Full wwPDB EM Validation Report ⓘ

Dec 13, 2023 – 06:36 PM JST

PDB ID	:	8IZD
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:

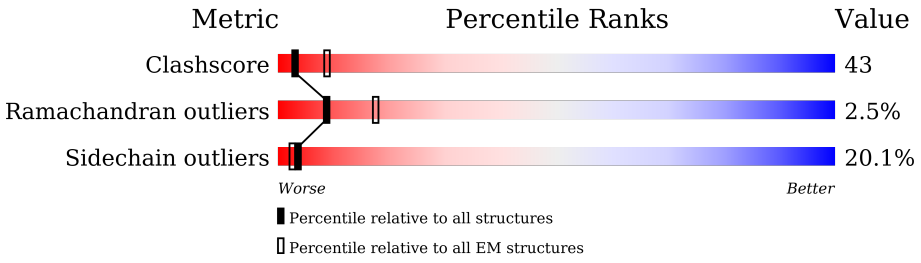
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	20% 25% 22% 7% 26%
1	C	428	21% 24% 23% 6% 26%
2	B	150	55% 23% 8% • 12%
2	D	150	54% 25% 7% • 12%

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	-

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

2 Entry composition (i)

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 2670	C 1809	N 424	O 424	S 13	0	0
1	C	315	Total 2670	C 1809	N 424	O 424	S 13	0	0

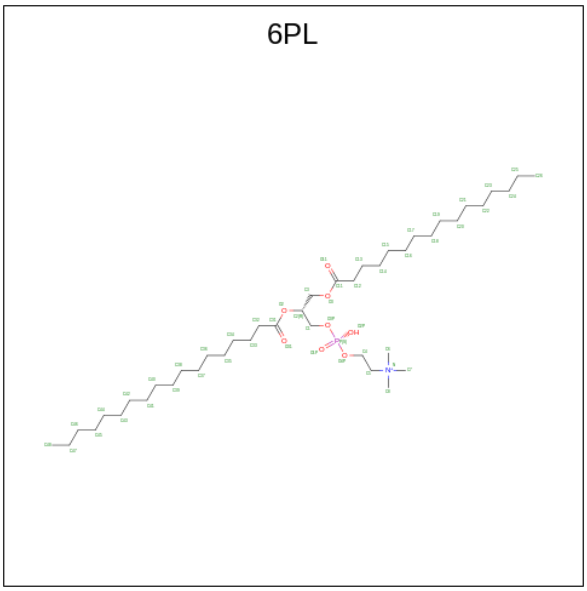
There are 20 discrepancies between the modelled and reference sequences:

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.

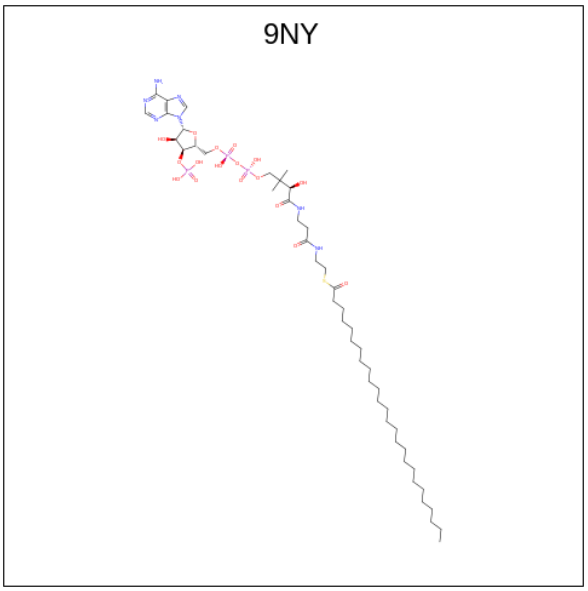
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1082	698	177	201	6		
2	D	132	Total	C	N	O	S	0	0
			1082	698	177	201	6		

- 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 (three-letter code: 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 (three-letter code: 9NY) (formula: $C_{47}H_{86}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



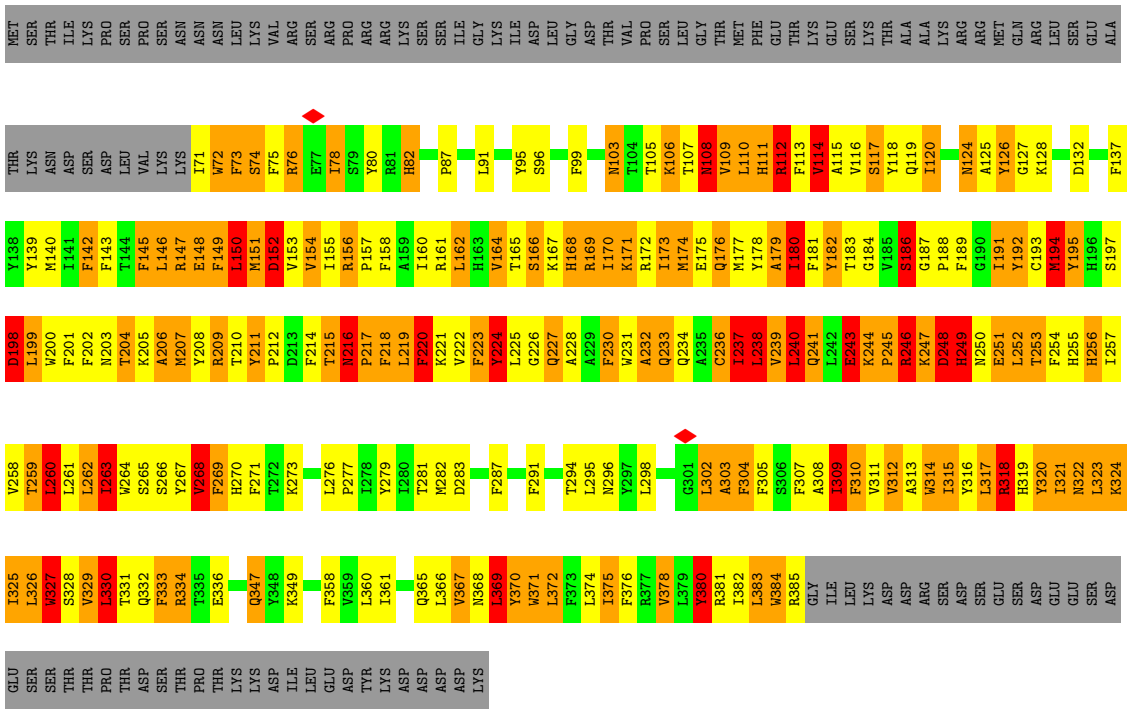
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	N	O	P	S	0
			75	47	7	17	3	1	
4	C	1	Total	C	N	O	P	S	0
			75	47	7	17	3	1	

3 Residue-property plots (i)

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

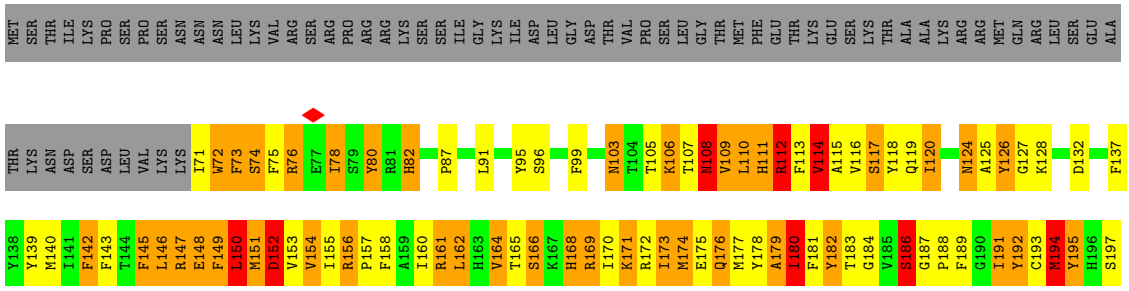
- Molecule 1: Ceramide synthase LAC1

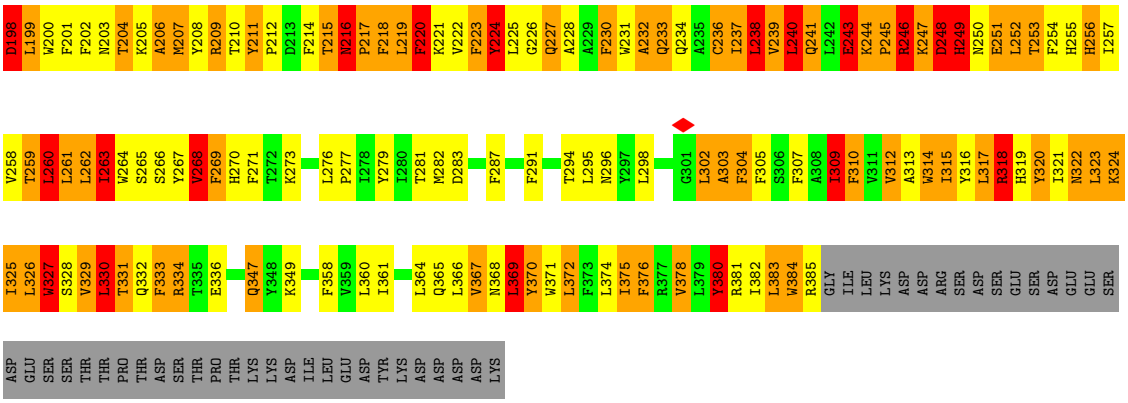
Chain A:



- Molecule 1: Ceramide synthase LAC1

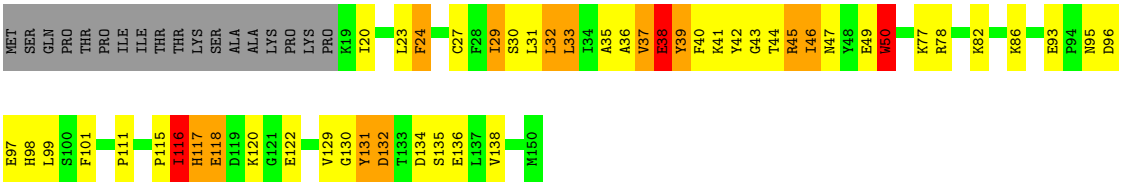
Chain C:





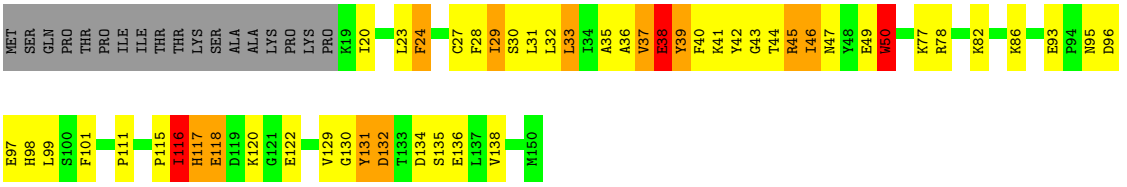
• Molecule 2: Ceramide synthase subunit LIP1

Chain B:



• Molecule 2: Ceramide synthase subunit LIP1

Chain D:



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	274.432, 274.432, 274.432	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 9NY, 6PL

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	2.90	282/2764 (10.2%)	1.67	72/3760 (1.9%)
1	C	2.90	278/2764 (10.1%)	1.67	72/3760 (1.9%)
2	B	1.91	41/1114 (3.7%)	1.12	8/1512 (0.5%)
2	D	1.91	42/1114 (3.8%)	1.12	9/1512 (0.6%)
All	All	2.66	643/7756 (8.3%)	1.53	161/10544 (1.5%)

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 (643) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	TRP	CB-CG	-13.84	1.25	1.50
1	A	327	TRP	CB-CG	-13.79	1.25	1.50
1	C	139	TYR	CE1-CZ	-13.34	1.21	1.38
1	A	139	TYR	CE1-CZ	-13.28	1.21	1.38
1	A	127	GLY	C-O	-12.84	1.03	1.23
1	C	127	GLY	C-O	-12.82	1.03	1.23
2	D	43	GLY	C-O	-12.41	1.03	1.23
2	B	43	GLY	C-O	-12.40	1.03	1.23
1	A	320	TYR	CE1-CZ	-12.28	1.22	1.38
1	C	320	TYR	CE1-CZ	-12.24	1.22	1.38
2	D	50	TRP	CB-CG	-11.85	1.28	1.50
2	B	50	TRP	CB-CG	-11.83	1.28	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	PHE	C-O	-11.50	1.01	1.23
1	C	230	PHE	C-O	-11.46	1.01	1.23
1	A	182	TYR	CB-CG	-11.43	1.34	1.51
1	C	182	TYR	CB-CG	-11.40	1.34	1.51
1	C	126	TYR	CG-CD1	-11.28	1.24	1.39
1	A	126	TYR	CG-CD1	-11.26	1.24	1.39
1	C	126	TYR	CE2-CZ	-11.17	1.24	1.38
1	A	126	TYR	CE2-CZ	-11.12	1.24	1.38
1	A	227	GLN	C-O	-11.09	1.02	1.23
1	C	227	GLN	C-O	-11.09	1.02	1.23
1	A	314	TRP	CG-CD1	-10.99	1.21	1.36
1	C	314	TRP	CG-CD1	-10.95	1.21	1.36
1	C	139	TYR	C-O	-10.72	1.02	1.23
1	A	139	TYR	C-O	-10.70	1.03	1.23
2	B	50	TRP	CG-CD1	-10.65	1.21	1.36
1	C	208	TYR	CE1-CZ	-10.61	1.24	1.38
1	A	208	TYR	CE1-CZ	-10.59	1.24	1.38
2	D	50	TRP	CG-CD1	-10.58	1.22	1.36
1	A	219	LEU	C-O	-10.48	1.03	1.23
1	C	219	LEU	C-O	-10.47	1.03	1.23
1	A	226	GLY	C-O	-10.36	1.07	1.23
1	C	126	TYR	CG-CD2	-10.32	1.25	1.39
1	C	226	GLY	C-O	-10.31	1.07	1.23
1	A	126	TYR	CG-CD2	-10.29	1.25	1.39
1	A	231	TRP	CB-CG	-10.27	1.31	1.50
1	C	231	TRP	CB-CG	-10.26	1.31	1.50
1	C	224	TYR	CB-CG	-10.15	1.36	1.51
1	A	224	TYR	CB-CG	-10.13	1.36	1.51
1	C	118	TYR	CE2-CZ	-10.07	1.25	1.38
1	A	139	TYR	CZ-OH	-10.03	1.20	1.37
1	C	139	TYR	CZ-OH	-10.02	1.20	1.37
1	A	118	TYR	CE2-CZ	-10.02	1.25	1.38
1	C	111	HIS	C-O	-10.01	1.04	1.23
1	A	111	HIS	C-O	-9.98	1.04	1.23
1	C	149	PHE	CG-CD1	-9.91	1.23	1.38
1	A	149	PHE	CG-CD1	-9.88	1.24	1.38
1	C	224	TYR	CZ-OH	-9.82	1.21	1.37
1	A	224	TYR	CZ-OH	-9.80	1.21	1.37
1	A	232	ALA	C-O	-9.80	1.04	1.23
1	C	232	ALA	C-O	-9.79	1.04	1.23
1	A	126	TYR	C-O	-9.77	1.04	1.23
1	C	126	TYR	C-O	-9.77	1.04	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	PHE	C-O	-9.76	1.04	1.23
1	A	142	PHE	C-O	-9.75	1.04	1.23
1	A	192	TYR	CB-CG	-9.69	1.37	1.51
1	C	192	TYR	CB-CG	-9.69	1.37	1.51
1	C	313	ALA	C-O	-9.66	1.04	1.23
1	A	313	ALA	C-O	-9.64	1.05	1.23
1	C	307	PHE	CB-CG	-9.62	1.34	1.51
1	A	139	TYR	CE2-CZ	-9.61	1.26	1.38
1	A	224	TYR	CE1-CZ	-9.59	1.26	1.38
1	A	307	PHE	CB-CG	-9.59	1.35	1.51
1	C	139	TYR	CE2-CZ	-9.59	1.26	1.38
1	C	224	TYR	CE1-CZ	-9.57	1.26	1.38
1	A	268	VAL	C-O	-9.51	1.05	1.23
1	C	268	VAL	C-O	-9.51	1.05	1.23
1	C	145	PHE	C-O	-9.48	1.05	1.23
1	A	145	PHE	C-O	-9.46	1.05	1.23
1	A	327	TRP	CG-CD1	-9.41	1.23	1.36
1	C	327	TRP	CG-CD1	-9.38	1.23	1.36
1	A	118	TYR	CE1-CZ	-9.38	1.26	1.38
1	A	178	TYR	CE1-CZ	-9.34	1.26	1.38
1	C	178	TYR	CE1-CZ	-9.33	1.26	1.38
1	C	118	TYR	CE1-CZ	-9.31	1.26	1.38
1	A	271	PHE	C-O	-9.30	1.05	1.23
1	C	271	PHE	C-O	-9.29	1.05	1.23
1	C	333	PHE	CG-CD1	-9.28	1.24	1.38
1	C	319	HIS	CA-C	-9.26	1.28	1.52
1	A	319	HIS	CA-C	-9.25	1.28	1.52
1	A	333	PHE	CG-CD1	-9.24	1.24	1.38
1	C	264	TRP	CB-CG	-9.22	1.33	1.50
1	A	264	TRP	CB-CG	-9.18	1.33	1.50
1	A	126	TYR	CB-CG	-9.18	1.37	1.51
1	C	126	TYR	CB-CG	-9.18	1.37	1.51
1	A	142	PHE	CG-CD2	-9.04	1.25	1.38
1	C	142	PHE	CG-CD2	-9.00	1.25	1.38
1	C	228	ALA	C-O	-8.87	1.06	1.23
1	A	228	ALA	C-O	-8.87	1.06	1.23
1	A	225	LEU	C-O	-8.64	1.06	1.23
1	A	320	TYR	CB-CG	-8.61	1.38	1.51
1	C	225	LEU	C-O	-8.59	1.07	1.23
1	C	320	TYR	CB-CG	-8.57	1.38	1.51
1	A	259	THR	CB-CG2	-8.55	1.24	1.52
1	C	224	TYR	CE2-CZ	-8.55	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TYR	CE2-CZ	-8.55	1.27	1.38
1	C	259	THR	CB-CG2	-8.53	1.24	1.52
1	C	208	TYR	CG-CD2	-8.46	1.28	1.39
1	A	371	TRP	CB-CG	-8.45	1.35	1.50
1	A	208	TYR	CG-CD2	-8.45	1.28	1.39
1	C	371	TRP	CB-CG	-8.44	1.35	1.50
1	A	149	PHE	CG-CD2	-8.40	1.26	1.38
1	A	231	TRP	CD2-CE2	-8.38	1.31	1.41
1	C	149	PHE	CG-CD2	-8.35	1.26	1.38
1	C	231	TRP	CD2-CE2	-8.34	1.31	1.41
1	A	371	TRP	CG-CD1	-8.34	1.25	1.36
1	C	118	TYR	CZ-OH	-8.33	1.23	1.37
1	C	371	TRP	CG-CD1	-8.32	1.25	1.36
1	A	118	TYR	CZ-OH	-8.30	1.23	1.37
1	C	314	TRP	C-O	-8.28	1.07	1.23
2	D	40	PHE	C-O	-8.28	1.07	1.23
1	A	208	TYR	CB-CG	-8.27	1.39	1.51
1	C	208	TYR	CB-CG	-8.26	1.39	1.51
1	A	314	TRP	C-O	-8.26	1.07	1.23
1	A	216	ASN	C-O	-8.25	1.07	1.23
2	B	44	THR	C-O	-8.25	1.07	1.23
2	B	40	PHE	C-O	-8.25	1.07	1.23
1	C	216	ASN	C-O	-8.25	1.07	1.23
2	D	44	THR	C-O	-8.24	1.07	1.23
1	A	208	TYR	CZ-OH	-8.21	1.23	1.37
1	C	208	TYR	CZ-OH	-8.20	1.24	1.37
1	C	316	TYR	CE1-CZ	-8.20	1.27	1.38
1	A	316	TYR	CE1-CZ	-8.18	1.27	1.38
1	C	220	PHE	C-O	-8.17	1.07	1.23
1	A	378	VAL	C-O	-8.17	1.07	1.23
1	C	126	TYR	CE1-CZ	-8.17	1.27	1.38
1	A	220	PHE	C-O	-8.16	1.07	1.23
1	A	126	TYR	CE1-CZ	-8.16	1.27	1.38
1	C	378	VAL	C-O	-8.15	1.07	1.23
1	A	145	PHE	CA-C	-8.09	1.31	1.52
1	A	232	ALA	CA-C	-8.08	1.31	1.52
1	C	232	ALA	CA-C	-8.08	1.31	1.52
1	C	145	PHE	CA-C	-8.08	1.31	1.52
1	C	231	TRP	C-O	-8.08	1.08	1.23
1	A	231	TRP	C-O	-8.08	1.08	1.23
1	C	215	THR	CB-CG2	-8.07	1.25	1.52
1	A	215	THR	CB-CG2	-8.06	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	TRP	CD2-CE2	-8.01	1.31	1.41
1	C	118	TYR	CB-CG	-8.00	1.39	1.51
1	A	118	TYR	CB-CG	-8.00	1.39	1.51
1	A	314	TRP	CB-CG	-8.00	1.35	1.50
1	C	264	TRP	CD2-CE2	-7.99	1.31	1.41
1	C	371	TRP	CD2-CE2	-7.99	1.31	1.41
1	A	119	GLN	C-O	-7.98	1.08	1.23
1	C	314	TRP	CB-CG	-7.98	1.35	1.50
1	C	119	GLN	C-O	-7.95	1.08	1.23
1	A	371	TRP	CD2-CE2	-7.92	1.31	1.41
1	A	126	TYR	CZ-OH	-7.88	1.24	1.37
1	C	126	TYR	CZ-OH	-7.86	1.24	1.37
1	A	319	HIS	C-O	-7.83	1.08	1.23
1	C	319	HIS	C-O	-7.83	1.08	1.23
1	A	264	TRP	CG-CD1	-7.82	1.25	1.36
1	C	170	ILE	C-O	-7.81	1.08	1.23
1	A	170	ILE	C-O	-7.81	1.08	1.23
1	C	264	TRP	CG-CD1	-7.77	1.25	1.36
1	C	192	TYR	CE1-CZ	-7.75	1.28	1.38
1	A	265	SER	CB-OG	-7.74	1.32	1.42
1	C	320	TYR	CG-CD1	-7.74	1.29	1.39
1	C	110	LEU	C-O	-7.74	1.08	1.23
1	C	265	SER	CB-OG	-7.72	1.32	1.42
1	A	110	LEU	C-O	-7.72	1.08	1.23
1	A	320	TYR	CG-CD1	-7.71	1.29	1.39
1	C	307	PHE	CG-CD1	-7.71	1.27	1.38
1	A	192	TYR	CE1-CZ	-7.70	1.28	1.38
1	C	72	TRP	CB-CG	-7.69	1.36	1.50
1	A	307	PHE	CG-CD1	-7.67	1.27	1.38
1	C	368	ASN	C-O	-7.67	1.08	1.23
1	A	72	TRP	CB-CG	-7.65	1.36	1.50
1	A	368	ASN	C-O	-7.64	1.08	1.23
1	A	334	ARG	C-O	-7.59	1.08	1.23
1	C	334	ARG	C-O	-7.59	1.08	1.23
2	D	50	TRP	CD2-CE2	-7.58	1.32	1.41
1	A	371	TRP	C-O	-7.56	1.08	1.23
1	C	371	TRP	C-O	-7.56	1.08	1.23
1	A	329	VAL	C-O	-7.51	1.09	1.23
1	C	182	TYR	CG-CD2	-7.51	1.29	1.39
2	B	50	TRP	CD2-CE2	-7.51	1.32	1.41
1	C	329	VAL	C-O	-7.50	1.09	1.23
1	C	264	TRP	C-O	-7.48	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ILE	C-O	-7.47	1.09	1.23
1	A	220	PHE	CB-CG	-7.47	1.38	1.51
1	C	180	ILE	C-O	-7.47	1.09	1.23
1	A	143	PHE	CG-CD2	-7.47	1.27	1.38
1	C	220	PHE	CB-CG	-7.47	1.38	1.51
1	A	264	TRP	C-O	-7.46	1.09	1.23
1	C	220	PHE	CA-CB	-7.46	1.37	1.53
1	C	147	ARG	C-O	-7.46	1.09	1.23
1	A	182	TYR	CG-CD2	-7.46	1.29	1.39
1	A	333	PHE	CB-CG	-7.45	1.38	1.51
1	A	147	ARG	C-O	-7.44	1.09	1.23
1	A	220	PHE	CA-CB	-7.44	1.37	1.53
1	C	333	PHE	CB-CG	-7.44	1.38	1.51
1	C	143	PHE	CG-CD2	-7.44	1.27	1.38
1	C	316	TYR	CB-CG	-7.43	1.40	1.51
1	A	224	TYR	CG-CD2	-7.42	1.29	1.39
1	A	118	TYR	C-O	-7.41	1.09	1.23
1	A	316	TYR	CB-CG	-7.39	1.40	1.51
1	C	118	TYR	C-O	-7.39	1.09	1.23
1	C	224	TYR	CG-CD2	-7.39	1.29	1.39
1	A	118	TYR	CG-CD1	-7.37	1.29	1.39
1	A	192	TYR	CG-CD2	-7.37	1.29	1.39
2	B	98	HIS	C-O	-7.37	1.09	1.23
2	D	98	HIS	C-O	-7.37	1.09	1.23
1	C	152	ASP	CB-CG	-7.33	1.36	1.51
1	C	118	TYR	CG-CD1	-7.32	1.29	1.39
1	C	208	TYR	CE2-CZ	-7.31	1.29	1.38
1	A	152	ASP	CB-CG	-7.31	1.36	1.51
1	C	192	TYR	CG-CD2	-7.30	1.29	1.39
1	A	203	ASN	C-O	-7.30	1.09	1.23
1	C	143	PHE	C-O	-7.30	1.09	1.23
1	A	208	TYR	CE2-CZ	-7.30	1.29	1.38
1	C	314	TRP	CD2-CE2	-7.29	1.32	1.41
1	A	269	PHE	C-O	-7.29	1.09	1.23
1	A	178	TYR	CB-CG	-7.27	1.40	1.51
1	A	314	TRP	CD2-CE2	-7.27	1.32	1.41
1	A	143	PHE	C-O	-7.26	1.09	1.23
1	C	178	TYR	CB-CG	-7.26	1.40	1.51
1	C	333	PHE	CA-CB	-7.24	1.38	1.53
1	C	269	PHE	C-O	-7.24	1.09	1.23
1	A	333	PHE	CA-CB	-7.22	1.38	1.53
1	C	203	ASN	C-O	-7.17	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	PHE	CB-CG	-7.17	1.39	1.51
1	A	149	PHE	CB-CG	-7.17	1.39	1.51
1	A	188	PRO	CA-C	-7.16	1.38	1.52
1	C	188	PRO	CA-C	-7.16	1.38	1.52
1	A	206	ALA	C-O	-7.15	1.09	1.23
1	C	206	ALA	C-O	-7.14	1.09	1.23
2	B	30	SER	C-O	-7.13	1.09	1.23
2	D	30	SER	C-O	-7.13	1.09	1.23
1	C	139	TYR	CG-CD2	-7.08	1.29	1.39
1	C	113	PHE	CG-CD2	-7.06	1.28	1.38
2	D	43	GLY	CA-C	-7.04	1.40	1.51
2	B	43	GLY	CA-C	-7.04	1.40	1.51
1	A	269	PHE	CG-CD1	-7.03	1.28	1.38
1	A	192	TYR	C-O	-7.03	1.09	1.23
1	A	139	TYR	CG-CD2	-7.03	1.30	1.39
1	C	192	TYR	C-O	-7.03	1.09	1.23
1	C	269	PHE	CG-CD1	-7.03	1.28	1.38
2	B	39	TYR	CB-CG	-7.01	1.41	1.51
2	D	39	TYR	CB-CG	-7.01	1.41	1.51
1	A	113	PHE	CG-CD2	-7.00	1.28	1.38
1	A	125	ALA	C-O	-7.00	1.10	1.23
1	C	125	ALA	C-O	-7.00	1.10	1.23
1	A	113	PHE	C-O	-7.00	1.10	1.23
2	D	44	THR	CB-CG2	-6.98	1.29	1.52
1	C	230	PHE	CG-CD2	-6.98	1.28	1.38
1	A	230	PHE	CG-CD2	-6.98	1.28	1.38
1	C	113	PHE	C-O	-6.98	1.10	1.23
1	A	200	TRP	CZ3-CH2	-6.97	1.28	1.40
1	C	264	TRP	CE3-CZ3	-6.97	1.26	1.38
1	A	264	TRP	CE3-CZ3	-6.97	1.26	1.38
2	B	44	THR	CB-CG2	-6.96	1.29	1.52
1	A	227	GLN	CA-CB	-6.95	1.38	1.53
1	C	227	GLN	CA-CB	-6.95	1.38	1.53
2	D	42	TYR	CE1-CZ	-6.93	1.29	1.38
1	C	316	TYR	C-O	-6.93	1.10	1.23
1	A	316	TYR	C-O	-6.92	1.10	1.23
2	B	42	TYR	CE1-CZ	-6.91	1.29	1.38
1	C	231	TRP	CG-CD1	-6.89	1.27	1.36
1	A	195	TYR	CE2-CZ	-6.89	1.29	1.38
1	A	231	TRP	CG-CD1	-6.89	1.27	1.36
1	C	200	TRP	CZ3-CH2	-6.88	1.29	1.40
1	C	265	SER	CA-CB	-6.87	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	TRP	CD2-CE2	-6.87	1.33	1.41
1	A	265	SER	CA-CB	-6.86	1.42	1.52
1	C	195	TYR	CE2-CZ	-6.84	1.29	1.38
2	B	39	TYR	C-O	-6.84	1.10	1.23
1	A	327	TRP	CD2-CE2	-6.84	1.33	1.41
2	D	39	TYR	C-O	-6.83	1.10	1.23
2	B	134	ASP	CB-CG	-6.82	1.37	1.51
2	D	134	ASP	CB-CG	-6.81	1.37	1.51
1	C	322	ASN	C-O	-6.81	1.10	1.23
1	A	322	ASN	C-O	-6.80	1.10	1.23
1	C	265	SER	C-O	-6.80	1.10	1.23
1	A	200	TRP	CG-CD1	-6.79	1.27	1.36
1	C	320	TYR	CG-CD2	-6.79	1.30	1.39
1	C	310	PHE	CG-CD1	-6.79	1.28	1.38
1	C	200	TRP	CG-CD1	-6.78	1.27	1.36
1	A	320	TYR	CG-CD2	-6.77	1.30	1.39
1	A	265	SER	C-O	-6.77	1.10	1.23
1	C	195	TYR	CG-CD2	-6.77	1.30	1.39
1	A	234	GLN	CA-CB	-6.76	1.39	1.53
2	B	97	GLU	CD-OE1	-6.76	1.18	1.25
1	C	236	CYS	CB-SG	-6.76	1.70	1.82
1	A	195	TYR	CG-CD2	-6.75	1.30	1.39
1	A	368	ASN	CA-C	-6.75	1.35	1.52
1	C	368	ASN	CA-C	-6.75	1.35	1.52
2	D	97	GLU	CD-OE1	-6.75	1.18	1.25
1	A	236	CYS	CB-SG	-6.75	1.70	1.82
1	A	320	TYR	C-O	-6.75	1.10	1.23
1	A	128	LYS	C-O	-6.75	1.10	1.23
1	C	218	PHE	CA-C	-6.75	1.35	1.52
1	C	234	GLN	CA-CB	-6.75	1.39	1.53
1	C	128	LYS	C-O	-6.74	1.10	1.23
1	A	218	PHE	CA-C	-6.74	1.35	1.52
1	A	310	PHE	CG-CD1	-6.74	1.28	1.38
1	C	320	TYR	C-O	-6.73	1.10	1.23
1	A	231	TRP	CZ3-CH2	-6.64	1.29	1.40
1	A	320	TYR	CA-C	-6.63	1.35	1.52
2	B	45	ARG	CA-C	-6.62	1.35	1.52
1	C	320	TYR	CA-C	-6.60	1.35	1.52
1	C	231	TRP	CZ3-CH2	-6.60	1.29	1.40
1	C	208	TYR	C-O	-6.59	1.10	1.23
2	D	45	ARG	CA-C	-6.59	1.35	1.52
1	A	265	SER	CA-C	-6.59	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	TYR	C-O	-6.58	1.10	1.23
1	A	150	LEU	CA-C	-6.57	1.35	1.52
1	C	150	LEU	CA-C	-6.57	1.35	1.52
1	C	265	SER	CA-C	-6.57	1.35	1.52
1	A	200	TRP	CD2-CE2	-6.55	1.33	1.41
2	B	42	TYR	CB-CG	-6.55	1.41	1.51
1	A	146	LEU	C-O	-6.55	1.10	1.23
1	C	200	TRP	CD2-CE2	-6.55	1.33	1.41
2	D	42	TYR	CB-CG	-6.53	1.41	1.51
1	C	145	PHE	CG-CD2	-6.53	1.28	1.38
1	C	147	ARG	CA-CB	-6.53	1.39	1.53
1	C	146	LEU	C-O	-6.53	1.10	1.23
1	A	261	LEU	C-O	-6.51	1.10	1.23
1	A	147	ARG	CA-CB	-6.51	1.39	1.53
1	C	261	LEU	C-O	-6.50	1.10	1.23
2	D	46	ILE	C-O	-6.50	1.11	1.23
2	B	46	ILE	C-O	-6.49	1.11	1.23
1	C	195	TYR	CE1-CZ	-6.49	1.30	1.38
1	A	145	PHE	CG-CD2	-6.48	1.29	1.38
1	A	195	TYR	CE1-CZ	-6.47	1.30	1.38
1	A	370	TYR	CB-CG	-6.46	1.42	1.51
1	A	332	GLN	C-O	-6.44	1.11	1.23
1	C	218	PHE	CG-CD1	-6.44	1.29	1.38
1	C	370	TYR	CB-CG	-6.44	1.42	1.51
1	A	218	PHE	CG-CD1	-6.44	1.29	1.38
1	C	332	GLN	C-O	-6.44	1.11	1.23
1	C	367	VAL	C-O	-6.42	1.11	1.23
1	C	182	TYR	CG-CD1	-6.40	1.30	1.39
1	A	367	VAL	C-O	-6.40	1.11	1.23
1	A	327	TRP	CE3-CZ3	-6.40	1.27	1.38
1	A	113	PHE	CB-CG	-6.39	1.40	1.51
1	A	146	LEU	CA-C	-6.38	1.36	1.52
1	A	182	TYR	CG-CD1	-6.38	1.30	1.39
1	C	146	LEU	CA-C	-6.37	1.36	1.52
1	A	200	TRP	CE2-CZ2	-6.37	1.28	1.39
1	C	178	TYR	CG-CD2	-6.37	1.30	1.39
1	A	178	TYR	CG-CD2	-6.37	1.30	1.39
1	C	113	PHE	CB-CG	-6.36	1.40	1.51
1	C	200	TRP	CE2-CZ2	-6.36	1.28	1.39
1	C	327	TRP	CE3-CZ3	-6.36	1.27	1.38
1	C	184	GLY	C-O	-6.35	1.13	1.23
1	A	184	GLY	C-O	-6.35	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	TRP	CE2-CZ2	-6.34	1.28	1.39
1	C	264	TRP	CE2-CZ2	-6.34	1.28	1.39
1	A	314	TRP	CA-C	-6.34	1.36	1.52
1	A	145	PHE	CG-CD1	-6.34	1.29	1.38
1	A	220	PHE	CG-CD2	-6.33	1.29	1.38
1	C	314	TRP	CA-C	-6.33	1.36	1.52
1	C	220	PHE	CG-CD2	-6.31	1.29	1.38
1	A	181	PHE	CA-C	-6.30	1.36	1.52
1	C	145	PHE	CG-CD1	-6.30	1.29	1.38
1	C	181	PHE	CA-C	-6.29	1.36	1.52
1	A	259	THR	C-O	-6.29	1.11	1.23
1	A	223	PHE	CG-CD1	-6.28	1.29	1.38
1	C	231	TRP	CE3-CZ3	-6.28	1.27	1.38
1	A	219	LEU	CA-C	-6.28	1.36	1.52
1	A	262	LEU	C-O	-6.28	1.11	1.23
1	C	219	LEU	CA-C	-6.28	1.36	1.52
1	C	224	TYR	C-O	-6.28	1.11	1.23
1	C	262	LEU	C-O	-6.27	1.11	1.23
1	C	259	THR	C-O	-6.27	1.11	1.23
1	C	230	PHE	CA-C	-6.26	1.36	1.52
1	C	263	ILE	C-O	-6.26	1.11	1.23
1	A	230	PHE	CA-C	-6.25	1.36	1.52
1	A	231	TRP	CE3-CZ3	-6.24	1.27	1.38
1	A	224	TYR	C-O	-6.24	1.11	1.23
1	C	223	PHE	CG-CD1	-6.24	1.29	1.38
1	A	263	ILE	C-O	-6.23	1.11	1.23
1	A	182	TYR	CA-CB	-6.22	1.40	1.53
1	C	142	PHE	CG-CD1	-6.20	1.29	1.38
1	C	195	TYR	CB-CG	-6.20	1.42	1.51
1	C	182	TYR	CA-CB	-6.20	1.40	1.53
1	A	268	VAL	CB-CG2	-6.19	1.39	1.52
2	D	32	LEU	C-O	-6.19	1.11	1.23
2	B	32	LEU	C-O	-6.18	1.11	1.23
1	A	126	TYR	CD2-CE2	-6.17	1.30	1.39
1	A	142	PHE	CG-CD1	-6.17	1.29	1.38
1	A	195	TYR	CB-CG	-6.17	1.42	1.51
1	C	268	VAL	CB-CG2	-6.16	1.40	1.52
1	C	312	VAL	CA-CB	-6.15	1.41	1.54
1	C	314	TRP	CE2-CZ2	-6.14	1.29	1.39
1	A	317	LEU	C-O	-6.14	1.11	1.23
1	A	312	VAL	CA-CB	-6.14	1.41	1.54
1	C	221	LYS	C-O	-6.13	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	PHE	C-O	-6.13	1.11	1.23
1	A	221	LYS	C-O	-6.13	1.11	1.23
1	A	314	TRP	CE2-CZ2	-6.13	1.29	1.39
1	C	126	TYR	CD2-CE2	-6.13	1.30	1.39
1	A	332	GLN	CA-C	-6.12	1.37	1.52
1	C	317	LEU	C-O	-6.12	1.11	1.23
1	A	223	PHE	C-O	-6.11	1.11	1.23
1	C	217	PRO	CA-C	-6.10	1.40	1.52
2	D	42	TYR	C-O	-6.10	1.11	1.23
2	B	42	TYR	C-O	-6.09	1.11	1.23
1	C	175	GLU	C-O	-6.09	1.11	1.23
1	C	186	SER	CA-CB	-6.08	1.43	1.52
1	C	332	GLN	CA-C	-6.08	1.37	1.52
1	A	175	GLU	C-O	-6.07	1.11	1.23
1	C	231	TRP	CA-C	-6.07	1.37	1.52
1	A	231	TRP	CA-C	-6.06	1.37	1.52
1	C	230	PHE	CG-CD1	-6.06	1.29	1.38
1	A	186	SER	CA-CB	-6.06	1.43	1.52
1	A	217	PRO	CA-C	-6.04	1.40	1.52
1	A	271	PHE	CG-CD2	-6.04	1.29	1.38
1	C	193	CYS	C-O	-6.02	1.11	1.23
1	A	264	TRP	CZ3-CH2	-6.02	1.30	1.40
1	A	230	PHE	CG-CD1	-6.01	1.29	1.38
1	C	315	ILE	C-O	-6.01	1.11	1.23
1	A	193	CYS	C-O	-6.01	1.11	1.23
1	C	271	PHE	CG-CD2	-6.01	1.29	1.38
1	A	315	ILE	C-O	-6.00	1.11	1.23
2	B	37	VAL	C-O	-6.00	1.11	1.23
1	C	264	TRP	CZ3-CH2	-6.00	1.30	1.40
1	A	325	ILE	C-O	-5.99	1.11	1.23
1	C	197	SER	CB-OG	-5.99	1.34	1.42
1	C	143	PHE	CG-CD1	-5.98	1.29	1.38
2	D	37	VAL	C-O	-5.98	1.11	1.23
1	C	325	ILE	C-O	-5.96	1.12	1.23
2	B	50	TRP	C-O	-5.96	1.12	1.23
1	C	233	GLN	CA-CB	-5.96	1.40	1.53
1	A	269	PHE	CG-CD2	-5.96	1.29	1.38
1	C	269	PHE	CG-CD2	-5.95	1.29	1.38
1	C	369	LEU	C-O	-5.95	1.12	1.23
1	A	197	SER	CB-OG	-5.95	1.34	1.42
1	A	233	GLN	CA-CB	-5.94	1.40	1.53
2	B	134	ASP	C-O	-5.94	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	50	TRP	C-O	-5.94	1.12	1.23
1	A	143	PHE	CG-CD1	-5.94	1.29	1.38
2	D	50	TRP	CA-C	-5.93	1.37	1.52
2	D	134	ASP	C-O	-5.93	1.12	1.23
2	D	50	TRP	CZ3-CH2	-5.93	1.30	1.40
2	B	50	TRP	CA-C	-5.92	1.37	1.52
1	A	369	LEU	C-O	-5.91	1.12	1.23
1	A	327	TRP	CA-CB	-5.91	1.41	1.53
1	A	307	PHE	CG-CD2	-5.90	1.29	1.38
2	B	50	TRP	CZ3-CH2	-5.89	1.30	1.40
1	C	327	TRP	CA-CB	-5.89	1.41	1.53
1	A	264	TRP	CA-C	-5.88	1.37	1.52
1	C	371	TRP	CZ3-CH2	-5.88	1.30	1.40
1	A	371	TRP	CZ3-CH2	-5.88	1.30	1.40
1	C	264	TRP	CA-C	-5.88	1.37	1.52
2	B	36	ALA	CA-C	-5.87	1.37	1.52
1	C	178	TYR	CG-CD1	-5.86	1.31	1.39
2	D	36	ALA	CA-C	-5.85	1.37	1.52
1	C	307	PHE	CG-CD2	-5.84	1.29	1.38
1	A	176	GLN	CA-C	-5.84	1.37	1.52
1	C	179	ALA	C-O	-5.83	1.12	1.23
2	B	39	TYR	CG-CD1	-5.83	1.31	1.39
1	A	178	TYR	CG-CD1	-5.83	1.31	1.39
1	C	176	GLN	CA-C	-5.82	1.37	1.52
1	C	371	TRP	CA-CB	-5.82	1.41	1.53
1	A	179	ALA	C-O	-5.82	1.12	1.23
1	C	112	ARG	CA-C	-5.81	1.37	1.52
1	C	310	PHE	CG-CD2	-5.81	1.30	1.38
2	D	42	TYR	CG-CD2	-5.80	1.31	1.39
1	A	112	ARG	CA-C	-5.80	1.37	1.52
1	C	170	ILE	C-N	-5.80	1.20	1.34
2	D	45	ARG	CD-NE	-5.80	1.36	1.46
1	A	170	ILE	C-N	-5.79	1.20	1.34
1	C	176	GLN	C-O	-5.79	1.12	1.23
1	A	176	GLN	C-O	-5.78	1.12	1.23
2	B	45	ARG	CD-NE	-5.78	1.36	1.46
2	B	39	TYR	CE1-CZ	-5.78	1.31	1.38
2	B	42	TYR	CG-CD2	-5.78	1.31	1.39
1	A	371	TRP	CA-CB	-5.77	1.41	1.53
1	A	189	PHE	C-O	-5.77	1.12	1.23
1	C	189	PHE	C-O	-5.77	1.12	1.23
2	D	39	TYR	CG-CD1	-5.77	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	TYR	CG-CD1	-5.76	1.31	1.39
2	D	132	ASP	N-CA	-5.76	1.34	1.46
1	C	119	GLN	CA-C	-5.76	1.38	1.52
2	D	97	GLU	CA-CB	-5.75	1.41	1.53
1	A	327	TRP	C-O	-5.75	1.12	1.23
1	A	310	PHE	CG-CD2	-5.75	1.30	1.38
1	A	139	TYR	CG-CD1	-5.75	1.31	1.39
2	B	132	ASP	N-CA	-5.75	1.34	1.46
1	C	327	TRP	C-O	-5.74	1.12	1.23
1	C	375	ILE	C-O	-5.74	1.12	1.23
2	B	97	GLU	CA-CB	-5.73	1.41	1.53
1	A	119	GLN	CA-C	-5.73	1.38	1.52
1	A	150	LEU	C-O	-5.72	1.12	1.23
2	D	39	TYR	CE1-CZ	-5.71	1.31	1.38
1	C	313	ALA	CA-C	-5.71	1.38	1.52
1	A	375	ILE	C-O	-5.70	1.12	1.23
1	C	150	LEU	C-O	-5.69	1.12	1.23
1	A	313	ALA	CA-C	-5.69	1.38	1.52
1	A	172	ARG	CA-CB	-5.69	1.41	1.53
1	C	172	ARG	CA-CB	-5.68	1.41	1.53
1	A	217	PRO	CA-CB	-5.68	1.42	1.53
1	A	231	TRP	CE2-CZ2	-5.68	1.30	1.39
2	B	38	GLU	CA-CB	-5.68	1.41	1.53
1	C	217	PRO	CA-CB	-5.68	1.42	1.53
1	C	231	TRP	CE2-CZ2	-5.67	1.30	1.39
1	C	233	GLN	C-O	-5.67	1.12	1.23
1	A	233	GLN	C-O	-5.67	1.12	1.23
2	D	38	GLU	CA-CB	-5.67	1.41	1.53
1	A	310	PHE	C-O	-5.67	1.12	1.23
1	C	323	LEU	C-O	-5.67	1.12	1.23
1	A	323	LEU	C-O	-5.67	1.12	1.23
1	C	380	TYR	CE1-CZ	-5.66	1.31	1.38
1	A	380	TYR	CE1-CZ	-5.65	1.31	1.38
2	B	46	ILE	CB-CG1	-5.64	1.38	1.54
2	D	46	ILE	CB-CG1	-5.64	1.38	1.54
1	C	310	PHE	C-O	-5.63	1.12	1.23
1	A	310	PHE	CB-CG	-5.63	1.41	1.51
1	C	310	PHE	CB-CG	-5.63	1.41	1.51
1	A	111	HIS	CA-C	-5.63	1.38	1.52
1	C	111	HIS	CA-C	-5.62	1.38	1.52
1	A	147	ARG	CA-C	-5.62	1.38	1.52
1	A	260	LEU	C-O	-5.61	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	260	LEU	C-O	-5.61	1.12	1.23
1	A	217	PRO	C-O	-5.61	1.12	1.23
1	C	370	TYR	CG-CD2	-5.61	1.31	1.39
1	A	370	TYR	CG-CD2	-5.60	1.31	1.39
1	C	147	ARG	CA-C	-5.59	1.38	1.52
1	C	227	GLN	CA-C	-5.59	1.38	1.52
1	C	217	PRO	C-O	-5.59	1.12	1.23
1	A	227	GLN	CA-C	-5.58	1.38	1.52
2	D	46	ILE	CA-CB	-5.56	1.42	1.54
2	B	46	ILE	CA-CB	-5.56	1.42	1.54
1	C	178	TYR	CE2-CZ	-5.54	1.31	1.38
1	A	113	PHE	CG-CD1	-5.54	1.30	1.38
1	A	206	ALA	CA-C	-5.54	1.38	1.52
1	C	309	ILE	C-O	-5.54	1.12	1.23
1	A	204	THR	CB-CG2	-5.54	1.34	1.52
1	C	206	ALA	CA-C	-5.53	1.38	1.52
2	B	42	TYR	CE2-CZ	-5.53	1.31	1.38
1	C	113	PHE	CG-CD1	-5.52	1.30	1.38
1	A	178	TYR	N-CA	-5.51	1.35	1.46
2	B	42	TYR	CZ-OH	-5.51	1.28	1.37
1	A	309	ILE	C-O	-5.51	1.12	1.23
2	D	42	TYR	CZ-OH	-5.51	1.28	1.37
2	D	35	ALA	C-O	-5.51	1.12	1.23
1	C	178	TYR	N-CA	-5.50	1.35	1.46
1	C	204	THR	CB-CG2	-5.50	1.34	1.52
1	A	178	TYR	CE2-CZ	-5.50	1.31	1.38
1	C	193	CYS	CB-SG	-5.50	1.72	1.81
1	A	148	GLU	CA-C	-5.49	1.38	1.52
2	B	35	ALA	C-O	-5.49	1.12	1.23
1	A	143	PHE	CA-C	-5.49	1.38	1.52
2	D	42	TYR	CE2-CZ	-5.48	1.31	1.38
1	C	143	PHE	CA-C	-5.48	1.38	1.52
1	C	317	LEU	CA-C	-5.48	1.38	1.52
1	A	193	CYS	CB-SG	-5.48	1.72	1.81
1	A	317	LEU	CA-C	-5.48	1.38	1.52
1	A	178	TYR	CA-CB	-5.48	1.42	1.53
1	C	331	THR	C-O	-5.47	1.12	1.23
2	D	36	ALA	C-O	-5.47	1.12	1.23
1	A	256	HIS	CA-CB	-5.47	1.42	1.53
1	C	192	TYR	CG-CD1	-5.47	1.32	1.39
1	C	148	GLU	CA-C	-5.46	1.38	1.52
1	A	148	GLU	C-O	-5.46	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	256	HIS	CA-CB	-5.46	1.42	1.53
1	A	331	THR	C-O	-5.46	1.12	1.23
1	A	182	TYR	C-O	-5.46	1.12	1.23
1	C	370	TYR	CG-CD1	-5.46	1.32	1.39
1	A	370	TYR	CG-CD1	-5.45	1.32	1.39
2	B	36	ALA	C-O	-5.45	1.13	1.23
1	C	178	TYR	CA-CB	-5.45	1.42	1.53
1	C	182	TYR	C-O	-5.45	1.13	1.23
1	A	192	TYR	CG-CD1	-5.44	1.32	1.39
1	A	147	ARG	N-CA	-5.44	1.35	1.46
1	A	324	LYS	CA-CB	-5.43	1.42	1.53
1	C	147	ARG	N-CA	-5.42	1.35	1.46
1	C	324	LYS	CA-CB	-5.42	1.42	1.53
1	C	148	GLU	C-O	-5.42	1.13	1.23
1	C	118	TYR	CG-CD2	-5.40	1.32	1.39
1	A	192	TYR	CA-CB	-5.39	1.42	1.53
1	C	192	TYR	CA-CB	-5.39	1.42	1.53
2	B	41	LYS	C-O	-5.38	1.13	1.23
1	C	271	PHE	CB-CG	-5.38	1.42	1.51
2	D	41	LYS	C-O	-5.38	1.13	1.23
1	A	271	PHE	CB-CG	-5.38	1.42	1.51
1	A	318	ARG	C-O	-5.37	1.13	1.23
1	A	216	ASN	CG-ND2	-5.37	1.19	1.32
1	A	118	TYR	CG-CD2	-5.36	1.32	1.39
1	A	234	GLN	C-O	-5.36	1.13	1.23
1	A	316	TYR	CA-C	-5.36	1.39	1.52
1	A	316	TYR	CZ-OH	-5.35	1.28	1.37
1	C	216	ASN	CG-ND2	-5.35	1.19	1.32
1	C	318	ARG	C-O	-5.35	1.13	1.23
1	C	316	TYR	CZ-OH	-5.34	1.28	1.37
1	C	316	TYR	CA-C	-5.33	1.39	1.52
1	A	148	GLU	CA-CB	-5.33	1.42	1.53
2	B	45	ARG	C-O	-5.33	1.13	1.23
2	D	45	ARG	C-O	-5.33	1.13	1.23
1	C	148	GLU	CA-CB	-5.33	1.42	1.53
1	C	234	GLN	C-O	-5.32	1.13	1.23
1	C	237	ILE	C-O	-5.31	1.13	1.23
1	C	199	LEU	C-O	-5.30	1.13	1.23
1	A	188	PRO	CA-CB	-5.30	1.43	1.53
1	A	112	ARG	C-O	-5.30	1.13	1.23
1	A	237	ILE	C-O	-5.29	1.13	1.23
1	C	188	PRO	CA-CB	-5.28	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	ARG	C-O	-5.26	1.13	1.23
1	A	203	ASN	CB-CG	-5.21	1.39	1.51
1	A	257	ILE	CA-CB	-5.21	1.42	1.54
1	C	257	ILE	CA-CB	-5.21	1.42	1.54
1	A	320	TYR	CA-CB	-5.20	1.42	1.53
1	C	203	ASN	CB-CG	-5.20	1.39	1.51
1	A	234	GLN	CB-CG	-5.19	1.38	1.52
1	C	320	TYR	CA-CB	-5.19	1.42	1.53
1	A	199	LEU	C-O	-5.19	1.13	1.23
1	C	234	GLN	CB-CG	-5.18	1.38	1.52
1	A	269	PHE	CA-CB	-5.15	1.42	1.53
1	A	230	PHE	CA-CB	-5.14	1.42	1.53
1	C	230	PHE	CA-CB	-5.13	1.42	1.53
1	C	269	PHE	CA-CB	-5.13	1.42	1.53
1	A	173	ILE	C-O	-5.09	1.13	1.23
1	A	218	PHE	CG-CD2	-5.09	1.31	1.38
1	C	173	ILE	C-O	-5.09	1.13	1.23
1	C	194	MET	C-O	-5.08	1.13	1.23
1	A	318	ARG	CZ-NH1	-5.08	1.26	1.33
1	A	371	TRP	CE3-CZ3	-5.08	1.29	1.38
1	A	206	ALA	CA-CB	-5.08	1.41	1.52
1	C	218	PHE	CG-CD2	-5.08	1.31	1.38
1	C	206	ALA	CA-CB	-5.07	1.41	1.52
1	C	234	GLN	CG-CD	-5.07	1.39	1.51
1	A	194	MET	C-O	-5.07	1.13	1.23
1	A	333	PHE	CE2-CZ	-5.07	1.27	1.37
1	C	333	PHE	CE2-CZ	-5.06	1.27	1.37
1	A	234	GLN	CG-CD	-5.05	1.39	1.51
1	C	371	TRP	CE3-CZ3	-5.04	1.29	1.38
1	C	189	PHE	CA-C	-5.04	1.39	1.52
1	A	367	VAL	CB-CG1	-5.04	1.42	1.52
1	A	189	PHE	CA-C	-5.03	1.39	1.52
1	C	221	LYS	CA-C	-5.02	1.39	1.52
2	D	31	LEU	C-O	-5.02	1.13	1.23
1	A	171	LYS	CA-CB	-5.02	1.43	1.53
1	A	327	TRP	CE2-CZ2	-5.02	1.31	1.39
1	A	370	TYR	C-O	-5.02	1.13	1.23
1	C	171	LYS	CA-CB	-5.01	1.43	1.53
1	A	221	LYS	CA-C	-5.01	1.40	1.52
1	A	117	SER	C-O	-5.01	1.13	1.23
1	C	318	ARG	CZ-NH1	-5.01	1.26	1.33
1	C	117	SER	C-O	-5.01	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	PHE	CG-CD1	-5.00	1.31	1.38

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	318	ARG	NE-CZ-NH2	10.33	125.46	120.30
1	A	318	ARG	NE-CZ-NH2	10.25	125.43	120.30
1	C	173	ILE	CB-CA-C	-10.23	91.14	111.60
1	A	173	ILE	CB-CA-C	-10.21	91.18	111.60
1	A	317	LEU	CB-CG-CD2	-10.06	93.89	111.00
1	C	317	LEU	CB-CG-CD2	-10.04	93.92	111.00
1	A	187	GLY	C-N-CD	-9.62	99.44	120.60
1	C	187	GLY	C-N-CD	-9.62	99.44	120.60
2	B	116	ILE	CB-CA-C	-9.15	93.29	111.60
2	D	116	ILE	CB-CA-C	-9.15	93.30	111.60
1	A	263	ILE	CG1-CB-CG2	-9.11	91.36	111.40
1	C	263	ILE	CG1-CB-CG2	-9.11	91.36	111.40
1	C	326	LEU	CB-CG-CD2	-9.02	95.66	111.00
1	A	326	LEU	CB-CG-CD2	-9.02	95.67	111.00
1	A	374	LEU	CB-CG-CD2	-7.90	97.57	111.00
1	C	374	LEU	CB-CG-CD2	-7.90	97.57	111.00
1	A	128	LYS	CD-CE-NZ	7.62	129.24	111.70
1	A	334	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	C	128	LYS	CD-CE-NZ	7.61	129.21	111.70
1	C	334	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	230	PHE	CB-CA-C	-7.48	95.43	110.40
1	C	230	PHE	CB-CA-C	-7.46	95.48	110.40
1	C	333	PHE	CB-CA-C	-7.43	95.53	110.40
1	A	333	PHE	CB-CA-C	-7.42	95.56	110.40
1	C	307	PHE	CB-CA-C	-7.42	95.56	110.40
1	A	307	PHE	CB-CA-C	-7.42	95.57	110.40
1	A	176	GLN	CB-CA-C	-7.38	95.64	110.40
1	C	176	GLN	CB-CA-C	-7.38	95.65	110.40
2	D	31	LEU	CB-CG-CD2	-7.17	98.81	111.00
2	B	31	LEU	CB-CG-CD2	-7.16	98.83	111.00
1	A	261	LEU	CB-CG-CD2	-7.10	98.93	111.00
1	C	261	LEU	CB-CG-CD2	-7.08	98.97	111.00
1	C	199	LEU	CA-CB-CG	7.07	131.57	115.30
1	A	199	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	147	ARG	CG-CD-NE	-7.03	97.04	111.80
1	C	147	ARG	CG-CD-NE	-7.01	97.07	111.80
1	A	170	ILE	CG1-CB-CG2	-6.90	96.22	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	170	ILE	CG1-CB-CG2	-6.88	96.26	111.40
1	C	170	ILE	O-C-N	-6.87	111.71	122.70
1	A	170	ILE	O-C-N	-6.86	111.72	122.70
2	D	38	GLU	CB-CA-C	-6.84	96.73	110.40
1	A	149	PHE	CB-CA-C	-6.83	96.73	110.40
2	B	38	GLU	CB-CA-C	-6.83	96.75	110.40
1	C	149	PHE	CB-CA-C	-6.82	96.76	110.40
1	A	161	ARG	CB-CA-C	-6.74	96.93	110.40
1	C	161	ARG	CB-CA-C	-6.71	96.97	110.40
1	A	145	PHE	CB-CA-C	-6.59	97.22	110.40
1	C	145	PHE	CB-CA-C	-6.57	97.26	110.40
1	C	225	LEU	CB-CG-CD1	-6.54	99.88	111.00
1	A	225	LEU	CB-CG-CD1	-6.54	99.89	111.00
1	A	265	SER	CB-CA-C	-6.50	97.75	110.10
1	C	265	SER	CB-CA-C	-6.50	97.75	110.10
1	C	113	PHE	CB-CA-C	-6.41	97.57	110.40
1	A	113	PHE	CB-CA-C	-6.40	97.59	110.40
1	C	226	GLY	N-CA-C	-6.31	97.32	113.10
1	C	188	PRO	CA-N-CD	-6.31	102.67	111.50
1	A	188	PRO	CA-N-CD	-6.31	102.67	111.50
1	A	114	VAL	CG1-CB-CG2	-6.30	100.81	110.90
1	A	226	GLY	N-CA-C	-6.30	97.34	113.10
1	C	114	VAL	CG1-CB-CG2	-6.27	100.86	110.90
1	C	118	TYR	N-CA-C	6.27	127.92	111.00
1	C	261	LEU	CB-CG-CD1	-6.26	100.35	111.00
1	A	118	TYR	N-CA-C	6.26	127.91	111.00
1	A	261	LEU	CB-CG-CD1	-6.26	100.36	111.00
1	C	199	LEU	CB-CG-CD1	-6.24	100.39	111.00
1	C	333	PHE	N-CA-C	-6.22	94.19	111.00
1	A	333	PHE	N-CA-C	-6.21	94.23	111.00
1	A	150	LEU	CB-CG-CD2	-6.20	100.46	111.00
1	C	150	LEU	CB-CG-CD2	-6.20	100.46	111.00
1	A	199	LEU	CB-CG-CD1	-6.19	100.48	111.00
1	A	170	ILE	C-N-CA	-6.16	106.31	121.70
1	C	170	ILE	C-N-CA	-6.15	106.32	121.70
2	D	32	LEU	CB-CG-CD2	-6.09	100.65	111.00
2	B	32	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	A	367	VAL	CB-CA-C	-6.07	99.86	111.40
1	C	367	VAL	CB-CA-C	-6.07	99.86	111.40
1	C	384	TRP	CA-CB-CG	-5.95	102.39	113.70
1	A	384	TRP	CA-CB-CG	-5.95	102.40	113.70
1	C	211	TYR	C-N-CA	-5.91	97.16	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	TRP	N-CA-C	5.91	126.95	111.00
1	A	211	TYR	C-N-CA	-5.91	97.19	122.00
1	C	72	TRP	N-CA-C	5.89	126.92	111.00
1	C	271	PHE	O-C-N	-5.88	113.29	122.70
1	A	271	PHE	O-C-N	-5.86	113.32	122.70
1	C	230	PHE	CA-C-N	5.86	130.10	117.20
1	A	230	PHE	CA-C-N	5.85	130.06	117.20
2	B	32	LEU	CB-CA-C	-5.84	99.10	110.20
1	C	173	ILE	CG1-CB-CG2	-5.84	98.55	111.40
2	D	32	LEU	CB-CA-C	-5.84	99.11	110.20
1	A	173	ILE	CG1-CB-CG2	-5.83	98.58	111.40
1	C	262	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	A	262	LEU	CB-CG-CD1	-5.75	101.22	111.00
1	A	238	LEU	CB-CG-CD1	5.68	120.66	111.00
1	C	238	LEU	CB-CG-CD1	5.67	120.64	111.00
1	C	128	LYS	CG-CD-CE	-5.65	94.94	111.90
1	A	128	LYS	CG-CD-CE	-5.64	94.97	111.90
1	C	372	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	C	168	HIS	N-CA-C	-5.64	95.78	111.00
1	A	372	LEU	CB-CG-CD1	-5.63	101.42	111.00
1	C	204	THR	O-C-N	-5.63	113.69	122.70
1	A	168	HIS	N-CA-C	-5.62	95.83	111.00
1	A	317	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	C	164	VAL	N-CA-C	-5.57	95.96	111.00
1	A	164	VAL	N-CA-C	-5.56	95.98	111.00
1	C	317	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	A	204	THR	O-C-N	-5.54	113.83	122.70
1	A	307	PHE	N-CA-CB	5.53	120.55	110.60
2	D	96	ASP	N-CA-C	-5.53	96.07	111.00
1	C	120	ILE	CG1-CB-CG2	-5.53	99.24	111.40
2	B	96	ASP	N-CA-C	-5.52	96.10	111.00
1	C	307	PHE	N-CA-CB	5.52	120.53	110.60
1	A	120	ILE	CG1-CB-CG2	-5.51	99.27	111.40
1	C	78	ILE	CB-CA-C	-5.43	100.73	111.60
1	A	78	ILE	CB-CA-C	-5.43	100.74	111.60
1	A	330	LEU	CB-CG-CD2	5.43	120.22	111.00
1	C	330	LEU	CB-CG-CD2	5.42	120.22	111.00
1	A	172	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	98	HIS	N-CA-CB	-5.40	100.88	110.60
2	D	98	HIS	N-CA-CB	-5.39	100.90	110.60
1	A	162	LEU	CA-CB-CG	-5.38	102.92	115.30
1	C	147	ARG	N-CA-CB	-5.38	100.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	ARG	N-CA-CB	-5.38	100.92	110.60
1	C	172	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	162	LEU	CA-CB-CG	-5.37	102.95	115.30
2	B	43	GLY	CA-C-O	-5.36	110.95	120.60
2	D	43	GLY	CA-C-O	-5.35	110.98	120.60
1	A	110	LEU	N-CA-C	-5.34	96.57	111.00
1	C	207	MET	CB-CG-SD	-5.34	96.38	112.40
1	C	110	LEU	N-CA-C	-5.33	96.60	111.00
1	A	207	MET	CB-CG-SD	-5.33	96.43	112.40
1	A	110	LEU	CA-C-N	5.32	128.91	117.20
1	C	184	GLY	N-CA-C	-5.32	99.80	113.10
1	A	184	GLY	N-CA-C	-5.32	99.81	113.10
1	C	139	TYR	CA-CB-CG	-5.31	103.31	113.40
1	A	139	TYR	CA-CB-CG	-5.31	103.32	113.40
1	C	110	LEU	CA-C-N	5.31	128.88	117.20
1	C	224	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	C	74	SER	N-CA-C	-5.30	96.70	111.00
1	A	74	SER	N-CA-C	-5.29	96.70	111.00
1	A	224	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	247	LYS	O-C-N	5.26	131.11	122.70
1	C	247	LYS	O-C-N	5.25	131.10	122.70
1	A	193	CYS	CB-CA-C	-5.24	99.92	110.40
1	A	220	PHE	N-CA-CB	-5.24	101.17	110.60
1	C	193	CYS	CB-CA-C	-5.24	99.92	110.40
1	C	220	PHE	N-CA-CB	-5.24	101.17	110.60
1	A	247	LYS	C-N-CA	5.22	134.76	121.70
1	A	323	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	C	247	LYS	C-N-CA	5.22	134.74	121.70
1	C	191	ILE	CB-CA-C	-5.20	101.20	111.60
1	A	191	ILE	CB-CA-C	-5.20	101.20	111.60
1	C	323	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	C	162	LEU	N-CA-C	5.16	124.92	111.00
1	A	162	LEU	N-CA-C	5.14	124.89	111.00
1	A	147	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	174	MET	CB-CG-SD	-5.13	97.00	112.40
1	C	174	MET	CB-CG-SD	-5.12	97.03	112.40
1	C	147	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	A	198	ASP	CB-CA-C	-5.08	100.25	110.40
1	C	198	ASP	CB-CA-C	-5.07	100.26	110.40
2	D	45	ARG	CB-CA-C	-5.01	100.39	110.40

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
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	284	0
1	C	2670	0	2667	288	0
2	B	1082	0	1037	44	0
2	D	1082	0	1037	45	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	668	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 43.

All (668) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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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: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: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:A:154:VAL:C	1:A:157:PRO:HD2	2.03	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:C:204:THR:O	1:C:205:LYS:C	2.17	0.78
1:C:132:ASP:OD1	1:C:267:TYR:OH	2.03	0.77
1:C:154:VAL:C	1:C:157:PRO:HD2	2.03	0.77
1:A:204:THR:O	1:A:205:LYS:C	2.14	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: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
2:D:132:ASP:OD1	2:D:135:SER:HB2	1.85	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:C:248:ASP:C	1:C:250:ASN:H	1.90	0.75
1:A:137:PHE:HA	1:A:140:MET:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:CE2	1:A:279:TYR:CD2	2.75	0.74
1:A:106:LYS:HB3	1:A:106:LYS:HZ2	1.49	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:C:137:PHE:HA	1:C:140:MET:HG3	1.69	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:A:204:THR:HG21	1:A:328:SER:HB2	1.70	0.73
1:A:248:ASP:C	1:A:250:ASN:H	1.90	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: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:248:ASP:C	1:C:250:ASN:N	2.42	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:C:295:LEU:HD22	1:C:303:ALA:CA	2.19	0.71
2:D:50:TRP:HE1	3:D:201:6PL:H32	1.54	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
1:A:248:ASP:C	1:A:250:ASN:N	2.42	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
1:A:211:TYR:O	1:A:212:PRO:C	2.27	0.70
1:C:309:ILE:HD13	1:C:309:ILE:N	2.06	0.70
1:A:239:VAL:C	1:A:241:GLN:H	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:239:VAL:C	1:C:241:GLN:N	2.45	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:C:239:VAL:C	1:C:241:GLN:H	1.94	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: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: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
1:A:252:LEU:C	1:A:252:LEU:HD23	2.16	0.67
2:D:45:ARG:HG2	2:D:45:ARG:O	1.93	0.67
1:C:238:LEU:C	1:C:238:LEU:HD23	2.16	0.66
1:C:252:LEU:C	1:C:252:LEU:HD23	2.16	0.66
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:C:251:GLU:CG	1:C:370:TYR:CD2	2.78	0.66
1:A:176:GLN:HA	1:A:176:GLN:OE1	1.96	0.66
1:A:238:LEU:C	1:A:238:LEU:HD23	2.16	0.66
1:C:156:ARG:N	1:C:157:PRO:CD	2.59	0.66
1:A:239:VAL:C	1:A:241:GLN:N	2.45	0.65
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:C:147:ARG:HH11	1:C:151:MET:HE1	1.60	0.65
1:C:211:TYR:O	1:C:212:PRO:C	2.27	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:233:GLN:O	1:C:233:GLN:HG2	1.99	0.63
1:A:140:MET:HE1	1:A:232:ALA:HB1	1.80	0.63
1:A:224:TYR:OH	1:A:266:SER:OG	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:204:THR:HG21	1:A:328:SER:CB	2.31	0.60
1:A:302:LEU:C	1:A:304:PHE:H	2.05	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:HG12	1:C:312:VAL:O	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:A:302:LEU:C	1:A:304:PHE:N	2.53	0.59
1:C:176:GLN:CB	1:C:294:THR:HG22	2.33	0.59
1:C:302:LEU:C	1:C:304:PHE:N	2.53	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
1:A:317:LEU:HA	1:A:321:ILE:HG12	1.84	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:C:147:ARG:HE	1:C:151:MET:HE2	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:C	1:C:304:PHE:H	2.05	0.58
2:B:130:GLY:HA3	2:B:138:VAL:HG21	1.86	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: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:140:MET:HE3	1:C:232:ALA:HB1	1.87	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: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
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
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:C:219:LEU:C	1:C:222:VAL:HG12	2.18	0.56
1:A:87:PRO:HB2	1:A:145:PHE:HB2	1.86	0.55
1:A:106:LYS:HB3	1:A:106:LYS:HZ3	1.71	0.55
1:A:204:THR:CG2	1:A:328:SER:OG	2.54	0.55
1:A:219:LEU:C	1:A:222:VAL:HG12	2.18	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
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:A:183:THR:HG21	1:A:287:PHE:HB2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:147:ARG:NE	1:C:151:MET:HE2	2.21	0.55
1:C:383:LEU:HD23	1:C:383:LEU:O	2.07	0.55
1:A:383:LEU:HD23	1:A:383:LEU:O	2.07	0.54
1:C:204:THR:HA	1:C:207:MET:HG3	1.89	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: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
1:C:148:GLU:OE2	1:C:148:GLU:HA	2.07	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:214:PHE:C	1:A:215:THR:HG23	2.27	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:214:PHE:C	1:C:215:THR:HG23	2.27	0.54
1:C:309:ILE:N	1:C:309:ILE:CD1	2.71	0.54
1:C:320:TYR:CD1	1:C:320:TYR:C	2.81	0.54
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:A:336:GLU:O	1:A:349:LYS:NZ	2.26	0.53
2:D:50:TRP:HE1	3:D:201:6PL:H12	1.61	0.53
1:A:320:TYR:CD1	1:A:320:TYR:C	2.81	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
1:A:173:ILE:O	1:A:173:ILE:HG22	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HG2	1:A:147:ARG:HH21	1.73	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:325:ILE:O	1:A:325:ILE:HG22	2.08	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
2:B:24:PHE:C	2:B:24:PHE:CD2	2.83	0.52
1:C:195:TYR:C	1:C:195:TYR:CD2	2.83	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: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
2:D:24:PHE:C	2:D:24:PHE:CD2	2.83	0.51
1:A:239:VAL:O	1:A:241:GLN:N	2.43	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:C:116:VAL:CG2	1:C:218:PHE:HE1	2.23	0.51
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:195:TYR:C	1:A:195:TYR:CD2	2.83	0.51
1:A:214:PHE:C	1:A:215:THR:CG2	2.78	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:372:LEU:HD12	1:A:372:LEU:O	2.11	0.51
1:C:325:ILE:HG22	1:C:325:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:HIS:CD2	1:C:111:HIS:C	2.84	0.50
1:C:214:PHE:C	1:C:215:THR:CG2	2.78	0.50
1:C:334:ARG:CZ	1:C:334:ARG:HB2	2.41	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
1:A:111:HIS:C	1:A:111:HIS:CD2	2.84	0.50
2:D:115:PRO:HB2	2:D:117:HIS:CD2	2.47	0.50
1:C:194:MET:HB2	1:C:276:LEU:HD21	1.94	0.50
1:A:182:TYR:CD1	1:A:182:TYR:C	2.84	0.50
2:B:115:PRO:HB2	2:B:117:HIS:CD2	2.47	0.50
1:C:220:PHE:HD2	1:C:220:PHE:O	1.95	0.50
2:D:23:LEU:HD12	2:D:23:LEU:C	2.32	0.50
1:A:309:ILE:O	1:A:309:ILE:HG22	2.11	0.49
1:A:262:LEU:HD21	1:A:360:LEU:HB3	1.94	0.49
1:C:268:VAL:HG13	1:C:268:VAL:O	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: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
1:C:220:PHE:C	1:C:220:PHE:CD2	2.84	0.49
1:C:375:ILE:HG13	4:C:502:9NY:C31	2.38	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:314:TRP:CD1	1:C:314:TRP:C	2.85	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: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:C:215:THR:O	1:C:215:THR:OG1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:238:LEU:HD23	1:A:238:LEU:O	2.13	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
1:A:220:PHE:C	1:A:220:PHE:CD2	2.84	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
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:182:TYR:CD1	1:C:182:TYR:C	2.84	0.47
1:C:251:GLU:CD	1:C:370:TYR:CE2	2.87	0.47
1:C:378:VAL:HG13	1:C:382:ILE:HG12	1.96	0.47
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:142:PHE:O	1:C:142:PHE:CG	2.66	0.47
1:C:214:PHE:O	1:C:215:THR:HG22	2.15	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:A:140:MET:HE1	1:A:232:ALA:CB	2.43	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:A:251:GLU:CD	1:A:370:TYR:CE2	2.87	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:O	1:C:370:TYR:CD1	2.68	0.47
1:C:262:LEU:CB	4:C:502:9NY:C19	2.91	0.47
1:A:192:TYR:CD2	1:A:192:TYR:C	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:327:TRP:CD1	1:A:327:TRP:C	2.85	0.46
1:A:183:THR:HG21	1:A:287:PHE:CA	2.45	0.46
1:A:370:TYR:O	1:A:370:TYR:CD1	2.68	0.46
1:C:109:VAL:HA	1:C:112:ARG:NH1	2.30	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: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:A:314:TRP:CD1	1:A:314:TRP:C	2.85	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:A:230:PHE:O	1:A:230:PHE:CG	2.68	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
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: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:O	1:C:380:TYR:CD2	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
2:D:46:ILE:CG1	2:D:47:ASN:N	2.79	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:C:192:TYR:CD2	1:C:192:TYR:C	2.85	0.45
1:A:156:ARG:HH21	1:A:156:ARG:CG	2.30	0.45
1:C:238:LEU:O	1:C:238:LEU:HG	2.16	0.45
1:C:310:PHE:O	1:C:310:PHE:CD1	2.69	0.45
1:C:320:TYR:CD1	1:C:320:TYR:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:140:MET:HE2	1:C:232:ALA:HB3	1.99	0.45
1:A:380:TYR:CD2	1:A:380:TYR:C	2.86	0.45
1:A:334:ARG:NH2	1:A:334:ARG:HB3	2.32	0.45
1:A:383:LEU:C	1:A:383:LEU:CD2	2.85	0.45
1:A:238:LEU:O	1:A:238:LEU:HG	2.16	0.45
1:C:249:HIS:O	1:C:249:HIS:CG	2.68	0.45
1:C:327:TRP:CD1	1:C:327:TRP:C	2.85	0.45
1:C:380:TYR:CD2	1:C:380:TYR:C	2.86	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
2:B:23:LEU:HD12	2:B:23:LEU:C	2.32	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
1:C:383:LEU:C	1:C:383:LEU:CD2	2.85	0.45
4:C:502:9NY:C31	4:C:502:9NY:O15	2.65	0.45
1:C:251:GLU:CD	1:C:370:TYR:HE2	2.20	0.45
1:A:327:TRP:O	1:A:327:TRP:CG	2.69	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:A:103:ASN:ND2	1:A:103:ASN:C	2.70	0.44
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.53	0.44
1:C:147:ARG:NE	1:C:151:MET:CE	2.70	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:A:147:ARG:HE	1:A:151:MET:CE	2.30	0.44
1:C:103:ASN:ND2	1:C:103:ASN:C	2.70	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:251:GLU:CD	1:A:370:TYR:HE2	2.20	0.44
1:C:302:LEU:O	1:C:304:PHE:N	2.51	0.44
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
1:A:302:LEU:O	1:A:304:PHE:N	2.51	0.44
2:B:32:LEU:HD12	2:B:32:LEU:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ARG:HH11	1:C:151:MET:CE	2.30	0.44
1:C:220:PHE:HD2	1:C:220:PHE:C	2.22	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:O	1:A:220:PHE:CD2	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:241:GLN:OE1	1:A:241:GLN:HA	2.14	0.43
1:A:370:TYR:CD1	1:A:370:TYR:C	2.84	0.43
1:C:245:PRO:HB2	1:C:249:HIS:HB3	2.01	0.43
1:C:327:TRP:O	1:C:327:TRP:CG	2.69	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
1:C:310:PHE:O	1:C:310:PHE:CG	2.68	0.43
2:D:29:ILE:N	2:D:29:ILE:CD1	2.81	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
1:C:370:TYR:CD1	1:C:370:TYR:C	2.84	0.43
1:A:73:PHE:CE2	1:A:76:ARG:HB2	2.54	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.86	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:326:LEU:HG	1:C:361:ILE:HG22	2.02	0.42
1:A:220:PHE:HD2	1:A:220:PHE:C	2.22	0.42
1:A:238:LEU:O	1:A:238:LEU:CG	2.67	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: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
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:C:238:LEU:C	1:C:238:LEU:CD2	2.84	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:152:ASP:OD1	1:C:152:ASP:C	2.59	0.41
1:C:220:PHE:O	1:C:220:PHE:CD2	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
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:325:ILE:O	1:C:325:ILE:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:118:GLU:CA	2:B:118:GLU:OE2	2.67	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:194:MET:O	1:C:194:MET:CG	2.68	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:152:ASP:OD1	1:A:152:ASP:C	2.59	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:194:MET:O	1:A:194:MET:CG	2.68	0.41
1:A:320:TYR:O	1:A:320:TYR:CG	2.68	0.41
1:A:372:LEU:O	1:A:372:LEU:CG	2.69	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: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
1:A:126:TYR:N	1:A:126:TYR:HD2	2.14	0.40
2:B:33:LEU:HD23	2:B:33:LEU:C	2.42	0.40
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:THR:O	1:C:253:THR:CG2	2.66	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
3:D:201:6PL:H361	3:D:201:6PL:H391	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	313/428 (73%)	266 (85%)	37 (12%)	10 (3%)	4 22
1	C	313/428 (73%)	267 (85%)	36 (12%)	10 (3%)	4 22
2	B	130/150 (87%)	120 (92%)	9 (7%)	1 (1%)	19 54
2	D	130/150 (87%)	120 (92%)	9 (7%)	1 (1%)	19 54
All	All	886/1156 (77%)	773 (87%)	91 (10%)	22 (2%)	9 27

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

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Mol	Chain	Res	Type
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 (i)

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%)	214 (75%)	70 (25%)	0 2
1	C	284/391 (73%)	215 (76%)	69 (24%)	0 2
2	B	119/135 (88%)	108 (91%)	11 (9%)	9 33
2	D	119/135 (88%)	107 (90%)	12 (10%)	7 28
All	All	806/1052 (77%)	644 (80%)	162 (20%)	3 5

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	72	TRP
1	A	73	PHE
1	A	74	SER
1	A	76	ARG
1	A	78	ILE
1	A	80	TYR

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Mol	Chain	Res	Type
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	124	ASN
1	A	150	LEU
1	A	151	MET
1	A	152	ASP
1	A	154	VAL
1	A	156	ARG
1	A	158	PHE
1	A	160	ILE
1	A	165	THR
1	A	166	SER
1	A	168	HIS
1	A	169	ARG
1	A	177	MET
1	A	180	ILE
1	A	186	SER
1	A	194	MET
1	A	198	ASP
1	A	199	LEU
1	A	201	PHE
1	A	209	ARG
1	A	216	ASN
1	A	217	PRO
1	A	220	PHE
1	A	224	TYR
1	A	236	CYS
1	A	237	ILE
1	A	238	LEU
1	A	240	LEU
1	A	241	GLN
1	A	243	GLU
1	A	244	LYS
1	A	246	ARG
1	A	248	ASP
1	A	249	HIS

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Mol	Chain	Res	Type
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	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	27	CYS
2	B	29	ILE
2	B	33	LEU
2	B	38	GLU
2	B	50	TRP
2	B	116	ILE
2	B	117	HIS
2	B	118	GLU
2	B	131	TYR
2	B	136	GLU
1	C	71	ILE
1	C	72	TRP
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

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Mol	Chain	Res	Type
1	C	106	LYS
1	C	108	ASN
1	C	112	ARG
1	C	114	VAL
1	C	117	SER
1	C	124	ASN
1	C	150	LEU
1	C	151	MET
1	C	152	ASP
1	C	154	VAL
1	C	156	ARG
1	C	158	PHE
1	C	160	ILE
1	C	165	THR
1	C	166	SER
1	C	168	HIS
1	C	169	ARG
1	C	177	MET
1	C	180	ILE
1	C	186	SER
1	C	194	MET
1	C	198	ASP
1	C	199	LEU
1	C	201	PHE
1	C	209	ARG
1	C	216	ASN
1	C	217	PRO
1	C	220	PHE
1	C	224	TYR
1	C	236	CYS
1	C	237	ILE
1	C	238	LEU
1	C	240	LEU
1	C	241	GLN
1	C	243	GLU
1	C	244	LYS
1	C	246	ARG
1	C	248	ASP
1	C	249	HIS
1	C	251	GLU
1	C	252	LEU
1	C	253	THR

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Mol	Chain	Res	Type
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	315	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	27	CYS
2	D	28	PHE
2	D	29	ILE
2	D	33	LEU
2	D	38	GLU
2	D	50	TRP
2	D	116	ILE
2	D	117	HIS
2	D	118	GLU
2	D	131	TYR
2	D	136	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	117	HIS
1	C	108	ASN
1	C	111	HIS
1	C	131	ASN

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Mol	Chain	Res	Type
1	C	256	HIS
1	C	319	HIS
1	C	365	GLN
2	D	117	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	201	-	39,39,51	1.53	6 (15%)	43,44,59	1.86	8 (18%)
3	6PL	A	501	-	17,17,51	0.22	0	16,16,59	0.63	0
3	6PL	B	202	-	17,17,51	0.29	0	16,16,59	0.85	0
3	6PL	D	202	-	17,17,51	0.29	0	16,16,59	0.85	0
3	6PL	C	501	-	17,17,51	0.22	0	16,16,59	0.63	0
4	9NY	A	502	-	69,77,77	2.34	17 (24%)	80,103,103	2.29	24 (30%)
4	9NY	C	502	-	69,77,77	2.34	17 (24%)	80,103,103	2.28	24 (30%)
3	6PL	B	201	-	39,39,51	1.53	6 (15%)	43,44,59	1.87	8 (18%)

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	D	201	-	-	21/41/41/55	-
3	6PL	A	501	-	-	8/15/15/55	-
3	6PL	B	202	-	-	6/15/15/55	-
3	6PL	D	202	-	-	6/15/15/55	-
3	6PL	C	501	-	-	8/15/15/55	-
4	9NY	A	502	-	-	35/72/92/92	0/3/3/3
4	9NY	C	502	-	-	35/72/92/92	0/3/3/3
3	6PL	B	201	-	-	21/41/41/55	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	9NY	C44-S1	9.36	1.98	1.76
4	C	502	9NY	C44-S1	9.35	1.98	1.76
4	C	502	9NY	C40-C44	7.41	1.58	1.50
4	A	502	9NY	C40-C44	7.39	1.58	1.50
4	C	502	9NY	O12-C25	-5.72	1.31	1.42
4	A	502	9NY	O12-C25	-5.72	1.31	1.42
4	A	502	9NY	C6-N2	5.30	1.40	1.32
4	C	502	9NY	C6-N2	5.27	1.40	1.32
3	D	201	6PL	O2-C31	5.27	1.49	1.34
3	B	201	6PL	O2-C31	5.25	1.49	1.34
4	A	502	9NY	O3-C9	-4.78	1.34	1.45
4	C	502	9NY	O3-C9	-4.78	1.34	1.45
4	A	502	9NY	O3-C5	4.06	1.46	1.41
4	C	502	9NY	O3-C5	4.05	1.46	1.41
4	C	502	9NY	O15-C36	-3.76	1.15	1.23
4	A	502	9NY	O15-C36	-3.74	1.16	1.23
3	D	201	6PL	O2-C2	-3.63	1.37	1.46
3	B	201	6PL	O2-C2	-3.61	1.37	1.46
3	D	201	6PL	O3-C11	3.44	1.43	1.33
3	B	201	6PL	O3-C11	3.43	1.43	1.33
4	A	502	9NY	P2-O9	-3.25	1.39	1.50
4	C	502	9NY	P2-O9	-3.24	1.39	1.50
3	D	201	6PL	P-O2P	-3.23	1.42	1.54
3	B	201	6PL	P-O2P	-3.22	1.42	1.54
3	B	201	6PL	P-O1P	-3.05	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	6PL	P-O1P	-3.02	1.40	1.50
4	A	502	9NY	C36-N6	-2.94	1.27	1.33
4	C	502	9NY	C36-N6	-2.92	1.27	1.33
4	A	502	9NY	C31-C11	-2.89	1.47	1.53
4	C	502	9NY	C31-C11	-2.87	1.47	1.53
3	B	201	6PL	O11-C11	-2.86	1.14	1.22
3	D	201	6PL	O11-C11	-2.84	1.14	1.22
4	C	502	9NY	C3-C2	-2.70	1.33	1.43
4	A	502	9NY	C3-C2	-2.69	1.33	1.43
4	A	502	9NY	C2-C1	-2.59	1.34	1.40
4	C	502	9NY	C2-C1	-2.59	1.34	1.40
4	C	502	9NY	P2-O10	-2.24	1.44	1.55
4	A	502	9NY	P2-O10	-2.24	1.44	1.55
4	A	502	9NY	C45-N7	-2.16	1.28	1.33
4	C	502	9NY	C45-N7	-2.16	1.28	1.33
4	C	502	9NY	C7-C5	-2.13	1.50	1.53
4	A	502	9NY	C7-C5	-2.12	1.50	1.53
4	C	502	9NY	C41-C43	2.12	1.58	1.51
4	A	502	9NY	C41-C43	2.11	1.58	1.51
4	A	502	9NY	C2-N4	-2.01	1.32	1.39
4	C	502	9NY	C2-N4	-2.00	1.32	1.39

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	9NY	C5-N5-C1	6.27	137.66	126.64
4	A	502	9NY	C5-N5-C1	6.27	137.65	126.64
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
4	A	502	9NY	N2-C6-N1	-6.10	119.15	128.68
4	C	502	9NY	N2-C6-N1	-6.09	119.15	128.68
3	B	201	6PL	O2-C31-C32	6.06	124.57	111.50
3	D	201	6PL	O2-C31-C32	6.04	124.53	111.50
3	B	201	6PL	P-O3P-C1	5.31	132.92	118.30
3	D	201	6PL	P-O3P-C1	5.31	132.92	118.30
4	A	502	9NY	C30-C11-C24	-4.90	100.25	108.23
4	C	502	9NY	C30-C11-C24	-4.87	100.29	108.23
4	C	502	9NY	O4-P2-O9	-4.84	90.14	109.07
4	A	502	9NY	O4-P2-O9	-4.83	90.18	109.07
4	C	502	9NY	C31-C11-C24	4.73	115.94	108.23
4	A	502	9NY	C31-C11-C24	4.72	115.93	108.23
4	A	502	9NY	O11-P3-O13	-4.60	91.08	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	9NY	O11-P3-O13	-4.60	91.10	109.07
4	A	502	9NY	C40-C44-S1	4.50	118.69	113.46
4	C	502	9NY	C40-C44-S1	4.49	118.68	113.46
3	D	201	6PL	O3-C11-C12	4.41	125.75	111.91
3	B	201	6PL	O3-C11-C12	4.40	125.73	111.91
4	A	502	9NY	C38-C40-C44	4.33	121.94	112.33
4	C	502	9NY	C38-C40-C44	4.32	121.92	112.33
4	A	502	9NY	O14-P3-O13	4.03	132.18	112.24
4	C	502	9NY	O14-P3-O13	4.03	132.16	112.24
4	A	502	9NY	C31-C11-C25	3.83	115.46	108.82
4	C	502	9NY	C31-C11-C25	3.81	115.42	108.82
4	A	502	9NY	P3-O8-P2	-3.79	119.83	132.83
4	C	502	9NY	P3-O8-P2	-3.78	119.84	132.83
4	C	502	9NY	O14-P3-O11	-3.59	91.07	107.75
4	A	502	9NY	O14-P3-O11	-3.58	91.11	107.75
3	B	201	6PL	O4P-P-O3P	-3.55	97.30	106.73
3	D	201	6PL	O4P-P-O3P	-3.52	97.35	106.73
3	D	201	6PL	C3-O3-C11	3.11	128.64	117.12
3	B	201	6PL	C3-O3-C11	3.11	128.63	117.12
3	B	201	6PL	O3-C3-C2	2.97	117.09	108.43
3	D	201	6PL	O3-C3-C2	2.97	117.09	108.43
4	C	502	9NY	O3-C5-C7	-2.93	102.64	106.93
4	A	502	9NY	O3-C5-C7	-2.91	102.67	106.93
4	A	502	9NY	C41-C43-C45	2.84	117.09	112.36
4	C	502	9NY	C41-C43-C45	2.81	117.04	112.36
4	C	502	9NY	O10-P2-O4	2.70	120.28	107.75
4	A	502	9NY	O10-P2-O4	2.69	120.24	107.75
4	A	502	9NY	O16-C44-C40	-2.68	120.82	123.99
4	C	502	9NY	O16-C44-C40	-2.68	120.83	123.99
4	C	502	9NY	C28-C26-C22	-2.53	101.59	114.42
4	A	502	9NY	C28-C26-C22	-2.52	101.62	114.42
4	C	502	9NY	C43-C41-N6	-2.49	106.87	111.90
4	A	502	9NY	C43-C41-N6	-2.48	106.90	111.90
4	C	502	9NY	O3-C9-C8	-2.45	99.61	104.87
4	C	502	9NY	C1-C2-N4	-2.45	106.84	109.40
4	A	502	9NY	C2-C3-N3	-2.44	116.64	120.35
4	C	502	9NY	C2-C3-N3	-2.44	116.64	120.35
4	A	502	9NY	O3-C9-C8	-2.43	99.66	104.87
4	A	502	9NY	C1-C2-N4	-2.42	106.88	109.40
4	A	502	9NY	P2-O4-C10	2.21	134.62	121.68
4	C	502	9NY	P2-O4-C10	2.21	134.62	121.68
3	D	201	6PL	O11-C11-C12	-2.15	115.36	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	9NY	O4-C10-C9	2.14	116.36	108.99
4	C	502	9NY	O4-C10-C9	2.14	116.36	108.99
3	B	201	6PL	O11-C11-C12	-2.14	115.40	123.73
3	B	201	6PL	O31-C31-C32	-2.12	115.48	123.73
3	D	201	6PL	O31-C31-C32	-2.10	115.53	123.73

There are no chirality outliers.

All (140) 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	C24-C11-C25-C36
4	A	502	9NY	C24-C11-C25-O12
4	A	502	9NY	C31-C11-C25-C36
4	A	502	9NY	C11-C25-C36-N6
4	A	502	9NY	C11-C25-C36-O15
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	C24-O11-P3-O8
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	C11-C25-C36-N6
4	C	502	9NY	C11-C25-C36-O15
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	C24-O11-P3-O8
3	B	201	6PL	C34-C35-C36-C37
3	D	201	6PL	C34-C35-C36-C37
3	B	201	6PL	C21-C22-C23-C24
3	B	201	6PL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	B	201	6PL	C36-C37-C38-C39
3	D	201	6PL	C21-C22-C23-C24
3	D	201	6PL	C14-C15-C16-C17
3	D	201	6PL	C36-C37-C38-C39
4	A	502	9NY	O4-C10-C9-C8
4	A	502	9NY	O4-C10-C9-O3
4	C	502	9NY	O4-C10-C9-C8
4	C	502	9NY	O4-C10-C9-O3
3	B	201	6PL	C19-C20-C21-C22
3	D	201	6PL	C19-C20-C21-C22
4	A	502	9NY	C7-C8-O2-P1
4	C	502	9NY	C7-C8-O2-P1
3	B	201	6PL	O2-C2-C3-O3
3	D	201	6PL	O2-C2-C3-O3
3	B	202	6PL	C41-C42-C43-C44
3	C	501	6PL	C44-C45-C46-C47
3	D	202	6PL	C41-C42-C43-C44
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	B	202	6PL	C36-C37-C38-C39
3	C	501	6PL	C32-C33-C34-C35
3	D	202	6PL	C35-C36-C37-C38
3	D	202	6PL	C36-C37-C38-C39
3	A	501	6PL	C40-C41-C42-C43
3	C	501	6PL	C40-C41-C42-C43
4	A	502	9NY	C13-C12-C14-C16
4	C	502	9NY	C13-C12-C14-C16
3	A	501	6PL	C33-C34-C35-C36
3	C	501	6PL	C33-C34-C35-C36
3	B	201	6PL	C22-C23-C24-C25
3	D	201	6PL	C22-C23-C24-C25
4	A	502	9NY	C14-C12-C13-C15
4	C	502	9NY	C14-C12-C13-C15
3	B	201	6PL	C17-C18-C19-C20
3	D	201	6PL	C17-C18-C19-C20
4	A	502	9NY	C12-C14-C16-C18
4	C	502	9NY	C12-C14-C16-C18
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	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
3	B	201	6PL	C18-C19-C20-C21
3	D	201	6PL	C18-C19-C20-C21
3	B	201	6PL	C32-C33-C34-C35
3	D	201	6PL	C32-C33-C34-C35
3	B	201	6PL	C1-C2-C3-O3
3	D	201	6PL	C1-C2-C3-O3
3	A	501	6PL	C34-C35-C36-C37
3	C	501	6PL	C34-C35-C36-C37
4	A	502	9NY	C9-C10-O4-P2
4	C	502	9NY	C9-C10-O4-P2
3	B	202	6PL	C31-C32-C33-C34
3	D	202	6PL	C31-C32-C33-C34
3	B	202	6PL	C38-C39-C40-C41
3	D	202	6PL	C38-C39-C40-C41
4	A	502	9NY	P2-O8-P3-O13
4	C	502	9NY	P2-O8-P3-O13
3	B	202	6PL	C45-C46-C47-C48
3	D	202	6PL	C45-C46-C47-C48
3	B	201	6PL	O3P-C1-C2-C3
3	D	201	6PL	O3P-C1-C2-C3
3	D	201	6PL	C37-C38-C39-C40
3	B	201	6PL	C37-C38-C39-C40
4	A	502	9NY	C29-C33-C35-C38
4	C	502	9NY	C29-C33-C35-C38
4	C	502	9NY	C32-C34-C37-C39
4	A	502	9NY	C32-C34-C37-C39
4	A	502	9NY	C8-O2-P1-O7
4	C	502	9NY	C8-O2-P1-O7
4	A	502	9NY	C15-C17-C19-C21
4	C	502	9NY	C15-C17-C19-C21
4	A	502	9NY	C17-C19-C21-C23
4	C	502	9NY	C17-C19-C21-C23
3	B	201	6PL	O3P-C1-C2-O2
3	D	201	6PL	O3P-C1-C2-O2
4	A	502	9NY	C30-C11-C25-C36
4	C	502	9NY	C30-C11-C25-C36
4	A	502	9NY	C10-O4-P2-O8
4	C	502	9NY	C10-O4-P2-O8
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

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Mol	Chain	Res	Type	Atoms
3	B	201	6PL	C15-C16-C17-C18
3	D	201	6PL	C15-C16-C17-C18
3	A	501	6PL	C37-C38-C39-C40
3	C	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	D	201	6PL	C16-C17-C18-C19
3	B	201	6PL	C16-C17-C18-C19
4	A	502	9NY	C8-O2-P1-O5
4	C	502	9NY	C8-O2-P1-O5
4	A	502	9NY	C10-O4-P2-O9
4	C	502	9NY	C10-O4-P2-O9
3	B	201	6PL	C23-C24-C25-C26
3	D	201	6PL	C23-C24-C25-C26
3	A	501	6PL	C38-C39-C40-C41
4	C	502	9NY	C27-C29-C33-C35
3	C	501	6PL	C38-C39-C40-C41
4	A	502	9NY	C27-C29-C33-C35

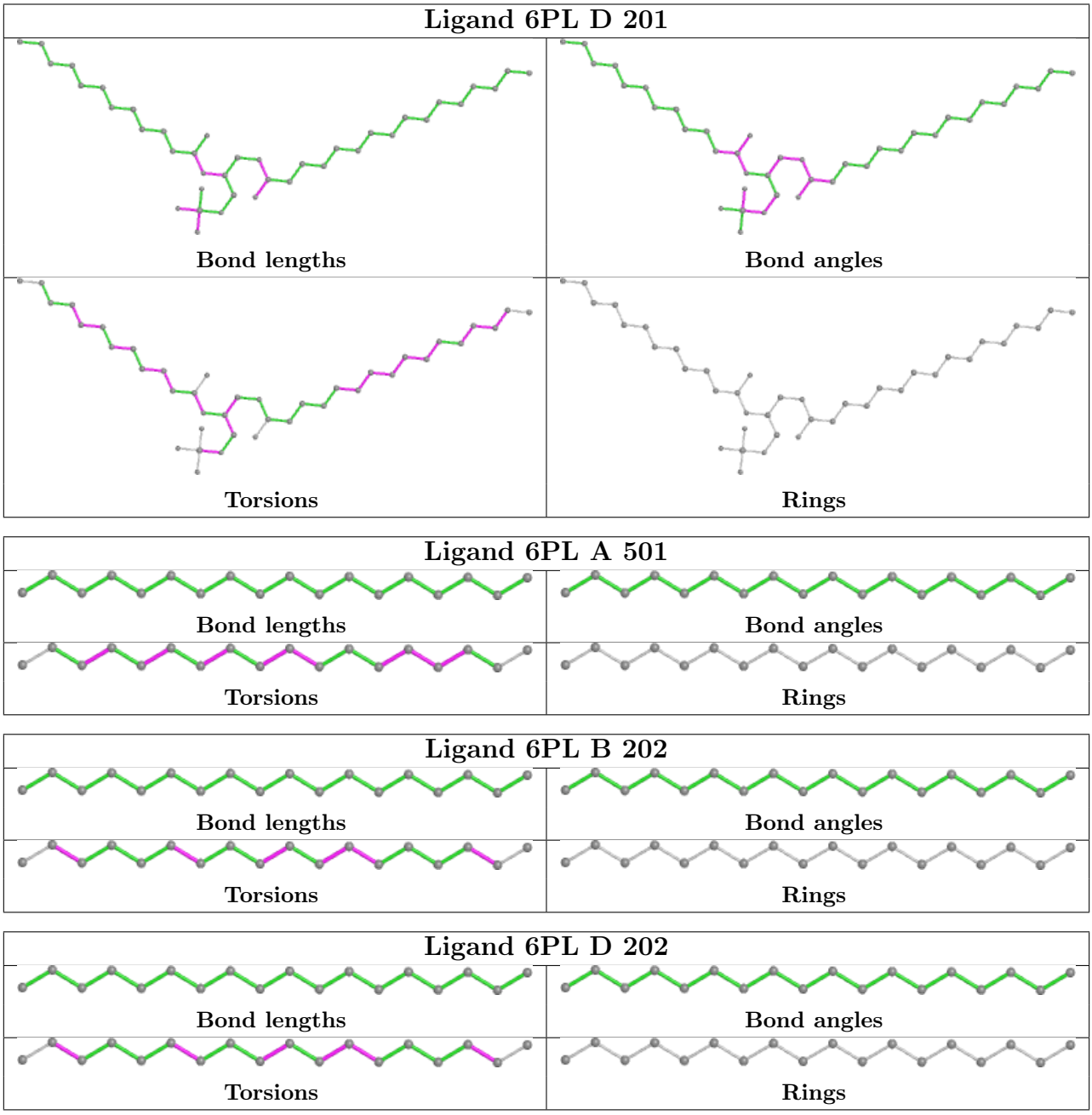
There are no ring outliers.

8 monomers are involved in 81 short contacts:

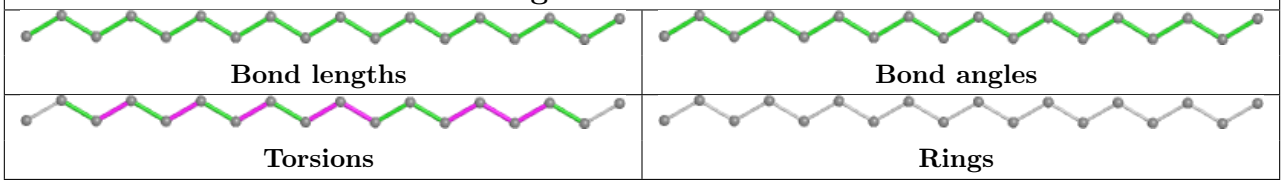
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	6PL	16	0
3	A	501	6PL	2	0
3	B	202	6PL	2	0
3	D	202	6PL	2	0
3	C	501	6PL	1	0
4	A	502	9NY	21	0
4	C	502	9NY	21	0
3	B	201	6PL	16	0

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 then 5% of the Mogul distribution of torsion angles is

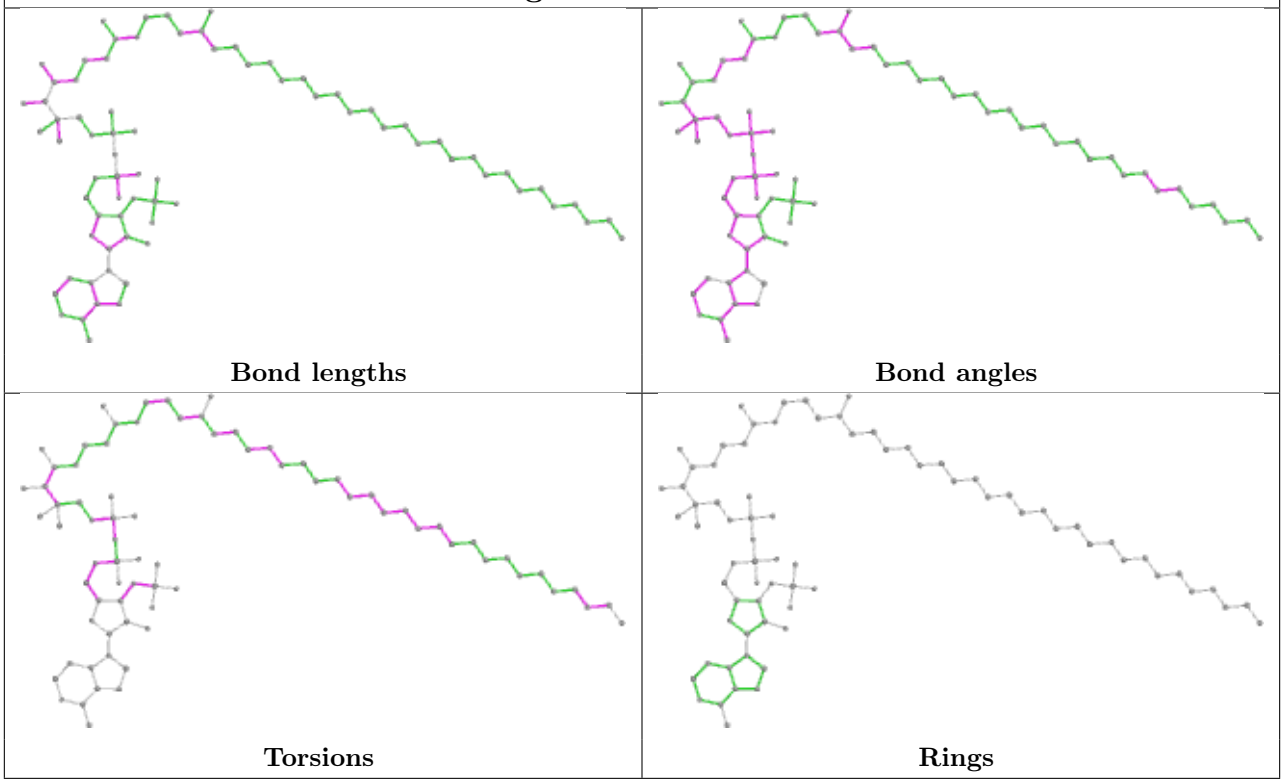
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



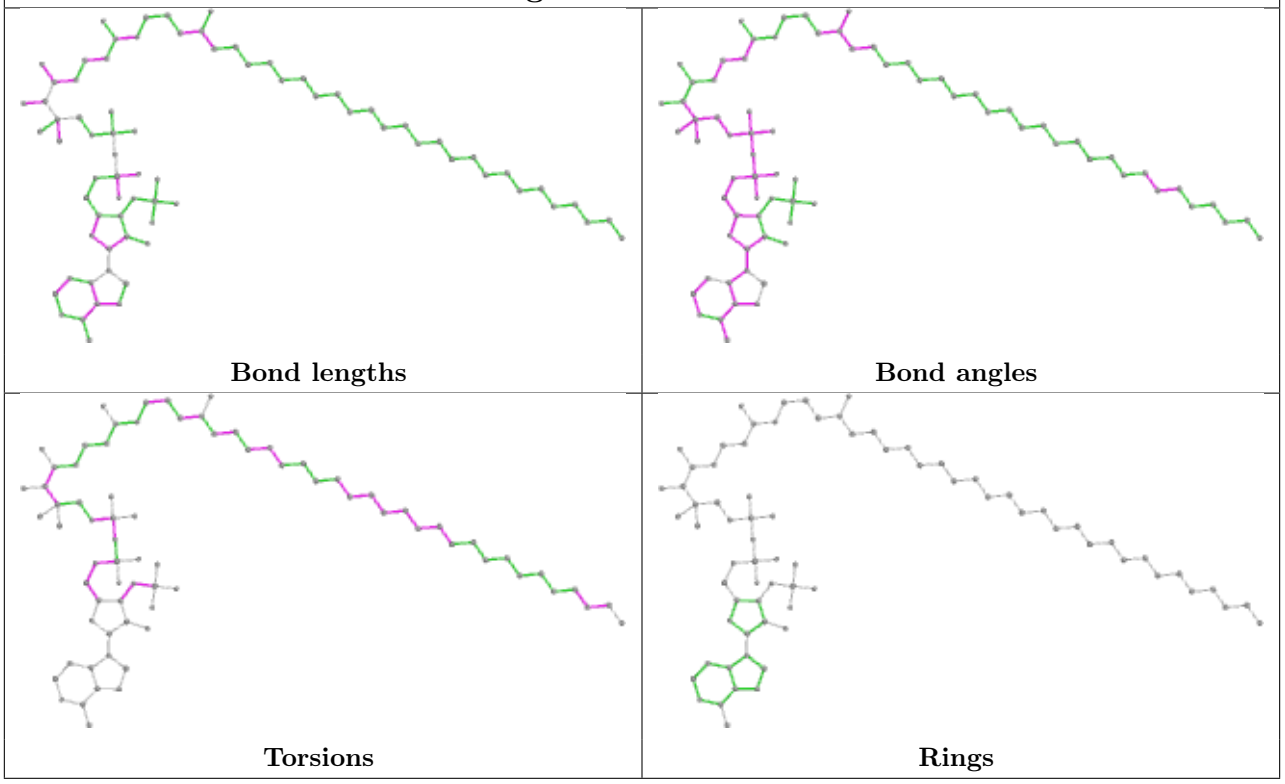
Ligand 6PL C 501



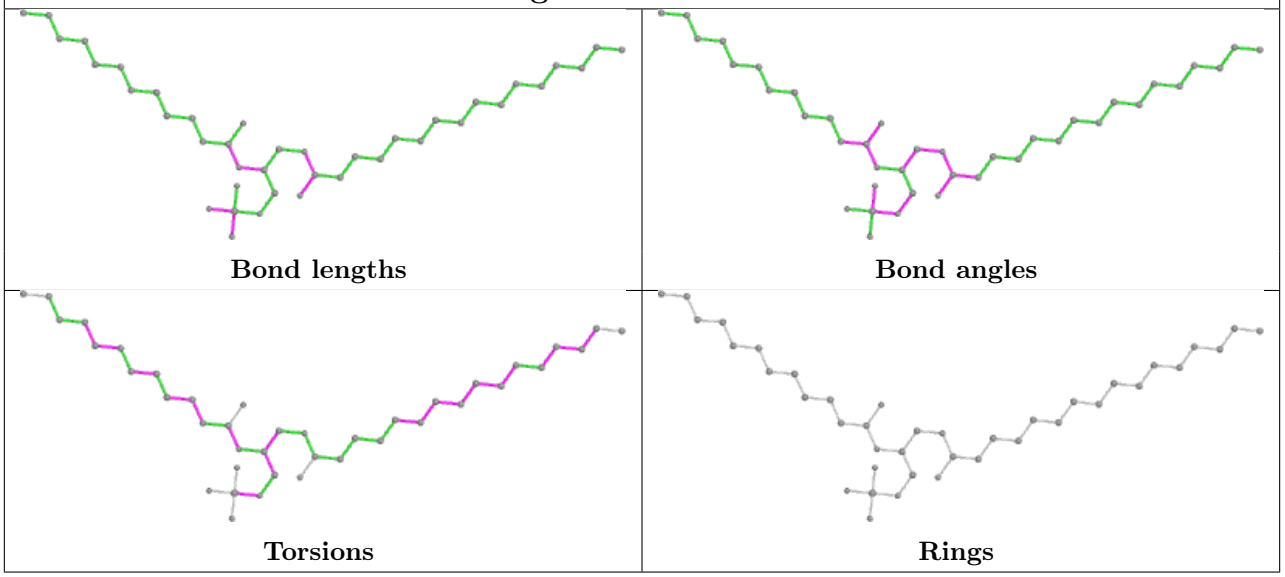
Ligand 9NY A 502



Ligand 9NY C 502



Ligand 6PL B 201



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.

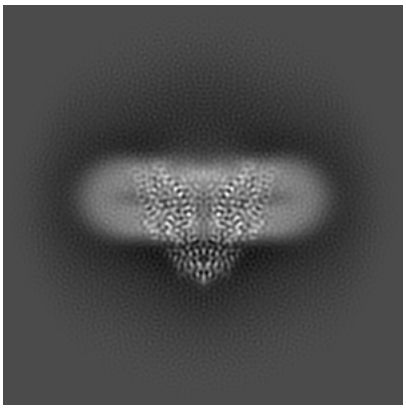
6 Map visualisation

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.

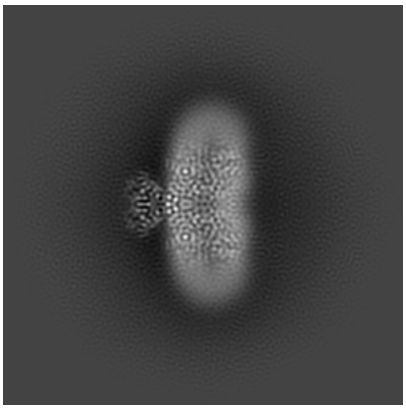
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

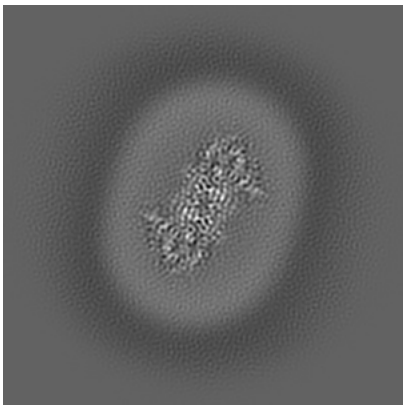
6.1.1 Primary map



X

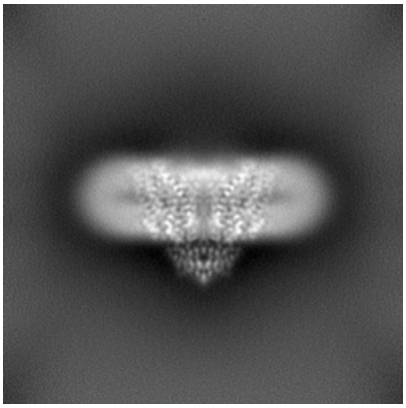


Y

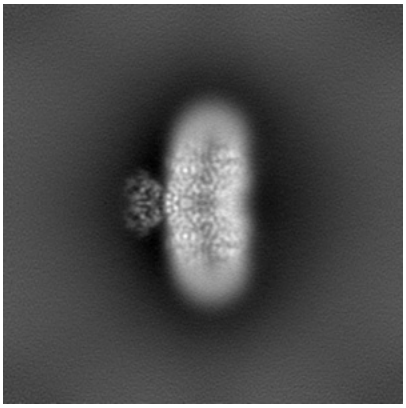


Z

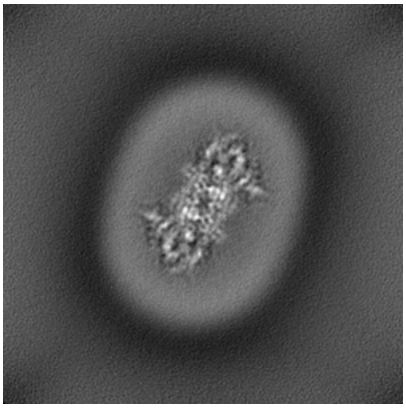
6.1.2 Raw map



X



Y

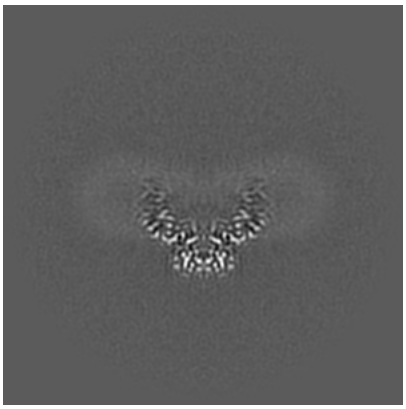


Z

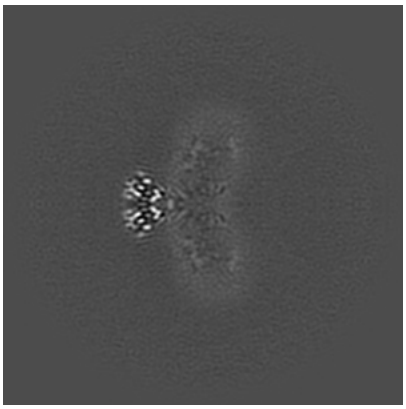
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

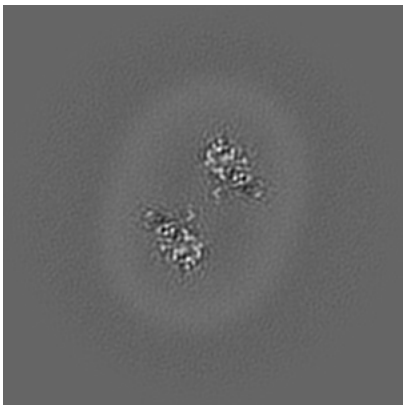
6.2.1 Primary map



X Index: 128

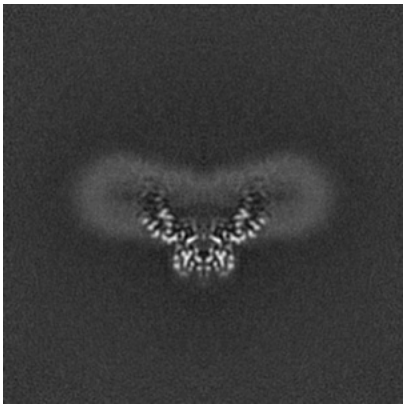


Y Index: 128

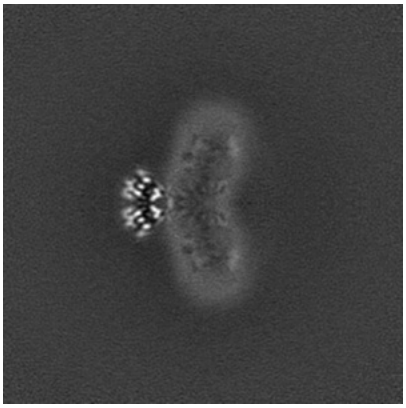


Z Index: 128

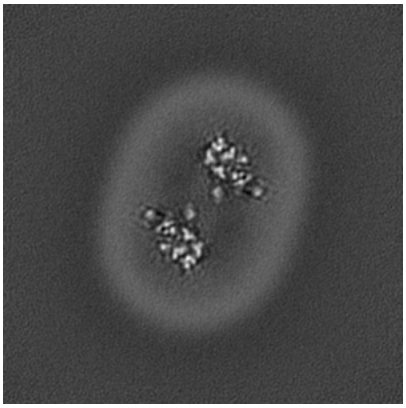
6.2.2 Raw map



X Index: 128



Y Index: 128

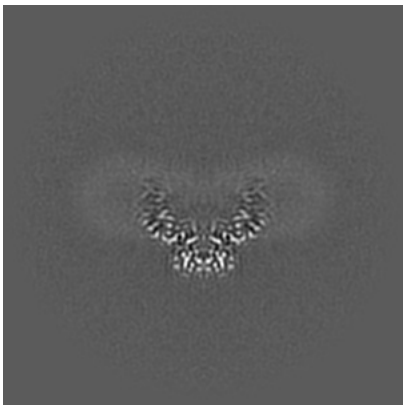


Z Index: 128

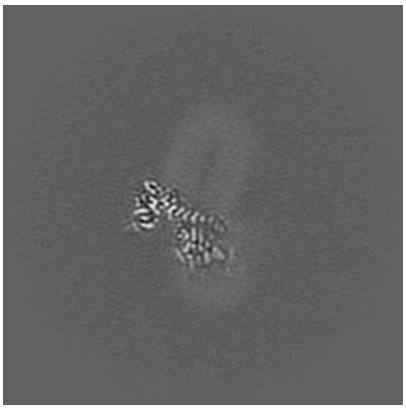
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

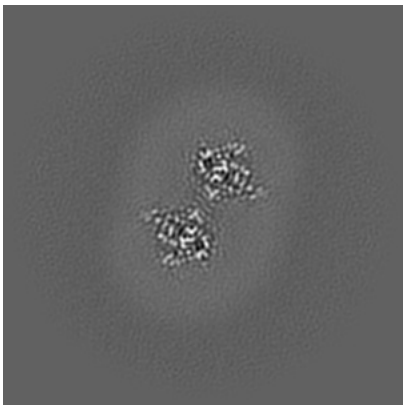
6.3.1 Primary map



X Index: 128

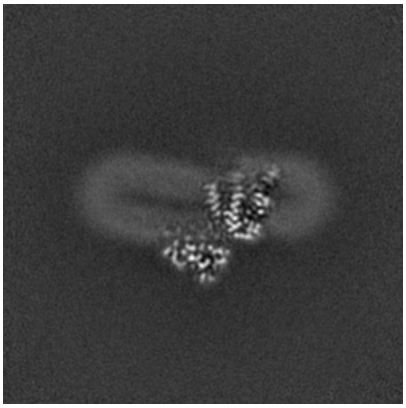


Y Index: 119

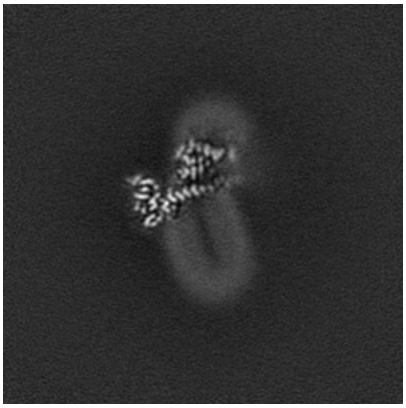


Z Index: 115

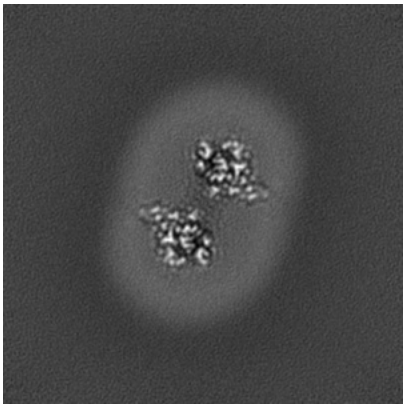
6.3.2 Raw map



X Index: 138



Y Index: 137

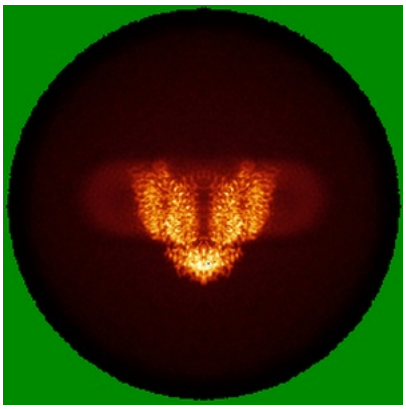


Z Index: 116

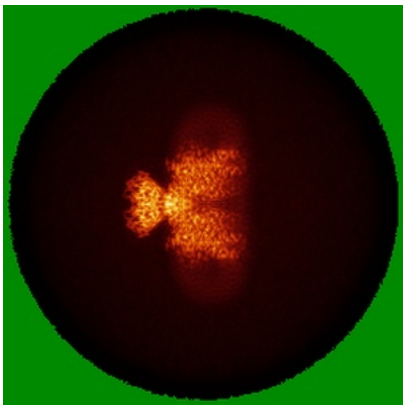
The images above show the largest variance slices of the map in three orthogonal directions.

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

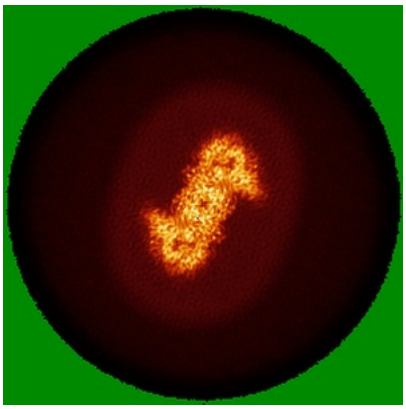
6.4.1 Primary map



X

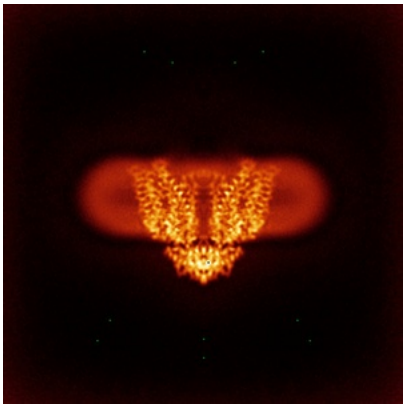


Y

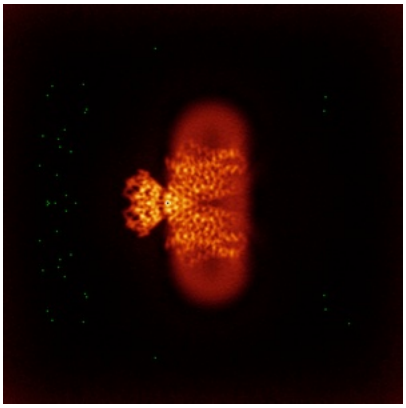


Z

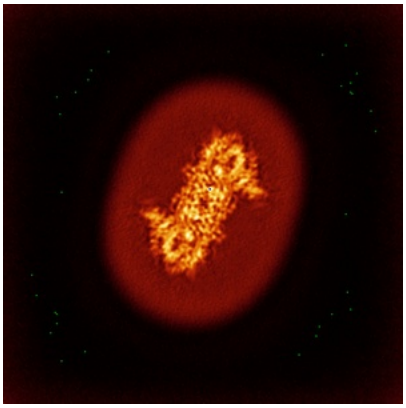
6.4.2 Raw map



X



Y

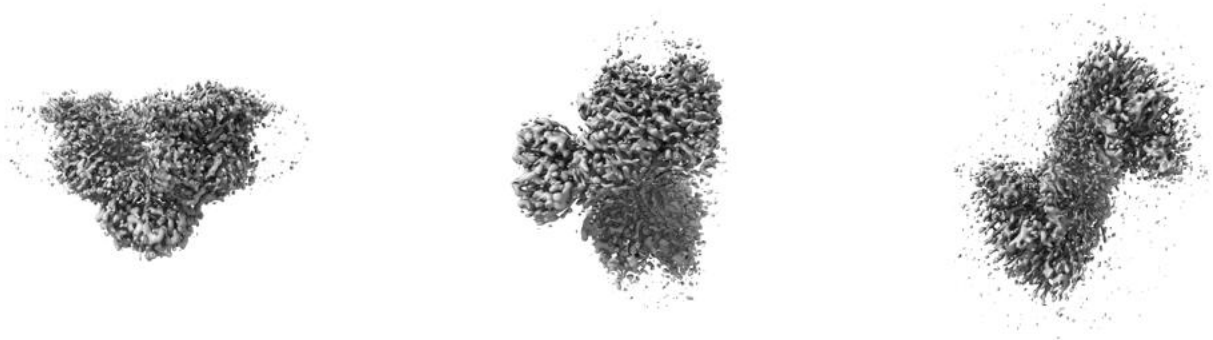


Z

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

6.5 Orthogonal surface views (i)

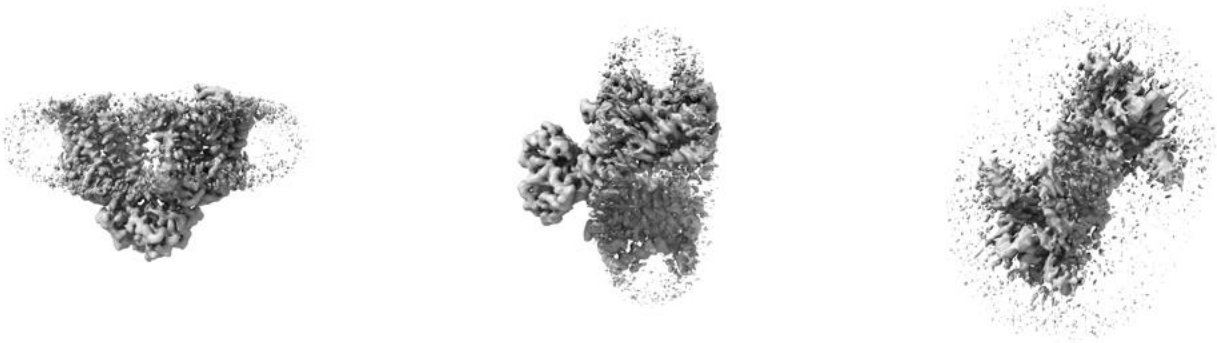
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.37. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

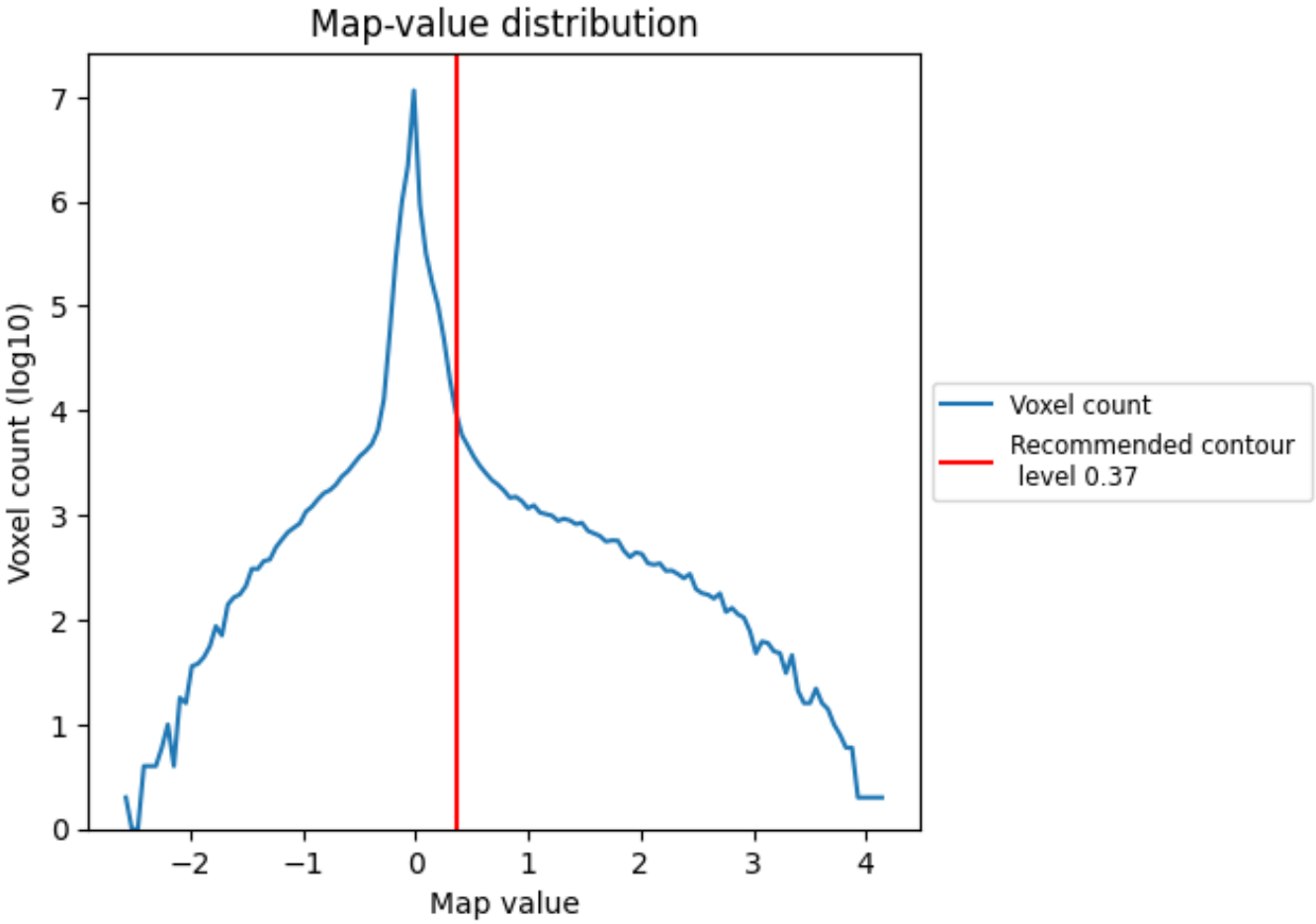
6.6 Mask visualisation (i)

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

7 Map analysis

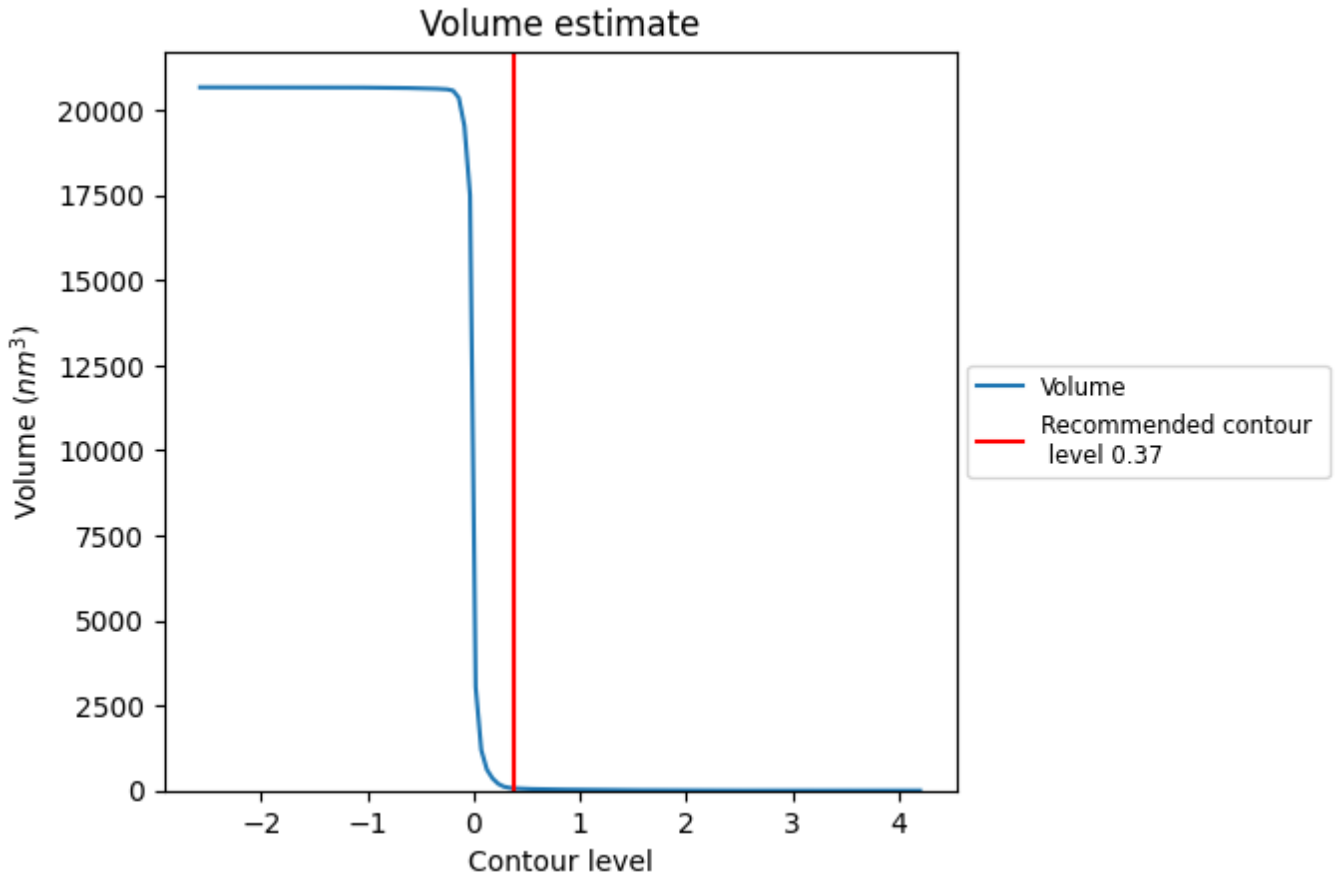
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

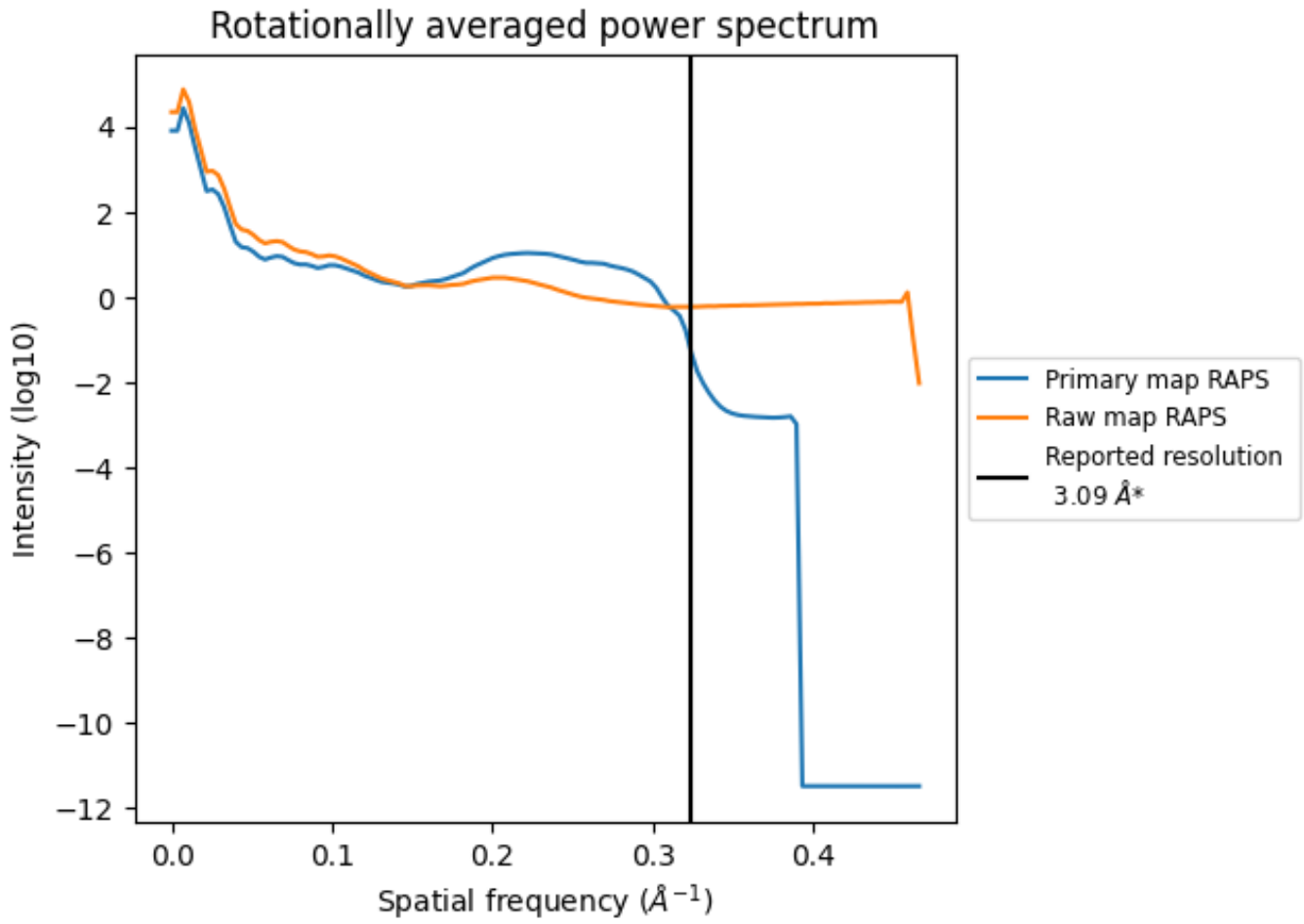
7.2 Volume estimate



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 (i)

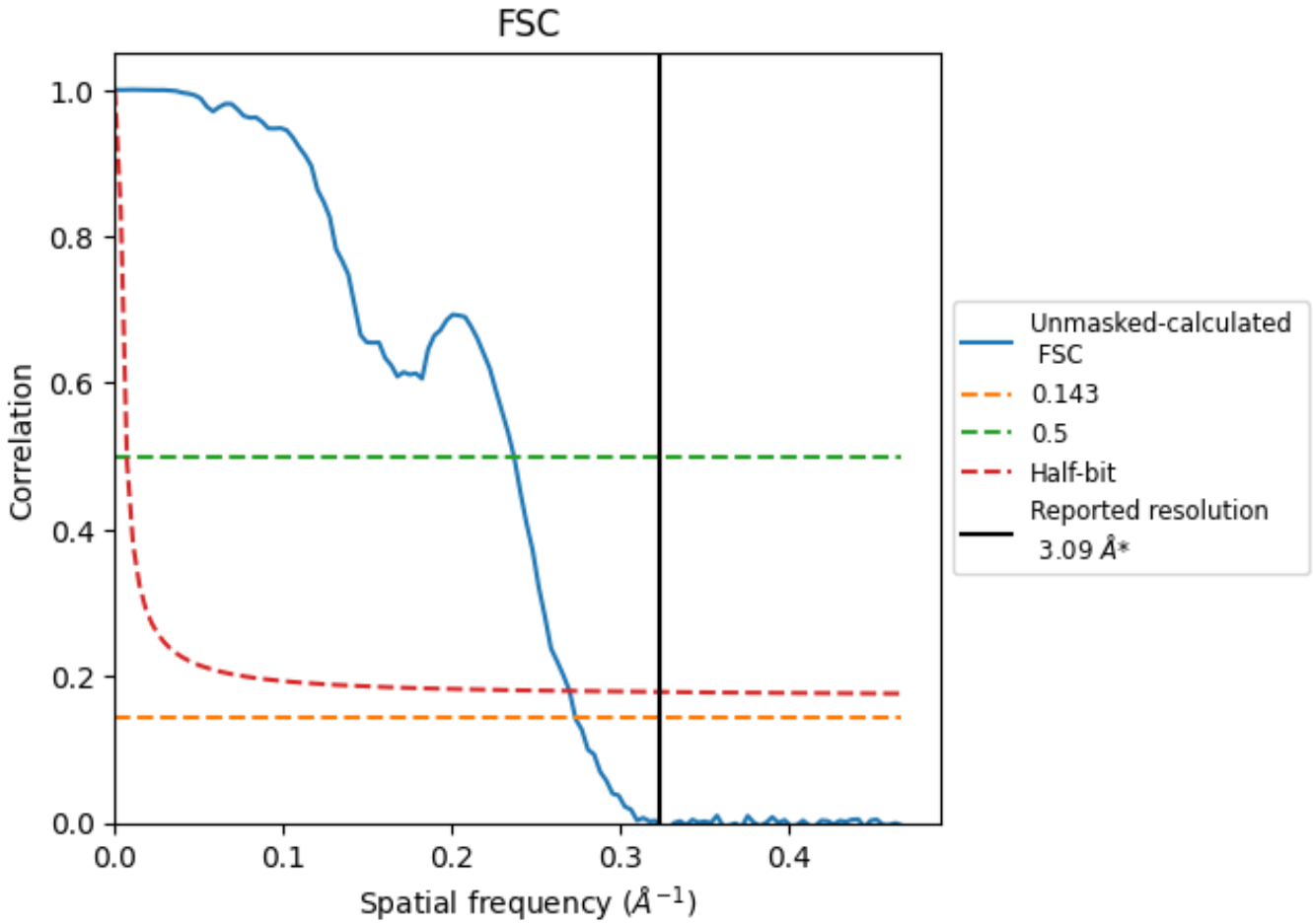


*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

8.2 Resolution estimates (i)

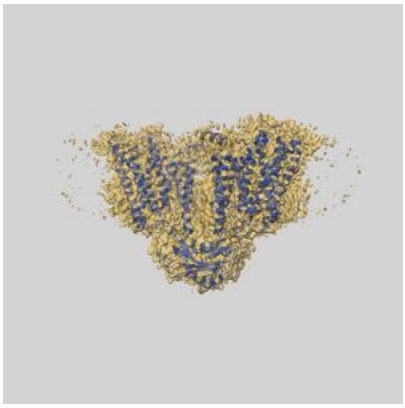
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.22	3.71

*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 %

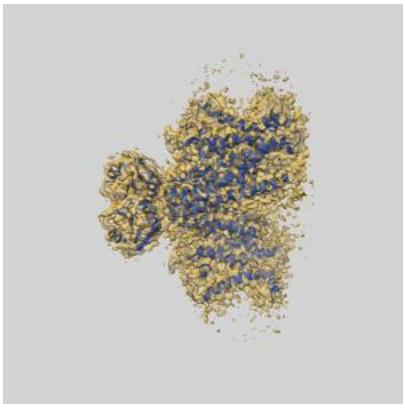
9 Map-model fit

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.

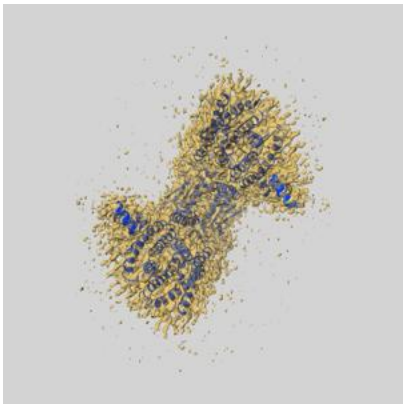
9.1 Map-model overlay



X



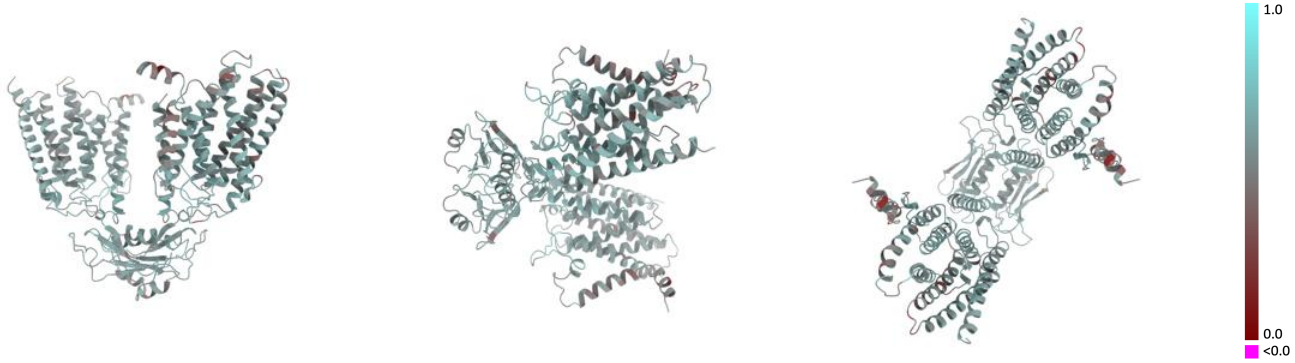
Y



Z

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.

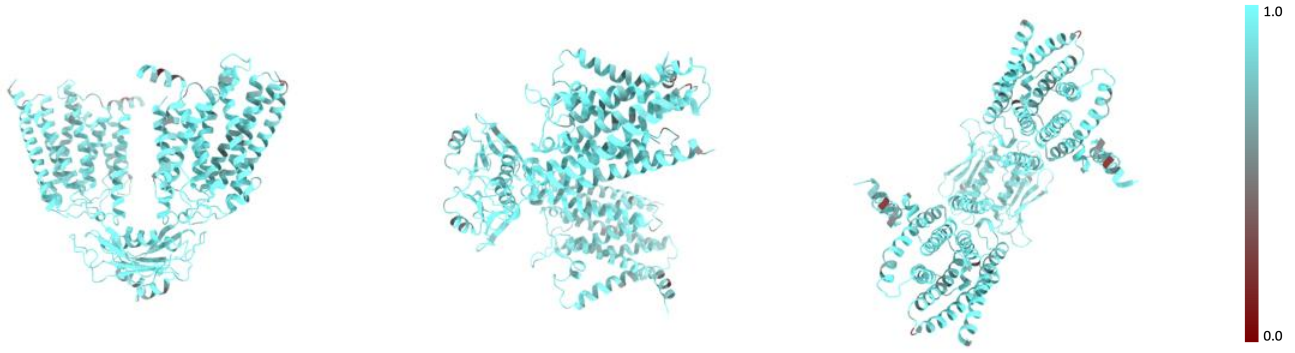
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

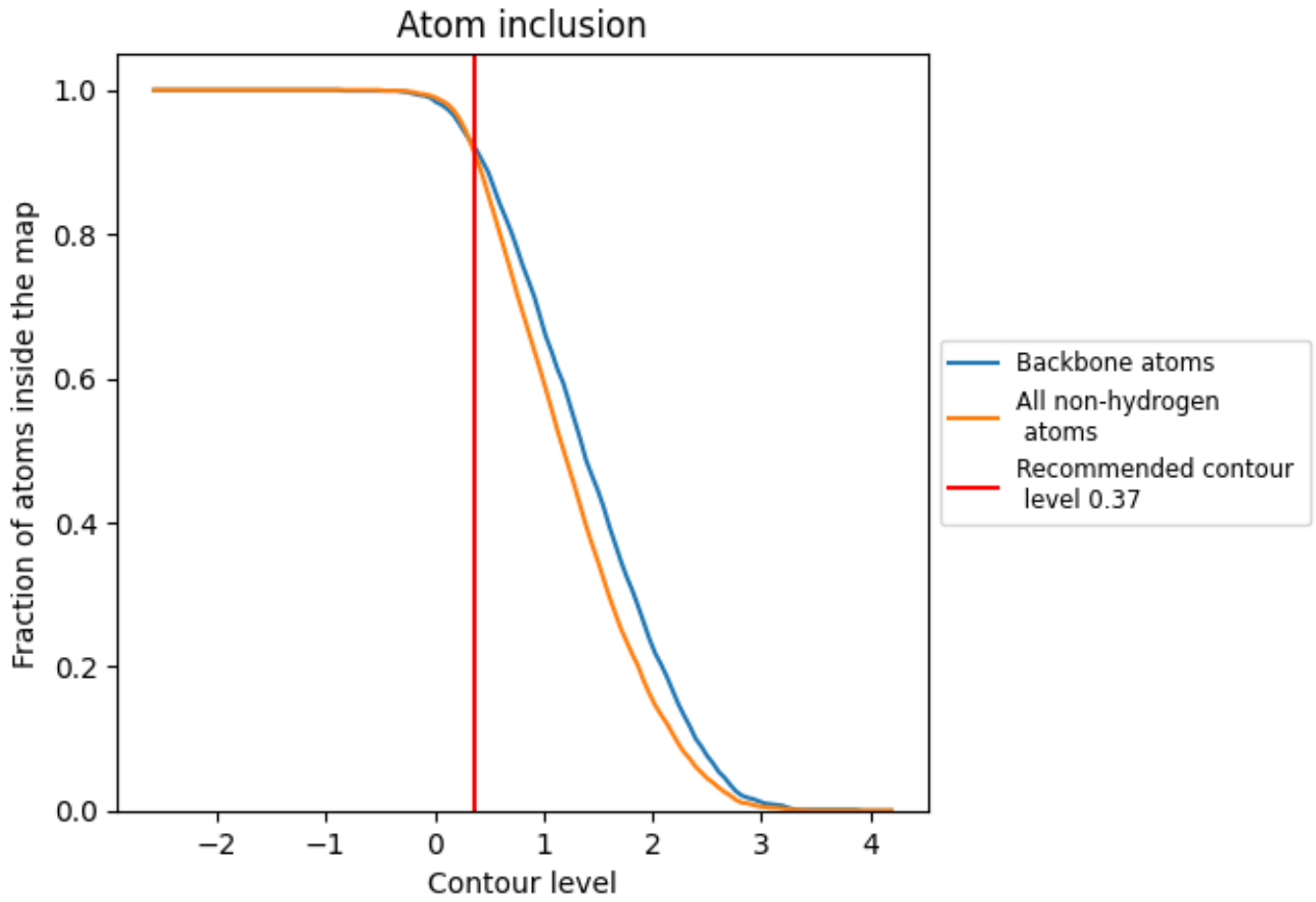
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.37).

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