



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:57 PM UTC

PDB ID : 8IZD / pdb_00008izd
EMDB ID : EMD-35862
Title : Cryo-EM structure of the C26-CoA-bound Lac1-Lip1 complex
Authors : Xie, T.; Fang, Q.; Gong, X.
Deposited on : 2023-04-07
Resolution : 3.09 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

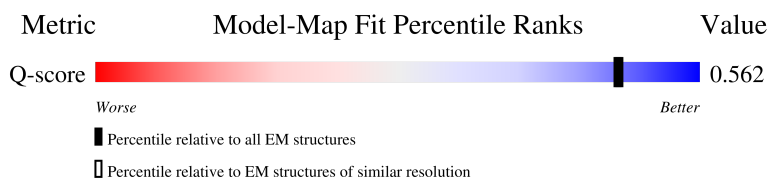
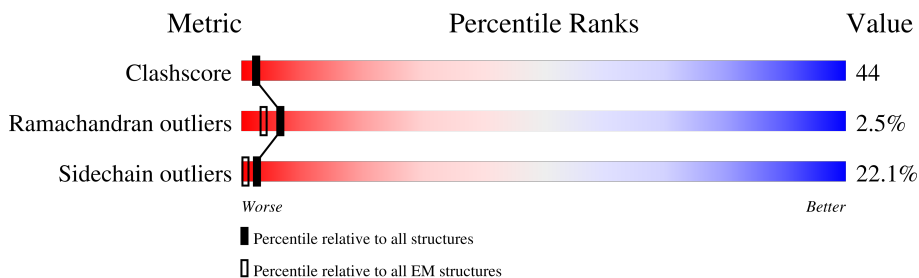
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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	14003 (2.59 - 3.59)

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	428	
1	C	428	
2	B	150	
2	D	150	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	9NY	A	502	-	-	X	-
4	9NY	C	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7806 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ceramide synthase LAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	315	Total	C	N	O	S	0	0
			2670	1809	424	424	13		
1	C	315	Total	C	N	O	S	0	0
			2670	1809	424	424	13		

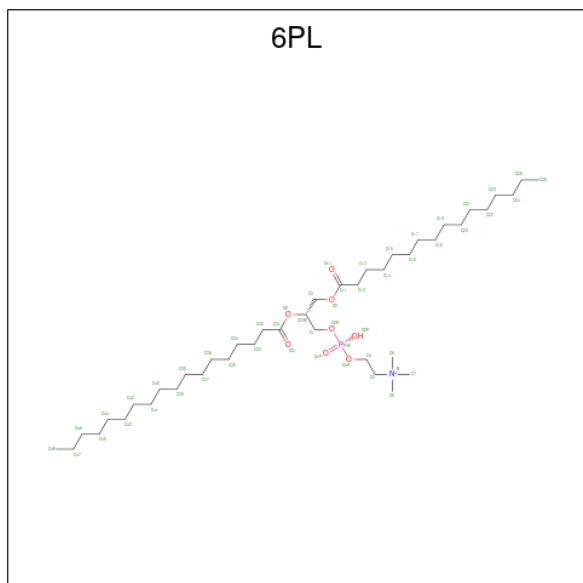
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P28496
A	420	GLU	-	expression tag	UNP P28496
A	421	ASP	-	expression tag	UNP P28496
A	422	TYR	-	expression tag	UNP P28496
A	423	LYS	-	expression tag	UNP P28496
A	424	ASP	-	expression tag	UNP P28496
A	425	ASP	-	expression tag	UNP P28496
A	426	ASP	-	expression tag	UNP P28496
A	427	ASP	-	expression tag	UNP P28496
A	428	LYS	-	expression tag	UNP P28496
C	419	LEU	-	expression tag	UNP P28496
C	420	GLU	-	expression tag	UNP P28496
C	421	ASP	-	expression tag	UNP P28496
C	422	TYR	-	expression tag	UNP P28496
C	423	LYS	-	expression tag	UNP P28496
C	424	ASP	-	expression tag	UNP P28496
C	425	ASP	-	expression tag	UNP P28496
C	426	ASP	-	expression tag	UNP P28496
C	427	ASP	-	expression tag	UNP P28496
C	428	LYS	-	expression tag	UNP P28496

- Molecule 2 is a protein called Ceramide synthase subunit LIP1.

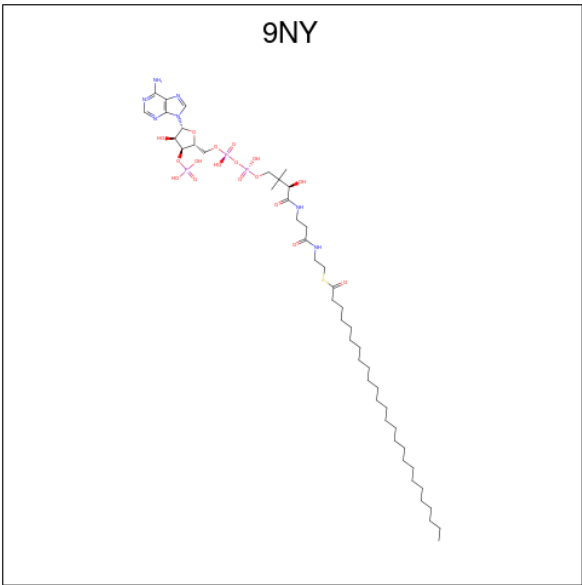
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1082	698	177	201	6		
2	D	132	Total	C	N	O	S	0	0
			1082	698	177	201	6		

- Molecule 3 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: $C_{42}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C			0
			18	18			
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C			0
			18	18			
3	C	1	Total	C			0
			18	18			
3	D	1	Total	C	O	P	0
			40	31	8	1	
3	D	1	Total	C			0
			18	18			

- Molecule 4 is Hexacosanoyl-CoA (CCD ID: 9NY) (formula: $C_{47}H_{86}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).

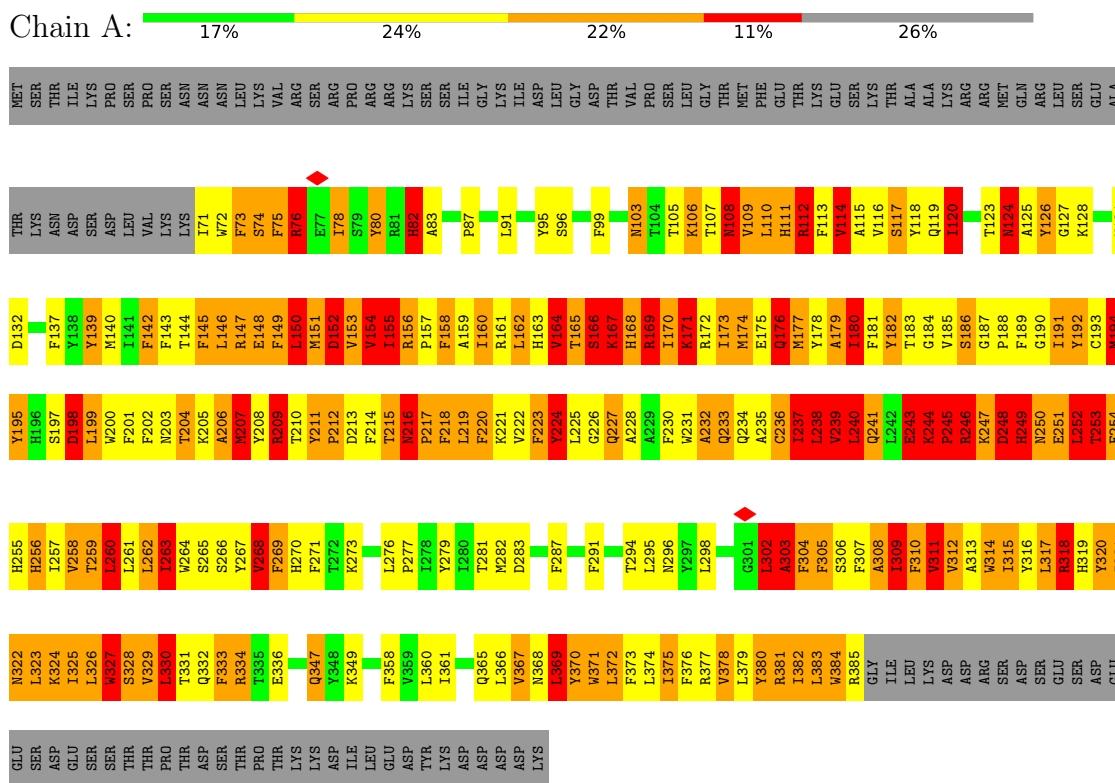


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
4	A	1	75	47	7	17	3	1	0
4	C	1	75	47	7	17	3	1	0

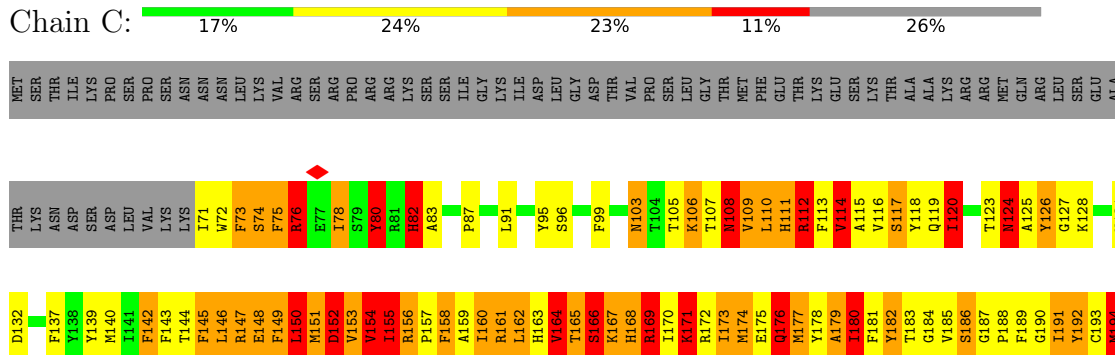
3 Residue-property plots

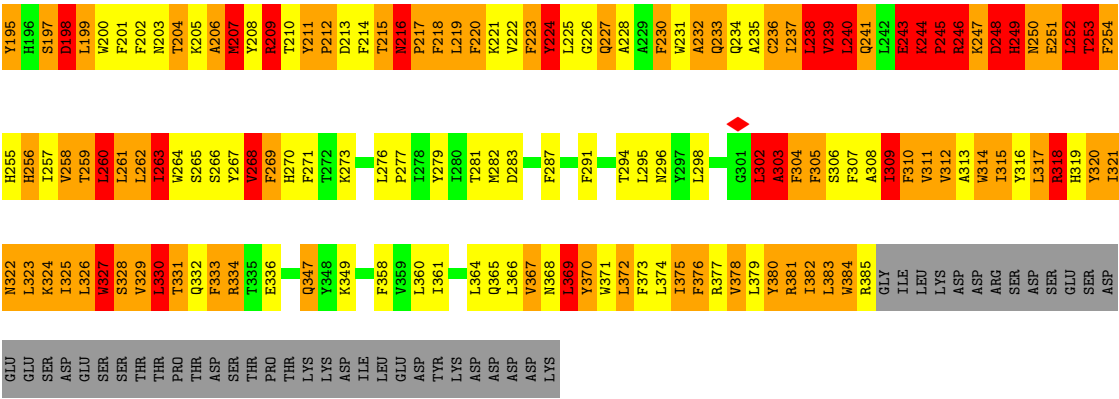
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ceramide synthase LAC1

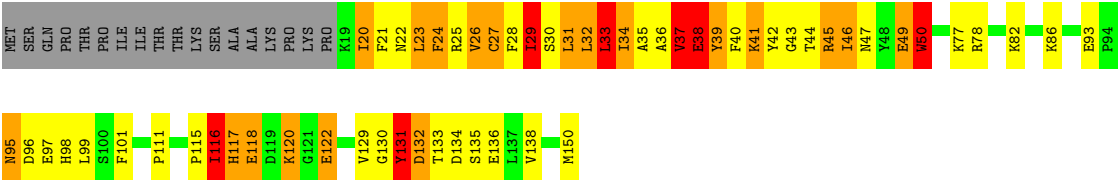


• Molecule 1: Ceramide synthase LAC1

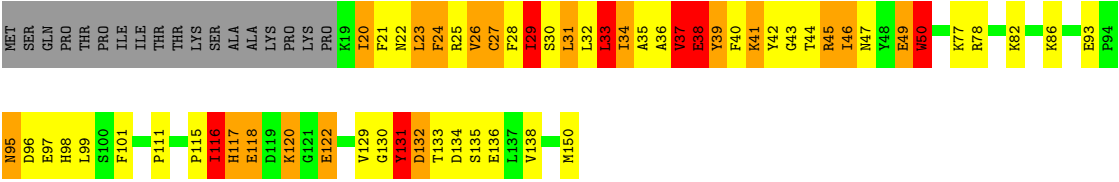




• Molecule 2: Ceramide synthase subunit LIP1



• Molecule 2: Ceramide synthase subunit LIP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.198	Depositor
Minimum map value	-2.577	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.37	Depositor
Map size ($\text{\AA}$)	274.432, 274.432, 274.432	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6PL, 9NY

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	3.71	407/2764 (14.7%)	2.17	173/3760 (4.6%)
1	C	3.71	406/2764 (14.7%)	2.17	175/3760 (4.7%)
2	B	2.56	89/1114 (8.0%)	1.35	24/1512 (1.6%)
2	D	2.56	89/1114 (8.0%)	1.35	24/1512 (1.6%)
All	All	3.42	991/7756 (12.8%)	1.97	396/10544 (3.8%)

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	3
1	C	0	4
All	All	0	7

All (991) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLY	C-O	-21.12	1.03	1.23
1	C	127	GLY	C-O	-21.10	1.03	1.23
1	C	319	HIS	CA-C	-20.05	1.28	1.53
1	A	319	HIS	CA-C	-20.03	1.28	1.53
1	A	230	PHE	C-O	-18.49	1.01	1.24
1	C	230	PHE	C-O	-18.43	1.01	1.24
1	A	219	LEU	C-O	-17.94	1.03	1.24
1	C	219	LEU	C-O	-17.92	1.03	1.24
1	A	227	GLN	C-O	-16.85	1.02	1.24
1	C	227	GLN	C-O	-16.84	1.02	1.24
1	A	232	ALA	C-O	-16.84	1.04	1.24
1	C	232	ALA	C-O	-16.82	1.04	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	43	GLY	C-O	-16.67	1.03	1.23
2	B	43	GLY	C-O	-16.65	1.03	1.23
1	C	218	PHE	CA-C	-16.52	1.35	1.53
1	A	218	PHE	CA-C	-16.49	1.35	1.53
1	C	313	ALA	C-O	-16.48	1.04	1.24
1	A	313	ALA	C-O	-16.45	1.05	1.24
1	A	232	ALA	CA-C	-16.45	1.31	1.52
1	C	232	ALA	CA-C	-16.45	1.31	1.52
1	C	139	TYR	C-O	-16.34	1.02	1.24
1	A	139	TYR	C-O	-16.30	1.03	1.24
1	C	145	PHE	C-O	-15.91	1.05	1.24
1	A	126	TYR	C-O	-15.89	1.04	1.24
1	C	126	TYR	C-O	-15.89	1.04	1.24
1	A	145	PHE	C-O	-15.86	1.05	1.24
1	C	111	HIS	C-O	-15.81	1.04	1.24
1	A	111	HIS	C-O	-15.77	1.04	1.24
1	A	145	PHE	CA-C	-15.42	1.31	1.52
1	C	145	PHE	CA-C	-15.41	1.31	1.52
1	C	142	PHE	C-O	-14.56	1.04	1.24
1	A	142	PHE	C-O	-14.55	1.04	1.24
1	A	268	VAL	C-O	-14.34	1.05	1.24
1	C	268	VAL	C-O	-14.34	1.05	1.24
1	A	319	HIS	C-O	-14.07	1.08	1.24
1	C	319	HIS	C-O	-14.07	1.08	1.24
1	C	314	TRP	C-O	-13.86	1.07	1.24
1	A	314	TRP	C-O	-13.82	1.07	1.24
2	D	40	PHE	C-O	-13.79	1.07	1.24
2	B	40	PHE	C-O	-13.75	1.07	1.24
1	C	150	LEU	CA-C	-13.71	1.35	1.52
1	A	150	LEU	CA-C	-13.71	1.35	1.52
1	A	378	VAL	C-O	-13.70	1.07	1.24
1	C	378	VAL	C-O	-13.68	1.07	1.24
1	C	228	ALA	C-O	-13.62	1.06	1.24
1	A	228	ALA	C-O	-13.62	1.06	1.24
1	A	265	SER	CA-C	-13.49	1.35	1.52
1	C	265	SER	CA-C	-13.45	1.35	1.52
1	A	320	TYR	CA-C	-13.24	1.35	1.52
1	A	329	VAL	C-O	-13.21	1.09	1.24
1	C	320	TYR	CA-C	-13.20	1.35	1.52
1	C	329	VAL	C-O	-13.19	1.09	1.24
1	A	334	ARG	C-O	-13.18	1.08	1.24
1	C	334	ARG	C-O	-13.17	1.08	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	GLN	C-O	-13.14	1.08	1.24
1	C	119	GLN	C-O	-13.09	1.08	1.24
1	C	220	PHE	C-O	-13.02	1.07	1.24
1	A	220	PHE	C-O	-13.00	1.07	1.24
1	C	110	LEU	C-O	-12.99	1.08	1.24
1	C	147	ARG	C-O	-12.98	1.09	1.24
1	A	110	LEU	C-O	-12.96	1.08	1.24
1	A	147	ARG	C-O	-12.95	1.09	1.24
1	A	216	ASN	C-O	-12.94	1.07	1.24
1	C	216	ASN	C-O	-12.93	1.07	1.24
1	A	181	PHE	CA-C	-12.91	1.36	1.52
1	C	181	PHE	CA-C	-12.88	1.36	1.52
1	A	146	LEU	CA-C	-12.75	1.36	1.52
1	A	225	LEU	C-O	-12.74	1.06	1.24
1	C	146	LEU	CA-C	-12.72	1.36	1.52
1	C	225	LEU	C-O	-12.67	1.07	1.24
1	A	314	TRP	CA-C	-12.66	1.36	1.52
1	A	368	ASN	CA-C	-12.66	1.35	1.52
1	C	368	ASN	CA-C	-12.66	1.35	1.52
1	C	314	TRP	CA-C	-12.64	1.36	1.52
1	C	264	TRP	C-O	-12.59	1.09	1.24
1	A	264	TRP	C-O	-12.56	1.09	1.24
1	A	226	GLY	C-O	-12.48	1.07	1.23
2	B	45	ARG	CA-C	-12.46	1.35	1.52
1	C	231	TRP	C-O	-12.45	1.08	1.24
1	A	231	TRP	C-O	-12.45	1.08	1.24
1	C	226	GLY	C-O	-12.42	1.07	1.23
2	D	45	ARG	CA-C	-12.40	1.35	1.52
2	B	44	THR	C-O	-12.39	1.07	1.24
2	D	44	THR	C-O	-12.38	1.07	1.24
2	B	30	SER	C-O	-12.34	1.09	1.24
2	D	30	SER	C-O	-12.33	1.09	1.24
1	A	219	LEU	CA-C	-12.28	1.36	1.52
1	A	332	GLN	CA-C	-12.28	1.37	1.52
1	C	219	LEU	CA-C	-12.27	1.36	1.52
1	C	230	PHE	CA-C	-12.24	1.36	1.52
1	A	230	PHE	CA-C	-12.21	1.36	1.52
1	C	332	GLN	CA-C	-12.21	1.37	1.52
1	A	203	ASN	C-O	-12.20	1.09	1.24
1	A	192	TYR	C-O	-12.08	1.09	1.24
2	B	98	HIS	C-O	-12.07	1.09	1.24
2	D	98	HIS	C-O	-12.07	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	TYR	C-O	-12.07	1.09	1.24
1	C	316	TYR	C-O	-12.00	1.10	1.24
1	A	316	TYR	C-O	-11.99	1.10	1.24
1	C	203	ASN	C-O	-11.99	1.09	1.24
1	C	368	ASN	C-O	-11.84	1.08	1.24
2	D	50	TRP	CA-C	-11.80	1.37	1.52
1	A	368	ASN	C-O	-11.80	1.08	1.24
1	C	265	SER	C-O	-11.79	1.10	1.24
1	A	125	ALA	C-O	-11.78	1.10	1.23
2	B	50	TRP	CA-C	-11.77	1.37	1.52
1	A	264	TRP	CA-C	-11.74	1.37	1.52
1	A	265	SER	C-O	-11.74	1.10	1.24
1	C	264	TRP	CA-C	-11.72	1.37	1.52
2	B	36	ALA	CA-C	-11.71	1.37	1.52
1	C	313	ALA	CA-C	-11.69	1.38	1.52
2	D	36	ALA	CA-C	-11.67	1.37	1.52
1	A	176	GLN	CA-C	-11.65	1.37	1.52
1	A	371	TRP	C-O	-11.65	1.08	1.24
1	A	313	ALA	CA-C	-11.65	1.38	1.52
1	C	371	TRP	C-O	-11.64	1.08	1.24
1	C	176	GLN	CA-C	-11.62	1.37	1.52
1	C	112	ARG	CA-C	-11.60	1.37	1.52
1	A	112	ARG	CA-C	-11.58	1.37	1.52
1	C	170	ILE	C-O	-11.54	1.08	1.24
1	A	170	ILE	C-O	-11.54	1.08	1.24
1	A	320	TYR	C-O	-11.42	1.10	1.24
1	A	147	ARG	CA-C	-11.40	1.38	1.52
1	C	320	TYR	C-O	-11.38	1.10	1.24
1	A	206	ALA	C-O	-11.36	1.09	1.24
1	C	231	TRP	CA-C	-11.36	1.37	1.52
1	A	231	TRP	CA-C	-11.34	1.37	1.52
1	C	206	ALA	C-O	-11.34	1.09	1.24
1	C	147	ARG	CA-C	-11.34	1.38	1.52
1	C	125	ALA	C-O	-11.23	1.10	1.24
1	C	317	LEU	CA-C	-11.22	1.38	1.52
1	A	317	LEU	CA-C	-11.21	1.38	1.52
1	C	143	PHE	C-O	-11.17	1.09	1.24
1	A	143	PHE	C-O	-11.12	1.09	1.24
1	A	146	LEU	C-O	-11.10	1.10	1.24
1	A	180	ILE	C-O	-11.07	1.09	1.24
1	C	180	ILE	C-O	-11.07	1.09	1.24
1	C	146	LEU	C-O	-11.06	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	GLU	CA-C	-10.96	1.38	1.52
1	A	316	TYR	CA-C	-10.96	1.39	1.52
1	A	259	THR	C-O	-10.95	1.11	1.24
1	C	259	THR	C-O	-10.93	1.11	1.24
1	C	316	TYR	CA-C	-10.91	1.39	1.52
1	C	148	GLU	CA-C	-10.90	1.38	1.52
1	A	113	PHE	C-O	-10.85	1.10	1.24
1	C	224	TYR	C-O	-10.85	1.11	1.24
1	C	113	PHE	C-O	-10.83	1.10	1.24
1	A	224	TYR	C-O	-10.79	1.11	1.24
1	A	317	LEU	C-O	-10.71	1.11	1.24
1	C	223	PHE	C-O	-10.70	1.11	1.24
1	C	317	LEU	C-O	-10.67	1.11	1.24
1	C	263	ILE	C-O	-10.66	1.11	1.24
1	A	223	PHE	C-O	-10.65	1.11	1.24
2	D	42	TYR	C-O	-10.65	1.11	1.24
2	B	42	TYR	C-O	-10.63	1.11	1.24
1	A	263	ILE	C-O	-10.61	1.11	1.24
1	A	111	HIS	CA-C	-10.58	1.38	1.52
1	C	111	HIS	CA-C	-10.56	1.38	1.52
1	A	269	PHE	C-O	-10.53	1.09	1.24
2	D	32	LEU	C-O	-10.52	1.11	1.24
1	A	206	ALA	CA-C	-10.52	1.38	1.52
2	B	32	LEU	C-O	-10.50	1.11	1.24
1	C	206	ALA	CA-C	-10.50	1.38	1.52
1	C	208	TYR	C-O	-10.49	1.10	1.23
1	A	208	TYR	C-O	-10.46	1.10	1.23
1	C	269	PHE	C-O	-10.46	1.09	1.24
1	C	322	ASN	C-O	-10.40	1.10	1.24
1	C	119	GLN	CA-C	-10.39	1.38	1.52
1	A	322	ASN	C-O	-10.38	1.10	1.24
2	B	39	TYR	C-O	-10.36	1.10	1.24
1	A	119	GLN	CA-C	-10.35	1.38	1.52
2	D	39	TYR	C-O	-10.35	1.10	1.24
1	C	189	PHE	CA-C	-10.31	1.39	1.52
1	A	128	LYS	C-O	-10.31	1.10	1.23
1	C	128	LYS	C-O	-10.29	1.10	1.23
1	A	189	PHE	CA-C	-10.28	1.39	1.52
2	D	43	GLY	CA-C	-10.27	1.40	1.52
1	C	315	ILE	C-O	-10.27	1.11	1.24
2	B	43	GLY	CA-C	-10.26	1.40	1.52
1	A	315	ILE	C-O	-10.25	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	GLN	CA-C	-10.19	1.38	1.52
1	A	227	GLN	CA-C	-10.18	1.38	1.52
1	A	261	LEU	C-O	-10.14	1.10	1.24
1	C	261	LEU	C-O	-10.13	1.10	1.24
1	A	189	PHE	C-O	-10.10	1.12	1.24
1	C	189	PHE	C-O	-10.10	1.12	1.24
1	C	367	VAL	C-O	-10.09	1.11	1.24
1	A	150	LEU	C-O	-10.08	1.12	1.24
1	A	367	VAL	C-O	-10.06	1.11	1.24
1	A	262	LEU	C-O	-10.04	1.11	1.24
1	C	262	LEU	C-O	-10.04	1.11	1.24
1	C	150	LEU	C-O	-10.04	1.12	1.24
1	A	117	SER	C-O	-10.01	1.13	1.23
1	C	117	SER	C-O	-10.00	1.13	1.23
1	A	143	PHE	CA-C	-9.94	1.38	1.52
1	C	143	PHE	CA-C	-9.93	1.38	1.52
1	C	149	PHE	CA-C	-9.93	1.40	1.52
1	A	149	PHE	CA-C	-9.91	1.40	1.52
1	C	176	GLN	C-O	-9.88	1.12	1.24
1	A	176	GLN	C-O	-9.87	1.12	1.24
1	C	221	LYS	C-O	-9.83	1.11	1.24
1	A	221	LYS	C-O	-9.82	1.11	1.24
1	C	175	GLU	C-O	-9.76	1.11	1.24
1	C	193	CYS	C-O	-9.74	1.11	1.24
1	A	175	GLU	C-O	-9.73	1.11	1.24
1	A	193	CYS	C-O	-9.72	1.11	1.24
2	D	46	ILE	C-O	-9.70	1.11	1.24
2	B	46	ILE	C-O	-9.69	1.11	1.24
1	C	312	VAL	CA-CB	-9.68	1.41	1.54
1	C	220	PHE	CA-CB	-9.63	1.37	1.53
1	C	323	LEU	C-O	-9.63	1.12	1.24
1	A	323	LEU	C-O	-9.62	1.12	1.24
2	B	32	LEU	CA-C	-9.61	1.40	1.52
1	C	170	ILE	C-N	-9.60	1.20	1.34
1	A	220	PHE	CA-CB	-9.60	1.37	1.53
2	D	32	LEU	CA-C	-9.60	1.40	1.52
1	A	170	ILE	C-N	-9.58	1.20	1.34
1	A	271	PHE	C-O	-9.58	1.05	1.23
1	C	271	PHE	C-O	-9.56	1.05	1.23
1	A	155	ILE	CA-C	-9.53	1.40	1.52
1	C	155	ILE	CA-C	-9.53	1.40	1.52
2	B	50	TRP	C-O	-9.53	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	221	LYS	CA-C	-9.52	1.39	1.52
2	B	41	LYS	C-O	-9.51	1.13	1.24
2	D	41	LYS	C-O	-9.51	1.13	1.24
1	A	221	LYS	CA-C	-9.49	1.40	1.52
2	D	50	TRP	C-O	-9.49	1.12	1.23
1	A	197	SER	C-O	-9.46	1.14	1.24
1	A	325	ILE	C-O	-9.46	1.11	1.24
1	C	309	ILE	C-O	-9.45	1.12	1.24
1	C	333	PHE	CA-CB	-9.45	1.38	1.53
1	C	197	SER	C-O	-9.43	1.14	1.24
1	C	325	ILE	C-O	-9.42	1.12	1.24
1	A	333	PHE	CA-CB	-9.42	1.38	1.53
1	A	309	ILE	C-O	-9.41	1.12	1.24
2	D	42	TYR	CA-C	-9.39	1.41	1.52
1	A	332	GLN	C-O	-9.37	1.11	1.24
1	C	179	ALA	C-O	-9.37	1.12	1.24
1	C	331	THR	C-O	-9.37	1.12	1.24
2	D	36	ALA	C-O	-9.37	1.12	1.24
1	C	332	GLN	C-O	-9.37	1.11	1.24
1	A	148	GLU	C-O	-9.36	1.12	1.24
1	A	218	PHE	N-CA	-9.36	1.36	1.46
1	A	331	THR	C-O	-9.35	1.12	1.24
1	C	218	PHE	N-CA	-9.35	1.36	1.46
1	A	179	ALA	C-O	-9.35	1.12	1.24
2	B	42	TYR	CA-C	-9.34	1.41	1.52
2	B	36	ALA	C-O	-9.34	1.13	1.24
1	C	148	GLU	C-O	-9.29	1.13	1.24
1	A	118	TYR	C-O	-9.24	1.09	1.24
1	C	118	TYR	C-O	-9.22	1.09	1.24
1	C	233	GLN	C-O	-9.21	1.12	1.24
1	A	233	GLN	C-O	-9.21	1.12	1.24
1	A	217	PRO	C-O	-9.18	1.12	1.24
1	A	147	ARG	N-CA	-9.17	1.35	1.46
1	C	217	PRO	C-O	-9.14	1.12	1.24
1	C	147	ARG	N-CA	-9.14	1.35	1.46
1	A	112	ARG	C-O	-9.10	1.13	1.24
1	C	375	ILE	C-O	-9.08	1.12	1.24
1	C	369	LEU	C-O	-9.08	1.12	1.24
1	A	83	ALA	CA-C	-9.07	1.41	1.53
1	C	83	ALA	CA-C	-9.07	1.41	1.53
1	A	188	PRO	CA-C	-9.05	1.38	1.52
1	C	188	PRO	CA-C	-9.05	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	LEU	C-O	-9.04	1.12	1.24
1	C	260	LEU	C-O	-9.04	1.12	1.24
1	C	112	ARG	C-O	-9.04	1.13	1.24
1	A	375	ILE	C-O	-9.03	1.12	1.24
1	A	369	LEU	C-O	-9.03	1.12	1.24
2	B	37	VAL	C-O	-9.00	1.11	1.24
2	D	34	ILE	CA-C	-8.98	1.41	1.52
2	D	37	VAL	C-O	-8.98	1.11	1.24
2	B	34	ILE	CA-C	-8.97	1.41	1.52
1	A	257	ILE	CA-CB	-8.94	1.42	1.54
1	C	257	ILE	CA-CB	-8.94	1.42	1.54
2	D	46	ILE	CA-CB	-8.91	1.42	1.54
1	A	310	PHE	C-O	-8.90	1.12	1.24
2	B	46	ILE	CA-CB	-8.90	1.42	1.54
1	A	179	ALA	CA-C	-8.89	1.40	1.52
1	C	147	ARG	CA-CB	-8.88	1.39	1.53
1	C	179	ALA	CA-C	-8.87	1.40	1.52
1	A	147	ARG	CA-CB	-8.85	1.39	1.53
1	C	310	PHE	C-O	-8.85	1.12	1.24
1	A	173	ILE	C-O	-8.80	1.13	1.24
1	A	327	TRP	C-O	-8.79	1.12	1.24
1	C	173	ILE	C-O	-8.79	1.13	1.24
1	C	327	TRP	C-O	-8.78	1.12	1.24
1	A	234	GLN	CA-CB	-8.78	1.39	1.53
1	C	234	GLN	CA-CB	-8.76	1.39	1.53
1	C	239	VAL	C-O	-8.71	1.14	1.23
1	A	239	VAL	C-O	-8.70	1.14	1.23
1	A	312	VAL	CA-CB	-8.70	1.41	1.54
1	A	370	TYR	C-O	-8.65	1.13	1.24
1	C	195	TYR	C-O	-8.64	1.14	1.24
1	A	195	TYR	C-O	-8.64	1.14	1.24
1	C	197	SER	CA-C	-8.63	1.43	1.53
2	D	35	ALA	C-O	-8.62	1.12	1.24
1	A	259	THR	CB-CG2	-8.62	1.24	1.52
1	C	370	TYR	C-O	-8.61	1.13	1.24
1	A	154	VAL	CA-C	-8.60	1.43	1.53
2	B	35	ALA	C-O	-8.60	1.12	1.24
1	A	197	SER	CA-C	-8.60	1.43	1.53
1	C	154	VAL	CA-C	-8.60	1.43	1.53
1	A	182	TYR	CA-C	-8.59	1.40	1.52
1	A	184	GLY	C-O	-8.59	1.13	1.23
1	C	184	GLY	C-O	-8.59	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259	THR	CB-CG2	-8.59	1.24	1.52
1	C	182	TYR	CA-C	-8.58	1.40	1.52
1	C	228	ALA	CA-C	-8.56	1.41	1.52
1	A	114	VAL	C-O	-8.54	1.14	1.24
1	A	228	ALA	CA-C	-8.54	1.41	1.52
1	C	114	VAL	C-O	-8.53	1.14	1.24
1	A	236	CYS	C-O	-8.51	1.14	1.24
2	D	34	ILE	C-O	-8.50	1.14	1.24
1	C	199	LEU	C-O	-8.50	1.13	1.24
1	C	236	CYS	C-O	-8.48	1.14	1.24
2	D	44	THR	CA-C	-8.46	1.41	1.52
1	A	315	ILE	CA-C	-8.46	1.41	1.52
1	A	318	ARG	C-O	-8.46	1.13	1.24
1	C	237	ILE	C-O	-8.46	1.13	1.24
1	A	125	ALA	CA-C	-8.45	1.43	1.52
2	B	44	THR	CA-C	-8.45	1.41	1.52
1	C	315	ILE	CA-C	-8.45	1.41	1.52
2	D	21	PHE	CA-C	-8.45	1.42	1.52
1	A	227	GLN	CA-CB	-8.45	1.38	1.53
2	B	45	ARG	C-O	-8.44	1.13	1.24
1	C	227	GLN	CA-CB	-8.44	1.38	1.53
1	A	234	GLN	C-O	-8.44	1.13	1.24
2	D	45	ARG	C-O	-8.44	1.13	1.24
1	C	223	PHE	CA-C	-8.44	1.42	1.52
1	C	318	ARG	C-O	-8.43	1.13	1.24
1	A	237	ILE	C-O	-8.43	1.13	1.24
1	A	223	PHE	CA-C	-8.42	1.42	1.52
2	B	21	PHE	CA-C	-8.42	1.42	1.52
2	B	134	ASP	C-O	-8.40	1.12	1.23
2	B	34	ILE	C-O	-8.40	1.14	1.24
2	D	134	ASP	C-O	-8.39	1.12	1.23
1	C	234	GLN	C-O	-8.39	1.13	1.24
1	A	182	TYR	C-O	-8.37	1.12	1.24
1	A	117	SER	N-CA	-8.36	1.36	1.46
1	A	371	TRP	CA-C	-8.35	1.41	1.52
1	C	182	TYR	C-O	-8.35	1.13	1.24
1	C	371	TRP	CA-C	-8.35	1.41	1.52
1	C	218	PHE	C-O	-8.34	1.15	1.23
1	A	160	ILE	C-O	-8.34	1.14	1.24
1	A	193	CYS	CA-C	-8.34	1.41	1.52
1	C	378	VAL	CA-C	-8.33	1.42	1.52
1	C	160	ILE	C-O	-8.33	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	CYS	CA-C	-8.33	1.41	1.52
1	A	218	PHE	C-O	-8.31	1.15	1.23
1	A	191	ILE	CA-CB	-8.31	1.43	1.54
1	C	191	ILE	CA-CB	-8.31	1.43	1.54
1	C	117	SER	N-CA	-8.30	1.36	1.46
1	A	333	PHE	C-O	-8.30	1.14	1.24
1	C	333	PHE	C-O	-8.30	1.14	1.24
2	D	21	PHE	C-O	-8.29	1.14	1.24
1	A	378	VAL	CA-C	-8.28	1.42	1.52
2	B	21	PHE	C-O	-8.28	1.14	1.24
1	C	217	PRO	CA-C	-8.28	1.40	1.52
1	C	257	ILE	C-O	-8.24	1.14	1.24
1	A	256	HIS	CA-C	-8.23	1.42	1.52
2	B	23	LEU	C-O	-8.22	1.14	1.24
1	A	139	TYR	CZ-OH	-8.22	1.20	1.38
1	C	256	HIS	CA-C	-8.22	1.42	1.52
1	C	139	TYR	CZ-OH	-8.21	1.20	1.38
1	A	217	PRO	CA-C	-8.20	1.40	1.52
2	D	23	LEU	C-O	-8.20	1.14	1.24
1	A	257	ILE	C-O	-8.19	1.14	1.24
1	A	217	PRO	CA-CB	-8.16	1.42	1.53
1	A	208	TYR	CA-C	-8.15	1.42	1.52
2	D	31	LEU	C-O	-8.15	1.13	1.24
1	C	217	PRO	CA-CB	-8.15	1.42	1.53
1	C	215	THR	CB-CG2	-8.14	1.25	1.52
1	C	311	VAL	C-O	-8.13	1.14	1.24
1	C	203	ASN	CA-C	-8.13	1.42	1.52
1	A	311	VAL	C-O	-8.13	1.14	1.24
1	A	215	THR	CB-CG2	-8.12	1.25	1.52
1	C	208	TYR	CA-C	-8.12	1.42	1.52
2	B	31	LEU	C-O	-8.10	1.13	1.24
1	A	203	ASN	CA-C	-8.09	1.42	1.52
1	A	178	TYR	N-CA	-8.07	1.35	1.46
1	C	178	TYR	N-CA	-8.06	1.35	1.46
1	C	224	TYR	CZ-OH	-8.05	1.21	1.38
2	D	41	LYS	CA-C	-8.05	1.42	1.52
1	A	145	PHE	N-CA	-8.05	1.36	1.46
1	C	327	TRP	CB-CG	-8.04	1.25	1.50
2	D	132	ASP	N-CA	-8.03	1.34	1.45
1	A	224	TYR	CZ-OH	-8.03	1.21	1.38
1	C	261	LEU	CA-C	-8.02	1.41	1.52
2	B	132	ASP	N-CA	-8.02	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	LEU	CA-C	-8.01	1.41	1.52
1	A	327	TRP	CB-CG	-8.01	1.25	1.50
2	B	41	LYS	CA-C	-8.00	1.42	1.52
1	A	142	PHE	CA-C	-8.00	1.41	1.52
1	A	252	LEU	C-O	-8.00	1.14	1.24
1	C	145	PHE	N-CA	-7.99	1.36	1.46
1	C	142	PHE	CA-C	-7.98	1.41	1.52
1	C	252	LEU	C-O	-7.97	1.14	1.24
1	C	326	LEU	C-O	-7.95	1.14	1.24
1	A	326	LEU	C-O	-7.94	1.14	1.24
1	C	191	ILE	CA-C	-7.94	1.42	1.52
1	A	191	ILE	CA-C	-7.92	1.42	1.52
1	C	256	HIS	C-O	-7.90	1.14	1.24
1	A	256	HIS	C-O	-7.89	1.14	1.24
1	A	182	TYR	CA-CB	-7.84	1.40	1.53
1	C	194	MET	C-O	-7.83	1.13	1.24
1	A	368	ASN	CA-CB	-7.82	1.40	1.53
1	C	125	ALA	CA-C	-7.82	1.43	1.52
1	C	182	TYR	CA-CB	-7.82	1.40	1.53
1	A	194	MET	C-O	-7.81	1.13	1.24
1	A	182	TYR	CB-CG	-7.79	1.34	1.51
2	B	30	SER	CA-C	-7.79	1.43	1.52
2	D	33	LEU	C-O	-7.78	1.14	1.24
2	B	33	LEU	C-O	-7.78	1.14	1.24
1	C	368	ASN	CA-CB	-7.78	1.40	1.53
1	C	182	TYR	CB-CG	-7.78	1.34	1.51
1	A	372	LEU	CA-C	-7.76	1.42	1.52
2	D	46	ILE	CA-C	-7.76	1.40	1.52
2	B	46	ILE	CA-C	-7.75	1.40	1.52
1	C	372	LEU	CA-C	-7.74	1.42	1.52
2	D	30	SER	CA-C	-7.73	1.43	1.52
1	A	215	THR	CA-C	-7.69	1.43	1.52
1	C	148	GLU	N-CA	-7.68	1.36	1.46
2	B	26	VAL	C-O	-7.67	1.14	1.24
1	C	215	THR	CA-C	-7.67	1.43	1.52
2	D	26	VAL	C-O	-7.67	1.14	1.24
1	A	148	GLU	N-CA	-7.65	1.36	1.46
1	C	233	GLN	CA-CB	-7.61	1.40	1.53
2	B	46	ILE	CB-CG1	-7.59	1.38	1.53
2	D	46	ILE	CB-CG1	-7.59	1.38	1.53
1	A	233	GLN	CA-CB	-7.59	1.40	1.53
1	C	209	ARG	C-O	-7.54	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ARG	C-O	-7.50	1.14	1.24
1	A	191	ILE	C-O	-7.45	1.15	1.24
1	C	159	ALA	CA-C	-7.45	1.43	1.52
1	C	318	ARG	CA-C	-7.44	1.42	1.52
1	A	327	TRP	CA-CB	-7.43	1.41	1.53
1	A	159	ALA	CA-C	-7.43	1.43	1.52
1	C	191	ILE	C-O	-7.43	1.15	1.24
1	C	327	TRP	CA-CB	-7.42	1.41	1.53
1	C	234	GLN	CA-C	-7.41	1.42	1.52
1	A	234	GLN	CA-C	-7.39	1.42	1.52
1	A	306	SER	C-O	-7.38	1.14	1.24
1	A	318	ARG	CA-C	-7.38	1.42	1.52
1	C	311	VAL	CA-C	-7.37	1.43	1.52
1	C	306	SER	C-O	-7.36	1.14	1.24
1	A	311	VAL	CA-C	-7.34	1.43	1.52
2	B	46	ILE	C-N	-7.32	1.24	1.33
2	B	97	GLU	CA-C	-7.31	1.43	1.52
1	A	256	HIS	CA-CB	-7.29	1.42	1.53
1	C	256	HIS	CA-CB	-7.28	1.42	1.53
2	D	97	GLU	CA-C	-7.28	1.43	1.52
2	D	46	ILE	C-N	-7.27	1.24	1.33
1	C	172	ARG	C-O	-7.24	1.14	1.24
1	A	215	THR	C-O	-7.24	1.15	1.24
1	A	269	PHE	CA-CB	-7.22	1.42	1.53
1	A	172	ARG	C-O	-7.20	1.14	1.24
1	C	204	THR	C-N	-7.20	1.23	1.33
1	C	269	PHE	CA-CB	-7.20	1.42	1.53
1	A	192	TYR	CA-CB	-7.19	1.42	1.53
1	C	192	TYR	CA-CB	-7.19	1.42	1.53
1	A	224	TYR	CA-C	-7.19	1.43	1.52
1	C	215	THR	C-O	-7.18	1.15	1.24
1	C	224	TYR	CA-C	-7.16	1.43	1.52
1	A	172	ARG	CA-CB	-7.15	1.41	1.53
2	B	98	HIS	N-CA	-7.15	1.37	1.46
1	C	172	ARG	CA-CB	-7.15	1.41	1.53
2	B	38	GLU	CA-C	-7.14	1.42	1.52
1	A	149	PHE	C-O	-7.13	1.15	1.24
1	C	149	PHE	CG-CD1	-7.13	1.23	1.38
2	D	38	GLU	CA-C	-7.13	1.42	1.52
1	A	219	LEU	CA-CB	-7.12	1.42	1.53
2	B	97	GLU	C-O	-7.11	1.14	1.23
2	D	97	GLU	C-O	-7.11	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	98	HIS	N-CA	-7.11	1.37	1.46
1	A	178	TYR	CA-CB	-7.11	1.42	1.53
1	C	149	PHE	C-O	-7.11	1.16	1.24
1	C	308	ALA	CA-C	-7.11	1.44	1.52
1	A	149	PHE	CG-CD1	-7.10	1.24	1.38
1	C	219	LEU	CA-CB	-7.10	1.42	1.53
1	C	139	TYR	CE1-CZ	-7.10	1.21	1.38
2	B	95	ASN	C-O	-7.10	1.14	1.24
1	A	308	ALA	CA-C	-7.09	1.44	1.52
1	A	186	SER	C-O	-7.09	1.15	1.24
1	C	186	SER	C-O	-7.09	1.15	1.24
1	A	204	THR	C-N	-7.08	1.23	1.33
1	A	334	ARG	CA-C	-7.08	1.44	1.52
1	C	173	ILE	CA-C	-7.08	1.43	1.52
1	A	173	ILE	CA-C	-7.08	1.43	1.52
1	C	126	TYR	CG-CD1	-7.08	1.24	1.39
1	A	139	TYR	CE1-CZ	-7.07	1.21	1.38
1	C	178	TYR	CA-CB	-7.07	1.42	1.53
1	A	126	TYR	CG-CD1	-7.07	1.24	1.39
1	C	308	ALA	C-O	-7.06	1.16	1.24
1	C	334	ARG	CA-C	-7.05	1.44	1.52
2	D	95	ASN	C-O	-7.05	1.14	1.24
2	D	44	THR	CB-CG2	-7.04	1.29	1.52
1	A	373	PHE	C-O	-7.04	1.15	1.24
1	C	373	PHE	C-O	-7.04	1.15	1.24
2	B	44	THR	CB-CG2	-7.02	1.29	1.52
1	C	371	TRP	CA-CB	-7.02	1.41	1.53
1	C	215	THR	N-CA	-7.01	1.38	1.46
1	A	215	THR	N-CA	-7.00	1.38	1.46
1	A	308	ALA	C-O	-7.00	1.16	1.24
1	C	110	LEU	N-CA	-6.99	1.37	1.46
1	C	192	TYR	CA-C	-6.98	1.43	1.52
1	A	371	TRP	CA-CB	-6.96	1.41	1.53
1	A	148	GLU	CA-CB	-6.96	1.42	1.53
1	C	148	GLU	CA-CB	-6.95	1.42	1.53
1	A	192	TYR	CA-C	-6.95	1.43	1.52
1	C	269	PHE	C-N	-6.94	1.23	1.33
1	A	269	PHE	C-N	-6.94	1.23	1.33
1	C	185	VAL	CA-CB	-6.94	1.45	1.54
1	A	375	ILE	CA-C	-6.93	1.42	1.52
1	A	206	ALA	CA-CB	-6.93	1.41	1.53
1	C	310	PHE	CA-C	-6.93	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	ALA	CA-CB	-6.92	1.41	1.53
1	C	224	TYR	CB-CG	-6.92	1.36	1.51
1	A	110	LEU	N-CA	-6.92	1.37	1.46
1	A	381	ARG	CA-C	-6.92	1.44	1.52
1	A	185	VAL	CA-CB	-6.91	1.45	1.54
1	A	224	TYR	CB-CG	-6.91	1.36	1.51
1	A	310	PHE	CA-C	-6.91	1.43	1.52
1	C	381	ARG	CA-C	-6.91	1.44	1.52
1	C	375	ILE	CA-C	-6.90	1.42	1.52
1	A	324	LYS	CA-CB	-6.90	1.42	1.53
2	D	45	ARG	CD-NE	-6.90	1.36	1.46
1	A	258	VAL	CA-CB	-6.89	1.45	1.54
1	C	258	VAL	CA-CB	-6.89	1.45	1.54
1	C	322	ASN	CA-C	-6.89	1.43	1.52
1	A	322	ASN	CA-C	-6.89	1.43	1.52
1	C	324	LYS	CA-CB	-6.88	1.42	1.53
2	D	50	TRP	CB-CG	-6.88	1.28	1.50
2	B	45	ARG	CD-NE	-6.88	1.36	1.46
1	C	162	LEU	CA-C	-6.87	1.43	1.52
2	B	50	TRP	CB-CG	-6.87	1.28	1.50
1	A	198	ASP	CA-C	-6.85	1.43	1.52
2	B	38	GLU	CA-CB	-6.84	1.41	1.53
1	C	118	TYR	CZ-OH	-6.84	1.23	1.38
1	C	198	ASP	CA-C	-6.84	1.43	1.52
2	D	38	GLU	CA-CB	-6.83	1.41	1.53
1	C	220	PHE	CA-C	-6.83	1.43	1.52
1	C	152	ASP	C-O	-6.82	1.16	1.24
1	C	312	VAL	C-O	-6.82	1.15	1.24
1	A	162	LEU	CA-C	-6.81	1.43	1.52
1	A	118	TYR	CZ-OH	-6.81	1.23	1.38
1	A	152	ASP	C-O	-6.81	1.16	1.24
1	A	220	PHE	CA-C	-6.81	1.43	1.52
1	C	307	PHE	CB-CG	-6.81	1.34	1.50
1	A	307	PHE	CB-CG	-6.79	1.35	1.50
2	D	37	VAL	CA-C	-6.79	1.42	1.52
2	B	37	VAL	CA-C	-6.78	1.42	1.52
1	A	320	TYR	CA-CB	-6.77	1.42	1.53
1	C	265	SER	CA-CB	-6.77	1.42	1.53
1	C	228	ALA	CA-CB	-6.76	1.42	1.53
1	C	320	TYR	CA-CB	-6.76	1.42	1.53
1	A	265	SER	CA-CB	-6.76	1.42	1.53
1	A	262	LEU	CA-C	-6.76	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	20	ILE	CA-C	-6.75	1.44	1.52
1	A	228	ALA	CA-CB	-6.75	1.42	1.53
2	B	20	ILE	CA-C	-6.74	1.44	1.52
2	D	40	PHE	CA-C	-6.74	1.44	1.52
1	A	208	TYR	CZ-OH	-6.74	1.23	1.38
1	C	208	TYR	CZ-OH	-6.74	1.24	1.38
1	C	262	LEU	CA-C	-6.72	1.43	1.52
2	B	40	PHE	CA-C	-6.72	1.44	1.52
1	C	313	ALA	CA-CB	-6.71	1.42	1.53
1	C	225	LEU	CA-C	-6.70	1.43	1.52
1	C	333	PHE	CG-CD1	-6.68	1.24	1.38
1	A	313	ALA	CA-CB	-6.67	1.42	1.53
1	A	225	LEU	CA-C	-6.67	1.43	1.52
1	C	240	LEU	C-O	-6.67	1.15	1.24
2	D	23	LEU	CA-C	-6.67	1.44	1.52
2	B	23	LEU	CA-C	-6.66	1.44	1.52
2	B	132	ASP	CA-C	-6.65	1.43	1.52
1	A	333	PHE	CG-CD1	-6.65	1.24	1.38
2	D	132	ASP	CA-C	-6.65	1.43	1.52
1	C	261	LEU	CA-CB	-6.64	1.42	1.53
1	A	240	LEU	C-O	-6.64	1.15	1.24
1	A	382	ILE	CA-C	-6.63	1.45	1.52
1	A	200	TRP	C-O	-6.62	1.16	1.24
1	C	382	ILE	CA-C	-6.62	1.45	1.52
1	A	261	LEU	CA-CB	-6.62	1.42	1.53
1	A	230	PHE	CA-CB	-6.61	1.42	1.53
1	A	192	TYR	CB-CG	-6.61	1.37	1.51
1	A	312	VAL	C-O	-6.61	1.15	1.24
1	C	192	TYR	CB-CG	-6.61	1.37	1.51
1	C	200	TRP	C-O	-6.60	1.16	1.24
1	C	230	PHE	CA-CB	-6.60	1.42	1.53
1	A	334	ARG	CA-CB	-6.58	1.43	1.53
1	A	216	ASN	CG-ND2	-6.58	1.19	1.33
1	C	322	ASN	CA-CB	-6.57	1.42	1.53
1	C	216	ASN	CG-ND2	-6.56	1.19	1.33
1	A	218	PHE	CA-CB	-6.56	1.45	1.53
1	C	330	LEU	N-CA	6.55	1.54	1.46
1	A	322	ASN	CA-CB	-6.55	1.42	1.53
1	C	334	ARG	CA-CB	-6.55	1.43	1.53
1	A	320	TYR	CE1-CZ	-6.53	1.22	1.38
1	C	218	PHE	CA-CB	-6.51	1.45	1.53
1	C	240	LEU	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	PHE	CG-CD2	-6.51	1.25	1.38
1	C	320	TYR	CE1-CZ	-6.50	1.22	1.38
1	C	367	VAL	CA-CB	-6.50	1.45	1.54
1	C	374	LEU	C-O	-6.50	1.16	1.24
1	C	257	ILE	CA-C	-6.50	1.44	1.52
1	A	374	LEU	C-O	-6.49	1.16	1.24
1	A	367	VAL	CA-CB	-6.49	1.45	1.54
1	A	240	LEU	CA-C	-6.49	1.44	1.52
1	A	330	LEU	N-CA	6.49	1.53	1.46
1	C	126	TYR	CG-CD2	-6.48	1.25	1.39
2	B	98	HIS	CA-C	-6.48	1.44	1.52
2	D	98	HIS	CA-C	-6.48	1.44	1.52
1	A	257	ILE	CA-C	-6.48	1.44	1.52
2	B	36	ALA	CA-CB	-6.48	1.43	1.53
1	C	142	PHE	CG-CD2	-6.47	1.25	1.38
1	A	126	TYR	CZ-OH	-6.47	1.24	1.38
1	A	126	TYR	CG-CD2	-6.47	1.25	1.39
1	C	325	ILE	CA-CB	-6.47	1.45	1.54
1	A	325	ILE	CA-CB	-6.46	1.45	1.54
2	D	36	ALA	CA-CB	-6.46	1.43	1.53
1	C	126	TYR	CZ-OH	-6.46	1.24	1.38
1	C	180	ILE	CB-CG1	-6.45	1.40	1.53
2	D	25	ARG	C-O	-6.45	1.16	1.24
2	B	25	ARG	C-O	-6.44	1.16	1.24
1	C	269	PHE	CA-C	-6.44	1.44	1.52
2	D	35	ALA	CA-C	-6.44	1.43	1.52
1	A	78	ILE	CA-C	-6.43	1.45	1.52
1	A	190	GLY	C-O	-6.43	1.16	1.23
1	C	78	ILE	CA-C	-6.43	1.45	1.52
1	A	332	GLN	CA-CB	-6.43	1.43	1.53
1	C	334	ARG	N-CA	-6.43	1.38	1.46
1	A	180	ILE	CB-CG1	-6.42	1.40	1.53
1	A	269	PHE	CA-C	-6.42	1.44	1.52
2	B	35	ALA	CA-C	-6.42	1.43	1.52
1	A	334	ARG	N-CA	-6.41	1.38	1.46
1	C	190	GLY	C-O	-6.40	1.16	1.23
1	C	332	GLN	CA-CB	-6.39	1.43	1.53
1	A	253	THR	C-O	-6.39	1.15	1.24
1	C	253	THR	C-O	-6.38	1.15	1.24
1	A	264	TRP	CA-CB	-6.38	1.43	1.53
1	A	329	VAL	CA-C	-6.37	1.45	1.52
1	C	207	MET	C-O	-6.36	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	MET	C-O	-6.36	1.16	1.24
1	A	372	LEU	C-O	-6.35	1.16	1.24
1	C	372	LEU	C-O	-6.35	1.16	1.24
1	A	370	TYR	CA-CB	-6.34	1.43	1.53
1	C	329	VAL	CA-C	-6.34	1.45	1.52
1	C	370	TYR	CA-CB	-6.34	1.43	1.53
1	C	188	PRO	C-O	-6.33	1.16	1.24
1	A	188	PRO	C-O	-6.32	1.16	1.24
1	C	264	TRP	CA-CB	-6.31	1.43	1.53
1	C	238	LEU	C-O	-6.31	1.15	1.24
1	A	238	LEU	C-O	-6.29	1.15	1.24
1	C	208	TYR	CA-CB	-6.28	1.45	1.54
1	C	152	ASP	CB-CG	-6.28	1.36	1.52
1	A	152	ASP	CB-CG	-6.26	1.36	1.52
1	A	126	TYR	CB-CG	-6.26	1.37	1.51
1	A	171	LYS	CA-CB	-6.26	1.43	1.53
1	C	126	TYR	CB-CG	-6.26	1.37	1.51
1	A	208	TYR	CA-CB	-6.25	1.45	1.54
1	C	171	LYS	CA-CB	-6.25	1.43	1.53
1	A	314	TRP	CG-CD1	-6.23	1.21	1.36
1	A	184	GLY	CA-C	-6.22	1.45	1.52
1	C	184	GLY	CA-C	-6.22	1.45	1.52
1	C	334	ARG	C-N	-6.22	1.25	1.33
1	C	314	TRP	CG-CD1	-6.21	1.21	1.36
1	A	307	PHE	C-O	-6.21	1.16	1.24
1	C	120	ILE	C-O	-6.19	1.18	1.23
1	A	334	ARG	C-N	-6.18	1.25	1.33
1	A	324	LYS	C-O	-6.16	1.16	1.24
2	B	22	ASN	C-O	-6.15	1.17	1.24
2	D	22	ASN	C-O	-6.15	1.17	1.24
1	C	259	THR	N-CA	-6.13	1.39	1.46
1	A	120	ILE	C-O	-6.13	1.18	1.23
1	C	307	PHE	C-O	-6.12	1.16	1.24
2	D	97	GLU	CA-CB	-6.12	1.41	1.54
1	A	259	THR	N-CA	-6.11	1.39	1.46
1	C	324	LYS	C-O	-6.11	1.16	1.24
2	B	97	GLU	CA-CB	-6.10	1.41	1.54
1	A	155	ILE	C-O	-6.09	1.16	1.23
1	A	188	PRO	CA-CB	-6.09	1.43	1.53
2	B	117	HIS	C-O	-6.09	1.16	1.24
2	B	42	TYR	CA-CB	-6.09	1.43	1.53
2	D	42	TYR	CA-CB	-6.08	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	ILE	CA-CB	-6.08	1.46	1.54
2	D	117	HIS	C-O	-6.08	1.16	1.24
2	B	28	PHE	C-O	-6.08	1.16	1.24
1	C	188	PRO	CA-CB	-6.08	1.43	1.53
1	A	263	ILE	CA-CB	-6.07	1.46	1.54
1	C	155	ILE	C-O	-6.06	1.16	1.23
1	C	227	GLN	CD-NE2	-6.05	1.20	1.33
1	A	149	PHE	CG-CD2	-6.05	1.26	1.38
2	B	50	TRP	CG-CD1	-6.04	1.21	1.36
1	C	370	TYR	CA-C	-6.04	1.45	1.52
2	D	45	ARG	N-CA	-6.04	1.38	1.46
1	A	232	ALA	CA-CB	-6.03	1.44	1.53
2	B	45	ARG	N-CA	-6.03	1.38	1.46
1	A	227	GLN	CD-NE2	-6.03	1.20	1.33
1	A	370	TYR	CA-C	-6.03	1.45	1.52
2	D	28	PHE	C-O	-6.02	1.16	1.24
1	C	149	PHE	CG-CD2	-6.01	1.26	1.38
1	C	232	ALA	CA-CB	-6.01	1.44	1.53
2	D	50	TRP	CG-CD1	-6.01	1.22	1.36
1	A	174	MET	CA-C	-6.00	1.45	1.52
1	C	154	VAL	CA-CB	-6.00	1.47	1.54
1	C	331	THR	N-CA	-6.00	1.39	1.46
1	C	263	ILE	CA-C	-6.00	1.45	1.52
1	A	331	THR	N-CA	-5.99	1.39	1.46
1	A	253	THR	CA-C	-5.99	1.44	1.52
1	A	263	ILE	CA-C	-5.98	1.45	1.52
1	A	154	VAL	CA-CB	-5.97	1.47	1.54
1	C	174	MET	CA-C	-5.97	1.45	1.52
1	A	231	TRP	CB-CG	-5.96	1.31	1.50
1	C	231	TRP	CB-CG	-5.96	1.31	1.50
1	C	253	THR	CA-C	-5.94	1.44	1.52
1	C	189	PHE	N-CA	-5.93	1.39	1.46
1	A	118	TYR	CA-CB	-5.93	1.44	1.53
2	D	50	TRP	CA-CB	-5.93	1.45	1.54
1	A	221	LYS	CA-CB	-5.93	1.43	1.53
1	C	126	TYR	CE2-CZ	-5.93	1.24	1.38
1	A	189	PHE	N-CA	-5.92	1.39	1.46
1	C	221	LYS	CA-CB	-5.92	1.43	1.53
1	A	256	HIS	CB-CG	-5.92	1.41	1.50
1	A	231	TRP	CD2-CE2	-5.92	1.31	1.41
1	C	260	LEU	CA-CB	-5.92	1.43	1.53
2	D	133	THR	N-CA	-5.91	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	133	THR	N-CA	-5.91	1.38	1.46
1	A	318	ARG	CA-CB	-5.91	1.43	1.53
1	A	327	TRP	CA-C	-5.91	1.44	1.52
2	B	50	TRP	CA-CB	-5.91	1.45	1.54
1	A	260	LEU	CA-CB	-5.90	1.43	1.53
1	C	118	TYR	CA-CB	-5.90	1.44	1.53
1	A	126	TYR	CE2-CZ	-5.90	1.24	1.38
1	A	175	GLU	CA-C	-5.89	1.44	1.52
2	D	44	THR	CB-OG1	-5.89	1.34	1.43
1	C	256	HIS	CB-CG	-5.89	1.42	1.50
1	C	231	TRP	CD2-CE2	-5.89	1.31	1.41
2	B	44	THR	CB-OG1	-5.88	1.34	1.43
1	C	318	ARG	CA-CB	-5.88	1.43	1.53
1	C	327	TRP	CA-C	-5.88	1.44	1.52
1	C	175	GLU	CA-C	-5.87	1.44	1.52
1	A	320	TYR	CB-CG	-5.87	1.38	1.51
1	A	199	LEU	C-O	-5.87	1.13	1.23
2	D	97	GLU	N-CA	-5.86	1.38	1.45
1	C	186	SER	CA-CB	-5.86	1.43	1.53
1	C	118	TYR	CA-C	-5.86	1.43	1.52
1	A	118	TYR	CA-C	-5.85	1.43	1.52
2	B	134	ASP	CB-CG	-5.85	1.37	1.52
1	C	320	TYR	CB-CG	-5.84	1.38	1.51
2	D	134	ASP	CB-CG	-5.84	1.37	1.52
1	A	186	SER	CA-CB	-5.84	1.43	1.53
1	C	147	ARG	CD-NE	-5.83	1.38	1.46
1	A	254	PHE	C-O	-5.83	1.17	1.24
2	B	97	GLU	N-CA	-5.83	1.38	1.45
1	C	161	ARG	CA-C	-5.83	1.45	1.53
1	C	232	ALA	C-N	-5.82	1.26	1.34
1	A	375	ILE	CA-CB	-5.81	1.46	1.54
1	A	139	TYR	CA-C	-5.79	1.44	1.52
1	A	147	ARG	CD-NE	-5.78	1.38	1.46
1	C	254	PHE	C-O	-5.78	1.17	1.24
1	C	139	TYR	CA-C	-5.77	1.44	1.52
1	A	161	ARG	CA-C	-5.77	1.45	1.53
1	C	375	ILE	CA-CB	-5.77	1.46	1.54
1	A	232	ALA	C-N	-5.76	1.26	1.34
1	C	149	PHE	CA-CB	-5.76	1.44	1.53
1	A	149	PHE	CA-CB	-5.76	1.44	1.53
1	A	307	PHE	CA-CB	-5.75	1.44	1.53
1	C	260	LEU	N-CA	-5.73	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	PHE	CA-CB	-5.73	1.44	1.53
1	A	373	PHE	CA-C	-5.72	1.45	1.52
2	B	134	ASP	C-N	-5.72	1.26	1.34
2	D	27	CYS	C-O	-5.72	1.16	1.24
1	C	305	PHE	CA-CB	-5.71	1.44	1.53
1	C	310	PHE	CA-CB	-5.71	1.44	1.53
2	D	134	ASP	C-N	-5.71	1.26	1.34
2	B	27	CYS	C-O	-5.71	1.16	1.24
2	D	122	GLU	CA-C	-5.70	1.45	1.52
2	B	95	ASN	CG-ND2	-5.70	1.21	1.33
1	C	373	PHE	CA-C	-5.70	1.45	1.52
1	A	82	HIS	C-O	-5.69	1.16	1.23
1	A	268	VAL	CA-C	-5.69	1.45	1.52
1	C	307	PHE	CA-CB	-5.69	1.44	1.53
2	D	95	ASN	CG-ND2	-5.68	1.21	1.33
1	A	271	PHE	C-N	-5.68	1.25	1.33
1	A	305	PHE	CA-CB	-5.68	1.44	1.53
1	A	326	LEU	CA-C	-5.67	1.45	1.52
1	C	326	LEU	CA-C	-5.67	1.45	1.52
1	C	82	HIS	C-O	-5.67	1.16	1.23
1	C	169	ARG	CA-C	-5.67	1.45	1.52
1	C	271	PHE	C-N	-5.66	1.25	1.33
1	A	169	ARG	CA-C	-5.66	1.45	1.52
2	B	122	GLU	CA-C	-5.66	1.45	1.52
1	C	323	LEU	CA-C	-5.66	1.45	1.52
1	A	260	LEU	N-CA	-5.65	1.39	1.46
1	A	264	TRP	CD2-CE2	-5.65	1.31	1.41
1	C	268	VAL	CA-C	-5.65	1.46	1.52
2	D	134	ASP	CG-OD1	-5.64	1.14	1.25
1	A	231	TRP	CA-CB	-5.64	1.44	1.53
1	C	264	TRP	CD2-CE2	-5.64	1.31	1.41
1	C	371	TRP	CD2-CE2	-5.64	1.31	1.41
2	D	29	ILE	C-O	-5.64	1.17	1.24
1	A	208	TYR	CB-CG	-5.63	1.39	1.51
1	C	208	TYR	CB-CG	-5.63	1.39	1.51
2	D	116	ILE	CA-C	-5.63	1.44	1.52
2	B	134	ASP	CG-OD1	-5.62	1.14	1.25
2	B	29	ILE	C-O	-5.62	1.17	1.24
1	C	208	TYR	CE1-CZ	-5.62	1.24	1.38
1	C	231	TRP	CA-CB	-5.62	1.44	1.53
1	A	208	TYR	CE1-CZ	-5.61	1.24	1.38
2	B	20	ILE	N-CA	-5.61	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	LEU	CA-C	-5.61	1.45	1.52
1	A	204	THR	CB-CG2	-5.60	1.34	1.52
1	A	212	PRO	C-O	-5.59	1.17	1.24
1	A	371	TRP	CD2-CE2	-5.59	1.31	1.41
2	B	116	ILE	CA-C	-5.59	1.44	1.52
2	B	31	LEU	CA-C	-5.59	1.45	1.52
2	D	20	ILE	N-CA	-5.59	1.39	1.46
2	D	35	ALA	CA-CB	-5.59	1.43	1.53
2	B	35	ALA	CA-CB	-5.58	1.43	1.53
1	A	187	GLY	CA-C	-5.58	1.44	1.51
1	C	212	PRO	C-O	-5.58	1.17	1.24
1	A	331	THR	CA-CB	-5.57	1.44	1.53
1	C	331	THR	CA-CB	-5.57	1.44	1.53
2	D	22	ASN	N-CA	-5.57	1.39	1.46
1	C	258	VAL	C-O	-5.57	1.16	1.24
2	B	22	ASN	N-CA	-5.57	1.39	1.46
2	D	31	LEU	CA-C	-5.57	1.45	1.52
1	C	204	THR	CB-CG2	-5.56	1.34	1.52
1	A	368	ASN	N-CA	-5.56	1.39	1.46
1	C	307	PHE	CG-CD1	-5.55	1.27	1.38
1	A	258	VAL	C-O	-5.55	1.16	1.24
1	C	187	GLY	CA-C	-5.54	1.44	1.51
1	A	307	PHE	CG-CD1	-5.53	1.27	1.38
1	C	303	ALA	CA-C	-5.53	1.45	1.52
1	A	303	ALA	CA-C	-5.52	1.45	1.52
1	A	124	ASN	C-O	-5.52	1.16	1.23
1	C	125	ALA	N-CA	-5.52	1.40	1.46
2	D	37	VAL	CA-CB	-5.52	1.46	1.54
1	C	368	ASN	N-CA	-5.51	1.39	1.46
1	A	198	ASP	C-O	-5.51	1.16	1.23
1	C	198	ASP	C-O	-5.50	1.16	1.23
1	C	124	ASN	C-O	-5.50	1.16	1.23
1	C	223	PHE	CA-CB	-5.50	1.44	1.53
1	A	223	PHE	CA-CB	-5.49	1.44	1.53
2	B	122	GLU	CA-CB	-5.49	1.44	1.53
2	D	122	GLU	CA-CB	-5.49	1.44	1.53
1	A	208	TYR	N-CA	-5.48	1.38	1.45
2	B	37	VAL	CA-CB	-5.48	1.46	1.54
1	A	319	HIS	C-N	-5.48	1.26	1.33
1	C	208	TYR	N-CA	-5.48	1.38	1.45
1	C	319	HIS	C-N	-5.46	1.26	1.33
1	C	118	TYR	CB-CG	-5.46	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	TYR	CB-CG	-5.45	1.39	1.51
1	A	224	TYR	CA-CB	-5.45	1.44	1.53
1	C	189	PHE	CA-CB	-5.43	1.44	1.53
1	A	185	VAL	C-O	-5.42	1.17	1.24
1	A	125	ALA	N-CA	-5.42	1.40	1.46
1	C	185	VAL	C-O	-5.41	1.17	1.24
1	C	204	THR	C-O	-5.41	1.17	1.24
1	C	367	VAL	CA-C	-5.40	1.44	1.52
1	A	189	PHE	CA-CB	-5.40	1.44	1.53
1	C	167	LYS	C-N	-5.39	1.26	1.33
1	C	178	TYR	C-O	-5.39	1.17	1.24
1	A	367	VAL	CA-C	-5.39	1.44	1.52
1	C	82	HIS	CA-CB	-5.39	1.44	1.53
1	A	143	PHE	CG-CD2	-5.38	1.27	1.38
1	C	262	LEU	CA-CB	-5.38	1.44	1.53
1	C	224	TYR	CA-CB	-5.38	1.45	1.53
1	A	178	TYR	C-O	-5.38	1.17	1.24
1	A	167	LYS	C-N	-5.37	1.26	1.33
1	A	262	LEU	CA-CB	-5.37	1.44	1.53
2	B	134	ASP	CA-CB	-5.37	1.45	1.53
1	C	143	PHE	CG-CD2	-5.36	1.27	1.38
1	C	264	TRP	CB-CG	-5.35	1.33	1.50
1	C	119	GLN	CA-CB	-5.35	1.45	1.53
1	A	119	GLN	CA-CB	-5.35	1.45	1.53
2	D	50	TRP	CD2-CE2	-5.35	1.32	1.41
1	A	327	TRP	CG-CD1	-5.35	1.23	1.36
1	C	208	TYR	CG-CD2	-5.33	1.28	1.39
1	A	82	HIS	CA-CB	-5.33	1.45	1.53
1	C	327	TRP	CG-CD1	-5.33	1.23	1.36
1	A	264	TRP	CB-CG	-5.33	1.33	1.50
1	C	118	TYR	CE2-CZ	-5.33	1.25	1.38
1	A	208	TYR	CG-CD2	-5.33	1.28	1.39
1	C	305	PHE	C-O	-5.33	1.17	1.24
2	B	20	ILE	CA-CB	-5.32	1.47	1.54
1	A	83	ALA	C-N	-5.32	1.26	1.33
1	A	305	PHE	C-O	-5.31	1.17	1.24
1	A	316	TYR	N-CA	-5.31	1.40	1.46
1	C	146	LEU	C-N	-5.31	1.27	1.33
1	C	316	TYR	N-CA	-5.31	1.40	1.46
1	C	83	ALA	C-N	-5.31	1.26	1.33
1	A	74	SER	C-O	-5.30	1.18	1.24
1	A	118	TYR	CE2-CZ	-5.30	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	50	TRP	CD2-CE2	-5.30	1.32	1.41
2	D	134	ASP	CA-CB	-5.30	1.45	1.53
1	C	113	PHE	N-CA	5.30	1.53	1.46
1	C	74	SER	C-O	-5.28	1.18	1.24
1	A	319	HIS	CA-CB	-5.27	1.46	1.53
1	A	126	TYR	CA-C	-5.27	1.46	1.52
1	A	368	ASN	CG-ND2	-5.27	1.22	1.33
1	A	235	ALA	CA-C	-5.27	1.46	1.52
2	B	50	TRP	C-N	-5.27	1.26	1.33
2	D	20	ILE	CA-CB	-5.27	1.47	1.54
1	A	172	ARG	CA-C	-5.26	1.45	1.52
1	C	317	LEU	CB-CG	-5.26	1.43	1.53
1	A	146	LEU	C-N	-5.26	1.27	1.33
1	C	235	ALA	CA-C	-5.26	1.46	1.52
1	C	368	ASN	CG-ND2	-5.26	1.22	1.33
1	A	113	PHE	N-CA	5.25	1.53	1.46
1	C	319	HIS	CA-CB	-5.25	1.46	1.53
1	C	126	TYR	CA-C	-5.25	1.46	1.52
1	A	317	LEU	CB-CG	-5.24	1.43	1.53
1	A	249	HIS	CA-C	-5.23	1.45	1.52
2	D	50	TRP	C-N	-5.23	1.26	1.33
1	C	172	ARG	CA-C	-5.22	1.45	1.52
1	A	220	PHE	CB-CG	-5.22	1.38	1.50
2	D	118	GLU	C-O	-5.22	1.18	1.24
1	C	176	GLN	CA-CB	-5.22	1.45	1.53
1	C	220	PHE	CB-CG	-5.21	1.38	1.50
1	C	249	HIS	CA-C	-5.21	1.45	1.52
1	A	200	TRP	CE2-CZ2	-5.20	1.28	1.39
1	A	203	ASN	CB-CG	-5.20	1.39	1.52
1	A	333	PHE	CB-CG	-5.20	1.38	1.50
1	C	200	TRP	CE2-CZ2	-5.20	1.28	1.39
1	C	333	PHE	CB-CG	-5.20	1.38	1.50
1	A	176	GLN	CA-CB	-5.19	1.45	1.53
2	B	122	GLU	C-O	-5.19	1.17	1.23
2	B	118	GLU	C-O	-5.18	1.18	1.24
1	C	203	ASN	CB-CG	-5.18	1.39	1.52
1	A	264	TRP	CE2-CZ2	-5.18	1.28	1.39
1	C	264	TRP	CE2-CZ2	-5.18	1.28	1.39
1	C	149	PHE	N-CA	-5.15	1.40	1.46
1	A	152	ASP	N-CA	-5.15	1.40	1.46
1	A	333	PHE	CA-C	-5.15	1.46	1.52
1	C	166	SER	C-O	-5.15	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	TYR	CA-CB	-5.15	1.45	1.53
1	A	149	PHE	N-CA	-5.14	1.40	1.46
1	C	314	TRP	CD2-CE2	-5.14	1.32	1.41
1	C	152	ASP	N-CA	-5.14	1.40	1.46
2	B	38	GLU	C-O	-5.14	1.17	1.24
1	A	161	ARG	N-CA	-5.13	1.39	1.46
1	C	117	SER	CA-C	-5.13	1.47	1.53
1	A	314	TRP	CD2-CE2	-5.13	1.32	1.41
1	A	316	TYR	CA-CB	-5.12	1.45	1.53
1	C	161	ARG	N-CA	-5.12	1.39	1.46
1	A	166	SER	C-O	-5.12	1.17	1.24
1	C	333	PHE	CA-C	-5.12	1.46	1.52
2	D	38	GLU	C-O	-5.12	1.17	1.24
2	D	122	GLU	C-O	-5.11	1.17	1.23
1	C	329	VAL	CA-CB	-5.10	1.48	1.54
1	C	113	PHE	CG-CD2	-5.09	1.28	1.38
1	C	237	ILE	CA-C	-5.09	1.45	1.52
1	A	117	SER	CA-C	-5.08	1.47	1.53
1	A	139	TYR	CE2-CZ	-5.08	1.26	1.38
1	A	271	PHE	N-CA	-5.08	1.40	1.46
1	A	237	ILE	CA-C	-5.08	1.45	1.52
1	A	259	THR	CA-CB	-5.07	1.45	1.53
1	A	224	TYR	CE1-CZ	-5.07	1.26	1.38
1	A	269	PHE	CG-CD1	-5.07	1.28	1.38
1	C	139	TYR	CE2-CZ	-5.07	1.26	1.38
1	C	368	ASN	CG-OD1	-5.07	1.14	1.23
1	A	144	THR	C-N	-5.07	1.27	1.33
1	C	234	GLN	CG-CD	-5.07	1.39	1.52
1	C	269	PHE	CG-CD1	-5.07	1.28	1.38
1	C	316	TYR	CB-CG	-5.06	1.40	1.51
1	A	329	VAL	CA-CB	-5.06	1.48	1.54
2	D	34	ILE	CA-CB	-5.06	1.48	1.54
1	C	224	TYR	CE1-CZ	-5.06	1.26	1.38
1	C	259	THR	CA-CB	-5.06	1.45	1.53
1	C	307	PHE	CA-C	-5.06	1.46	1.52
1	A	325	ILE	CA-C	-5.06	1.45	1.52
1	C	144	THR	C-N	-5.06	1.27	1.33
2	B	34	ILE	CA-CB	-5.05	1.48	1.54
1	A	259	THR	CA-C	-5.05	1.46	1.52
1	A	368	ASN	CG-OD1	-5.05	1.14	1.23
1	A	113	PHE	CG-CD2	-5.05	1.28	1.38
1	C	259	THR	CA-C	-5.05	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GLN	CG-CD	-5.04	1.39	1.52
1	A	316	TYR	CB-CG	-5.04	1.40	1.51
1	C	271	PHE	N-CA	-5.04	1.40	1.46
1	A	204	THR	C-O	-5.04	1.18	1.24
1	C	230	PHE	CG-CD2	-5.03	1.28	1.38
1	A	230	PHE	CG-CD2	-5.03	1.28	1.38
1	C	325	ILE	CA-C	-5.02	1.45	1.52
1	C	314	TRP	CE2-CZ2	-5.02	1.29	1.39
1	A	307	PHE	CA-C	-5.02	1.46	1.52
1	A	314	TRP	CE2-CZ2	-5.01	1.29	1.39
1	A	209	ARG	C-N	-5.01	1.25	1.33
1	C	209	ARG	C-N	-5.00	1.25	1.33
1	A	220	PHE	N-CA	-5.00	1.40	1.46

All (396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	TYR	CA-C-N	-20.11	97.16	119.28
1	C	211	TYR	C-N-CA	-20.11	97.16	119.28
1	A	211	TYR	CA-C-N	-20.08	97.19	119.28
1	A	211	TYR	C-N-CA	-20.08	97.19	119.28
1	C	173	ILE	CB-CA-C	-15.28	91.14	112.22
1	A	173	ILE	CB-CA-C	-15.25	91.18	112.22
1	C	333	PHE	N-CA-C	-14.10	94.19	111.40
1	A	333	PHE	N-CA-C	-14.07	94.23	111.40
1	A	110	LEU	N-CA-C	-13.56	96.57	111.36
1	C	110	LEU	N-CA-C	-13.54	96.60	111.36
1	C	74	SER	N-CA-C	-13.37	96.70	111.14
1	A	74	SER	N-CA-C	-13.37	96.70	111.14
1	A	72	TRP	N-CA-C	13.20	126.95	111.11
1	C	72	TRP	N-CA-C	13.17	126.92	111.11
1	C	118	TYR	N-CA-C	12.46	127.92	112.47
1	A	118	TYR	N-CA-C	12.45	127.91	112.47
1	C	168	HIS	N-CA-C	-11.29	95.78	112.04
1	A	168	HIS	N-CA-C	-11.26	95.83	112.04
1	C	184	GLY	N-CA-C	-10.49	99.80	112.49
1	A	184	GLY	N-CA-C	-10.48	99.81	112.49
1	C	206	ALA	N-CA-C	10.06	123.49	111.82
1	A	206	ALA	N-CA-C	10.04	123.47	111.82
2	B	40	PHE	N-CA-C	-10.03	99.17	111.40
2	D	40	PHE	N-CA-C	-9.99	99.22	111.40
1	A	153	VAL	N-CA-C	9.88	120.69	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	VAL	N-CA-C	9.87	120.68	110.62
1	C	164	VAL	N-CA-C	-9.76	95.96	108.84
1	A	164	VAL	N-CA-C	-9.74	95.98	108.84
1	A	323	LEU	N-CA-C	-9.59	99.70	111.40
1	C	323	LEU	N-CA-C	-9.59	99.71	111.40
2	B	43	GLY	CA-C-O	-9.51	110.95	120.75
2	D	43	GLY	CA-C-O	-9.49	110.98	120.75
1	C	204	THR	CA-C-O	9.38	130.36	120.42
1	A	204	THR	CA-C-O	9.35	130.33	120.42
1	A	170	ILE	CA-C-N	-9.21	106.31	120.31
1	A	170	ILE	C-N-CA	-9.21	106.31	120.31
1	C	170	ILE	CA-C-N	-9.21	106.32	120.31
1	C	170	ILE	C-N-CA	-9.21	106.32	120.31
1	C	334	ARG	N-CA-C	9.20	121.00	110.97
1	A	334	ARG	N-CA-C	9.18	120.97	110.97
2	B	98	HIS	N-CA-C	9.13	124.28	109.76
2	D	98	HIS	N-CA-C	9.12	124.26	109.76
1	C	333	PHE	CB-CA-C	-9.08	95.53	110.79
1	A	333	PHE	CB-CA-C	-9.07	95.56	110.79
1	A	149	PHE	CB-CA-C	-9.01	96.73	110.88
1	C	307	PHE	CB-CA-C	-9.00	95.56	110.85
1	A	307	PHE	CB-CA-C	-8.99	95.57	110.85
1	C	149	PHE	CB-CA-C	-8.99	96.76	110.88
1	A	176	GLN	CB-CA-C	-8.95	95.64	110.85
1	C	176	GLN	CB-CA-C	-8.94	95.65	110.85
1	C	80	TYR	N-CA-C	-8.93	100.51	111.40
1	A	80	TYR	N-CA-C	-8.91	100.52	111.40
1	C	271	PHE	N-CA-C	-8.86	99.49	110.65
1	A	271	PHE	N-CA-C	-8.84	99.51	110.65
1	C	78	ILE	CB-CA-C	-8.78	100.73	111.97
1	A	78	ILE	CB-CA-C	-8.78	100.74	111.97
1	C	329	VAL	CA-C-O	-8.71	112.21	121.27
1	A	329	VAL	CA-C-O	-8.69	112.24	121.27
2	B	116	ILE	CB-CA-C	-8.59	93.29	111.32
2	D	116	ILE	CB-CA-C	-8.58	93.30	111.32
1	C	127	GLY	CA-C-O	-8.38	113.12	121.92
1	A	127	GLY	CA-C-O	-8.36	113.14	121.92
1	A	230	PHE	CB-CA-C	-8.34	95.43	110.70
1	A	265	SER	CB-CA-C	-8.32	97.75	110.90
1	C	265	SER	CB-CA-C	-8.32	97.75	110.90
1	C	230	PHE	CB-CA-C	-8.32	95.48	110.70
1	A	378	VAL	CA-C-O	-8.31	112.05	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	VAL	CA-C-O	-8.28	112.08	120.85
1	A	145	PHE	CA-C-O	-8.24	111.73	120.63
1	C	173	ILE	N-CA-C	-8.24	102.39	110.72
1	A	173	ILE	N-CA-C	-8.24	102.40	110.72
1	C	145	PHE	CA-C-O	-8.22	111.75	120.63
2	B	34	ILE	N-CA-C	-8.16	102.86	110.53
1	A	317	LEU	CA-C-O	-8.15	112.31	120.70
2	D	34	ILE	N-CA-C	-8.12	102.89	110.53
1	C	317	LEU	CA-C-O	-8.12	112.34	120.70
1	C	384	TRP	N-CA-C	8.10	123.27	112.25
1	A	384	TRP	N-CA-C	8.10	123.26	112.25
1	C	191	ILE	CB-CA-C	-7.99	101.20	112.22
1	A	191	ILE	CB-CA-C	-7.98	101.20	112.22
1	A	145	PHE	CB-CA-C	-7.92	97.22	110.68
1	C	145	PHE	CB-CA-C	-7.89	97.26	110.68
1	C	212	PRO	N-CA-C	7.81	124.20	113.65
1	A	212	PRO	N-CA-C	7.80	124.18	113.65
1	C	367	VAL	CB-CA-C	-7.66	99.86	112.26
1	A	367	VAL	CB-CA-C	-7.65	99.86	112.26
1	A	113	PHE	N-CA-C	7.61	121.82	112.23
1	C	113	PHE	N-CA-C	7.61	121.81	112.23
1	C	120	ILE	CB-CA-C	-7.49	103.19	111.35
1	C	331	THR	N-CA-C	7.45	119.48	111.36
1	A	161	ARG	CB-CA-C	-7.45	96.93	110.56
1	A	120	ILE	CB-CA-C	-7.44	103.24	111.35
1	A	331	THR	N-CA-C	7.43	119.46	111.36
1	C	161	ARG	CB-CA-C	-7.42	96.97	110.56
1	C	204	THR	O-C-N	-7.42	113.69	122.15
1	A	313	ALA	N-CA-C	-7.40	103.14	111.14
1	C	313	ALA	N-CA-C	-7.38	103.16	111.14
1	C	170	ILE	O-C-N	-7.38	111.71	121.82
1	A	170	ILE	O-C-N	-7.37	111.72	121.82
1	C	314	TRP	CA-C-O	-7.33	112.65	120.42
1	A	314	TRP	CA-C-O	-7.33	112.65	120.42
1	C	148	GLU	CA-C-O	-7.31	112.67	120.42
1	A	204	THR	O-C-N	-7.30	113.83	122.15
1	A	148	GLU	CA-C-O	-7.26	112.72	120.42
1	C	328	SER	N-CA-C	-7.17	103.39	111.14
1	A	377	ARG	N-CA-C	-7.16	103.41	111.14
1	A	328	SER	N-CA-C	-7.16	103.41	111.14
1	A	223	PHE	N-CA-C	-7.15	103.42	111.14
1	C	256	HIS	N-CA-C	7.14	119.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	HIS	N-CA-C	7.13	119.05	111.28
1	C	377	ARG	N-CA-C	-7.12	103.44	111.14
1	C	128	LYS	CG-CD-CE	-7.11	94.94	111.30
1	C	223	PHE	N-CA-C	-7.11	103.46	111.14
1	A	128	LYS	CG-CD-CE	-7.10	94.97	111.30
1	C	319	HIS	CA-C-O	-7.09	111.98	120.56
1	A	254	PHE	N-CA-C	-7.06	103.67	111.36
1	A	319	HIS	CA-C-O	-7.06	112.02	120.56
1	C	254	PHE	N-CA-C	-7.05	103.68	111.36
1	A	307	PHE	N-CA-CB	7.02	120.55	110.16
1	C	259	THR	N-CA-C	-7.01	103.56	111.14
1	A	161	ARG	N-CA-C	-7.01	101.94	112.04
1	A	259	THR	N-CA-C	-7.01	103.57	111.14
1	C	307	PHE	N-CA-CB	7.01	120.53	110.16
1	C	161	ARG	N-CA-C	-7.00	101.95	112.04
1	C	318	ARG	NE-CZ-NH2	6.96	125.46	119.20
1	A	228	ALA	N-CA-C	-6.93	103.50	112.23
1	A	247	LYS	CA-C-N	6.92	134.76	121.54
1	A	247	LYS	C-N-CA	6.92	134.76	121.54
1	A	318	ARG	NE-CZ-NH2	6.92	125.43	119.20
1	C	247	LYS	CA-C-N	6.91	134.74	121.54
1	C	247	LYS	C-N-CA	6.91	134.74	121.54
2	D	96	ASP	N-CA-C	-6.91	96.07	110.80
2	B	32	LEU	CB-CA-C	-6.91	99.10	110.85
2	D	32	LEU	CB-CA-C	-6.91	99.11	110.85
2	B	96	ASP	N-CA-C	-6.90	96.10	110.80
1	C	228	ALA	N-CA-C	-6.89	103.54	112.23
1	A	315	ILE	CA-C-O	-6.84	113.60	120.85
1	C	315	ILE	CA-C-O	-6.82	113.63	120.85
1	A	147	ARG	CG-CD-NE	-6.80	97.04	112.00
1	C	147	ARG	CG-CD-NE	-6.79	97.07	112.00
1	A	218	PHE	CA-C-O	-6.75	113.80	120.89
1	A	235	ALA	N-CA-C	-6.75	104.00	111.36
1	C	235	ALA	N-CA-C	-6.75	104.00	111.36
1	C	218	PHE	CA-C-O	-6.75	113.81	120.89
1	A	110	LEU	CA-C-O	-6.71	113.30	120.42
1	C	226	GLY	N-CA-C	-6.69	97.32	113.18
1	A	226	GLY	N-CA-C	-6.68	97.34	113.18
1	C	110	LEU	CA-C-O	-6.67	113.35	120.42
1	A	165	THR	CB-CA-C	-6.67	100.88	110.62
1	C	188	PRO	CA-N-CD	-6.67	102.67	112.00
1	A	188	PRO	CA-N-CD	-6.66	102.67	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	THR	CB-CA-C	-6.66	100.89	110.62
1	A	244	LYS	N-CA-C	6.64	121.79	109.10
1	C	244	LYS	N-CA-C	6.63	121.76	109.10
1	C	162	LEU	N-CA-C	6.63	124.92	110.80
1	A	162	LEU	N-CA-C	6.62	124.89	110.80
1	C	305	PHE	N-CA-C	-6.61	103.90	112.23
1	A	305	PHE	N-CA-C	-6.60	103.92	112.23
1	C	154	VAL	N-CA-C	-6.60	106.36	112.96
1	C	230	PHE	CA-C-O	-6.59	112.92	120.24
1	A	230	PHE	CA-C-O	-6.57	112.94	120.24
1	C	269	PHE	N-CA-C	-6.56	103.69	112.94
1	A	269	PHE	N-CA-C	-6.55	103.70	112.94
1	A	154	VAL	N-CA-C	-6.54	106.42	112.96
1	C	75	PHE	CA-C-O	-6.53	113.91	120.90
1	A	378	VAL	CB-CA-C	-6.52	103.22	112.22
1	C	378	VAL	CB-CA-C	-6.51	103.23	112.22
1	A	75	PHE	CA-C-O	-6.51	113.94	120.90
2	D	38	GLU	CB-CA-C	-6.50	96.73	110.31
2	B	38	GLU	CB-CA-C	-6.49	96.75	110.31
1	A	325	ILE	CB-CA-C	-6.49	101.75	112.26
1	C	325	ILE	CB-CA-C	-6.48	101.77	112.26
1	A	263	ILE	CG1-CB-CG2	-6.45	91.36	110.70
1	C	263	ILE	CG1-CB-CG2	-6.45	91.36	110.70
1	C	311	VAL	N-CA-C	-6.42	104.24	110.72
1	A	311	VAL	N-CA-C	-6.41	104.24	110.72
1	A	247	LYS	O-C-N	6.41	131.11	122.59
1	C	247	LYS	O-C-N	6.40	131.10	122.59
2	D	50	TRP	N-CA-CB	6.35	119.50	110.67
2	B	50	TRP	N-CA-CB	6.34	119.49	110.67
1	A	333	PHE	CA-C-O	-6.34	113.77	120.55
1	C	302	LEU	O-C-N	-6.34	115.18	122.09
1	C	333	PHE	CA-C-O	-6.33	113.78	120.55
1	A	302	LEU	O-C-N	-6.30	115.22	122.09
2	D	46	ILE	CB-CA-C	-6.29	101.90	112.16
1	C	239	VAL	N-CA-C	-6.28	105.61	111.45
1	C	113	PHE	CB-CA-C	-6.28	97.57	110.38
2	B	46	ILE	CB-CA-C	-6.27	101.93	112.16
1	C	147	ARG	N-CA-CB	-6.27	100.91	110.01
1	A	113	PHE	CB-CA-C	-6.27	97.59	110.38
1	A	147	ARG	N-CA-CB	-6.27	100.92	110.01
1	A	368	ASN	CA-C-O	-6.26	112.41	119.79
1	A	239	VAL	N-CA-C	-6.24	105.64	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	ASN	CA-C-O	-6.24	112.42	119.79
1	A	187	GLY	C-N-CD	-6.24	99.44	125.00
1	C	187	GLY	C-N-CD	-6.23	99.44	125.00
2	B	131	TYR	CA-C-N	-6.18	112.65	122.29
2	B	131	TYR	C-N-CA	-6.18	112.65	122.29
1	C	271	PHE	O-C-N	-6.17	113.29	122.67
2	D	131	TYR	CA-C-N	-6.17	112.66	122.29
2	D	131	TYR	C-N-CA	-6.17	112.66	122.29
1	A	271	PHE	O-C-N	-6.15	113.32	122.67
1	C	131	ASN	N-CA-C	-6.15	104.57	111.28
1	A	248	ASP	N-CA-C	6.13	123.86	110.80
1	C	248	ASP	N-CA-C	6.13	123.86	110.80
1	A	131	ASN	N-CA-C	-6.13	104.60	111.28
1	C	213	ASP	N-CA-C	6.12	118.67	111.02
1	A	200	TRP	CB-CA-C	6.10	119.78	109.84
1	A	213	ASP	N-CA-C	6.10	118.64	111.02
1	A	185	VAL	N-CA-C	6.08	116.82	110.62
1	C	268	VAL	N-CA-C	6.07	121.32	113.07
1	A	163	HIS	CB-CA-C	6.06	118.79	110.06
1	C	150	LEU	CA-C-O	-6.06	114.64	121.00
1	A	268	VAL	N-CA-C	6.06	121.31	113.07
1	C	163	HIS	CB-CA-C	6.06	118.78	110.06
1	C	178	TYR	N-CA-C	-6.06	105.72	113.23
1	C	185	VAL	N-CA-C	6.04	116.78	110.62
1	A	178	TYR	N-CA-C	-6.04	105.74	113.23
1	A	150	LEU	CA-C-O	-6.04	114.66	121.00
1	A	218	PHE	N-CA-C	-6.02	101.71	111.04
1	C	218	PHE	N-CA-C	-6.01	101.72	111.04
1	C	200	TRP	CB-CA-C	5.99	119.61	109.84
1	A	245	PRO	CA-C-N	5.97	132.95	121.54
1	A	245	PRO	C-N-CA	5.97	132.95	121.54
1	C	245	PRO	CA-C-N	5.96	132.93	121.54
1	C	245	PRO	C-N-CA	5.96	132.93	121.54
1	C	329	VAL	N-CA-CB	5.92	117.08	110.51
2	D	49	GLU	O-C-N	5.92	130.63	122.46
1	C	384	TRP	CA-CB-CG	-5.90	102.39	113.60
1	A	384	TRP	CA-CB-CG	-5.90	102.40	113.60
1	A	212	PRO	CA-C-O	-5.89	110.59	119.55
1	A	198	ASP	CB-CA-C	-5.89	100.25	110.09
1	A	329	VAL	N-CA-CB	5.89	117.05	110.51
2	B	49	GLU	O-C-N	5.89	130.58	122.46
1	C	139	TYR	CA-CB-CG	-5.88	103.31	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	ASP	CB-CA-C	-5.88	100.26	110.09
1	A	139	TYR	CA-CB-CG	-5.88	103.32	113.90
1	A	220	PHE	N-CA-CB	-5.88	101.17	110.22
1	C	212	PRO	CA-C-O	-5.88	110.61	119.55
1	C	220	PHE	N-CA-CB	-5.88	101.17	110.22
1	C	169	ARG	O-C-N	-5.87	116.03	122.07
1	A	307	PHE	N-CA-C	5.86	117.75	111.36
1	A	123	THR	O-C-N	-5.86	116.40	122.84
1	A	169	ARG	O-C-N	-5.86	116.04	122.07
1	C	123	THR	O-C-N	-5.86	116.40	122.84
1	C	307	PHE	N-CA-C	5.85	117.74	111.36
2	B	98	HIS	N-CA-CB	-5.85	100.88	109.95
1	C	152	ASP	CA-C-O	-5.84	114.88	120.90
2	D	98	HIS	N-CA-CB	-5.84	100.90	109.95
1	A	152	ASP	CA-C-O	-5.83	114.90	120.90
1	C	170	ILE	CB-CA-C	-5.82	102.67	112.16
1	A	126	TYR	O-C-N	-5.81	116.43	123.29
1	A	170	ILE	CB-CA-C	-5.81	102.69	112.16
1	A	193	CYS	CB-CA-C	-5.79	99.92	110.63
1	C	193	CYS	CB-CA-C	-5.79	99.92	110.63
1	A	231	TRP	CA-C-N	5.78	127.95	120.44
1	A	231	TRP	C-N-CA	5.78	127.95	120.44
1	C	126	TYR	O-C-N	-5.78	116.47	123.29
1	C	158	PHE	N-CA-C	-5.77	104.96	112.23
1	C	112	ARG	CA-C-O	-5.76	114.31	120.42
2	B	41	LYS	N-CA-C	5.76	118.02	111.11
1	C	231	TRP	CA-C-N	5.76	127.93	120.44
1	C	231	TRP	C-N-CA	5.76	127.93	120.44
1	A	158	PHE	N-CA-C	-5.75	104.99	112.23
1	A	112	ARG	CA-C-O	-5.74	114.33	120.42
2	D	41	LYS	N-CA-C	5.74	118.00	111.11
1	C	208	TYR	CA-C-O	-5.72	112.85	118.97
1	A	208	TYR	CA-C-O	-5.72	112.85	118.97
1	A	309	ILE	CB-CA-C	-5.67	102.00	111.29
1	C	309	ILE	CB-CA-C	-5.66	102.01	111.29
1	C	311	VAL	CA-C-O	-5.66	114.85	120.85
1	A	311	VAL	CA-C-O	-5.66	114.85	120.85
1	A	150	LEU	O-C-N	5.63	127.89	122.03
1	C	150	LEU	O-C-N	5.63	127.89	122.03
2	D	36	ALA	CA-C-O	-5.63	114.46	120.42
2	B	36	ALA	CA-C-O	-5.61	114.48	120.42
1	A	317	LEU	CB-CG-CD2	-5.60	93.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	ASN	N-CA-CB	5.60	118.41	110.13
1	C	317	LEU	CB-CG-CD2	-5.59	93.92	110.70
1	A	250	ASN	N-CA-CB	5.59	118.40	110.13
1	A	160	ILE	CB-CA-C	5.57	120.43	111.29
1	A	199	LEU	CA-C-N	-5.57	113.53	121.50
1	A	199	LEU	C-N-CA	-5.57	113.53	121.50
1	C	160	ILE	CB-CA-C	5.57	120.43	111.29
1	C	155	ILE	CA-C-O	-5.57	114.28	120.46
1	A	143	PHE	N-CA-C	-5.54	105.64	112.90
1	A	155	ILE	CA-C-O	-5.54	114.31	120.46
1	C	143	PHE	N-CA-C	-5.53	105.66	112.90
1	A	193	CYS	CA-C-O	-5.52	113.86	120.10
1	C	146	LEU	CB-CA-C	-5.52	101.47	110.85
1	A	310	PHE	CA-C-O	-5.52	113.28	119.79
1	A	146	LEU	CB-CA-C	-5.51	101.48	110.85
1	A	150	LEU	CB-CA-C	-5.51	102.47	110.96
2	D	30	SER	N-CA-C	-5.51	105.19	111.14
1	C	252	LEU	N-CA-C	-5.50	105.44	111.82
1	A	154	VAL	CA-C-N	-5.49	112.44	121.34
1	A	154	VAL	C-N-CA	-5.49	112.44	121.34
1	C	189	PHE	N-CA-C	-5.49	105.21	111.14
1	C	154	VAL	CA-C-N	-5.49	112.44	121.34
1	C	154	VAL	C-N-CA	-5.49	112.44	121.34
1	C	310	PHE	CA-C-O	-5.49	113.31	119.79
2	D	21	PHE	N-CA-CB	5.49	118.28	110.16
1	C	150	LEU	CB-CA-C	-5.49	102.51	110.96
1	A	189	PHE	N-CA-C	-5.48	105.22	111.14
1	C	320	TYR	CB-CA-C	-5.48	101.53	110.85
1	A	252	LEU	N-CA-C	-5.48	105.47	111.82
2	B	42	TYR	CB-CA-C	-5.47	102.25	110.90
1	C	193	CYS	CA-C-O	-5.47	113.92	120.10
2	B	21	PHE	N-CA-CB	5.47	118.26	110.16
2	B	30	SER	N-CA-C	-5.46	105.24	111.14
2	D	42	TYR	CB-CA-C	-5.46	102.27	110.90
1	A	320	TYR	CB-CA-C	-5.46	101.56	110.85
1	C	181	PHE	CA-C-N	-5.46	111.59	121.14
1	C	181	PHE	C-N-CA	-5.46	111.59	121.14
1	A	76	ARG	N-CA-CB	5.46	118.14	110.12
1	C	256	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	181	PHE	CA-C-N	-5.45	111.61	121.14
1	A	181	PHE	C-N-CA	-5.45	111.61	121.14
1	C	207	MET	CB-CG-SD	-5.44	96.38	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ARG	N-CA-CB	5.43	118.11	110.12
1	A	207	MET	CB-CG-SD	-5.42	96.43	112.70
1	C	209	ARG	N-CA-C	5.42	119.39	112.34
1	A	128	LYS	CD-CE-NZ	5.42	129.24	111.90
1	A	192	TYR	CB-CA-C	-5.42	101.80	110.79
1	A	256	HIS	CA-CB-CG	-5.42	108.39	113.80
1	C	128	LYS	CD-CE-NZ	5.41	129.21	111.90
1	C	192	TYR	CB-CA-C	-5.41	101.81	110.79
1	A	209	ARG	N-CA-C	5.41	119.37	112.34
1	A	308	ALA	N-CA-C	-5.36	105.13	110.97
1	C	199	LEU	CA-C-N	-5.33	113.88	121.50
1	C	199	LEU	C-N-CA	-5.33	113.88	121.50
1	C	244	LYS	CB-CA-C	-5.32	104.26	110.17
1	C	308	ALA	N-CA-C	-5.32	105.18	110.97
1	A	244	LYS	CB-CA-C	-5.31	104.28	110.17
1	C	331	THR	CA-C-O	-5.31	114.79	120.42
1	C	233	GLN	N-CA-C	5.30	117.81	111.71
2	B	122	GLU	N-CA-CB	-5.30	102.47	109.78
1	C	373	PHE	N-CA-CB	5.29	118.00	110.16
2	D	122	GLU	N-CA-CB	-5.29	102.47	109.78
1	C	155	ILE	CB-CA-C	5.29	118.61	111.94
1	A	233	GLN	N-CA-C	5.29	117.79	111.71
1	C	372	LEU	CD1-CG-CD2	-5.28	99.18	110.80
1	A	373	PHE	N-CA-CB	5.28	117.97	110.16
1	A	155	ILE	CB-CA-C	5.27	118.58	111.94
1	A	372	LEU	CD1-CG-CD2	-5.27	99.20	110.80
1	A	331	THR	CA-C-O	-5.26	114.84	120.42
1	A	204	THR	N-CA-CB	-5.26	102.37	110.16
1	C	111	HIS	CA-C-O	-5.26	114.16	120.10
1	C	177	MET	CA-C-N	-5.25	112.42	121.66
1	C	177	MET	C-N-CA	-5.25	112.42	121.66
1	A	177	MET	CA-C-N	-5.24	112.44	121.66
1	A	177	MET	C-N-CA	-5.24	112.44	121.66
1	A	174	MET	CB-CG-SD	-5.23	97.00	112.70
1	A	111	HIS	CA-C-O	-5.23	114.19	120.10
1	C	174	MET	CB-CG-SD	-5.22	97.03	112.70
1	C	219	LEU	CA-C-N	5.22	127.80	120.28
1	C	219	LEU	C-N-CA	5.22	127.80	120.28
1	A	219	LEU	CA-C-N	5.21	127.78	120.28
1	A	219	LEU	C-N-CA	5.21	127.78	120.28
1	A	257	ILE	CB-CA-C	-5.21	105.03	112.22
1	C	257	ILE	CB-CA-C	-5.20	105.05	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	THR	N-CA-CB	-5.19	102.48	110.16
1	C	259	THR	OG1-CB-CG2	-5.18	98.93	109.30
1	A	259	THR	OG1-CB-CG2	-5.17	98.95	109.30
1	C	271	PHE	CA-C-N	5.17	129.43	120.58
1	C	271	PHE	C-N-CA	5.17	129.43	120.58
2	B	34	ILE	CB-CA-C	-5.17	105.25	112.02
2	D	34	ILE	CB-CA-C	-5.15	105.28	112.02
1	A	271	PHE	CA-C-N	5.15	129.38	120.58
1	A	271	PHE	C-N-CA	5.15	129.38	120.58
2	D	45	ARG	CB-CA-C	-5.14	100.39	110.11
2	D	120	LYS	N-CA-C	5.14	121.76	110.80
1	A	269	PHE	CA-C-O	5.14	125.55	119.48
2	B	120	LYS	N-CA-C	5.14	121.74	110.80
1	C	379	LEU	O-C-N	-5.14	116.69	122.03
1	A	173	ILE	N-CA-CB	5.13	118.28	110.58
1	C	369	LEU	N-CA-C	-5.13	106.52	112.89
2	B	45	ARG	CB-CA-C	-5.13	100.41	110.11
1	C	173	ILE	N-CA-CB	5.13	118.28	110.58
1	A	369	LEU	N-CA-C	-5.13	106.53	112.89
1	A	379	LEU	O-C-N	-5.12	116.71	122.03
1	C	203	ASN	CA-C-N	5.12	127.56	120.29
1	C	203	ASN	C-N-CA	5.12	127.56	120.29
1	C	182	TYR	N-CA-CB	5.11	118.72	110.40
1	C	208	TYR	CB-CA-C	-5.10	100.50	109.07
1	A	208	TYR	CB-CA-C	-5.10	100.50	109.07
1	A	182	TYR	N-CA-CB	5.10	118.71	110.40
1	C	269	PHE	CA-C-O	5.09	125.49	119.48
1	A	268	VAL	CA-C-O	-5.07	113.14	119.43
1	C	169	ARG	CA-C-O	-5.07	115.50	120.82
2	B	37	VAL	N-CA-CB	5.05	121.66	111.05
2	D	37	VAL	N-CA-CB	5.05	121.66	111.05
1	A	169	ARG	CA-C-O	-5.05	115.52	120.82
1	C	268	VAL	CA-C-O	-5.03	113.19	119.43
1	C	326	LEU	CB-CG-CD2	-5.01	95.66	110.70
1	A	326	LEU	CB-CG-CD2	-5.01	95.67	110.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	VAL	Mainchain
1	A	302	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	318	ARG	Mainchain
1	C	239	VAL	Mainchain
1	C	302	LEU	Mainchain
1	C	318	ARG	Mainchain
1	C	331	THR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2670	0	2667	288	0
1	C	2670	0	2667	294	0
2	B	1082	0	1037	45	0
2	D	1082	0	1037	47	0
3	A	18	0	35	2	0
3	B	58	0	91	18	0
3	C	18	0	35	1	0
3	D	58	0	91	18	0
4	A	75	0	0	21	0
4	C	75	0	0	21	0
All	All	7806	0	7660	681	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 44.

All (681) 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:C:323:LEU:CD2	1:C:365:GLN:HE21	1.43	1.31
1:A:323:LEU:CD2	1:A:365:GLN:HE21	1.43	1.29
1:C:323:LEU:HD21	1:C:365:GLN:NE2	1.48	1.26
1:A:251:GLU:HG2	1:A:370:TYR:CE2	1.69	1.26
1:A:323:LEU:HD21	1:A:365:GLN:NE2	1.48	1.26
1:C:251:GLU:HG2	1:C:370:TYR:CE2	1.70	1.25
1:C:330:LEU:HD21	1:C:358:PHE:CE1	1.75	1.22
1:A:330:LEU:HD21	1:A:358:PHE:CE1	1.75	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:CD2	1:C:303:ALA:HB2	1.69	1.20
1:A:255:HIS:CE1	4:A:502:9NY:C46	2.25	1.20
1:A:295:LEU:CD2	1:A:303:ALA:HB2	1.69	1.20
1:C:255:HIS:CE1	4:C:502:9NY:C46	2.25	1.19
1:A:153:VAL:O	1:A:157:PRO:HG2	1.43	1.19
1:A:323:LEU:CD2	1:A:365:GLN:NE2	2.05	1.16
1:C:295:LEU:HD22	1:C:303:ALA:HB2	1.22	1.16
1:C:153:VAL:O	1:C:157:PRO:HG2	1.43	1.15
1:C:330:LEU:HD21	1:C:358:PHE:HE1	1.05	1.15
1:C:219:LEU:O	1:C:222:VAL:HG12	1.45	1.14
1:C:323:LEU:CD2	1:C:365:GLN:NE2	2.05	1.13
1:A:219:LEU:O	1:A:222:VAL:HG12	1.45	1.12
1:A:317:LEU:O	1:A:321:ILE:HB	1.49	1.11
2:D:50:TRP:HE1	3:D:201:6PL:C1	1.65	1.10
1:C:281:THR:HG21	1:C:321:ILE:HG21	1.29	1.09
1:A:281:THR:HG21	1:A:321:ILE:HG21	1.26	1.09
1:A:295:LEU:HD22	1:A:303:ALA:HB2	1.22	1.09
1:C:375:ILE:HG12	4:C:502:9NY:C31	1.83	1.08
1:C:317:LEU:O	1:C:321:ILE:HB	1.51	1.08
1:A:375:ILE:HG12	4:A:502:9NY:C31	1.83	1.08
1:A:330:LEU:HD21	1:A:358:PHE:HE1	1.05	1.06
2:B:50:TRP:HE1	3:B:201:6PL:C1	1.66	1.06
2:B:50:TRP:NE1	3:B:201:6PL:H11	1.73	1.03
2:D:50:TRP:NE1	3:D:201:6PL:H11	1.72	1.03
1:C:248:ASP:O	1:C:250:ASN:N	1.91	1.03
1:A:248:ASP:O	1:A:250:ASN:N	1.91	1.02
1:C:282:MET:CB	4:C:502:9NY:C35	2.38	1.02
1:A:282:MET:CB	4:A:502:9NY:C35	2.38	1.01
1:A:295:LEU:HD22	1:A:303:ALA:CB	1.90	1.01
1:A:255:HIS:NE2	4:A:502:9NY:C46	2.24	1.01
2:B:38:GLU:OE2	3:B:202:6PL:H332	1.61	1.00
1:C:255:HIS:NE2	4:C:502:9NY:C46	2.24	1.00
1:C:295:LEU:HD22	1:C:303:ALA:CB	1.90	1.00
1:A:281:THR:CG2	1:A:321:ILE:HG21	1.91	1.00
1:C:281:THR:CG2	1:C:321:ILE:HG21	1.92	0.99
1:C:330:LEU:CD2	1:C:358:PHE:CE1	2.47	0.98
2:B:50:TRP:NE1	3:B:201:6PL:C1	2.26	0.98
1:A:330:LEU:CD2	1:A:358:PHE:CE1	2.47	0.97
2:D:38:GLU:OE2	3:D:202:6PL:H332	1.63	0.96
2:D:50:TRP:NE1	3:D:201:6PL:C1	2.26	0.96
1:C:251:GLU:HG2	1:C:370:TYR:HE2	1.26	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ARG:HG3	1:C:169:ARG:HH11	1.33	0.93
1:C:282:MET:HB3	4:C:502:9NY:C35	2.00	0.92
1:A:323:LEU:HD21	1:A:365:GLN:HE21	0.76	0.92
1:A:282:MET:HB3	4:A:502:9NY:C35	2.00	0.92
1:C:106:LYS:NZ	1:C:106:LYS:HB3	1.85	0.92
2:D:50:TRP:CD1	3:D:201:6PL:H11	2.05	0.92
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.33	0.91
2:B:50:TRP:CD1	3:B:201:6PL:H11	2.05	0.91
1:A:251:GLU:HG2	1:A:370:TYR:HE2	1.26	0.91
1:C:251:GLU:CG	1:C:370:TYR:CE2	2.54	0.90
1:C:323:LEU:HD21	1:C:365:GLN:HE21	0.76	0.90
1:A:106:LYS:NZ	1:A:106:LYS:HB3	1.85	0.90
1:A:251:GLU:HG2	1:A:370:TYR:CD2	2.07	0.90
1:A:251:GLU:CG	1:A:370:TYR:CE2	2.54	0.90
1:C:147:ARG:HH11	1:C:151:MET:HE1	1.37	0.90
1:C:251:GLU:HG2	1:C:370:TYR:CD2	2.07	0.89
1:A:295:LEU:HD23	1:A:303:ALA:HB2	1.53	0.89
1:C:262:LEU:HD22	4:C:502:9NY:C15	2.03	0.89
1:A:375:ILE:CG1	4:A:502:9NY:C31	2.51	0.89
1:C:295:LEU:HD23	1:C:303:ALA:HB2	1.53	0.89
1:A:112:ARG:HH11	1:A:112:ARG:HB3	1.36	0.88
1:C:124:ASN:O	1:C:124:ASN:ND2	2.06	0.88
1:C:375:ILE:CG1	4:C:502:9NY:C31	2.51	0.88
1:C:112:ARG:HH11	1:C:112:ARG:HB3	1.36	0.88
1:C:244:LYS:O	1:C:244:LYS:NZ	2.05	0.88
1:A:244:LYS:O	1:A:244:LYS:NZ	2.05	0.88
1:A:124:ASN:O	1:A:124:ASN:ND2	2.06	0.88
1:A:262:LEU:HD22	4:A:502:9NY:C15	2.03	0.87
1:A:223:PHE:HE2	1:A:279:TYR:CD2	1.94	0.86
1:C:223:PHE:HE2	1:C:279:TYR:CD2	1.94	0.86
1:C:262:LEU:HD13	4:C:502:9NY:C15	2.07	0.85
1:C:281:THR:HA	1:C:317:LEU:HD22	1.57	0.85
1:A:282:MET:HG3	4:A:502:9NY:C33	2.07	0.84
1:C:282:MET:HG3	4:C:502:9NY:C33	2.07	0.84
1:A:281:THR:HA	1:A:317:LEU:HD22	1.57	0.84
1:A:262:LEU:HD13	4:A:502:9NY:C15	2.07	0.83
2:D:50:TRP:HE1	3:D:201:6PL:H11	1.29	0.83
1:A:154:VAL:C	1:A:157:PRO:HD2	2.03	0.83
1:A:183:THR:CG2	1:A:287:PHE:HB2	2.09	0.82
1:C:149:PHE:CE1	1:C:153:VAL:HG21	2.14	0.82
1:C:204:THR:O	1:C:205:LYS:C	2.17	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:CE1	1:A:153:VAL:HG21	2.15	0.82
1:C:154:VAL:C	1:C:157:PRO:HD2	2.03	0.82
1:A:204:THR:O	1:A:205:LYS:C	2.14	0.82
1:C:183:THR:CG2	1:C:287:PHE:HB2	2.09	0.82
1:A:223:PHE:HE2	1:A:279:TYR:HD2	1.25	0.82
1:C:223:PHE:HE2	1:C:279:TYR:HD2	1.25	0.81
1:A:176:GLN:HB3	1:A:294:THR:CG2	2.11	0.81
1:C:251:GLU:CG	1:C:370:TYR:HE2	1.92	0.81
1:A:154:VAL:O	1:A:157:PRO:HD2	1.81	0.81
1:A:323:LEU:HD23	1:A:365:GLN:NE2	1.94	0.81
1:A:169:ARG:HG3	1:A:169:ARG:NH1	1.90	0.80
1:C:176:GLN:HB3	1:C:294:THR:CG2	2.11	0.80
1:A:251:GLU:CG	1:A:370:TYR:HE2	1.92	0.80
1:C:147:ARG:HE	1:C:151:MET:CE	1.94	0.80
1:C:323:LEU:HD23	1:C:365:GLN:NE2	1.94	0.80
1:C:154:VAL:O	1:C:157:PRO:HD2	1.81	0.80
1:C:248:ASP:C	1:C:250:ASN:H	1.90	0.79
1:C:147:ARG:HE	1:C:151:MET:HE1	1.48	0.79
1:A:183:THR:HG22	1:A:287:PHE:HB2	1.65	0.79
1:A:382:ILE:HD12	4:A:502:9NY:N2	1.99	0.78
1:C:382:ILE:HD12	4:C:502:9NY:N2	1.99	0.78
1:A:321:ILE:HG22	1:A:322:ASN:OD1	1.83	0.78
1:C:183:THR:HG22	1:C:287:PHE:HB2	1.65	0.78
1:A:149:PHE:HE1	1:A:153:VAL:HG21	1.49	0.78
1:A:106:LYS:HB3	1:A:106:LYS:HZ2	1.45	0.78
1:A:248:ASP:C	1:A:250:ASN:H	1.90	0.78
1:C:132:ASP:OD1	1:C:267:TYR:OH	2.03	0.77
1:C:149:PHE:HE1	1:C:153:VAL:HG21	1.48	0.77
1:C:169:ARG:HG3	1:C:169:ARG:NH1	1.90	0.77
1:C:248:ASP:C	1:C:250:ASN:N	2.42	0.77
1:A:330:LEU:CD2	1:A:358:PHE:CD1	2.68	0.77
1:A:132:ASP:OD1	1:A:267:TYR:OH	2.03	0.77
1:C:219:LEU:O	1:C:222:VAL:CG1	2.31	0.77
1:C:330:LEU:CD2	1:C:358:PHE:CD1	2.68	0.77
1:C:240:LEU:HD13	1:C:240:LEU:O	1.85	0.76
2:B:132:ASP:OD1	2:B:135:SER:HB2	1.85	0.76
1:A:240:LEU:HD13	1:A:240:LEU:O	1.85	0.76
1:C:262:LEU:HB3	4:C:502:9NY:C19	2.15	0.76
1:A:262:LEU:HB3	4:A:502:9NY:C19	2.15	0.76
1:A:248:ASP:C	1:A:250:ASN:N	2.42	0.75
2:D:132:ASP:OD1	2:D:135:SER:HB2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HH11	1:A:151:MET:HE1	1.52	0.75
1:C:204:THR:HG21	1:C:328:SER:HB2	1.67	0.75
1:C:223:PHE:CE2	1:C:279:TYR:CD2	2.75	0.75
1:A:137:PHE:HA	1:A:140:MET:HG3	1.69	0.74
1:A:223:PHE:CE2	1:A:279:TYR:CD2	2.75	0.74
1:C:106:LYS:HB3	1:C:106:LYS:HZ2	1.52	0.74
1:C:282:MET:HG3	4:C:502:9NY:C35	2.17	0.74
4:C:502:9NY:O5	4:C:502:9NY:O1	2.05	0.74
1:A:239:VAL:C	1:A:241:GLN:H	1.95	0.74
1:C:137:PHE:HA	1:C:140:MET:HG3	1.69	0.73
1:C:239:VAL:C	1:C:241:GLN:N	2.45	0.73
4:A:502:9NY:O5	4:A:502:9NY:O1	2.05	0.73
1:A:216:ASN:OD1	1:A:216:ASN:N	2.20	0.73
1:C:147:ARG:NH1	1:C:151:MET:HE1	2.02	0.73
1:A:204:THR:HG21	1:A:328:SER:HB2	1.70	0.73
1:A:282:MET:HG3	4:A:502:9NY:C35	2.17	0.73
2:B:50:TRP:HE1	3:B:201:6PL:H32	1.53	0.73
1:C:239:VAL:C	1:C:241:GLN:H	1.94	0.73
1:A:281:THR:HG21	1:A:321:ILE:CG2	2.13	0.73
1:A:295:LEU:HD22	1:A:303:ALA:CA	2.19	0.72
1:A:219:LEU:O	1:A:222:VAL:CG1	2.31	0.72
1:C:186:SER:OG	1:C:283:ASP:OD1	2.07	0.72
1:A:186:SER:OG	1:A:283:ASP:OD1	2.07	0.72
1:A:176:GLN:HB3	1:A:294:THR:HG22	1.71	0.72
1:A:153:VAL:O	1:A:157:PRO:CG	2.32	0.72
1:A:246:ARG:HD2	1:A:247:LYS:HG2	1.72	0.72
1:C:153:VAL:O	1:C:157:PRO:CG	2.33	0.72
1:C:281:THR:HG21	1:C:321:ILE:CG2	2.15	0.72
1:C:246:ARG:HD2	1:C:247:LYS:HG2	1.71	0.72
1:C:321:ILE:HG22	1:C:322:ASN:OD1	1.90	0.71
1:A:252:LEU:C	1:A:252:LEU:HD23	2.16	0.71
1:C:295:LEU:HD22	1:C:303:ALA:CA	2.19	0.71
1:C:252:LEU:C	1:C:252:LEU:HD23	2.16	0.71
2:D:50:TRP:HE1	3:D:201:6PL:H32	1.54	0.71
1:C:238:LEU:C	1:C:238:LEU:HD23	2.16	0.71
2:B:50:TRP:HE1	3:B:201:6PL:H11	1.31	0.71
2:D:47:ASN:OD1	3:D:201:6PL:H31	1.91	0.71
1:C:176:GLN:HB3	1:C:294:THR:HG22	1.72	0.71
1:C:282:MET:CG	4:C:502:9NY:C35	2.69	0.71
2:B:47:ASN:OD1	3:B:201:6PL:H31	1.90	0.71
1:A:330:LEU:HD23	1:A:358:PHE:CD1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:C	1:A:238:LEU:HD23	2.16	0.70
1:C:309:ILE:HD13	1:C:309:ILE:N	2.06	0.70
1:C:330:LEU:HD23	1:C:358:PHE:CD1	2.26	0.70
1:A:282:MET:CG	4:A:502:9NY:C35	2.69	0.70
2:D:50:TRP:NE1	3:D:201:6PL:H12	2.05	0.70
1:A:347:GLN:O	1:A:347:GLN:HG3	1.92	0.69
1:C:112:ARG:HB3	1:C:112:ARG:NH1	2.06	0.69
1:C:347:GLN:HG3	1:C:347:GLN:O	1.92	0.69
1:A:103:ASN:OD1	1:A:105:THR:HG22	1.92	0.69
1:C:103:ASN:OD1	1:C:105:THR:HG22	1.92	0.69
2:B:50:TRP:NE1	3:B:201:6PL:H12	2.06	0.69
1:A:202:PHE:HD1	1:A:277:PRO:HB3	1.57	0.69
1:A:239:VAL:C	1:A:241:GLN:N	2.45	0.69
1:C:140:MET:HE3	1:C:232:ALA:HB3	1.74	0.69
1:A:309:ILE:HD13	1:A:309:ILE:N	2.06	0.69
1:A:112:ARG:HB3	1:A:112:ARG:NH1	2.06	0.68
1:A:211:TYR:O	1:A:212:PRO:C	2.27	0.68
2:B:45:ARG:O	2:B:45:ARG:HG2	1.93	0.68
1:C:309:ILE:HD13	1:C:309:ILE:H	1.59	0.68
1:C:211:TYR:O	1:C:212:PRO:C	2.27	0.67
1:A:309:ILE:HD13	1:A:309:ILE:H	1.59	0.67
1:C:147:ARG:HG2	1:C:147:ARG:NH2	2.08	0.67
1:A:140:MET:HE3	1:A:232:ALA:HB3	1.74	0.67
1:A:282:MET:HB2	4:A:502:9NY:C35	2.23	0.67
1:C:202:PHE:HD1	1:C:277:PRO:HB3	1.59	0.67
2:D:45:ARG:HG2	2:D:45:ARG:O	1.93	0.67
1:A:91:LEU:O	1:A:95:TYR:HD2	1.77	0.66
1:A:147:ARG:HG2	1:A:147:ARG:NH2	2.08	0.66
1:C:91:LEU:O	1:C:95:TYR:HD2	1.77	0.66
1:A:140:MET:HE3	1:A:232:ALA:CB	2.26	0.66
1:C:147:ARG:NE	1:C:151:MET:HE1	2.09	0.66
1:C:251:GLU:CG	1:C:370:TYR:CD2	2.78	0.66
1:C:140:MET:HE3	1:C:232:ALA:CB	2.26	0.66
1:A:176:GLN:HA	1:A:176:GLN:OE1	1.96	0.66
1:C:156:ARG:N	1:C:157:PRO:CD	2.59	0.66
1:C:282:MET:HB2	4:C:502:9NY:C35	2.23	0.65
1:A:156:ARG:N	1:A:157:PRO:CD	2.59	0.65
1:C:116:VAL:HG21	1:C:218:PHE:HE1	1.62	0.65
1:C:176:GLN:OE1	1:C:176:GLN:HA	1.96	0.65
1:A:302:LEU:C	1:A:304:PHE:N	2.53	0.64
1:C:302:LEU:C	1:C:304:PHE:N	2.53	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:C	1:A:304:PHE:H	2.05	0.64
1:C:198:ASP:OD2	1:C:273:LYS:NZ	2.31	0.64
1:A:198:ASP:OD2	1:A:273:LYS:NZ	2.31	0.63
1:C:336:GLU:O	1:C:349:LYS:NZ	2.26	0.63
1:A:116:VAL:HG21	1:A:218:PHE:HE1	1.62	0.63
1:C:302:LEU:C	1:C:304:PHE:H	2.05	0.63
1:C:233:GLN:O	1:C:233:GLN:HG2	1.99	0.63
1:A:224:TYR:OH	1:A:266:SER:OG	2.16	0.62
1:A:169:ARG:HH11	1:A:169:ARG:CG	2.09	0.62
1:C:155:ILE:HG22	1:C:174:MET:CG	2.29	0.62
1:A:233:GLN:O	1:A:233:GLN:HG2	1.99	0.62
1:A:155:ILE:HG22	1:A:174:MET:CG	2.29	0.62
1:A:251:GLU:CG	1:A:370:TYR:CD2	2.78	0.62
1:C:224:TYR:OH	1:C:266:SER:OG	2.16	0.62
1:A:295:LEU:CD2	1:A:303:ALA:CB	2.58	0.62
1:A:282:MET:SD	1:A:318:ARG:NH1	2.73	0.62
1:A:330:LEU:HD23	1:A:358:PHE:HD1	1.64	0.62
1:A:240:LEU:HD21	2:B:20:ILE:HD13	1.82	0.62
1:C:171:LYS:HG3	1:C:171:LYS:O	2.00	0.62
1:C:282:MET:SD	1:C:318:ARG:NH1	2.73	0.62
1:A:95:TYR:O	1:A:99:PHE:HD2	1.83	0.62
1:C:95:TYR:O	1:C:99:PHE:HD2	1.83	0.61
1:C:204:THR:HG21	1:C:328:SER:CB	2.29	0.61
1:C:114:VAL:O	1:C:114:VAL:HG23	2.00	0.61
1:A:103:ASN:O	1:A:103:ASN:ND2	2.34	0.61
1:C:103:ASN:O	1:C:103:ASN:ND2	2.34	0.61
1:C:330:LEU:HD23	1:C:358:PHE:HD1	1.64	0.61
1:A:171:LYS:O	1:A:171:LYS:HG3	2.00	0.60
1:A:219:LEU:C	1:A:222:VAL:HG12	2.18	0.60
1:C:219:LEU:C	1:C:222:VAL:HG12	2.18	0.60
1:A:204:THR:HG21	1:A:328:SER:CB	2.31	0.60
1:C:216:ASN:OD1	1:C:216:ASN:N	2.21	0.60
1:C:367:VAL:O	1:C:367:VAL:HG12	2.00	0.60
1:A:114:VAL:HG23	1:A:114:VAL:O	2.00	0.60
1:C:240:LEU:HD21	2:D:20:ILE:HD13	1.82	0.60
1:C:312:VAL:O	1:C:312:VAL:HG12	2.02	0.60
1:A:367:VAL:HG12	1:A:367:VAL:O	2.00	0.59
1:C:116:VAL:HG21	1:C:218:PHE:CE1	2.37	0.59
1:C:176:GLN:CB	1:C:294:THR:HG22	2.33	0.59
1:A:176:GLN:CB	1:A:294:THR:HG22	2.32	0.59
1:A:312:VAL:O	1:A:312:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HA	1:A:321:ILE:HG12	1.84	0.59
1:C:214:PHE:C	1:C:215:THR:HG23	2.27	0.59
1:C:281:THR:HA	1:C:317:LEU:CD2	2.31	0.59
1:A:156:ARG:HD3	1:A:174:MET:SD	2.42	0.58
1:C:106:LYS:HB3	1:C:106:LYS:HZ3	1.68	0.58
1:A:262:LEU:HB3	4:A:502:9NY:C15	2.34	0.58
1:C:262:LEU:HB3	4:C:502:9NY:C15	2.34	0.58
1:A:214:PHE:C	1:A:215:THR:HG23	2.27	0.58
1:C:320:TYR:CD1	1:C:320:TYR:C	2.81	0.58
2:B:130:GLY:HA3	2:B:138:VAL:HG21	1.86	0.58
1:A:320:TYR:CD1	1:A:320:TYR:C	2.81	0.58
1:A:155:ILE:HG22	1:A:174:MET:HG2	1.86	0.57
2:D:130:GLY:HA3	2:D:138:VAL:HG21	1.86	0.57
1:A:116:VAL:HG21	1:A:218:PHE:CE1	2.37	0.57
1:A:296:ASN:O	1:A:298:LEU:O	2.22	0.57
2:B:99:LEU:H	2:B:99:LEU:HD23	1.70	0.57
2:B:39:TYR:CD1	3:B:201:6PL:H152	2.40	0.57
2:B:23:LEU:O	2:B:23:LEU:HD12	2.05	0.57
1:C:87:PRO:HB2	1:C:145:PHE:HB2	1.86	0.57
2:D:39:TYR:CD1	3:D:201:6PL:H152	2.39	0.57
1:C:334:ARG:CZ	1:C:334:ARG:CB	2.82	0.57
1:A:204:THR:HA	1:A:207:MET:HG3	1.87	0.56
1:A:330:LEU:CD2	1:A:358:PHE:HE1	1.93	0.56
1:C:156:ARG:HD3	1:C:174:MET:SD	2.45	0.56
1:C:296:ASN:O	1:C:298:LEU:O	2.22	0.56
2:B:24:PHE:C	2:B:24:PHE:CD2	2.83	0.56
1:C:195:TYR:C	1:C:195:TYR:CD2	2.83	0.56
2:D:93:GLU:OE2	2:D:95:ASN:ND2	2.38	0.56
2:B:116:ILE:O	2:B:116:ILE:HG22	2.05	0.56
1:C:155:ILE:HG22	1:C:174:MET:HG2	1.85	0.56
1:C:179:ALA:HA	1:C:182:TYR:CE2	2.41	0.56
2:D:24:PHE:C	2:D:24:PHE:CD2	2.83	0.56
1:A:336:GLU:O	1:A:349:LYS:NZ	2.26	0.56
2:D:116:ILE:HG22	2:D:116:ILE:O	2.05	0.56
1:A:179:ALA:HA	1:A:182:TYR:CE2	2.41	0.56
1:A:302:LEU:HB2	1:A:305:PHE:CD1	2.41	0.56
1:C:169:ARG:HH11	1:C:169:ARG:CG	2.09	0.56
1:C:204:THR:CG2	1:C:328:SER:OG	2.54	0.56
1:C:214:PHE:C	1:C:215:THR:CG2	2.78	0.56
2:D:23:LEU:HD12	2:D:23:LEU:O	2.05	0.56
1:A:281:THR:HA	1:A:317:LEU:CD2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:CB	1:A:334:ARG:CZ	2.82	0.56
1:C:302:LEU:HB2	1:C:305:PHE:CD1	2.41	0.56
1:A:126:TYR:N	1:A:126:TYR:CD2	2.70	0.56
1:A:195:TYR:C	1:A:195:TYR:CD2	2.83	0.56
1:A:87:PRO:HB2	1:A:145:PHE:HB2	1.86	0.55
1:A:204:THR:CG2	1:A:328:SER:OG	2.54	0.55
1:C:183:THR:HG21	1:C:287:PHE:HB2	1.86	0.55
2:D:99:LEU:HD23	2:D:99:LEU:H	1.70	0.55
1:A:214:PHE:C	1:A:215:THR:CG2	2.78	0.55
2:B:33:LEU:O	2:B:33:LEU:HG	2.07	0.55
2:B:50:TRP:NE1	3:B:201:6PL:H32	2.19	0.55
1:C:111:HIS:C	1:C:111:HIS:CD2	2.84	0.55
1:A:183:THR:HG21	1:A:287:PHE:HB2	1.86	0.55
1:A:156:ARG:HG2	1:A:156:ARG:NH2	2.22	0.55
1:A:112:ARG:NH1	1:A:112:ARG:CB	2.70	0.55
1:C:164:VAL:HG22	1:C:164:VAL:O	2.07	0.55
1:A:111:HIS:C	1:A:111:HIS:CD2	2.84	0.55
1:C:383:LEU:HD23	1:C:383:LEU:O	2.07	0.55
1:A:182:TYR:CD1	1:A:182:TYR:C	2.84	0.54
1:A:383:LEU:HD23	1:A:383:LEU:O	2.07	0.54
2:D:23:LEU:HD12	2:D:23:LEU:C	2.32	0.54
1:C:204:THR:HA	1:C:207:MET:HG3	1.89	0.54
2:B:23:LEU:HD12	2:B:23:LEU:C	2.32	0.54
2:D:38:GLU:OE2	3:D:202:6PL:C33	2.47	0.54
1:C:126:TYR:N	1:C:126:TYR:CD2	2.70	0.54
2:D:46:ILE:HG13	2:D:47:ASN:N	2.22	0.54
1:A:164:VAL:HG22	1:A:164:VAL:O	2.07	0.54
2:B:93:GLU:OE2	2:B:95:ASN:ND2	2.38	0.54
1:C:220:PHE:C	1:C:220:PHE:CD2	2.84	0.54
1:A:148:GLU:OE2	1:A:148:GLU:HA	2.07	0.54
2:B:101:PHE:HB3	2:B:129:VAL:HG23	1.90	0.54
2:D:101:PHE:HB3	2:D:129:VAL:HG23	1.90	0.54
1:A:95:TYR:O	1:A:99:PHE:CD2	2.61	0.54
1:A:176:GLN:CB	1:A:294:THR:CG2	2.86	0.54
1:A:212:PRO:O	1:A:270:HIS:HB3	2.07	0.54
1:A:309:ILE:N	1:A:309:ILE:CD1	2.71	0.54
1:C:112:ARG:NH1	1:C:112:ARG:CB	2.70	0.54
1:C:173:ILE:O	1:C:173:ILE:HG22	2.08	0.54
1:C:95:TYR:O	1:C:99:PHE:CD2	2.61	0.54
1:C:309:ILE:N	1:C:309:ILE:CD1	2.71	0.54
1:C:314:TRP:CD1	1:C:314:TRP:C	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:O	1:A:157:PRO:HD3	2.07	0.53
1:A:295:LEU:HD22	1:A:303:ALA:HA	1.90	0.53
1:C:147:ARG:CZ	1:C:151:MET:HE1	2.39	0.53
2:D:50:TRP:HE1	3:D:201:6PL:H12	1.61	0.53
1:C:152:ASP:O	1:C:157:PRO:HD3	2.07	0.53
2:D:33:LEU:O	2:D:33:LEU:HG	2.07	0.53
1:A:239:VAL:HG11	2:B:23:LEU:HA	1.91	0.53
1:C:212:PRO:O	1:C:270:HIS:HB3	2.07	0.53
2:B:46:ILE:HG13	2:B:47:ASN:N	2.22	0.53
1:C:281:THR:HG22	1:C:321:ILE:HG21	1.88	0.53
2:B:38:GLU:OE2	3:B:202:6PL:C33	2.45	0.53
2:B:99:LEU:HA	2:B:131:TYR:HA	1.91	0.53
1:A:147:ARG:HG2	1:A:147:ARG:HH21	1.73	0.52
1:C:182:TYR:CD1	1:C:182:TYR:C	2.84	0.52
1:C:219:LEU:HA	1:C:222:VAL:HG12	1.91	0.52
1:C:239:VAL:O	1:C:241:GLN:N	2.42	0.52
1:C:378:VAL:HG22	1:C:381:ARG:HH11	1.75	0.52
1:C:382:ILE:HG23	4:C:502:9NY:C1	2.40	0.52
2:D:99:LEU:HA	2:D:131:TYR:HA	1.91	0.52
1:A:173:ILE:O	1:A:173:ILE:HG22	2.08	0.52
1:A:325:ILE:O	1:A:325:ILE:HG22	2.08	0.52
1:C:148:GLU:OE2	1:C:148:GLU:HA	2.07	0.52
1:C:251:GLU:CD	1:C:370:TYR:CE2	2.87	0.52
1:A:147:ARG:NH1	1:A:151:MET:HE1	2.23	0.52
1:C:239:VAL:HG11	2:D:23:LEU:HA	1.91	0.52
2:D:50:TRP:HE1	3:D:201:6PL:C3	2.23	0.52
2:D:50:TRP:NE1	3:D:201:6PL:H32	2.21	0.52
1:A:382:ILE:HG23	4:A:502:9NY:C1	2.40	0.52
1:A:82:HIS:ND1	1:A:82:HIS:N	2.57	0.52
1:A:116:VAL:CG2	1:A:218:PHE:HE1	2.23	0.52
1:A:251:GLU:CD	1:A:370:TYR:CE2	2.87	0.52
1:C:145:PHE:O	1:C:145:PHE:CG	2.61	0.52
1:C:232:ALA:HA	1:C:260:LEU:HD21	1.91	0.52
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.10	0.52
1:A:239:VAL:O	1:A:241:GLN:N	2.43	0.51
1:A:192:TYR:CD2	1:A:192:TYR:C	2.85	0.51
1:A:305:PHE:N	1:A:305:PHE:CD2	2.73	0.51
1:A:375:ILE:HG13	4:A:502:9NY:C31	2.38	0.51
2:B:122:GLU:OE1	2:B:122:GLU:HA	2.10	0.51
1:A:327:TRP:CD1	1:A:327:TRP:C	2.85	0.51
1:C:116:VAL:CG2	1:C:218:PHE:HE1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:HG22	1:A:381:ARG:HH11	1.75	0.51
1:C:82:HIS:ND1	1:C:82:HIS:N	2.57	0.51
1:A:155:ILE:HG22	1:A:174:MET:HG3	1.93	0.51
1:A:366:LEU:HA	1:A:369:LEU:HD12	1.92	0.51
1:C:147:ARG:HG2	1:C:147:ARG:HH21	1.73	0.51
1:C:155:ILE:HG22	1:C:174:MET:HG3	1.93	0.51
1:C:176:GLN:CB	1:C:294:THR:CG2	2.86	0.51
1:A:219:LEU:HA	1:A:222:VAL:HG12	1.91	0.51
1:A:220:PHE:C	1:A:220:PHE:CD2	2.84	0.51
1:A:314:TRP:CD1	1:A:314:TRP:C	2.85	0.51
1:A:372:LEU:HD12	1:A:372:LEU:O	2.11	0.51
1:C:325:ILE:O	1:C:325:ILE:HG22	2.08	0.51
1:C:372:LEU:HD12	1:C:372:LEU:O	2.11	0.51
1:A:232:ALA:HA	1:A:260:LEU:HD21	1.92	0.50
1:C:205:LYS:HB3	1:C:209:ARG:NH2	2.26	0.50
1:C:295:LEU:CD2	1:C:303:ALA:CB	2.58	0.50
1:A:205:LYS:HB3	1:A:209:ARG:NH2	2.26	0.50
2:B:50:TRP:HE1	3:B:201:6PL:C3	2.21	0.50
1:C:91:LEU:O	1:C:95:TYR:CD2	2.63	0.50
1:C:334:ARG:CZ	1:C:334:ARG:HB2	2.41	0.50
1:C:192:TYR:CD2	1:C:192:TYR:C	2.85	0.50
1:A:383:LEU:C	1:A:383:LEU:CD2	2.85	0.50
1:C:295:LEU:HD22	1:C:303:ALA:HA	1.90	0.50
1:C:366:LEU:HA	1:C:369:LEU:HD12	1.92	0.50
2:D:115:PRO:HB2	2:D:117:HIS:CD2	2.47	0.50
1:A:380:TYR:CD2	1:A:380:TYR:C	2.86	0.50
1:C:194:MET:HB2	1:C:276:LEU:HD21	1.94	0.50
2:B:115:PRO:HB2	2:B:117:HIS:CD2	2.47	0.50
1:C:215:THR:O	1:C:215:THR:OG1	2.23	0.50
1:C:220:PHE:HD2	1:C:220:PHE:O	1.95	0.50
1:C:327:TRP:CD1	1:C:327:TRP:C	2.85	0.50
1:C:380:TYR:CD2	1:C:380:TYR:C	2.86	0.50
1:A:309:ILE:O	1:A:309:ILE:HG22	2.11	0.49
1:C:383:LEU:C	1:C:383:LEU:CD2	2.85	0.49
1:A:262:LEU:HD21	1:A:360:LEU:HB3	1.94	0.49
1:C:268:VAL:O	1:C:268:VAL:HG13	2.12	0.49
1:C:309:ILE:O	1:C:309:ILE:HG22	2.11	0.49
2:D:39:TYR:O	2:D:39:TYR:CG	2.65	0.49
1:C:251:GLU:CD	1:C:370:TYR:HE2	2.20	0.49
1:A:95:TYR:HD1	1:A:99:PHE:HE2	1.60	0.49
1:C:156:ARG:HG2	1:C:156:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ILE:HG13	4:C:502:9NY:C31	2.38	0.49
1:A:103:ASN:ND2	1:A:103:ASN:C	2.70	0.49
1:A:164:VAL:HG11	1:A:298:LEU:HD22	1.94	0.49
1:A:194:MET:HB2	1:A:276:LEU:HD21	1.94	0.49
1:A:220:PHE:HD2	1:A:220:PHE:O	1.95	0.49
1:C:95:TYR:HD1	1:C:99:PHE:HE2	1.60	0.49
1:C:191:ILE:O	1:C:191:ILE:HG22	2.12	0.49
1:C:255:HIS:ND1	1:C:256:HIS:CD2	2.81	0.49
1:C:262:LEU:HD21	1:C:360:LEU:HB3	1.94	0.49
1:C:103:ASN:ND2	1:C:103:ASN:C	2.70	0.49
1:A:145:PHE:O	1:A:145:PHE:CG	2.61	0.49
1:A:204:THR:O	1:A:206:ALA:N	2.46	0.49
1:A:251:GLU:CD	1:A:370:TYR:HE2	2.20	0.49
1:C:219:LEU:CA	1:C:222:VAL:HG12	2.43	0.49
1:A:255:HIS:ND1	1:A:256:HIS:CD2	2.81	0.48
1:A:304:PHE:O	1:A:304:PHE:CD1	2.66	0.48
1:A:334:ARG:CZ	1:A:334:ARG:HB2	2.41	0.48
1:A:156:ARG:N	1:A:157:PRO:HD3	2.28	0.48
2:D:37:VAL:O	2:D:37:VAL:HG23	2.13	0.48
1:A:145:PHE:O	1:A:145:PHE:CD1	2.67	0.48
1:A:156:ARG:HG2	1:A:156:ARG:HH21	1.77	0.48
1:A:219:LEU:CA	1:A:222:VAL:HG12	2.43	0.48
1:A:220:PHE:C	1:A:220:PHE:HD2	2.22	0.48
1:A:238:LEU:HD23	1:A:238:LEU:O	2.13	0.48
1:C:220:PHE:C	1:C:220:PHE:HD2	2.22	0.48
1:C:304:PHE:O	1:C:304:PHE:CD1	2.66	0.48
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.53	0.48
1:C:238:LEU:HD23	1:C:238:LEU:O	2.13	0.48
1:A:191:ILE:O	1:A:191:ILE:HG22	2.12	0.48
2:B:39:TYR:O	2:B:39:TYR:CG	2.65	0.48
1:C:145:PHE:O	1:C:145:PHE:CD1	2.67	0.48
1:C:173:ILE:HD11	1:C:298:LEU:HD23	1.96	0.48
1:C:214:PHE:O	1:C:215:THR:CG2	2.62	0.48
1:A:214:PHE:O	1:A:215:THR:CG2	2.62	0.48
1:A:268:VAL:O	1:A:268:VAL:HG13	2.12	0.48
1:A:378:VAL:HG13	1:A:382:ILE:HG12	1.96	0.48
1:C:180:ILE:HG21	1:C:180:ILE:HD13	1.54	0.48
1:A:370:TYR:CD1	1:A:370:TYR:C	2.84	0.48
2:B:37:VAL:O	2:B:37:VAL:HG23	2.13	0.48
1:A:281:THR:HG22	1:A:321:ILE:HG21	1.89	0.47
1:C:378:VAL:HG13	1:C:382:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG12	1:A:258:VAL:O	2.13	0.47
1:C:164:VAL:HG11	1:C:298:LEU:HD22	1.94	0.47
1:C:214:PHE:O	1:C:215:THR:HG22	2.15	0.47
1:C:370:TYR:CD1	1:C:370:TYR:C	2.84	0.47
1:A:269:PHE:O	1:A:270:HIS:CB	2.62	0.47
1:C:305:PHE:N	1:C:305:PHE:CD2	2.73	0.47
1:C:254:PHE:O	1:C:258:VAL:HG23	2.15	0.47
2:D:50:TRP:O	2:D:50:TRP:CE3	2.68	0.47
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.59	0.47
1:C:183:THR:HG21	1:C:287:PHE:CA	2.45	0.47
1:C:258:VAL:HG12	1:C:258:VAL:O	2.13	0.47
1:A:120:ILE:O	1:A:120:ILE:HG22	2.14	0.47
1:C:370:TYR:CD1	1:C:370:TYR:O	2.68	0.47
1:C:262:LEU:CB	4:C:502:9NY:C19	2.91	0.47
2:B:50:TRP:CE3	2:B:50:TRP:O	2.68	0.47
1:C:254:PHE:CD2	1:C:367:VAL:CG2	2.98	0.47
1:A:109:VAL:HA	1:A:112:ARG:NH1	2.30	0.46
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.55	0.46
1:A:214:PHE:O	1:A:215:THR:HG22	2.15	0.46
1:A:183:THR:HG21	1:A:287:PHE:CA	2.45	0.46
1:A:370:TYR:CD1	1:A:370:TYR:O	2.68	0.46
1:C:109:VAL:HA	1:C:112:ARG:NH1	2.30	0.46
1:C:238:LEU:C	1:C:238:LEU:CD2	2.84	0.46
1:A:173:ILE:HD11	1:A:298:LEU:HD23	1.96	0.46
1:A:238:LEU:HD11	1:A:253:THR:OG1	2.16	0.46
1:C:152:ASP:OD1	1:C:152:ASP:C	2.59	0.46
1:C:254:PHE:CD2	1:C:367:VAL:HG22	2.50	0.46
1:C:252:LEU:O	1:C:255:HIS:HB3	2.15	0.46
1:A:254:PHE:CD2	1:A:367:VAL:CG2	2.98	0.46
1:A:255:HIS:ND1	1:A:256:HIS:HD2	2.14	0.46
1:C:238:LEU:HD11	1:C:253:THR:OG1	2.16	0.46
1:A:252:LEU:O	1:A:255:HIS:HB3	2.15	0.46
1:A:255:HIS:CE1	4:A:502:9NY:S1	3.09	0.46
1:A:321:ILE:HG22	1:A:322:ASN:N	2.31	0.46
3:B:201:6PL:H242	3:B:201:6PL:H212	1.34	0.46
1:A:91:LEU:O	1:A:95:TYR:CD2	2.63	0.46
1:C:156:ARG:N	1:C:157:PRO:HD3	2.29	0.46
1:C:204:THR:O	1:C:206:ALA:N	2.49	0.46
1:C:255:HIS:ND1	1:C:256:HIS:HD2	2.14	0.46
1:A:173:ILE:HD13	1:A:173:ILE:HG21	1.56	0.46
1:A:254:PHE:CD2	1:A:367:VAL:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:GLU:OE2	2:B:86:LYS:HE2	2.16	0.46
1:C:240:LEU:HD22	1:C:240:LEU:HA	1.66	0.46
1:A:152:ASP:OD1	1:A:152:ASP:C	2.59	0.46
1:A:310:PHE:O	1:A:310:PHE:CD1	2.69	0.46
1:A:380:TYR:CD2	1:A:380:TYR:O	2.69	0.46
1:C:380:TYR:CD2	1:C:380:TYR:O	2.69	0.46
2:D:117:HIS:CD2	2:D:117:HIS:H	2.34	0.46
1:C:269:PHE:O	1:C:270:HIS:CB	2.62	0.46
1:A:254:PHE:O	1:A:258:VAL:HG23	2.15	0.45
2:B:117:HIS:CD2	2:B:117:HIS:H	2.34	0.45
1:C:75:PHE:N	1:C:75:PHE:CD2	2.82	0.45
1:A:156:ARG:HH21	1:A:156:ARG:CG	2.30	0.45
1:C:310:PHE:O	1:C:310:PHE:CD1	2.69	0.45
1:A:262:LEU:CB	4:A:502:9NY:C19	2.91	0.45
1:A:320:TYR:CD1	1:A:320:TYR:O	2.69	0.45
1:A:334:ARG:NH2	1:A:334:ARG:HB3	2.32	0.45
1:A:238:LEU:O	1:A:238:LEU:HG	2.16	0.45
2:B:33:LEU:HD23	2:B:33:LEU:C	2.42	0.45
1:C:249:HIS:O	1:C:249:HIS:CG	2.68	0.45
4:A:502:9NY:C31	4:A:502:9NY:O15	2.65	0.45
1:C:149:PHE:CE1	1:C:153:VAL:CG2	2.95	0.45
1:C:173:ILE:HD13	1:C:173:ILE:HG21	1.56	0.45
1:C:255:HIS:CE1	4:C:502:9NY:S1	3.09	0.45
1:C:108:ASN:HB3	1:C:109:VAL:H	1.21	0.45
1:C:120:ILE:O	1:C:120:ILE:HG22	2.14	0.45
4:C:502:9NY:C31	4:C:502:9NY:O15	2.65	0.45
2:D:33:LEU:HD23	2:D:33:LEU:C	2.42	0.45
1:C:254:PHE:HD2	1:C:367:VAL:CG2	2.30	0.45
1:C:320:TYR:O	1:C:320:TYR:CG	2.68	0.45
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.53	0.44
2:B:46:ILE:CG1	2:B:47:ASN:N	2.79	0.44
1:C:76:ARG:HA	1:C:76:ARG:HD2	1.27	0.44
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.59	0.44
1:C:174:MET:HE2	1:C:174:MET:HB3	1.77	0.44
1:A:147:ARG:HE	1:A:151:MET:CE	2.30	0.44
1:C:238:LEU:O	1:C:238:LEU:HG	2.16	0.44
1:C:320:TYR:CD1	1:C:320:TYR:O	2.69	0.44
1:A:75:PHE:N	1:A:75:PHE:CD2	2.82	0.44
1:C:334:ARG:NH2	1:C:334:ARG:HB3	2.32	0.44
2:D:49:GLU:OE2	2:D:86:LYS:HE2	2.16	0.44
1:A:139:TYR:O	1:A:140:MET:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HB3	1:A:109:VAL:H	1.21	0.44
1:A:142:PHE:O	1:A:142:PHE:CG	2.66	0.44
1:A:244:LYS:H	1:A:244:LYS:HG3	1.57	0.44
2:B:32:LEU:HD12	2:B:32:LEU:HA	1.72	0.44
1:C:302:LEU:O	1:C:304:PHE:N	2.51	0.44
1:A:254:PHE:HD2	1:A:367:VAL:CG2	2.30	0.43
1:C:245:PRO:CB	1:C:249:HIS:HB3	2.48	0.43
1:A:170:ILE:HG21	1:A:170:ILE:HD13	1.59	0.43
1:A:249:HIS:O	1:A:249:HIS:CG	2.68	0.43
1:C:80:TYR:HD1	1:C:80:TYR:HA	1.68	0.43
1:C:146:LEU:HA	1:C:146:LEU:HD23	1.59	0.43
1:C:317:LEU:O	1:C:321:ILE:CB	2.42	0.43
3:D:201:6PL:H141	3:D:201:6PL:H171	1.70	0.43
1:A:220:PHE:CD2	1:A:220:PHE:O	2.72	0.43
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.75	0.43
2:B:29:ILE:N	2:B:29:ILE:CD1	2.81	0.43
3:B:201:6PL:H221	3:B:201:6PL:H192	1.69	0.43
1:A:302:LEU:O	1:A:304:PHE:N	2.51	0.43
1:C:245:PRO:HB2	1:C:249:HIS:HB3	2.01	0.43
1:A:205:LYS:HE3	1:A:209:ARG:HH22	1.84	0.43
1:C:205:LYS:HE3	1:C:209:ARG:HH22	1.84	0.43
1:C:261:LEU:HA	1:C:261:LEU:HD12	1.83	0.43
2:D:29:ILE:N	2:D:29:ILE:CD1	2.81	0.43
1:A:124:ASN:ND2	1:A:124:ASN:C	2.71	0.43
1:C:142:PHE:O	1:C:142:PHE:CG	2.66	0.43
2:B:101:PHE:CE1	2:B:150:MET:HE3	2.54	0.43
1:C:150:LEU:HD12	1:C:150:LEU:HA	1.55	0.43
1:C:180:ILE:HD12	1:C:291:PHE:HD2	1.84	0.43
1:A:180:ILE:HD12	1:A:291:PHE:HD2	1.84	0.43
1:A:180:ILE:HG21	1:A:180:ILE:HD13	1.54	0.43
1:A:263:ILE:CG1	1:A:279:TYR:OH	2.67	0.43
1:C:73:PHE:CE2	1:C:76:ARG:HB2	2.54	0.43
1:C:156:ARG:HG2	1:C:156:ARG:HH21	1.83	0.43
1:C:238:LEU:O	1:C:238:LEU:CG	2.67	0.43
1:C:263:ILE:CG1	1:C:279:TYR:OH	2.67	0.43
2:D:46:ILE:CG1	2:D:47:ASN:N	2.79	0.43
1:A:140:MET:HE3	1:A:232:ALA:HB1	2.01	0.42
1:A:73:PHE:CE2	1:A:76:ARG:HB2	2.54	0.42
1:A:239:VAL:O	1:A:240:LEU:C	2.59	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.86	0.42
1:C:252:LEU:C	1:C:252:LEU:CD2	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:THR:HG23	1:A:107:THR:H	1.83	0.42
1:A:237:ILE:HD12	1:A:237:ILE:HA	1.41	0.42
1:C:126:TYR:N	1:C:126:TYR:HD2	2.14	0.42
1:C:239:VAL:O	1:C:240:LEU:C	2.59	0.42
1:A:227:GLN:HG2	3:A:501:6PL:H471	2.01	0.42
1:C:239:VAL:HG12	1:C:240:LEU:N	2.35	0.42
2:D:118:GLU:OE2	2:D:118:GLU:CA	2.67	0.42
3:D:201:6PL:H242	3:D:201:6PL:H212	1.34	0.42
1:A:152:ASP:OD1	1:A:153:VAL:N	2.53	0.42
1:A:256:HIS:CD2	1:A:256:HIS:N	2.84	0.42
3:B:201:6PL:H361	3:B:201:6PL:H391	1.86	0.42
1:C:110:LEU:HD23	1:C:110:LEU:HA	1.64	0.42
1:A:263:ILE:HG13	1:A:279:TYR:OH	2.20	0.42
1:A:304:PHE:CD1	1:A:304:PHE:C	2.98	0.42
1:A:326:LEU:HG	1:A:361:ILE:HG22	2.02	0.42
1:C:210:THR:HG23	1:C:210:THR:O	2.20	0.42
1:C:269:PHE:C	1:C:270:HIS:CG	2.97	0.42
1:C:326:LEU:HG	1:C:361:ILE:HG22	2.02	0.42
1:A:238:LEU:O	1:A:238:LEU:CG	2.67	0.42
1:A:269:PHE:C	1:A:270:HIS:CG	2.97	0.42
1:A:323:LEU:CD2	1:A:365:GLN:HE22	2.18	0.42
1:C:105:THR:HG23	1:C:107:THR:H	1.83	0.42
1:C:304:PHE:CD1	1:C:304:PHE:C	2.98	0.42
1:C:152:ASP:OD1	1:C:153:VAL:N	2.53	0.42
2:D:20:ILE:O	2:D:20:ILE:HG22	2.20	0.42
2:D:50:TRP:HE1	3:D:201:6PL:C2	2.29	0.42
2:D:101:PHE:CE1	2:D:150:MET:HE3	2.54	0.42
1:A:111:HIS:O	1:A:111:HIS:CG	2.70	0.42
1:A:210:THR:O	1:A:210:THR:HG23	2.20	0.42
1:C:114:VAL:O	1:C:115:ALA:HB2	2.20	0.42
1:A:244:LYS:O	1:A:244:LYS:CD	2.68	0.42
1:A:245:PRO:HB2	1:A:249:HIS:HB3	2.01	0.42
1:A:245:PRO:CB	1:A:249:HIS:HB3	2.48	0.42
1:A:371:TRP:HD1	1:A:371:TRP:HA	1.70	0.42
1:A:114:VAL:O	1:A:115:ALA:HB2	2.20	0.41
1:A:308:ALA:O	1:A:311:VAL:N	2.53	0.41
1:A:329:VAL:O	1:A:333:PHE:HB2	2.20	0.41
1:C:218:PHE:C	1:C:218:PHE:CD1	2.91	0.41
1:C:220:PHE:CD2	1:C:220:PHE:O	2.72	0.41
1:C:376:PHE:HD1	1:C:376:PHE:HA	1.55	0.41
1:C:111:HIS:O	1:C:111:HIS:CG	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LEU:HA	1:C:321:ILE:HG12	2.01	0.41
3:B:201:6PL:O31	3:B:201:6PL:C34	2.67	0.41
1:C:244:LYS:O	1:C:244:LYS:HD2	2.20	0.41
1:C:244:LYS:O	1:C:244:LYS:CD	2.68	0.41
1:C:364:LEU:HD23	1:C:364:LEU:HA	1.90	0.41
2:D:78:ARG:O	2:D:82:LYS:HG3	2.20	0.41
1:A:243:GLU:HB3	1:A:244:LYS:H	1.62	0.41
2:B:78:ARG:O	2:B:82:LYS:HG3	2.20	0.41
1:C:161:ARG:O	1:C:161:ARG:HG2	2.18	0.41
1:C:195:TYR:C	1:C:197:SER:H	2.29	0.41
1:C:230:PHE:O	1:C:230:PHE:CG	2.68	0.41
1:A:76:ARG:HD2	1:A:76:ARG:HA	1.27	0.41
1:A:241:GLN:OE1	1:A:241:GLN:CA	2.69	0.41
2:D:77:LYS:HD2	2:D:111:PRO:HA	2.02	0.41
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.58	0.41
1:A:325:ILE:HG21	1:A:325:ILE:HD13	1.76	0.41
1:C:263:ILE:HG13	1:C:279:TYR:OH	2.20	0.41
1:C:329:VAL:O	1:C:333:PHE:HB2	2.20	0.41
1:A:103:ASN:HD21	1:A:108:ASN:ND2	2.19	0.41
1:A:176:GLN:CG	1:A:294:THR:HG23	2.51	0.41
1:A:244:LYS:O	1:A:244:LYS:HD2	2.20	0.41
1:C:256:HIS:CD2	1:C:256:HIS:N	2.84	0.41
1:C:103:ASN:HD21	1:C:108:ASN:ND2	2.18	0.41
1:C:227:GLN:HG2	3:C:501:6PL:H471	2.03	0.41
1:A:173:ILE:O	1:A:173:ILE:CG2	2.66	0.41
1:A:320:TYR:O	1:A:320:TYR:CG	2.68	0.41
2:B:77:LYS:HD2	2:B:111:PRO:HA	2.02	0.41
1:C:176:GLN:CG	1:C:294:THR:HG23	2.51	0.41
1:C:323:LEU:CD2	1:C:365:GLN:HE22	2.18	0.41
1:A:167:LYS:NZ	1:A:171:LYS:HB2	2.36	0.41
1:A:239:VAL:HG12	1:A:240:LEU:N	2.34	0.41
1:A:240:LEU:HA	1:A:240:LEU:HD22	1.66	0.41
2:B:50:TRP:HE1	3:B:201:6PL:C2	2.28	0.41
2:B:115:PRO:HB2	2:B:117:HIS:HD2	1.84	0.41
1:A:106:LYS:HB3	1:A:106:LYS:HZ3	1.75	0.40
1:A:326:LEU:HA	1:A:326:LEU:HD23	1.59	0.40
1:C:156:ARG:HH21	1:C:156:ARG:CG	2.34	0.40
2:D:131:TYR:HA	2:D:131:TYR:HD2	1.71	0.40
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.64	0.40
2:B:118:GLU:OE2	2:B:118:GLU:CA	2.67	0.40
1:A:126:TYR:N	1:A:126:TYR:HD2	2.14	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ILE:HG22	1:C:322:ASN:N	2.35	0.40
2:D:20:ILE:O	2:D:20:ILE:CG2	2.68	0.40
1:A:174:MET:HE2	1:A:174:MET:HB3	1.77	0.40
1:C:111:HIS:CD2	1:C:111:HIS:O	2.75	0.40
1:C:173:ILE:HD13	1:C:298:LEU:HD21	2.04	0.40
1:C:241:GLN:OE1	1:C:241:GLN:HA	2.14	0.40
1:C:243:GLU:HB3	1:C:244:LYS:HG3	2.04	0.40
1:C:253:THR:O	1:C:253:THR:CG2	2.66	0.40
1:C:310:PHE:O	1:C:310:PHE:CG	2.68	0.40
1:C:372:LEU:HD12	1:C:372:LEU:HA	1.75	0.40
1:A:115:ALA:HB1	3:A:501:6PL:H322	2.04	0.40
1:A:183:THR:HG21	1:A:287:PHE:CB	2.50	0.40
1:A:310:PHE:O	1:A:310:PHE:CG	2.68	0.40
1:C:211:TYR:CD2	1:C:212:PRO:HD3	2.57	0.40
1:C:248:ASP:O	1:C:249:HIS:C	2.58	0.40
1:C:327:TRP:O	1:C:327:TRP:CG	2.69	0.40
3:D:201:6PL:H361	3:D:201:6PL:H391	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/428 (73%)	266 (85%)	37 (12%)	10 (3%)	3	18
1	C	313/428 (73%)	267 (85%)	36 (12%)	10 (3%)	3	18
2	B	130/150 (87%)	120 (92%)	9 (7%)	1 (1%)	16	47
2	D	130/150 (87%)	120 (92%)	9 (7%)	1 (1%)	16	47
All	All	886/1156 (77%)	773 (87%)	91 (10%)	22 (2%)	6	21

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	PRO
1	A	248	ASP
1	A	249	HIS
2	B	120	LYS
1	C	245	PRO
1	C	248	ASP
1	C	249	HIS
2	D	120	LYS
1	A	108	ASN
1	A	166	SER
1	A	240	LEU
1	A	243	GLU
1	A	246	ARG
1	C	108	ASN
1	C	166	SER
1	C	240	LEU
1	C	243	GLU
1	C	246	ARG
1	A	303	ALA
1	C	303	ALA
1	A	109	VAL
1	C	109	VAL

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	284/391 (73%)	209 (74%)	75 (26%)	0	2
1	C	284/391 (73%)	209 (74%)	75 (26%)	0	2
2	B	119/135 (88%)	105 (88%)	14 (12%)	5	21
2	D	119/135 (88%)	105 (88%)	14 (12%)	5	21
All	All	806/1052 (77%)	628 (78%)	178 (22%)	2	4

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	73	PHE
1	A	74	SER
1	A	76	ARG
1	A	78	ILE
1	A	80	TYR
1	A	82	HIS
1	A	96	SER
1	A	103	ASN
1	A	106	LYS
1	A	108	ASN
1	A	112	ARG
1	A	114	VAL
1	A	117	SER
1	A	120	ILE
1	A	124	ASN
1	A	150	LEU
1	A	151	MET
1	A	152	ASP
1	A	154	VAL
1	A	155	ILE
1	A	156	ARG
1	A	158	PHE
1	A	160	ILE
1	A	164	VAL
1	A	165	THR
1	A	166	SER
1	A	167	LYS
1	A	168	HIS
1	A	169	ARG
1	A	171	LYS
1	A	176	GLN
1	A	177	MET
1	A	180	ILE
1	A	194	MET
1	A	198	ASP
1	A	199	LEU
1	A	201	PHE
1	A	207	MET
1	A	209	ARG
1	A	216	ASN
1	A	217	PRO
1	A	224	TYR

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Mol	Chain	Res	Type
1	A	236	CYS
1	A	237	ILE
1	A	238	LEU
1	A	239	VAL
1	A	240	LEU
1	A	241	GLN
1	A	243	GLU
1	A	244	LYS
1	A	246	ARG
1	A	249	HIS
1	A	251	GLU
1	A	252	LEU
1	A	253	THR
1	A	259	THR
1	A	260	LEU
1	A	263	ILE
1	A	268	VAL
1	A	304	PHE
1	A	309	ILE
1	A	311	VAL
1	A	315	ILE
1	A	321	ILE
1	A	324	LYS
1	A	327	TRP
1	A	330	LEU
1	A	347	GLN
1	A	369	LEU
1	A	376	PHE
1	A	380	TYR
1	A	383	LEU
1	A	384	TRP
1	A	385	ARG
2	B	24	PHE
2	B	26	VAL
2	B	27	CYS
2	B	29	ILE
2	B	31	LEU
2	B	33	LEU
2	B	34	ILE
2	B	37	VAL
2	B	38	GLU
2	B	41	LYS

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Mol	Chain	Res	Type
2	B	50	TRP
2	B	116	ILE
2	B	131	TYR
2	B	136	GLU
1	C	71	ILE
1	C	73	PHE
1	C	74	SER
1	C	76	ARG
1	C	78	ILE
1	C	80	TYR
1	C	82	HIS
1	C	96	SER
1	C	103	ASN
1	C	106	LYS
1	C	108	ASN
1	C	112	ARG
1	C	114	VAL
1	C	117	SER
1	C	120	ILE
1	C	124	ASN
1	C	150	LEU
1	C	151	MET
1	C	152	ASP
1	C	154	VAL
1	C	155	ILE
1	C	156	ARG
1	C	158	PHE
1	C	160	ILE
1	C	164	VAL
1	C	165	THR
1	C	166	SER
1	C	167	LYS
1	C	168	HIS
1	C	169	ARG
1	C	171	LYS
1	C	176	GLN
1	C	177	MET
1	C	180	ILE
1	C	194	MET
1	C	198	ASP
1	C	199	LEU
1	C	201	PHE

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Mol	Chain	Res	Type
1	C	207	MET
1	C	209	ARG
1	C	216	ASN
1	C	217	PRO
1	C	224	TYR
1	C	236	CYS
1	C	237	ILE
1	C	238	LEU
1	C	239	VAL
1	C	240	LEU
1	C	241	GLN
1	C	243	GLU
1	C	244	LYS
1	C	246	ARG
1	C	249	HIS
1	C	251	GLU
1	C	252	LEU
1	C	253	THR
1	C	259	THR
1	C	260	LEU
1	C	263	ILE
1	C	268	VAL
1	C	304	PHE
1	C	309	ILE
1	C	311	VAL
1	C	315	ILE
1	C	321	ILE
1	C	324	LYS
1	C	327	TRP
1	C	330	LEU
1	C	347	GLN
1	C	369	LEU
1	C	376	PHE
1	C	380	TYR
1	C	383	LEU
1	C	384	TRP
1	C	385	ARG
2	D	24	PHE
2	D	26	VAL
2	D	27	CYS
2	D	29	ILE
2	D	31	LEU

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Mol	Chain	Res	Type
2	D	33	LEU
2	D	34	ILE
2	D	37	VAL
2	D	38	GLU
2	D	41	LYS
2	D	50	TRP
2	D	116	ILE
2	D	131	TYR
2	D	136	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	111	HIS
1	A	256	HIS
1	A	319	HIS
1	A	365	GLN
2	B	98	HIS
2	B	117	HIS
1	C	108	ASN
1	C	111	HIS
1	C	256	HIS
1	C	319	HIS
1	C	365	GLN
2	D	98	HIS
2	D	117	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

8 ligands are modelled in this entry.

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	6PL	C	501	-	17,17,51	0.21	0	16,16,59	0.63	0
4	9NY	C	502	-	75,77,77	2.79	23 (30%)	97,103,103	2.71	36 (37%)
3	6PL	A	501	-	17,17,51	0.21	0	16,16,59	0.62	0
3	6PL	B	201	-	39,39,51	1.56	6 (15%)	42,44,59	1.72	7 (16%)
3	6PL	D	201	-	39,39,51	1.56	6 (15%)	42,44,59	1.72	7 (16%)
3	6PL	B	202	-	17,17,51	0.32	0	16,16,59	0.86	0
3	6PL	D	202	-	17,17,51	0.32	0	16,16,59	0.86	0
4	9NY	A	502	-	75,77,77	2.79	22 (29%)	97,103,103	2.71	36 (37%)

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	6PL	C	501	-	-	7/15/15/55	-
4	9NY	C	502	-	-	35/76/92/92	0/3/3/3
3	6PL	A	501	-	-	7/15/15/55	-
3	6PL	B	201	-	-	21/41/41/55	-
3	6PL	D	201	-	-	20/41/41/55	-
3	6PL	B	202	-	-	6/15/15/55	-
3	6PL	D	202	-	-	6/15/15/55	-
4	9NY	A	502	-	-	35/76/92/92	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	9NY	P2-O8	-10.84	1.47	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	9NY	P2-O8	-10.83	1.47	1.59
4	A	502	9NY	C44-S1	9.60	1.98	1.76
4	C	502	9NY	C44-S1	9.59	1.98	1.76
4	C	502	9NY	C40-C44	7.57	1.58	1.50
4	A	502	9NY	C40-C44	7.54	1.58	1.50
4	C	502	9NY	P3-O8	-6.63	1.52	1.59
4	A	502	9NY	P3-O8	-6.62	1.52	1.59
4	C	502	9NY	O12-C25	-5.96	1.31	1.42
4	A	502	9NY	O12-C25	-5.96	1.31	1.42
3	D	201	6PL	O2-C31	5.26	1.49	1.34
3	B	201	6PL	O2-C31	5.25	1.49	1.34
4	A	502	9NY	O3-C9	-4.80	1.34	1.45
4	C	502	9NY	O3-C9	-4.80	1.34	1.45
4	A	502	9NY	C24-C11	-4.53	1.45	1.52
4	C	502	9NY	C24-C11	-4.51	1.45	1.52
4	A	502	9NY	C5-N5	4.42	1.58	1.46
4	C	502	9NY	C5-N5	4.41	1.58	1.46
4	C	502	9NY	O15-C36	-3.89	1.15	1.23
4	A	502	9NY	O15-C36	-3.87	1.16	1.23
3	D	201	6PL	O2-C2	-3.86	1.37	1.46
3	B	201	6PL	O2-C2	-3.85	1.37	1.46
4	A	502	9NY	C6-N2	3.77	1.40	1.33
4	C	502	9NY	C6-N2	3.75	1.40	1.33
4	A	502	9NY	C2-N4	-3.64	1.32	1.39
4	C	502	9NY	C2-N4	-3.63	1.32	1.39
3	D	201	6PL	O3-C11	3.44	1.43	1.33
3	B	201	6PL	O3-C11	3.44	1.43	1.33
3	D	201	6PL	P-O2P	-3.34	1.42	1.54
3	B	201	6PL	P-O2P	-3.33	1.42	1.54
4	A	502	9NY	P2-O9	-3.30	1.39	1.50
4	C	502	9NY	P2-O9	-3.28	1.39	1.50
3	B	201	6PL	P-O1P	-3.14	1.40	1.50
3	D	201	6PL	P-O1P	-3.11	1.40	1.50
4	A	502	9NY	C31-C11	-3.06	1.47	1.53
4	C	502	9NY	C31-C11	-3.04	1.47	1.53
3	B	201	6PL	O11-C11	-2.83	1.14	1.22
3	D	201	6PL	O11-C11	-2.81	1.14	1.22
4	A	502	9NY	C2-C1	-2.80	1.34	1.39
4	C	502	9NY	C2-C1	-2.80	1.34	1.39
4	C	502	9NY	C2-C3	-2.78	1.33	1.41
4	A	502	9NY	C2-C3	-2.77	1.33	1.41
4	A	502	9NY	C36-N6	-2.76	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	9NY	C36-N6	-2.74	1.27	1.33
4	A	502	9NY	C4-N5	-2.46	1.33	1.37
4	C	502	9NY	C4-N5	-2.43	1.33	1.37
4	C	502	9NY	P2-O10	-2.28	1.44	1.55
4	A	502	9NY	P2-O10	-2.27	1.44	1.55
4	C	502	9NY	C30-C11	-2.11	1.49	1.53
4	A	502	9NY	C30-C11	-2.08	1.49	1.53
4	A	502	9NY	C45-N7	-2.06	1.28	1.33
4	C	502	9NY	C45-N7	-2.06	1.28	1.33
4	A	502	9NY	O3-C5	2.05	1.46	1.42
4	C	502	9NY	O3-C5	2.05	1.46	1.42
4	C	502	9NY	C41-C43	2.03	1.58	1.51
4	A	502	9NY	C41-C43	2.02	1.58	1.51
4	C	502	9NY	C7-C8	-2.00	1.48	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	9NY	O14-P3-O8	7.93	128.71	107.27
4	C	502	9NY	O14-P3-O8	7.92	128.69	107.27
4	A	502	9NY	O8-P3-O13	-7.34	88.62	110.70
4	C	502	9NY	O8-P3-O13	-7.34	88.64	110.70
4	C	502	9NY	C2-C1-N2	-7.19	116.82	126.72
4	A	502	9NY	C2-C1-N2	-7.18	116.83	126.72
4	A	502	9NY	N2-C6-N1	-6.23	119.15	128.58
4	C	502	9NY	N2-C6-N1	-6.23	119.15	128.58
4	A	502	9NY	O11-C24-C11	6.16	120.45	110.55
4	C	502	9NY	O11-C24-C11	6.13	120.40	110.55
3	B	201	6PL	O2-C31-C32	6.05	124.57	111.48
3	D	201	6PL	O2-C31-C32	6.03	124.53	111.48
4	A	502	9NY	O3-C5-N5	5.34	118.35	108.09
4	C	502	9NY	O3-C5-N5	5.33	118.33	108.09
4	A	502	9NY	C30-C11-C24	-4.83	100.25	108.22
4	C	502	9NY	C30-C11-C24	-4.80	100.29	108.22
4	C	502	9NY	O4-P2-O9	-4.74	90.14	108.94
4	A	502	9NY	O4-P2-O9	-4.73	90.18	108.94
4	C	502	9NY	C1-N5-C5	4.71	137.66	126.63
4	A	502	9NY	C1-N5-C5	4.71	137.65	126.63
4	C	502	9NY	C31-C11-C24	4.67	115.94	108.22
4	A	502	9NY	C31-C11-C24	4.67	115.93	108.22
3	D	201	6PL	O3-C11-C12	4.56	125.75	111.83
3	B	201	6PL	O3-C11-C12	4.56	125.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	9NY	O11-P3-O13	-4.50	91.08	108.94
4	C	502	9NY	O11-P3-O13	-4.50	91.10	108.94
4	A	502	9NY	C40-C44-S1	4.44	118.69	113.40
4	C	502	9NY	C40-C44-S1	4.43	118.68	113.40
4	A	502	9NY	C38-C40-C44	4.38	121.94	112.27
4	C	502	9NY	C38-C40-C44	4.37	121.92	112.27
4	A	502	9NY	C5-N5-C4	-4.30	117.55	127.09
4	C	502	9NY	C5-N5-C4	-4.29	117.57	127.09
4	A	502	9NY	O14-P3-O13	4.24	132.18	112.44
4	C	502	9NY	O14-P3-O13	4.24	132.16	112.44
4	C	502	9NY	C3-C2-C1	3.94	122.56	117.18
4	A	502	9NY	C3-C2-C1	3.94	122.55	117.18
4	A	502	9NY	C31-C11-C25	3.92	115.46	108.77
4	C	502	9NY	C31-C11-C25	3.90	115.42	108.77
4	A	502	9NY	N2-C1-N5	3.84	133.71	127.17
4	C	502	9NY	N2-C1-N5	3.84	133.70	127.17
4	A	502	9NY	C9-O3-C5	-3.74	101.22	109.47
4	C	502	9NY	C9-O3-C5	-3.72	101.25	109.47
4	C	502	9NY	C6-N2-C1	3.72	120.91	111.83
4	A	502	9NY	C6-N2-C1	3.71	120.90	111.83
4	C	502	9NY	O14-P3-O11	-3.64	91.07	107.57
4	A	502	9NY	O14-P3-O11	-3.63	91.11	107.57
3	B	201	6PL	O4P-P-O3P	-3.59	97.30	106.67
3	D	201	6PL	O4P-P-O3P	-3.57	97.35	106.67
4	C	502	9NY	C2-N4-C4	3.41	108.81	103.45
4	A	502	9NY	C2-N4-C4	3.38	108.76	103.45
4	C	502	9NY	C2-C1-N5	3.36	109.48	105.81
4	A	502	9NY	C2-C1-N5	3.34	109.46	105.81
4	C	502	9NY	C1-C2-N4	-3.27	106.84	110.58
4	A	502	9NY	C1-C2-N4	-3.24	106.88	110.58
3	D	201	6PL	C3-O3-C11	3.15	128.64	117.12
3	B	201	6PL	C3-O3-C11	3.15	128.63	117.12
3	B	201	6PL	O3-C3-C2	3.02	117.09	108.40
3	D	201	6PL	O3-C3-C2	3.02	117.09	108.40
4	A	502	9NY	C41-C43-C45	2.82	117.09	112.39
4	C	502	9NY	O10-P2-O4	2.81	120.28	107.57
4	A	502	9NY	O10-P2-O4	2.80	120.24	107.57
4	C	502	9NY	C41-C43-C45	2.79	117.04	112.39
4	A	502	9NY	O16-C44-C40	-2.74	120.82	123.98
4	C	502	9NY	O16-C44-C40	-2.73	120.83	123.98
4	C	502	9NY	N5-C4-N4	-2.72	110.07	113.94
4	A	502	9NY	N5-C4-N4	-2.72	110.08	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	9NY	C2-C3-N3	-2.69	116.64	123.29
4	C	502	9NY	C2-C3-N3	-2.68	116.64	123.29
4	C	502	9NY	C28-C26-C22	-2.53	101.59	114.37
4	A	502	9NY	C28-C26-C22	-2.52	101.62	114.37
4	C	502	9NY	O3-C9-C8	-2.51	99.61	104.92
4	A	502	9NY	O3-C9-C8	-2.49	99.66	104.92
4	C	502	9NY	C43-C41-N6	-2.41	106.87	112.00
4	A	502	9NY	C43-C41-N6	-2.40	106.90	112.00
4	A	502	9NY	P2-O4-C10	2.32	134.62	121.35
4	C	502	9NY	P2-O4-C10	2.31	134.62	121.35
4	C	502	9NY	P1-O2-C8	2.31	129.59	123.43
4	A	502	9NY	P1-O2-C8	2.30	129.57	123.43
4	A	502	9NY	O4-C10-C9	2.16	116.36	108.99
4	C	502	9NY	O4-C10-C9	2.16	116.36	108.99
3	D	201	6PL	O11-C11-C12	-2.15	115.36	123.78
3	B	201	6PL	O11-C11-C12	-2.14	115.40	123.78
3	B	201	6PL	O31-C31-C32	-2.12	115.48	123.78
3	D	201	6PL	O31-C31-C32	-2.11	115.53	123.78
4	C	502	9NY	C2-C3-N1	2.07	122.77	117.51
4	A	502	9NY	C2-C3-N1	2.07	122.76	117.51

There are no chirality outliers.

All (137) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	6PL	O31-C31-O2-C2
3	B	201	6PL	C32-C31-O2-C2
3	D	201	6PL	O31-C31-O2-C2
3	D	201	6PL	C32-C31-O2-C2
4	A	502	9NY	C7-C5-N5-C1
4	A	502	9NY	C7-C5-N5-C4
4	A	502	9NY	C24-C11-C25-C36
4	A	502	9NY	C24-C11-C25-O12
4	A	502	9NY	C31-C11-C25-C36
4	A	502	9NY	O12-C25-C36-N6
4	A	502	9NY	O12-C25-C36-O15
4	A	502	9NY	C35-C38-C40-C44
4	A	502	9NY	C40-C44-S1-C46
4	A	502	9NY	O16-C44-S1-C46
4	A	502	9NY	S1-C46-C47-N7
4	A	502	9NY	C10-O4-P2-O8
4	A	502	9NY	C24-O11-P3-O8

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Mol	Chain	Res	Type	Atoms
4	C	502	9NY	C7-C5-N5-C1
4	C	502	9NY	C7-C5-N5-C4
4	C	502	9NY	C24-C11-C25-C36
4	C	502	9NY	C24-C11-C25-O12
4	C	502	9NY	C31-C11-C25-C36
4	C	502	9NY	O12-C25-C36-N6
4	C	502	9NY	O12-C25-C36-O15
4	C	502	9NY	C35-C38-C40-C44
4	C	502	9NY	C40-C44-S1-C46
4	C	502	9NY	O16-C44-S1-C46
4	C	502	9NY	S1-C46-C47-N7
4	C	502	9NY	C10-O4-P2-O8
4	C	502	9NY	C24-O11-P3-O8
3	D	201	6PL	C34-C35-C36-C37
3	B	201	6PL	C34-C35-C36-C37
4	A	502	9NY	C7-C8-O2-P1
4	C	502	9NY	C7-C8-O2-P1
3	B	201	6PL	C19-C20-C21-C22
3	D	201	6PL	C19-C20-C21-C22
3	B	201	6PL	C21-C22-C23-C24
3	B	201	6PL	C36-C37-C38-C39
3	D	201	6PL	C21-C22-C23-C24
3	D	201	6PL	C36-C37-C38-C39
3	B	201	6PL	C14-C15-C16-C17
3	D	201	6PL	C14-C15-C16-C17
3	B	201	6PL	O2-C2-C3-O3
3	D	201	6PL	O2-C2-C3-O3
4	A	502	9NY	O4-C10-C9-C8
4	C	502	9NY	O4-C10-C9-C8
3	D	202	6PL	C36-C37-C38-C39
3	B	202	6PL	C36-C37-C38-C39
3	B	202	6PL	C41-C42-C43-C44
3	D	202	6PL	C41-C42-C43-C44
3	C	501	6PL	C44-C45-C46-C47
3	D	202	6PL	C35-C36-C37-C38
3	A	501	6PL	C32-C33-C34-C35
3	A	501	6PL	C44-C45-C46-C47
3	B	202	6PL	C35-C36-C37-C38
3	C	501	6PL	C32-C33-C34-C35
3	A	501	6PL	C33-C34-C35-C36
3	C	501	6PL	C40-C41-C42-C43
3	A	501	6PL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
3	C	501	6PL	C33-C34-C35-C36
3	B	201	6PL	C17-C18-C19-C20
3	D	201	6PL	C17-C18-C19-C20
4	A	502	9NY	C13-C12-C14-C16
4	C	502	9NY	C13-C12-C14-C16
4	A	502	9NY	C12-C13-C15-C17
4	C	502	9NY	C12-C13-C15-C17
3	B	201	6PL	C31-C32-C33-C34
3	D	201	6PL	C22-C23-C24-C25
3	B	201	6PL	C22-C23-C24-C25
3	D	201	6PL	C31-C32-C33-C34
4	A	502	9NY	C14-C12-C13-C15
4	C	502	9NY	C14-C12-C13-C15
4	C	502	9NY	C12-C14-C16-C18
4	A	502	9NY	C12-C14-C16-C18
3	B	201	6PL	C18-C19-C20-C21
4	A	502	9NY	O4-C10-C9-O3
4	C	502	9NY	O4-C10-C9-O3
3	D	201	6PL	C18-C19-C20-C21
3	B	201	6PL	C1-C2-C3-O3
3	D	201	6PL	C1-C2-C3-O3
4	A	502	9NY	C9-C10-O4-P2
4	C	502	9NY	C9-C10-O4-P2
3	D	201	6PL	C32-C33-C34-C35
3	B	201	6PL	C32-C33-C34-C35
4	A	502	9NY	P2-O8-P3-O13
4	C	502	9NY	P2-O8-P3-O13
4	A	502	9NY	C11-C25-C36-O15
4	C	502	9NY	C11-C25-C36-O15
3	B	202	6PL	C38-C39-C40-C41
3	D	202	6PL	C38-C39-C40-C41
3	A	501	6PL	C34-C35-C36-C37
3	C	501	6PL	C34-C35-C36-C37
3	B	201	6PL	O3P-C1-C2-C3
3	D	201	6PL	O3P-C1-C2-C3
3	B	202	6PL	C31-C32-C33-C34
3	D	202	6PL	C31-C32-C33-C34
4	A	502	9NY	C11-C25-C36-N6
4	C	502	9NY	C11-C25-C36-N6
3	D	202	6PL	C45-C46-C47-C48
3	B	202	6PL	C45-C46-C47-C48
4	A	502	9NY	C29-C33-C35-C38

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Mol	Chain	Res	Type	Atoms
4	C	502	9NY	C29-C33-C35-C38
3	D	201	6PL	C37-C38-C39-C40
3	B	201	6PL	C37-C38-C39-C40
4	A	502	9NY	C32-C34-C37-C39
4	C	502	9NY	C32-C34-C37-C39
3	B	201	6PL	O3P-C1-C2-O2
3	D	201	6PL	O3P-C1-C2-O2
4	A	502	9NY	C15-C17-C19-C21
4	C	502	9NY	C15-C17-C19-C21
4	A	502	9NY	C30-C11-C25-C36
4	C	502	9NY	C30-C11-C25-C36
4	A	502	9NY	C17-C19-C21-C23
4	C	502	9NY	C17-C19-C21-C23
3	A	501	6PL	C42-C43-C44-C45
3	C	501	6PL	C42-C43-C44-C45
4	A	502	9NY	C34-C37-C39-C42
4	C	502	9NY	C34-C37-C39-C42
3	B	201	6PL	C15-C16-C17-C18
3	D	201	6PL	C15-C16-C17-C18
3	C	501	6PL	C37-C38-C39-C40
3	A	501	6PL	C37-C38-C39-C40
3	B	201	6PL	C1-O3P-P-O1P
3	D	201	6PL	C1-O3P-P-O1P
4	A	502	9NY	C31-C11-C25-O12
4	C	502	9NY	C31-C11-C25-O12
4	A	502	9NY	P2-O8-P3-O14
4	C	502	9NY	P2-O8-P3-O14
4	A	502	9NY	C13-C15-C17-C19
4	C	502	9NY	C13-C15-C17-C19
3	B	201	6PL	C16-C17-C18-C19
3	D	201	6PL	C16-C17-C18-C19
4	A	502	9NY	N6-C41-C43-C45
4	C	502	9NY	N6-C41-C43-C45
4	A	502	9NY	C8-O2-P1-O7
4	C	502	9NY	C8-O2-P1-O7
3	B	201	6PL	C23-C24-C25-C26

There are no ring outliers.

8 monomers are involved in 81 short contacts:

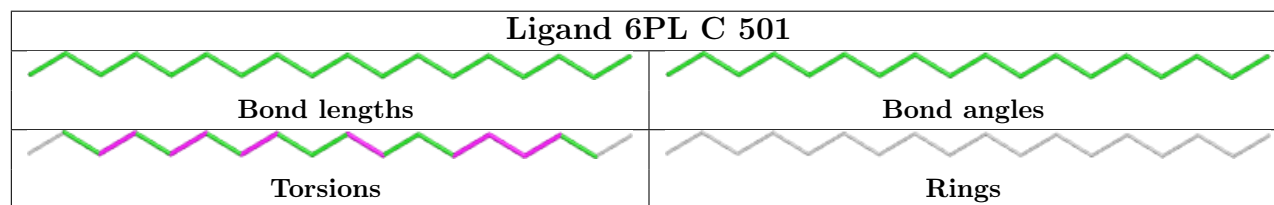
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	6PL	1	0

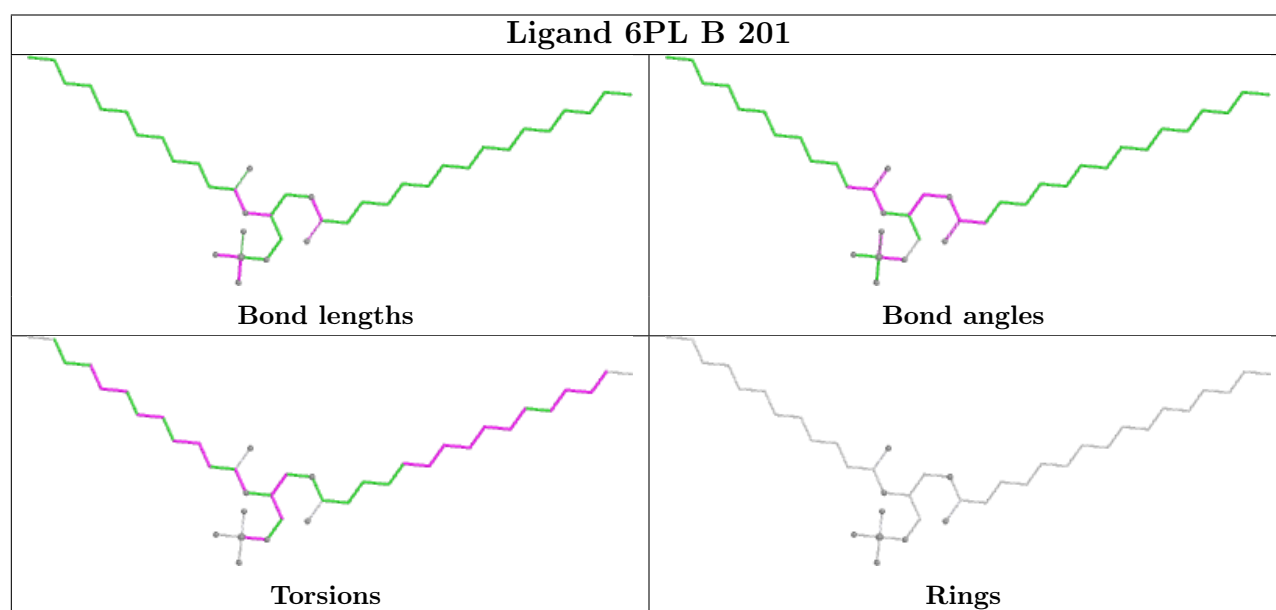
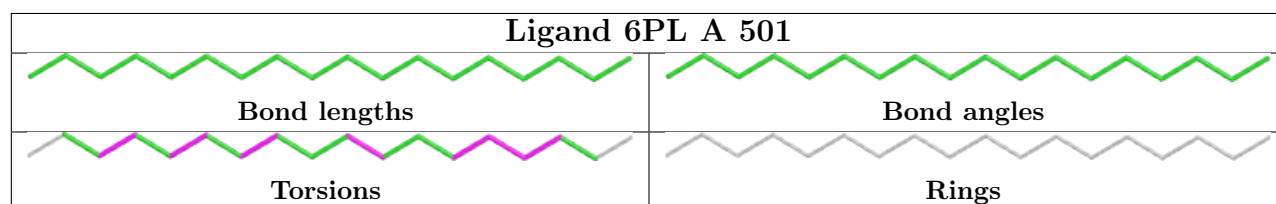
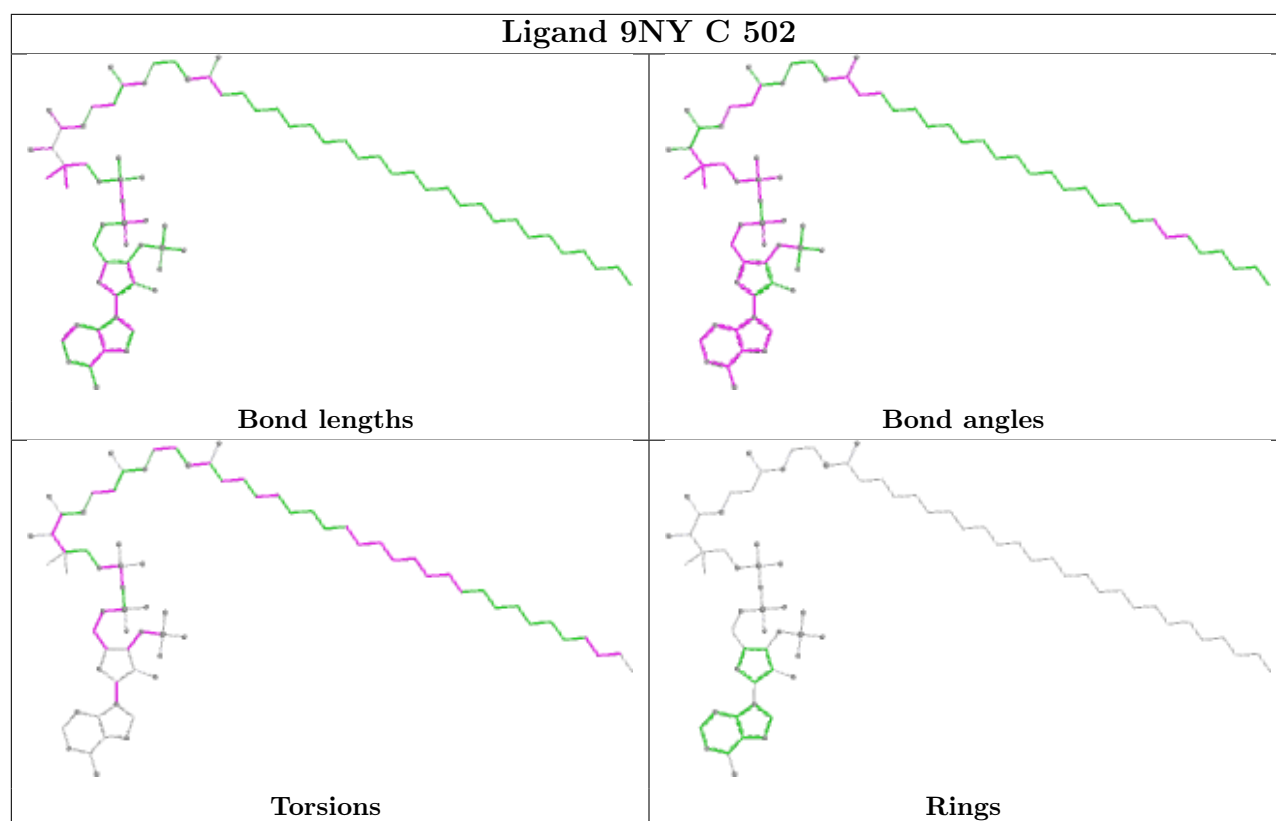
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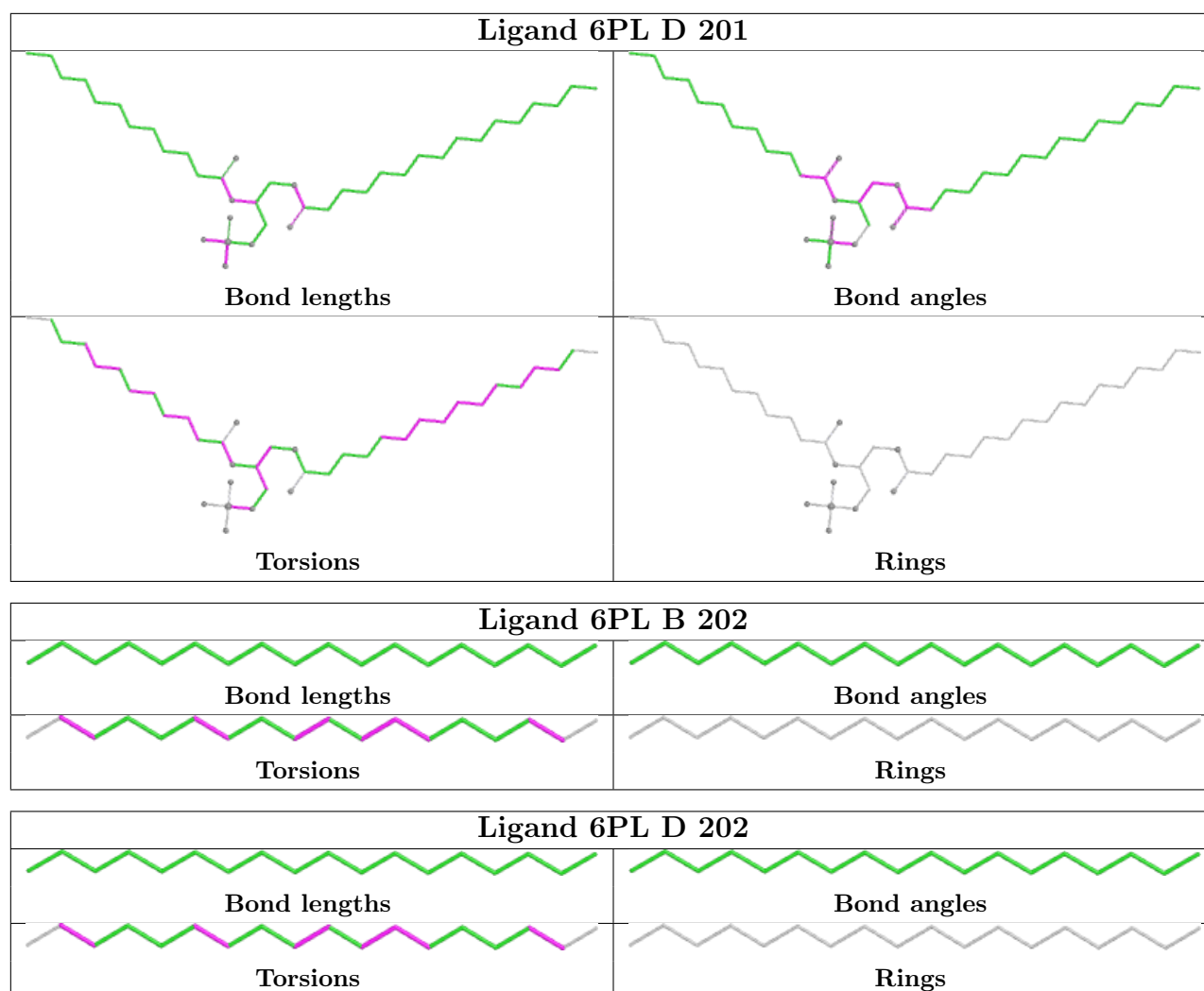
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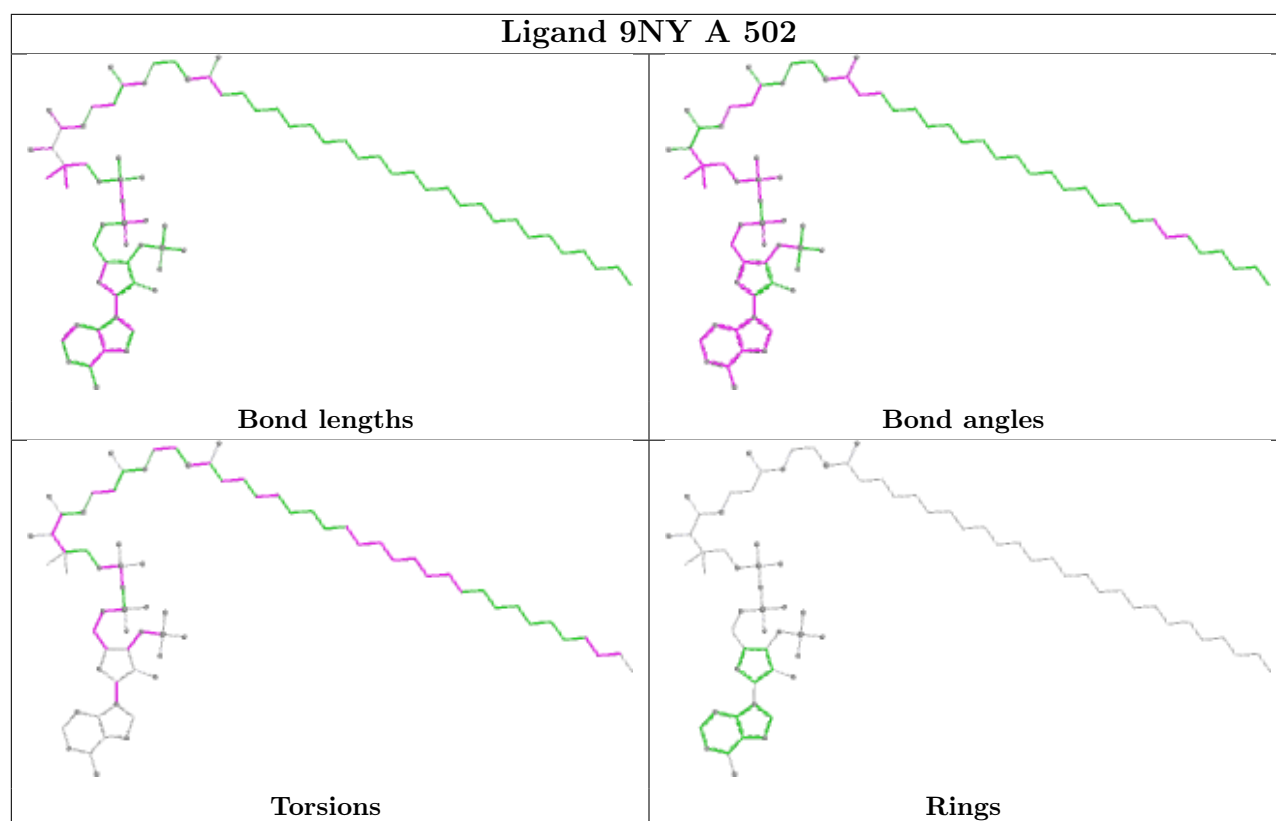
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	9NY	21	0
3	A	501	6PL	2	0
3	B	201	6PL	16	0
3	D	201	6PL	16	0
3	B	202	6PL	2	0
3	D	202	6PL	2	0
4	A	502	9NY	21	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

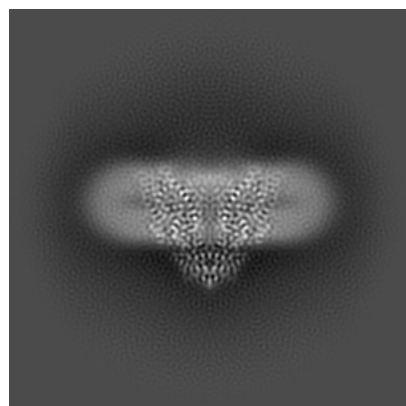
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35862. These allow visual inspection of the internal detail of the map and identification of artifacts.

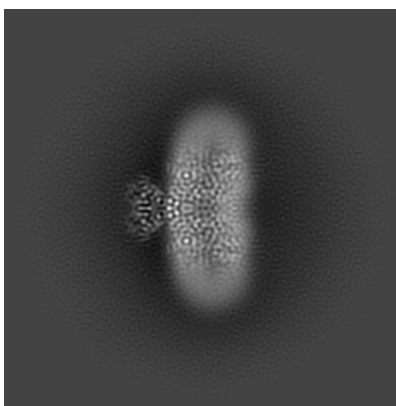
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

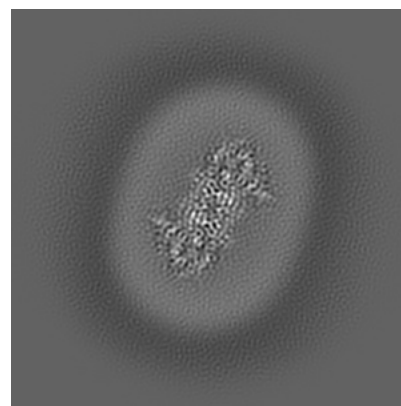
6.1.1 Primary map



X

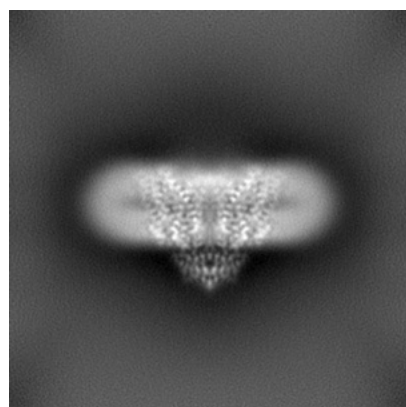


Y

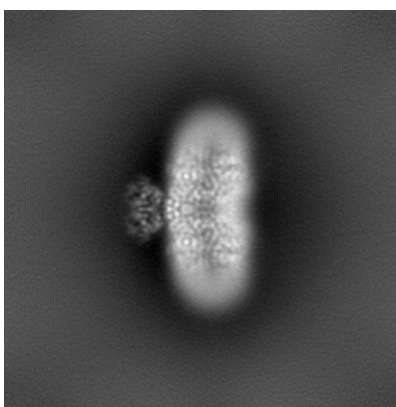


Z

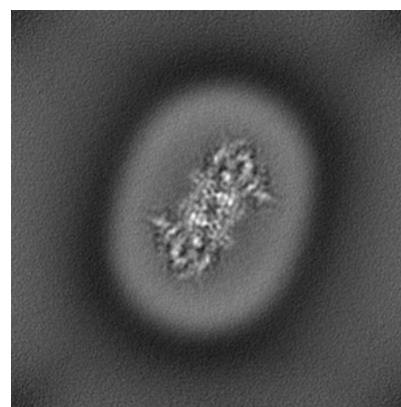
6.1.2 Raw map



X



Y

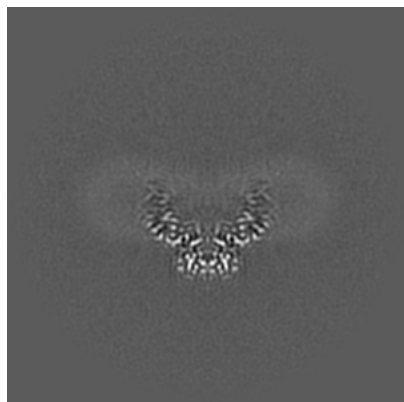


Z

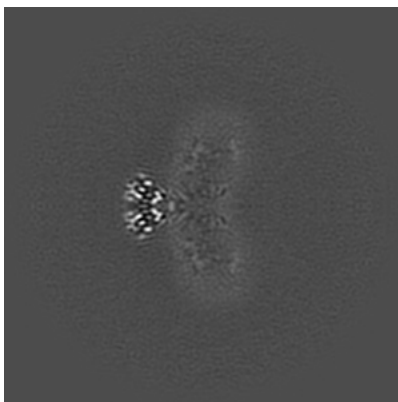
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

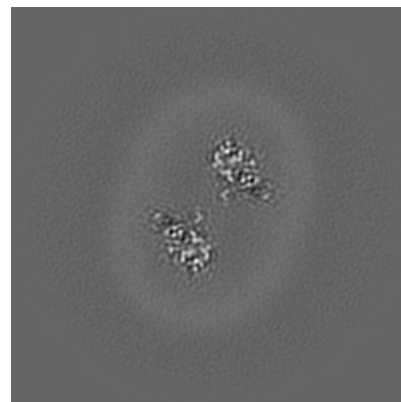
6.2.1 Primary map



X Index: 128

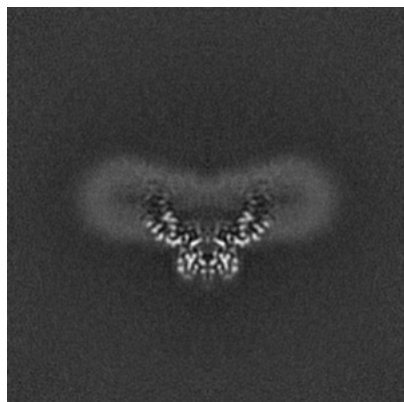


Y Index: 128

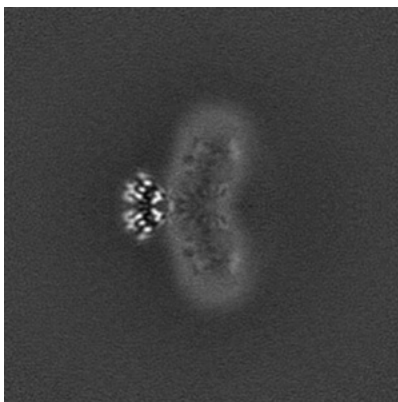


Z Index: 128

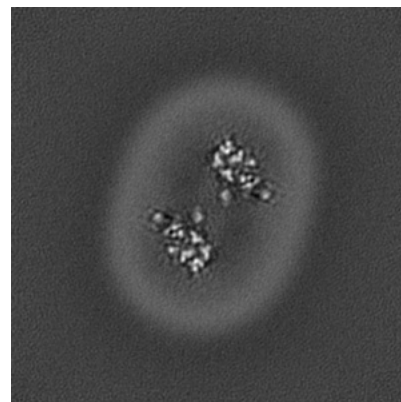
6.2.2 Raw map



X Index: 128



Y Index: 128

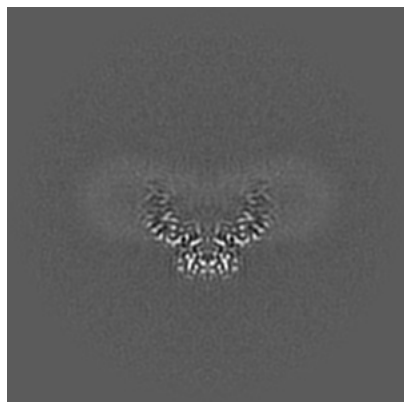


Z Index: 128

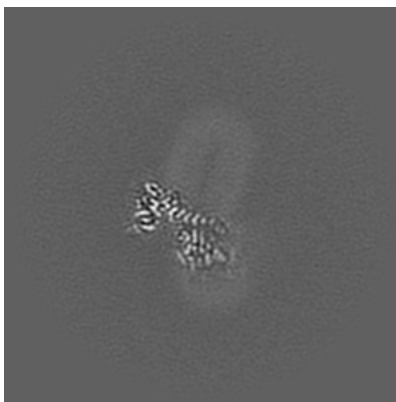
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

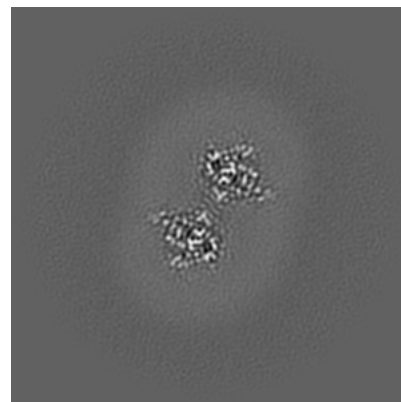
6.3.1 Primary map



X Index: 128

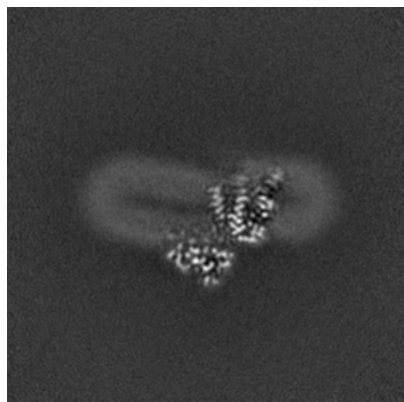


Y Index: 119

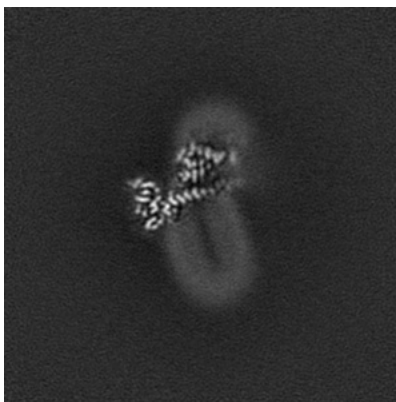


Z Index: 115

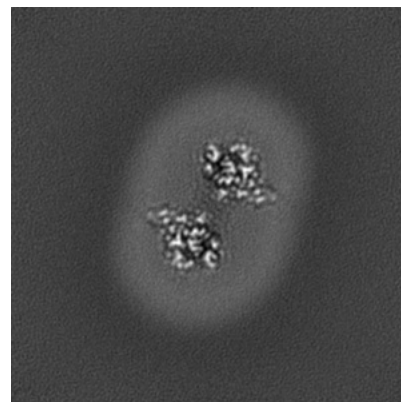
6.3.2 Raw map



X Index: 138



Y Index: 137

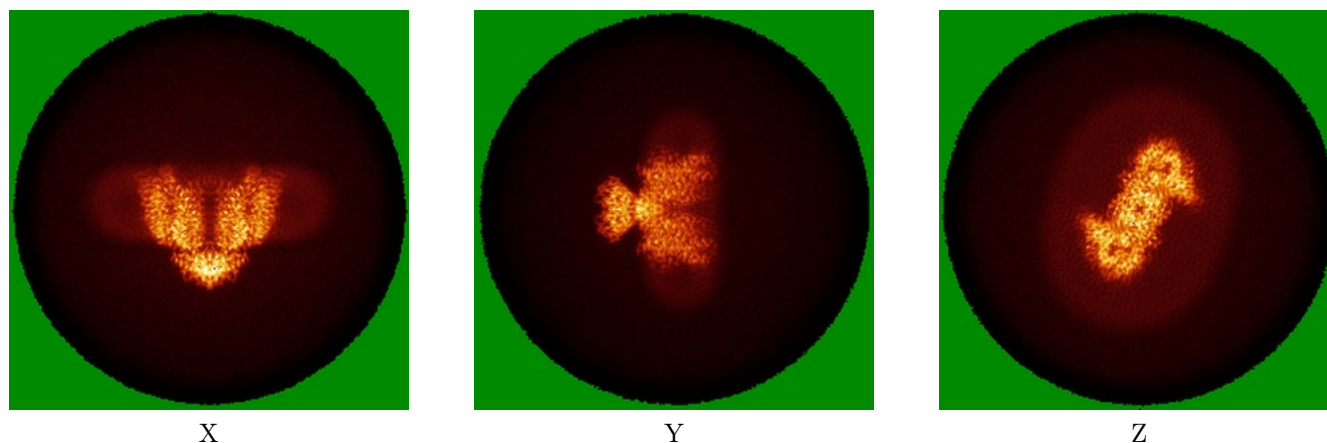


Z Index: 116

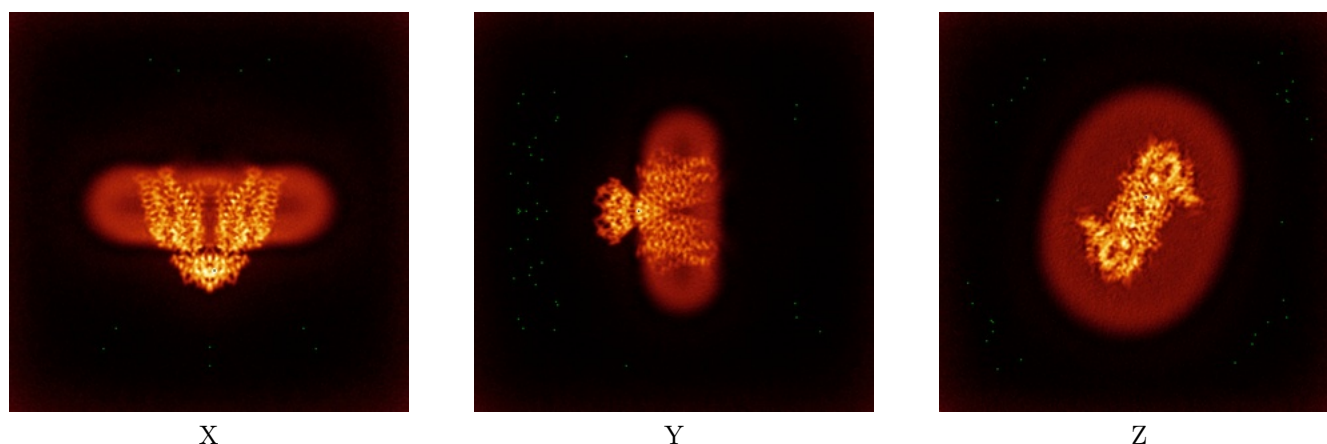
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

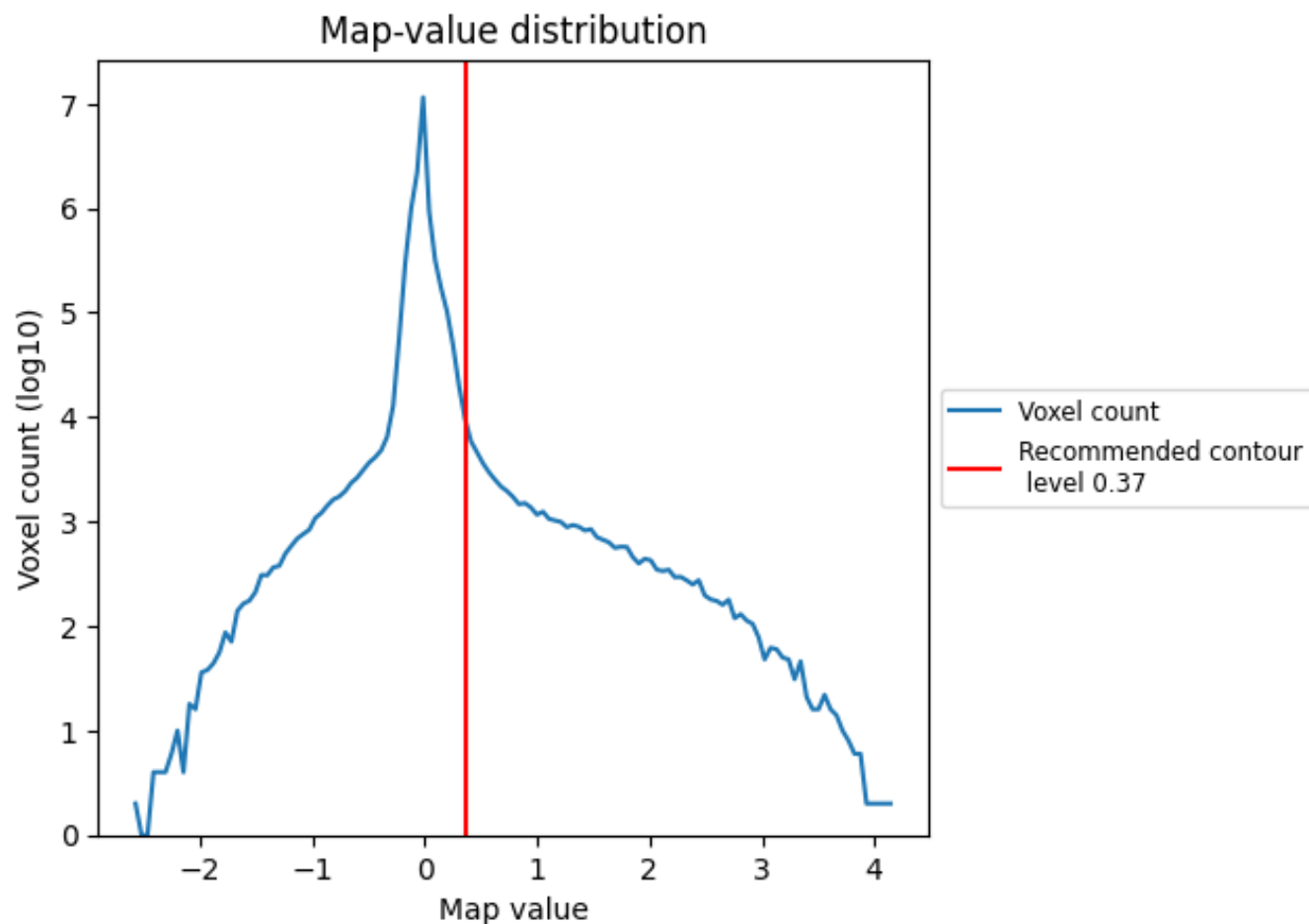
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

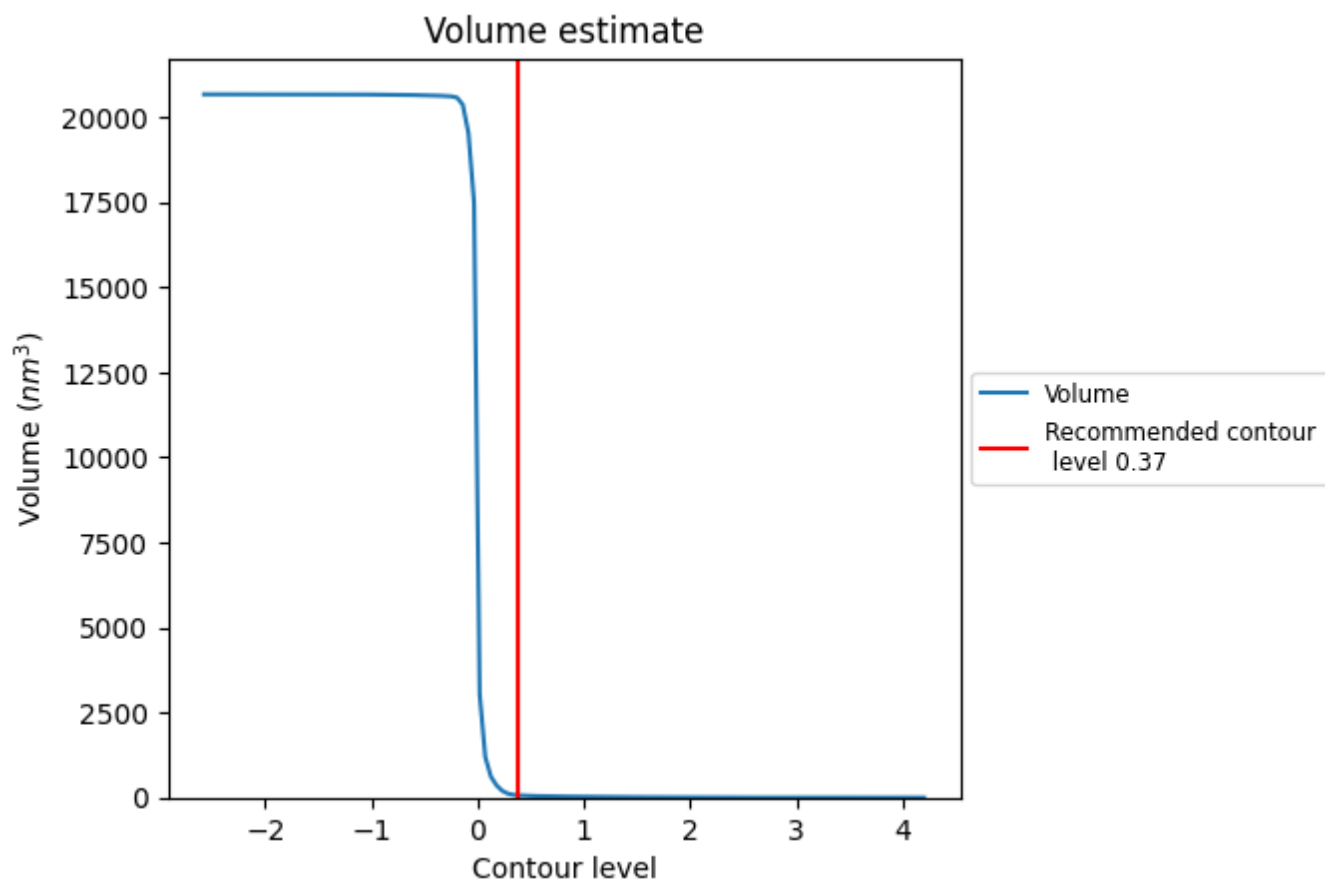
This section contains the results of statistical analysis of the map.

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.

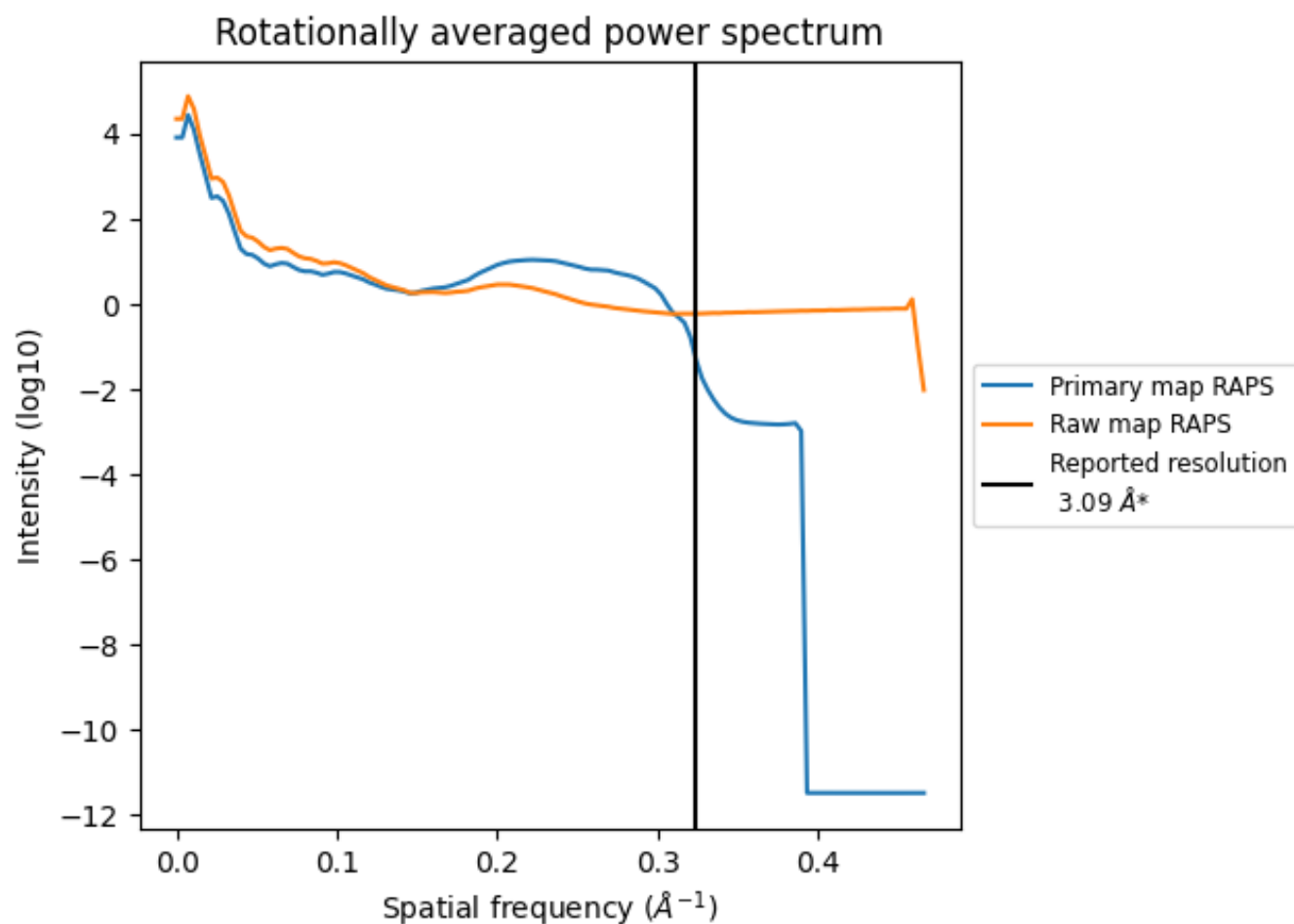
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 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 ⓘ

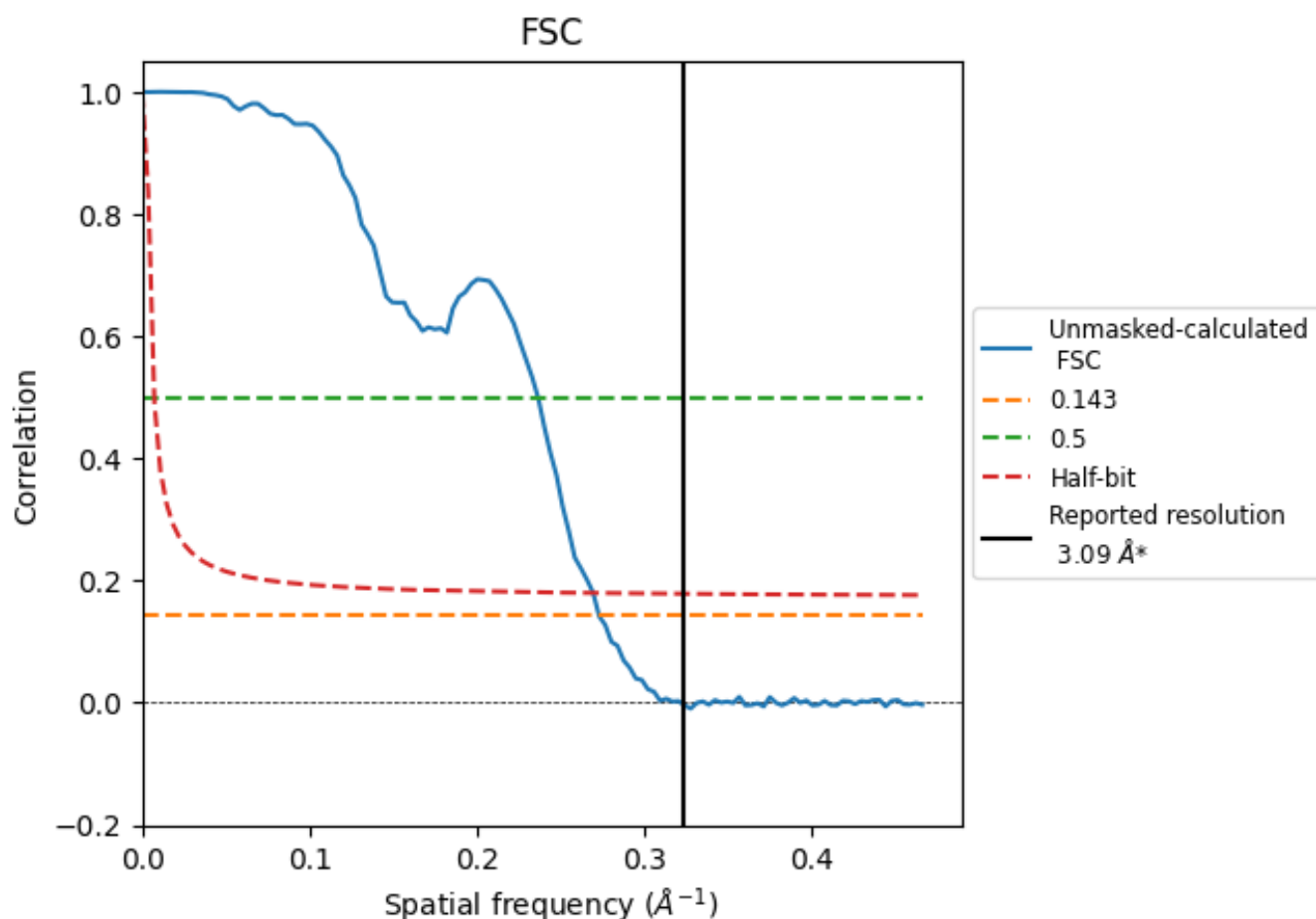


*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.324 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

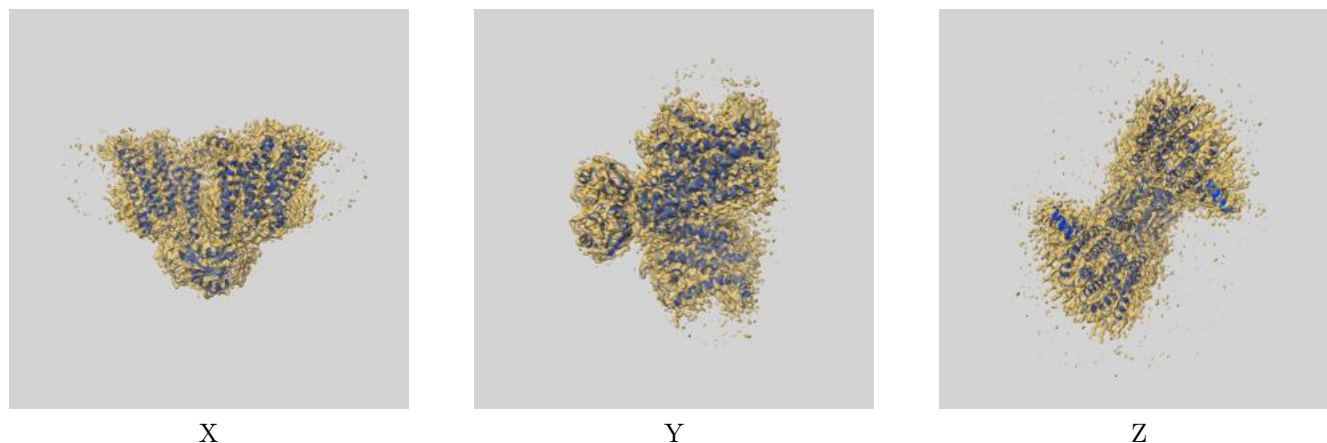
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.22	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

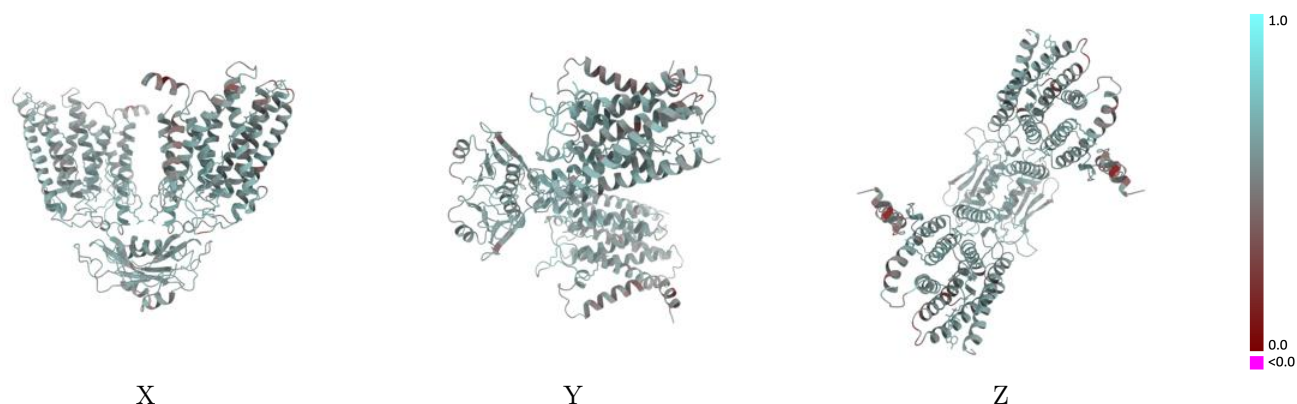
This section contains information regarding the fit between EMDB map EMD-35862 and PDB model 8IZD. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.37 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](#)

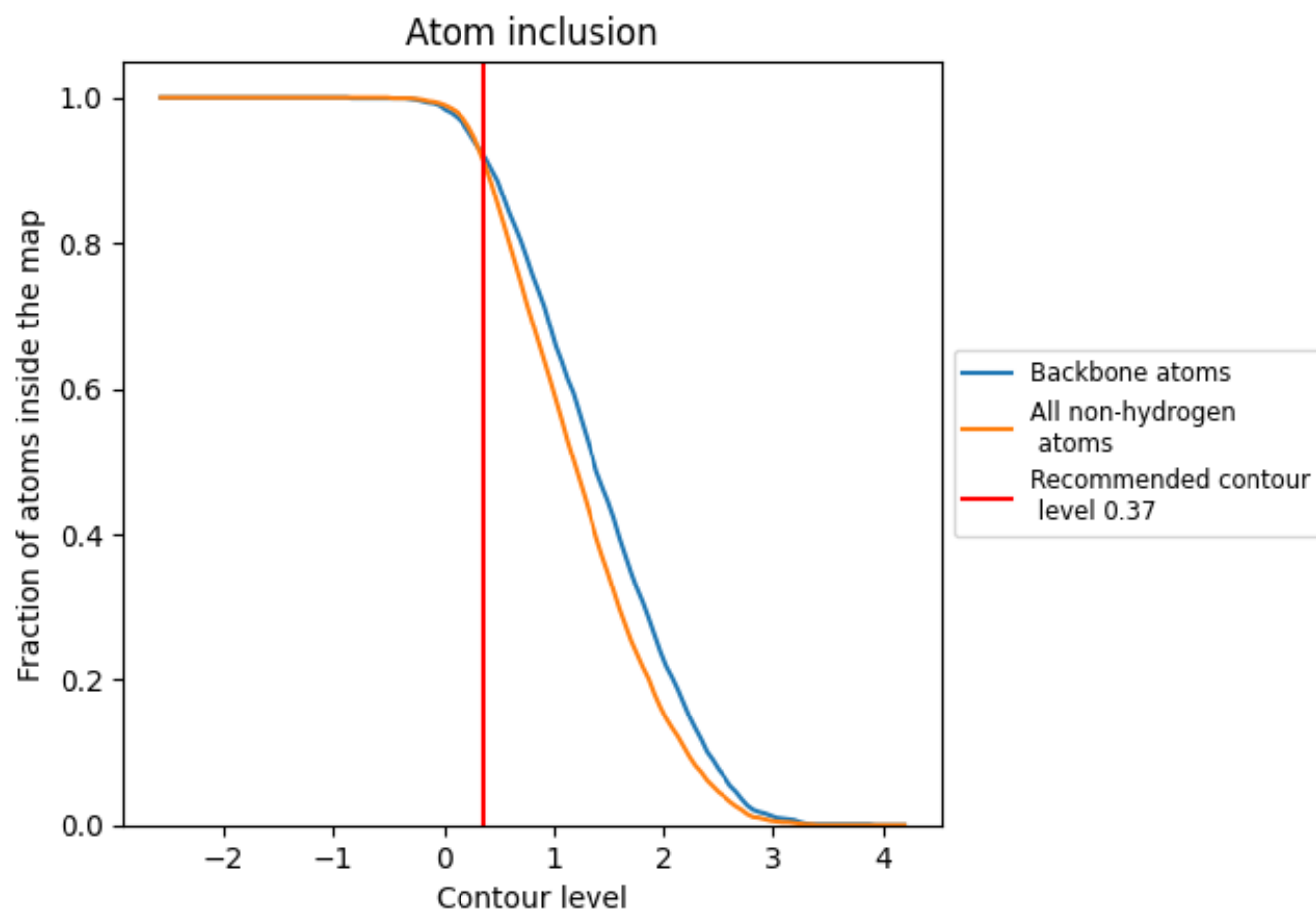


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.5620
A	0.9080	0.5570
B	0.9230	0.5750
C	0.9060	0.5560
D	0.9270	0.5770

