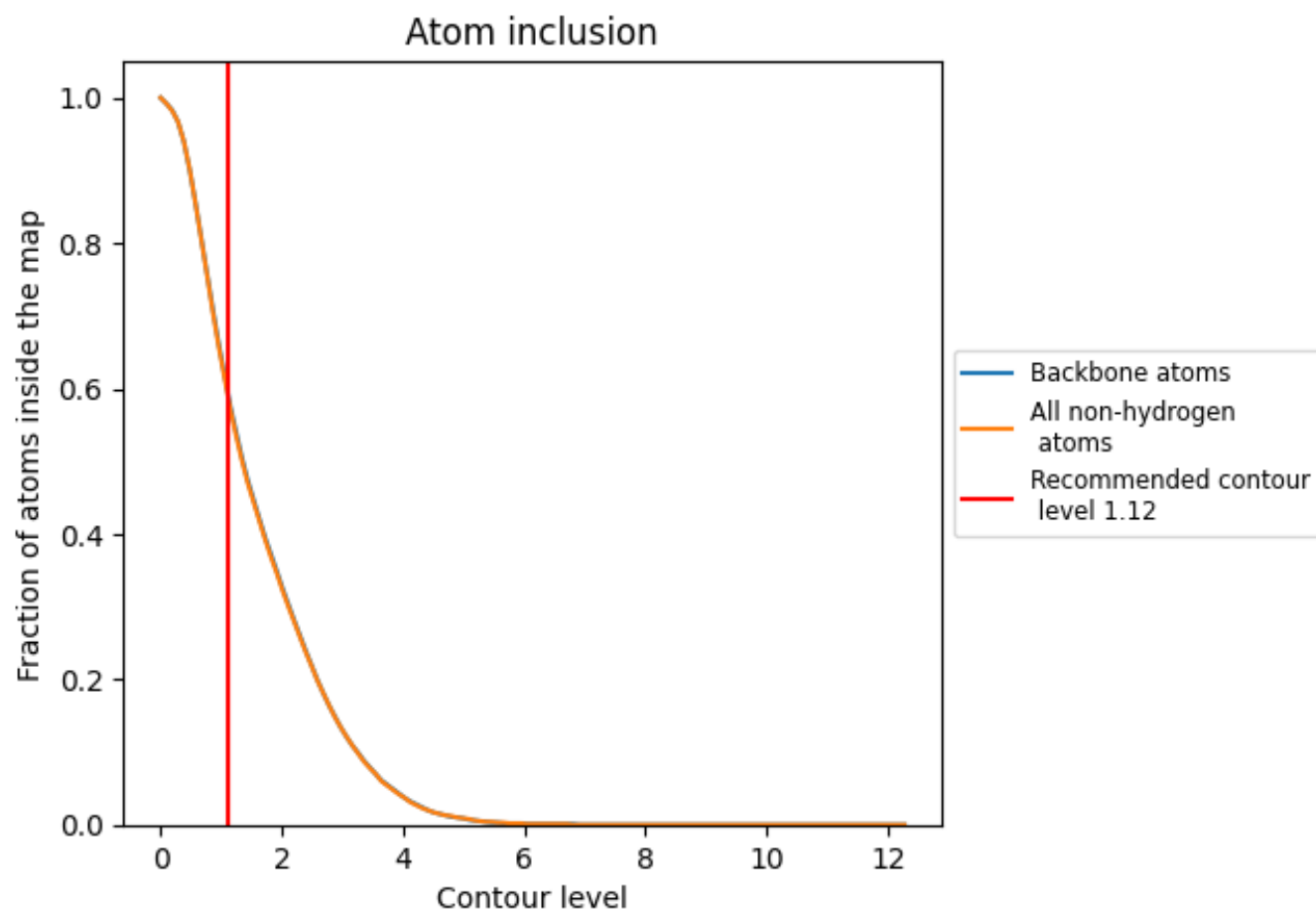
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 58% 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 (1.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5850	0.4050
A	0.5850	0.4040
B	0.5830	0.4040
C	0.5840	0.4040
D	0.5970	0.4020
E	0.7520	0.4880
F	0.7510	0.4890
G	0.7480	0.4910
H	0.7650	0.4850

1.0

0.0

<0.0