



Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 10:22 PM EDT

PDB ID : 5SV9
EMDB ID : EMD-8313
Title : Structure of the SLC4 transporter Bor1p in an inward-facing conformation
Authors : Coudray, N.; Seyler, S.; Lasala, R.; Zhang, Z.; Clark, K.M.; Dumont, M.E.; Rohou, A.; Beckstein, O.; Stokes, D.L.; Transcontinental EM Initiative for Membrane Protein Structure (TEMIMPS)
Deposited on : 2016-08-05
Resolution : 5.90 Å(reported)
Based on initial model : 4YZF

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.dev43
MolProbity : 4.02b-467
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) : 2.31.2

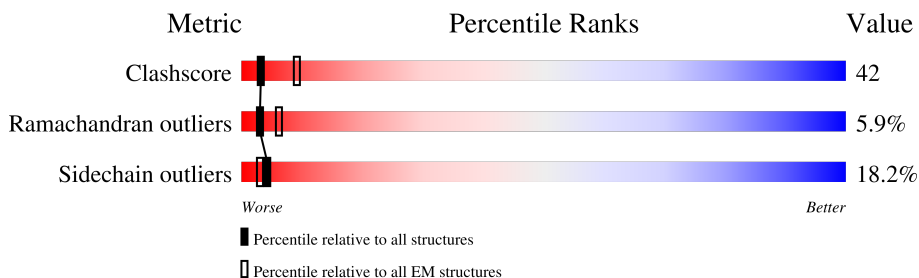
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	<div> <div>30%</div> <div>30%</div> <div>39%</div> <div>22%</div> <div>9%</div> </div>
1	B	476	<div> <div>28%</div> <div>26%</div> <div>40%</div> <div>24%</div> <div>10%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7612 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.

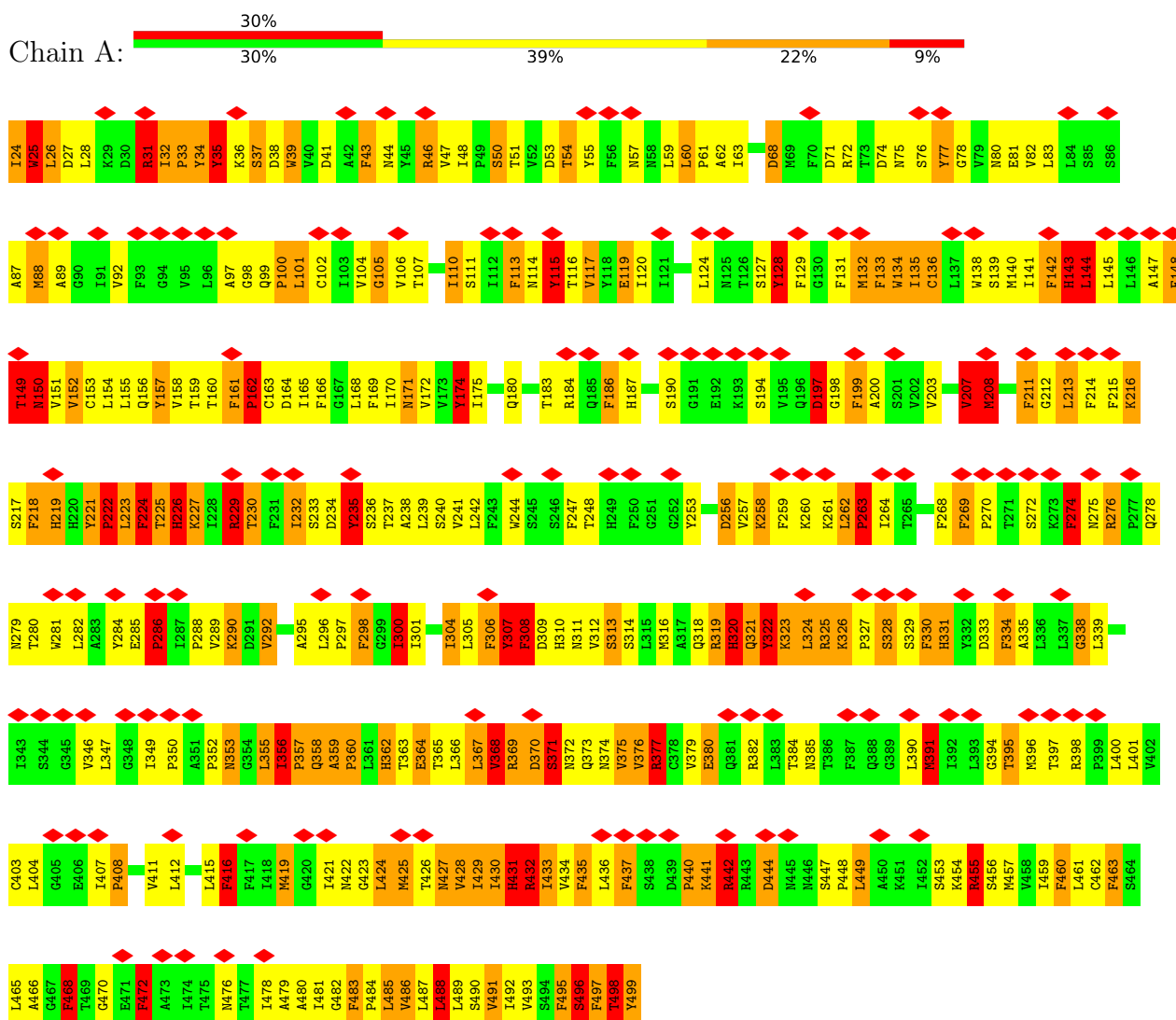
- Molecule 1 is a protein called Bor1p boron transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	476	Total	C	N	O	S	0	0
			3806	2527	608	652	19		
1	B	476	Total	C	N	O	S	0	0
			3806	2527	608	652	19		

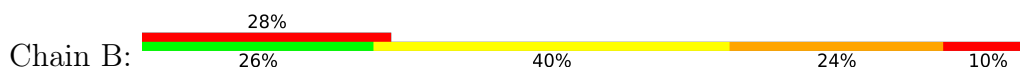
3 Residue-property plots

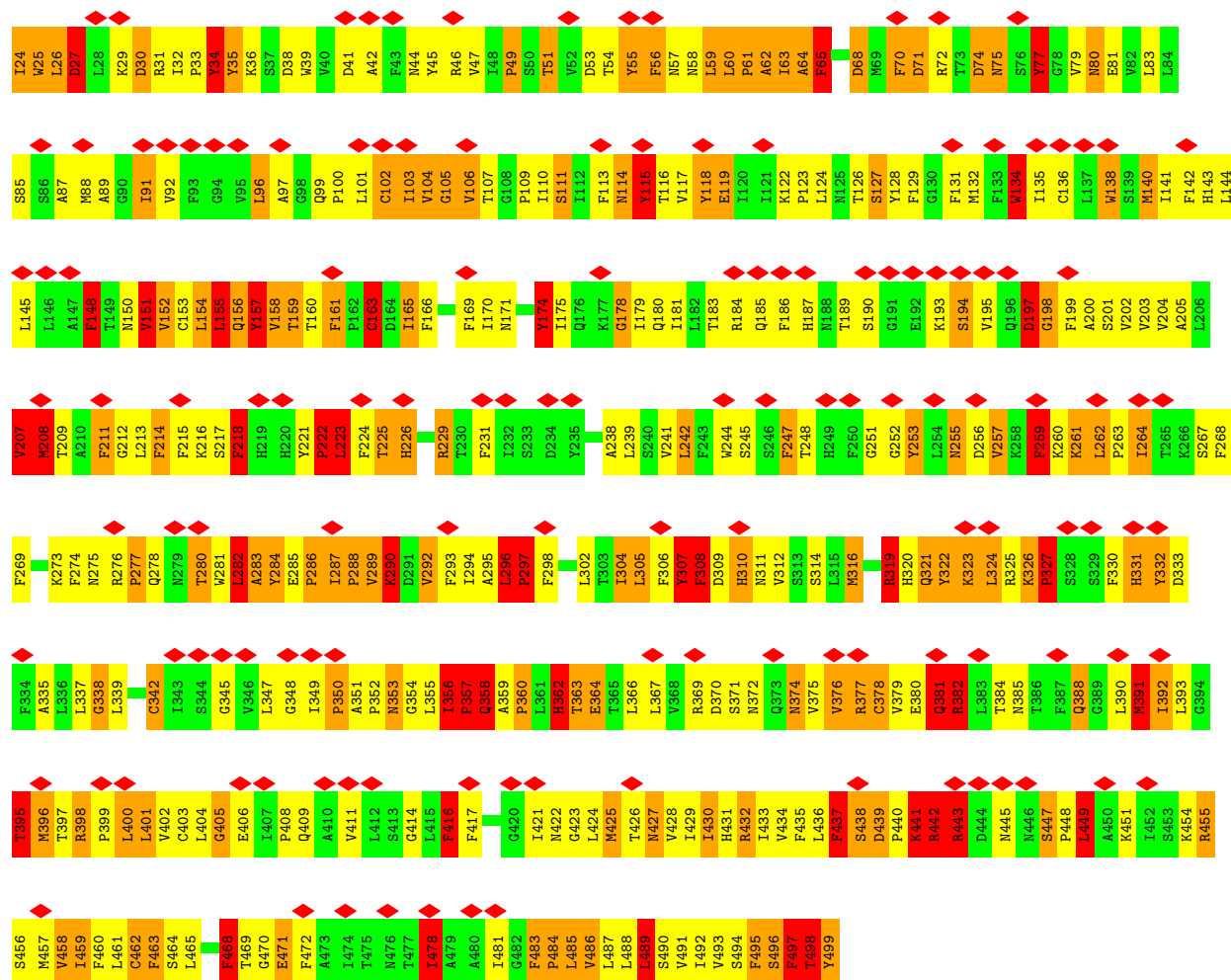
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Bor1p boron transporter



• Molecule 1: Bor1p boron transporter





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=37.35°, rise=4.8 Å, axial sym=C1	Depositor
Number of segments used	75	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	850	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	19000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	478.502	Depositor
Minimum map value	-365.121	Depositor
Average map value	0.789	Depositor
Map value standard deviation	24.341	Depositor
Recommended contour level	130.0	Depositor
Map size (Å)	183.82, 183.82, 183.82	wwPDB
Map dimensions	101, 101, 101	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.82, 1.82, 1.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.94	64/3917 (1.6%)	2.11	149/5333 (2.8%)
1	B	1.89	53/3917 (1.4%)	2.02	144/5333 (2.7%)
All	All	1.91	117/7834 (1.5%)	2.06	293/10666 (2.7%)

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	49
1	B	0	40
All	All	0	89

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	ARG	CD-NE	10.58	1.64	1.46
1	B	330	PHE	CB-CG	8.55	1.65	1.51
1	A	61	PRO	CA-C	-8.03	1.36	1.52
1	B	330	PHE	CA-CB	7.99	1.71	1.53
1	B	61	PRO	CA-C	-7.97	1.36	1.52
1	B	338	GLY	CA-C	-7.63	1.39	1.51
1	B	496	SER	N-CA	-7.42	1.31	1.46
1	A	320	HIS	CB-CG	7.08	1.62	1.50
1	B	432	ARG	CD-NE	7.04	1.58	1.46
1	B	308	PHE	CA-C	-7.01	1.34	1.52
1	B	309	ASP	CA-C	-6.74	1.35	1.52
1	A	432	ARG	NE-CZ	6.55	1.41	1.33
1	A	430	ILE	CA-C	-6.31	1.36	1.52
1	A	158	VAL	CA-CB	-6.31	1.41	1.54
1	A	460	PHE	CA-C	-6.28	1.36	1.52
1	A	162	PRO	CA-C	-6.22	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	430	ILE	CA-C	-6.21	1.36	1.52
1	B	134	TRP	CB-CG	-6.18	1.39	1.50
1	A	158	VAL	N-CA	-6.11	1.34	1.46
1	A	117	VAL	N-CA	-6.10	1.34	1.46
1	A	274	PHE	CB-CG	-6.10	1.41	1.51
1	A	408	PRO	CA-C	-6.03	1.40	1.52
1	B	357	PRO	CA-C	-6.03	1.40	1.52
1	A	486	VAL	N-CA	-6.02	1.34	1.46
1	A	221	TYR	CB-CG	6.02	1.60	1.51
1	A	432	ARG	CG-CD	5.95	1.66	1.51
1	B	60	LEU	C-N	-5.95	1.23	1.34
1	A	462	CYS	CA-C	-5.95	1.37	1.52
1	A	360	PRO	CA-C	-5.89	1.41	1.52
1	B	358	GLN	CA-C	-5.88	1.37	1.52
1	B	61	PRO	N-CD	-5.82	1.39	1.47
1	B	218	PHE	CA-C	-5.80	1.37	1.52
1	B	470	GLY	CA-C	-5.79	1.42	1.51
1	A	274	PHE	CA-C	-5.78	1.38	1.52
1	A	470	GLY	CA-C	-5.76	1.42	1.51
1	A	60	LEU	C-N	-5.75	1.23	1.34
1	A	491	VAL	N-CA	-5.70	1.34	1.46
1	B	100	PRO	CA-C	-5.63	1.41	1.52
1	A	239	LEU	CA-C	-5.61	1.38	1.52
1	B	65	PHE	CB-CG	-5.60	1.41	1.51
1	B	405	GLY	CA-C	-5.57	1.43	1.51
1	A	74	ASP	CA-C	-5.57	1.38	1.52
1	A	359	ALA	N-CA	-5.55	1.35	1.46
1	B	308	PHE	N-CA	-5.54	1.35	1.46
1	B	49	PRO	CA-C	-5.53	1.41	1.52
1	B	64	ALA	N-CA	-5.52	1.35	1.46
1	A	242	LEU	N-CA	-5.50	1.35	1.46
1	B	63	ILE	CA-C	-5.49	1.38	1.52
1	A	236	SER	N-CA	-5.48	1.35	1.46
1	B	208	MET	N-CA	-5.47	1.35	1.46
1	B	310	HIS	N-CA	-5.47	1.35	1.46
1	B	314	SER	CA-C	-5.46	1.38	1.52
1	B	308	PHE	CB-CG	-5.45	1.42	1.51
1	A	229	ARG	CA-C	-5.45	1.38	1.52
1	B	360	PRO	CA-C	-5.45	1.42	1.52
1	A	25	TRP	CA-C	-5.44	1.38	1.52
1	A	116	THR	CA-C	-5.44	1.38	1.52
1	A	226	HIS	CA-C	-5.44	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	LEU	N-CA	-5.44	1.35	1.46
1	B	486	VAL	N-CA	-5.44	1.35	1.46
1	A	240	SER	N-CA	-5.43	1.35	1.46
1	A	338	GLY	CA-C	-5.43	1.43	1.51
1	B	455	ARG	CA-C	-5.42	1.38	1.52
1	A	227	LYS	N-CA	-5.41	1.35	1.46
1	A	320	HIS	CA-CB	5.41	1.65	1.53
1	B	134	TRP	CA-C	-5.40	1.39	1.52
1	B	212	GLY	CA-C	-5.40	1.43	1.51
1	A	401	LEU	N-CA	-5.40	1.35	1.46
1	A	240	SER	CA-C	-5.39	1.39	1.52
1	A	314	SER	CA-C	-5.38	1.39	1.52
1	A	304	ILE	N-CA	-5.37	1.35	1.46
1	A	485	LEU	CA-C	-5.35	1.39	1.52
1	A	357	PRO	CA-C	-5.35	1.42	1.52
1	A	356	ILE	N-CA	-5.34	1.35	1.46
1	A	159	THR	N-CA	-5.33	1.35	1.46
1	B	311	ASN	N-CA	-5.33	1.35	1.46
1	A	429	ILE	N-CA	-5.30	1.35	1.46
1	B	65	PHE	CA-C	-5.29	1.39	1.52
1	A	498	THR	N-CA	-5.28	1.35	1.46
1	B	378	CYS	CA-C	-5.27	1.39	1.52
1	A	308	PHE	N-CA	-5.27	1.35	1.46
1	B	374	ASN	CA-C	-5.26	1.39	1.52
1	A	428	VAL	CA-C	-5.26	1.39	1.52
1	A	105	GLY	N-CA	-5.24	1.38	1.46
1	A	48	ILE	N-CA	-5.22	1.35	1.46
1	B	198	GLY	CA-C	-5.21	1.43	1.51
1	A	274	PHE	N-CA	-5.20	1.35	1.46
1	A	465	LEU	CA-C	-5.20	1.39	1.52
1	B	178	GLY	CA-C	-5.19	1.43	1.51
1	A	160	THR	CA-C	5.19	1.66	1.52
1	A	490	SER	CA-C	-5.18	1.39	1.52
1	B	222	PRO	CA-C	-5.17	1.42	1.52
1	A	313	SER	N-CA	-5.17	1.36	1.46
1	A	33	PRO	CA-C	-5.16	1.42	1.52
1	B	59	LEU	N-CA	-5.15	1.36	1.46
1	A	309	ASP	CA-C	-5.14	1.39	1.52
1	B	306	PHE	CA-C	-5.14	1.39	1.52
1	B	59	LEU	CA-C	-5.11	1.39	1.52
1	B	239	LEU	CA-C	-5.11	1.39	1.52
1	B	157	TYR	CA-C	-5.10	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	MET	N-CA	-5.09	1.36	1.46
1	A	355	LEU	CA-C	-5.09	1.39	1.52
1	B	405	GLY	N-CA	-5.09	1.38	1.46
1	B	157	TYR	N-CA	-5.08	1.36	1.46
1	B	62	ALA	N-CA	-5.08	1.36	1.46
1	B	362	HIS	CA-C	-5.07	1.39	1.52
1	B	363	THR	N-CA	-5.07	1.36	1.46
1	A	161	PHE	C-N	-5.06	1.24	1.34
1	B	105	GLY	N-CA	-5.05	1.38	1.46
1	B	140	MET	N-CA	-5.05	1.36	1.46
1	A	197	ASP	CA-C	-5.04	1.39	1.52
1	A	366	LEU	CA-C	-5.04	1.39	1.52
1	B	401	LEU	N-CA	-5.03	1.36	1.46
1	A	212	GLY	CA-C	-5.03	1.43	1.51
1	B	242	LEU	N-CA	-5.02	1.36	1.46
1	A	143	HIS	CB-CG	-5.01	1.41	1.50
1	A	440	PRO	CA-C	-5.00	1.42	1.52

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	TRP	CB-CG-CD2	-16.62	104.99	126.60
1	B	221	TYR	CB-CG-CD1	14.58	129.75	121.00
1	A	221	TYR	CB-CG-CD1	14.12	129.47	121.00
1	B	174	TYR	CB-CG-CD2	-12.92	113.25	121.00
1	A	499	TYR	CB-CG-CD1	12.44	128.46	121.00
1	A	496	SER	N-CA-CB	-12.30	92.05	110.50
1	A	499	TYR	CB-CG-CD2	-11.92	113.85	121.00
1	A	322	TYR	CB-CG-CD2	-11.76	113.94	121.00
1	B	330	PHE	CB-CG-CD1	11.71	128.99	120.80
1	B	416	PHE	CB-CG-CD2	-11.59	112.69	120.80
1	A	416	PHE	CB-CG-CD2	-11.52	112.74	120.80
1	B	221	TYR	CB-CG-CD2	-11.09	114.35	121.00
1	A	235	TYR	CB-CG-CD2	-10.60	114.64	121.00
1	B	463	PHE	CB-CG-CD1	10.50	128.15	120.80
1	A	290	LYS	N-CA-CB	-10.48	91.73	110.60
1	A	391	MET	CG-SD-CE	-10.48	83.44	100.20
1	B	391	MET	CG-SD-CE	-10.40	83.56	100.20
1	A	34	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	B	157	TYR	CB-CG-CD1	10.31	127.19	121.00
1	A	115	TYR	CB-CG-CD1	10.27	127.16	121.00
1	A	77	TYR	CB-CG-CD2	-10.26	114.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	TYR	CB-CG-CD1	10.17	127.10	121.00
1	A	330	PHE	CB-CG-CD1	10.16	127.91	120.80
1	B	157	TYR	CB-CG-CD2	-10.09	114.95	121.00
1	B	463	PHE	CB-CG-CD2	-10.03	113.78	120.80
1	A	207	VAL	CA-CB-CG1	9.99	125.89	110.90
1	A	377	ARG	N-CA-CB	9.76	128.17	110.60
1	B	218	PHE	CB-CG-CD2	-9.73	113.98	120.80
1	B	497	PHE	CA-C-N	-9.71	95.84	117.20
1	A	133	PHE	CB-CG-CD1	9.67	127.57	120.80
1	A	157	TYR	CB-CG-CD2	-9.65	115.21	121.00
1	A	128	TYR	CB-CG-CD1	-9.56	115.26	121.00
1	A	221	TYR	CB-CG-CD2	-9.47	115.32	121.00
1	A	320	HIS	CA-CB-CG	9.43	129.63	113.60
1	B	330	PHE	CA-CB-CG	9.41	136.49	113.90
1	A	427	ASN	N-CA-C	-9.37	85.69	111.00
1	A	219	HIS	CA-CB-CG	9.23	129.29	113.60
1	A	232	ILE	N-CA-C	9.05	135.44	111.00
1	A	115	TYR	CB-CG-CD2	-8.94	115.63	121.00
1	A	306	PHE	CB-CG-CD2	-8.90	114.57	120.80
1	A	435	PHE	CB-CG-CD1	8.68	126.88	120.80
1	A	330	PHE	CB-CG-CD2	-8.57	114.80	120.80
1	B	159	THR	N-CA-CB	8.54	126.53	110.30
1	A	157	TYR	CB-CG-CD1	8.50	126.10	121.00
1	B	115	TYR	CB-CG-CD1	8.45	126.07	121.00
1	A	221	TYR	CA-CB-CG	8.44	129.43	113.40
1	B	443	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	B	308	PHE	CB-CG-CD2	-8.38	114.93	120.80
1	B	161	PHE	N-CA-C	8.37	133.60	111.00
1	A	161	PHE	N-CA-C	8.35	133.55	111.00
1	A	77	TYR	CB-CG-CD1	8.35	126.01	121.00
1	A	462	CYS	CA-CB-SG	-8.33	99.00	114.00
1	A	133	PHE	CB-CG-CD2	-8.23	115.04	120.80
1	A	468	PHE	CB-CG-CD1	-8.19	115.07	120.80
1	A	435	PHE	CB-CG-CD2	-8.16	115.09	120.80
1	B	140	MET	CG-SD-CE	-8.10	87.24	100.20
1	B	34	TYR	CB-CG-CD2	-8.06	116.17	121.00
1	B	105	GLY	C-N-CA	8.02	141.76	121.70
1	A	159	THR	N-CA-C	-7.93	89.59	111.00
1	B	499	TYR	N-CA-CB	-7.88	96.42	110.60
1	B	372	ASN	N-CA-C	-7.84	89.82	111.00
1	A	171	ASN	CB-CA-C	-7.82	94.77	110.40
1	B	65	PHE	N-CA-CB	7.76	124.57	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	TYR	CB-CG-CD2	-7.69	116.39	121.00
1	A	186	PHE	CB-CG-CD1	7.60	126.12	120.80
1	A	463	PHE	CB-CG-CD2	-7.53	115.53	120.80
1	A	307	TYR	CB-CG-CD2	7.51	125.50	121.00
1	A	419	MET	N-CA-CB	-7.46	97.17	110.60
1	A	156	GLN	N-CA-CB	-7.45	97.20	110.60
1	B	253	TYR	CA-CB-CG	7.44	127.54	113.40
1	B	443	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	225	THR	N-CA-CB	7.43	124.42	110.30
1	B	215	PHE	CB-CG-CD1	7.42	125.99	120.80
1	B	155	LEU	CB-CG-CD1	7.38	123.55	111.00
1	B	379	VAL	N-CA-C	-7.38	91.08	111.00
1	A	376	VAL	N-CA-C	-7.34	91.17	111.00
1	B	218	PHE	CA-CB-CG	-7.33	96.31	113.90
1	B	27	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	322	TYR	C-N-CA	7.25	139.82	121.70
1	B	221	TYR	CA-CB-CG	7.22	127.12	113.40
1	B	151	VAL	C-N-CA	7.20	139.69	121.70
1	A	186	PHE	CB-CG-CD2	-7.18	115.77	120.80
1	B	174	TYR	CB-CG-CD1	7.18	125.31	121.00
1	B	262	LEU	CB-CA-C	-7.17	96.58	110.20
1	B	468	PHE	CB-CG-CD1	-7.14	115.80	120.80
1	B	194	SER	N-CA-CB	7.06	121.09	110.50
1	B	238	ALA	CB-CA-C	-7.02	99.57	110.10
1	A	194	SER	C-N-CA	6.94	139.05	121.70
1	A	235	TYR	CB-CA-C	-6.91	96.58	110.40
1	A	455	ARG	CD-NE-CZ	-6.89	113.95	123.60
1	B	437	PHE	CB-CG-CD2	-6.88	115.98	120.80
1	A	74	ASP	CA-CB-CG	-6.85	98.32	113.40
1	A	211	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	A	284	TYR	CA-CB-CG	-6.83	100.42	113.40
1	B	321	GLN	CB-CA-C	-6.82	96.76	110.40
1	B	289	VAL	N-CA-C	6.74	129.19	111.00
1	A	432	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	B	207	VAL	CA-CB-CG1	6.71	120.96	110.90
1	A	215	PHE	CB-CG-CD1	6.70	125.49	120.80
1	A	217	SER	CB-CA-C	-6.69	97.39	110.10
1	A	264	ILE	C-N-CA	6.68	138.39	121.70
1	A	486	VAL	N-CA-CB	-6.67	96.83	111.50
1	B	159	THR	N-CA-C	-6.66	93.02	111.00
1	A	329	SER	N-CA-CB	6.64	120.46	110.50
1	B	114	ASN	CA-CB-CG	-6.64	98.79	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	PHE	CB-CG-CD1	6.62	125.44	120.80
1	A	105	GLY	C-N-CA	6.62	138.26	121.70
1	A	368	VAL	N-CA-C	-6.62	93.14	111.00
1	B	215	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	A	274	PHE	CA-C-N	-6.57	102.75	117.20
1	B	437	PHE	CA-CB-CG	-6.52	98.25	113.90
1	A	34	TYR	CA-CB-CG	-6.52	101.01	113.40
1	A	488	LEU	CB-CG-CD1	6.51	122.06	111.00
1	A	197	ASP	CB-CA-C	-6.49	97.42	110.40
1	A	157	TYR	N-CA-CB	-6.45	98.99	110.60
1	B	496	SER	N-CA-CB	-6.45	100.83	110.50
1	A	89	ALA	CB-CA-C	-6.43	100.45	110.10
1	A	419	MET	CA-CB-CG	6.43	124.23	113.30
1	B	217	SER	N-CA-C	6.43	128.35	111.00
1	A	88	MET	N-CA-CB	6.41	122.14	110.60
1	B	499	TYR	CB-CG-CD1	6.40	124.84	121.00
1	A	160	THR	N-CA-C	6.39	128.26	111.00
1	B	25	TRP	CB-CG-CD2	-6.38	118.31	126.60
1	B	326	LYS	CB-CA-C	-6.38	97.65	110.40
1	B	70	PHE	CB-CG-CD2	-6.35	116.35	120.80
1	A	496	SER	N-CA-C	6.35	128.14	111.00
1	B	306	PHE	CB-CG-CD2	-6.35	116.36	120.80
1	B	283	ALA	C-N-CA	6.31	137.48	121.70
1	A	300	ILE	CA-CB-CG1	6.30	122.98	111.00
1	A	148	PHE	CB-CG-CD1	6.27	125.19	120.80
1	A	472	PHE	CB-CG-CD2	-6.26	116.42	120.80
1	A	224	PHE	CB-CG-CD1	6.25	125.17	120.80
1	B	124	LEU	N-CA-C	-6.24	94.14	111.00
1	B	208	MET	CG-SD-CE	-6.23	90.23	100.20
1	B	221	TYR	N-CA-C	-6.23	94.18	111.00
1	A	128	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	B	427	ASN	CB-CA-C	6.22	122.83	110.40
1	B	160	THR	N-CA-CB	-6.18	98.56	110.30
1	A	163	CYS	CA-CB-SG	-6.17	102.89	114.00
1	B	154	LEU	CB-CG-CD1	6.17	121.49	111.00
1	A	371	SER	N-CA-CB	6.17	119.75	110.50
1	B	189	THR	C-N-CA	6.11	136.96	121.70
1	B	321	GLN	N-CA-CB	6.11	121.59	110.60
1	B	438	SER	C-N-CA	6.08	136.90	121.70
1	A	31	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	258	LYS	N-CA-CB	6.07	121.53	110.60
1	B	432	ARG	NE-CZ-NH2	6.07	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	A	497	PHE	CA-C-N	-6.04	103.92	117.20
1	B	322	TYR	CB-CG-CD1	6.03	124.62	121.00
1	B	311	ASN	N-CA-CB	-6.02	99.76	110.60
1	A	148	PHE	CB-CG-CD2	-6.02	116.58	120.80
1	A	437	PHE	CA-CB-CG	-6.02	99.46	113.90
1	A	371	SER	N-CA-C	-6.01	94.76	111.00
1	A	325	ARG	C-N-CA	6.01	136.72	121.70
1	A	242	LEU	N-CA-CB	-6.00	98.41	110.40
1	B	208	MET	N-CA-CB	-5.99	99.82	110.60
1	B	134	TRP	CB-CA-C	-5.98	98.44	110.40
1	B	449	LEU	CB-CA-C	-5.97	98.86	110.20
1	B	400	LEU	N-CA-CB	5.96	122.31	110.40
1	B	88	MET	N-CA-CB	5.95	121.31	110.60
1	A	236	SER	N-CA-CB	-5.92	101.63	110.50
1	A	379	VAL	N-CA-C	-5.91	95.03	111.00
1	B	231	PHE	CB-CG-CD1	5.91	124.94	120.80
1	A	135	ILE	CB-CA-C	-5.90	99.79	111.60
1	B	96	LEU	N-CA-CB	5.89	122.18	110.40
1	A	307	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	A	401	LEU	N-CA-CB	-5.88	98.65	110.40
1	A	275	ASN	N-CA-C	-5.88	95.14	111.00
1	A	286	PRO	CA-N-CD	-5.87	103.28	111.50
1	A	229	ARG	N-CA-CB	5.86	121.14	110.60
1	B	381	GLN	N-CA-CB	5.85	121.13	110.60
1	B	441	LYS	CA-CB-CG	5.85	126.27	113.40
1	B	348	GLY	N-CA-C	-5.85	98.48	113.10
1	B	489	LEU	CB-CG-CD2	5.83	120.92	111.00
1	A	129	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	B	259	PHE	CB-CG-CD1	-5.82	116.72	120.80
1	B	88	MET	CG-SD-CE	5.81	109.49	100.20
1	B	217	SER	CB-CA-C	-5.81	99.06	110.10
1	B	92	VAL	CB-CA-C	5.80	122.43	111.40
1	A	282	LEU	CB-CA-C	-5.79	99.19	110.20
1	A	486	VAL	CB-CA-C	5.79	122.39	111.40
1	B	468	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	B	308	PHE	CB-CA-C	-5.76	98.88	110.40
1	B	160	THR	N-CA-C	5.74	126.49	111.00
1	A	150	ASN	CA-CB-CG	-5.74	100.78	113.40
1	B	378	CYS	N-CA-CB	5.73	120.92	110.60
1	B	171	ASN	CB-CA-C	-5.72	98.95	110.40
1	A	442	ARG	NE-CZ-NH1	5.72	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	LEU	CB-CA-C	-5.71	99.34	110.20
1	B	286	PRO	N-CA-C	5.71	126.96	112.10
1	A	35	TYR	CB-CG-CD1	5.71	124.42	121.00
1	A	110	ILE	CB-CA-C	-5.70	100.20	111.60
1	A	496	SER	CB-CA-C	-5.70	99.27	110.10
1	B	296	LEU	N-CA-CB	-5.69	99.01	110.40
1	B	290	LYS	CA-C-N	-5.69	104.68	117.20
1	B	152	VAL	N-CA-CB	-5.69	98.98	111.50
1	A	463	PHE	CB-CA-C	-5.69	99.03	110.40
1	B	77	TYR	CB-CG-CD1	5.68	124.41	121.00
1	A	198	GLY	N-CA-C	-5.67	98.93	113.10
1	A	449	LEU	N-CA-CB	5.62	121.65	110.40
1	B	25	TRP	CA-CB-CG	-5.62	103.03	113.70
1	B	292	VAL	CA-CB-CG2	5.61	119.32	110.90
1	A	432	ARG	CB-CG-CD	5.60	126.16	111.60
1	A	276	ARG	CB-CA-C	-5.59	99.21	110.40
1	A	322	TYR	CA-C-N	-5.58	104.91	117.20
1	A	346	VAL	CB-CA-C	-5.58	100.79	111.40
1	B	495	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	B	34	TYR	CB-CG-CD1	5.55	124.33	121.00
1	A	117	VAL	N-CA-CB	-5.54	99.31	111.50
1	A	480	ALA	C-N-CA	5.54	135.55	121.70
1	A	325	ARG	CA-CB-CG	5.54	125.58	113.40
1	A	432	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
1	B	332	TYR	CB-CG-CD1	5.48	124.29	121.00
1	A	155	LEU	CA-C-N	-5.48	105.15	117.20
1	B	88	MET	CA-CB-CG	5.46	122.59	113.30
1	A	396	MET	N-CA-CB	5.45	120.41	110.60
1	A	427	ASN	CA-CB-CG	-5.45	101.42	113.40
1	B	353	ASN	O-C-N	-5.43	113.97	123.20
1	B	27	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	432	ARG	CG-CD-NE	5.40	123.15	111.80
1	A	215	PHE	CB-CG-CD2	-5.39	117.02	120.80
1	B	356	ILE	CA-C-N	5.39	132.20	117.10
1	B	161	PHE	CB-CA-C	-5.38	99.63	110.40
1	B	447	SER	N-CA-CB	5.38	118.57	110.50
1	B	484	PRO	N-CA-CB	5.38	109.75	103.30
1	A	31	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	431	HIS	CA-CB-CG	-5.37	104.48	113.60
1	B	478	ILE	N-CA-C	-5.36	96.52	111.00
1	A	432	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	34	TYR	CA-CB-CG	-5.36	103.22	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ASP	C-N-CA	5.33	133.49	122.30
1	A	53	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	322	TYR	CB-CG-CD2	-5.33	117.81	121.00
1	B	374	ASN	CA-CB-CG	-5.32	101.69	113.40
1	B	211	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	B	458	VAL	CA-CB-CG1	-5.31	102.94	110.90
1	B	102	CYS	N-CA-CB	5.31	120.15	110.60
1	B	115	TYR	CB-CG-CD2	-5.31	117.82	121.00
1	B	342	CYS	CA-CB-SG	-5.30	104.46	114.00
1	B	462	CYS	CA-CB-SG	-5.30	104.46	114.00
1	B	400	LEU	CB-CA-C	-5.30	100.14	110.20
1	B	115	TYR	CA-CB-CG	5.29	123.46	113.40
1	A	396	MET	CA-C-N	-5.28	105.58	117.20
1	B	442	ARG	N-CA-CB	5.28	120.11	110.60
1	A	34	TYR	C-N-CA	5.28	134.90	121.70
1	B	158	VAL	CA-C-N	-5.27	105.60	117.20
1	B	395	THR	C-N-CA	5.27	134.88	121.70
1	B	35	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	A	101	LEU	C-N-CA	5.27	134.87	121.70
1	A	375	VAL	CA-CB-CG1	5.27	118.81	110.90
1	A	142	PHE	CB-CA-C	5.27	120.94	110.40
1	B	306	PHE	CB-CG-CD1	5.25	124.48	120.80
1	B	216	LYS	CB-CA-C	5.25	120.89	110.40
1	B	275	ASN	C-N-CA	5.24	134.81	121.70
1	B	91	ILE	CB-CA-C	-5.24	101.12	111.60
1	B	148	PHE	CA-CB-CG	-5.24	101.34	113.90
1	A	334	PHE	N-CA-CB	-5.23	101.18	110.60
1	A	449	LEU	CB-CG-CD1	5.23	119.89	111.00
1	A	43	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	A	174	TYR	N-CA-CB	-5.22	101.20	110.60
1	B	160	THR	O-C-N	-5.21	114.36	122.70
1	A	479	ALA	C-N-CA	5.21	134.73	121.70
1	B	498	THR	CA-C-N	-5.20	105.76	117.20
1	B	330	PHE	CD1-CG-CD2	-5.20	111.54	118.30
1	A	262	LEU	CB-CA-C	-5.19	100.33	110.20
1	B	441	LYS	N-CA-CB	5.17	119.90	110.60
1	A	298	PHE	CB-CG-CD1	5.16	124.42	120.80
1	A	432	ARG	CA-CB-CG	5.16	124.76	113.40
1	B	483	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	A	211	PHE	CB-CG-CD1	5.15	124.40	120.80
1	B	382	ARG	CB-CA-C	-5.15	100.11	110.40
1	A	54	THR	CB-CA-C	-5.14	97.71	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	PRO	CA-C-N	-5.12	105.93	117.20
1	B	218	PHE	N-CA-CB	5.09	119.77	110.60
1	A	369	ARG	N-CA-C	-5.09	97.25	111.00
1	B	207	VAL	CA-C-N	-5.09	106.00	117.20
1	A	159	THR	CB-CA-C	5.09	125.34	111.60
1	A	324	LEU	C-N-CA	5.08	134.41	121.70
1	B	282	LEU	N-CA-CB	5.08	120.56	110.40
1	A	433	ILE	CB-CA-C	-5.08	101.44	111.60
1	B	472	PHE	N-CA-CB	5.07	119.72	110.60
1	B	89	ALA	CB-CA-C	-5.06	102.51	110.10
1	A	163	CYS	N-CA-CB	5.05	119.70	110.60
1	B	214	PHE	CB-CG-CD2	-5.05	117.26	120.80
1	A	233	SER	C-N-CA	5.04	134.29	121.70
1	B	88	MET	CB-CG-SD	5.03	127.49	112.40
1	B	268	PHE	CB-CG-CD2	-5.02	117.28	120.80
1	A	159	THR	CA-C-N	5.01	128.23	117.20
1	B	347	LEU	CA-C-N	-5.01	106.19	116.20
1	B	498	THR	C-N-CA	5.01	134.21	121.70
1	B	163	CYS	C-N-CA	-5.00	109.19	121.70
1	B	469	THR	CA-C-N	-5.00	106.19	116.20

There are no chirality outliers.

All (89) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Sidechain
1	A	124	LEU	Mainchain
1	A	128	TYR	Sidechain
1	A	143	HIS	Sidechain
1	A	150	ASN	Mainchain
1	A	162	PRO	Peptide
1	A	174	TYR	Sidechain
1	A	197	ASP	Peptide,Mainchain
1	A	199	PHE	Sidechain
1	A	216	LYS	Mainchain
1	A	218	PHE	Sidechain
1	A	221	TYR	Sidechain
1	A	235	TYR	Sidechain
1	A	253	TYR	Peptide,Mainchain
1	A	263	PRO	Mainchain
1	A	268	PHE	Sidechain
1	A	274	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	306	PHE	Sidechain
1	A	31	ARG	Sidechain
1	A	320	HIS	Sidechain
1	A	322	TYR	Sidechain
1	A	326	LYS	Peptide
1	A	35	TYR	Sidechain
1	A	362	HIS	Sidechain
1	A	37	SER	Peptide,Mainchain
1	A	370	ASP	Peptide,Mainchain
1	A	374	ASN	Mainchain
1	A	375	VAL	Mainchain
1	A	377	ARG	Sidechain
1	A	398	ARG	Sidechain
1	A	416	PHE	Sidechain
1	A	423	GLY	Mainchain
1	A	43	PHE	Sidechain
1	A	432	ARG	Sidechain
1	A	442	ARG	Sidechain
1	A	455	ARG	Sidechain
1	A	46	ARG	Mainchain
1	A	468	PHE	Sidechain
1	A	472	PHE	Sidechain
1	A	476	ASN	Mainchain
1	A	483	PHE	Sidechain
1	A	496	SER	Peptide,Mainchain
1	A	55	TYR	Sidechain
1	A	72	ARG	Sidechain
1	B	104	VAL	Mainchain
1	B	115	TYR	Sidechain
1	B	118	TYR	Sidechain
1	B	148	PHE	Sidechain
1	B	156	GLN	Mainchain
1	B	157	TYR	Sidechain
1	B	158	VAL	Mainchain
1	B	174	TYR	Sidechain
1	B	218	PHE	Sidechain
1	B	226	HIS	Sidechain
1	B	229	ARG	Sidechain
1	B	247	PHE	Sidechain
1	B	253	TYR	Sidechain
1	B	259	PHE	Sidechain
1	B	297	PRO	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	B	307	TYR	Sidechain
1	B	308	PHE	Sidechain
1	B	319	ARG	Sidechain
1	B	320	HIS	Mainchain
1	B	325	ARG	Sidechain
1	B	331	HIS	Sidechain,Peptide,Mainchain
1	B	332	TYR	Sidechain
1	B	34	TYR	Sidechain
1	B	357	PRO	Peptide,Mainchain
1	B	398	ARG	Sidechain
1	B	416	PHE	Sidechain
1	B	435	PHE	Sidechain
1	B	437	PHE	Sidechain
1	B	441	LYS	Mainchain
1	B	443	ARG	Sidechain
1	B	468	PHE	Sidechain
1	B	497	PHE	Sidechain,Peptide,Mainchain
1	B	498	THR	Mainchain
1	B	56	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3806	0	3850	302	0
1	B	3806	0	3851	346	0
All	All	7612	0	7701	642	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 42.

All (642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:THR:HG23	1:B:110:ILE:H	1.40	0.87
1:B:331:HIS:HE1	1:B:335:ALA:HB2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:HA	1:A:187:HIS:CD2	2.12	0.84
1:B:143:HIS:CE1	1:B:338:GLY:HA3	2.16	0.79
1:B:331:HIS:CE1	1:B:335:ALA:HB2	2.20	0.77
1:B:154:LEU:HA	1:B:157:TYR:CE2	2.20	0.77
1:A:25:TRP:HA	1:A:25:TRP:CE2	2.19	0.76
1:A:60:LEU:HD13	1:A:412:LEU:HB3	1.65	0.76
1:A:459:ILE:HG22	1:A:463:PHE:CE1	2.21	0.76
1:B:288:PRO:O	1:B:292:VAL:HG13	1.85	0.75
1:A:496:SER:HA	1:A:499:TYR:CZ	2.23	0.74
1:A:203:VAL:HG22	1:B:203:VAL:HG22	1.69	0.74
1:A:140:MET:HA	1:A:143:HIS:CD2	2.24	0.72
1:A:262:LEU:HD12	1:A:404:LEU:O	1.89	0.72
1:A:207:VAL:HG13	1:A:211:PHE:CE2	2.24	0.72
1:A:138:TRP:HE1	1:A:295:ALA:HB3	1.54	0.72
1:A:496:SER:HA	1:A:499:TYR:CE2	2.25	0.72
1:B:105:GLY:C	1:B:353:ASN:H	1.93	0.72
1:A:356:ILE:N	1:A:358:GLN:HE22	1.87	0.72
1:A:261:LYS:HA	1:A:408:PRO:HA	1.71	0.71
1:B:199:PHE:O	1:B:203:VAL:HG23	1.90	0.71
1:B:113:PHE:O	1:B:117:VAL:HG23	1.90	0.71
1:A:223:LEU:H	1:A:229:ARG:HH12	1.38	0.71
1:B:218:PHE:CD1	1:B:223:LEU:HB2	2.25	0.71
1:B:497:PHE:CD2	1:B:498:THR:HA	2.26	0.70
1:A:431:HIS:CD2	1:A:431:HIS:N	2.57	0.70
1:B:198:GLY:O	1:B:202:VAL:HG23	1.91	0.70
1:B:154:LEU:HA	1:B:157:TYR:CZ	2.27	0.69
1:B:319:ARG:HG3	1:B:322:TYR:H	1.57	0.69
1:B:72:ARG:HH22	1:B:111:SER:HB3	1.57	0.69
1:B:359:ALA:HA	1:B:362:HIS:CD2	2.27	0.69
1:A:134:TRP:CD1	1:A:295:ALA:HB2	2.28	0.68
1:B:169:PHE:CE2	1:B:483:PHE:CD1	2.82	0.68
1:A:460:PHE:HA	1:A:463:PHE:CE2	2.29	0.67
1:B:455:ARG:O	1:B:458:VAL:HG22	1.93	0.67
1:B:135:ILE:HA	1:B:138:TRP:CD1	2.29	0.67
1:B:184:ARG:HH11	1:B:185:GLN:HG3	1.59	0.67
1:A:428:VAL:HA	1:A:431:HIS:ND1	2.09	0.67
1:B:280:THR:HG22	1:B:281:TRP:H	1.60	0.66
1:A:183:THR:HB	1:A:187:HIS:CE1	2.31	0.66
1:A:441:LYS:HD3	1:A:442:ARG:HH11	1.60	0.65
1:B:104:VAL:HG12	1:B:352:PRO:HB2	1.78	0.65
1:B:430:ILE:O	1:B:433:ILE:HB	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TRP:CD2	1:B:25:TRP:N	2.61	0.65
1:B:359:ALA:O	1:B:362:HIS:CG	2.50	0.65
1:A:415:LEU:O	1:A:419:MET:HB3	1.97	0.65
1:A:216:LYS:O	1:A:219:HIS:CD2	2.50	0.65
1:B:178:GLY:HA3	1:B:416:PHE:CG	2.32	0.64
1:B:226:HIS:CE1	1:B:370:ASP:O	2.49	0.64
1:A:356:ILE:HD12	1:A:356:ILE:H	1.63	0.64
1:A:138:TRP:HE1	1:A:295:ALA:CB	2.10	0.64
1:A:154:LEU:HA	1:A:157:TYR:CE2	2.32	0.64
1:A:38:ASP:HB2	1:A:382:ARG:HH11	1.62	0.64
1:A:218:PHE:HB3	1:A:229:ARG:HH11	1.63	0.64
1:A:134:TRP:HB2	1:A:138:TRP:CZ2	2.33	0.64
1:A:278:GLN:HA	1:A:281:TRP:CE3	2.33	0.64
1:A:359:ALA:HA	1:A:362:HIS:CD2	2.33	0.63
1:A:31:ARG:HH22	1:A:100:PRO:HD3	1.63	0.63
1:B:126:THR:HG22	1:B:127:SER:H	1.63	0.63
1:A:278:GLN:HA	1:A:281:TRP:CZ3	2.35	0.62
1:B:211:PHE:HA	1:B:214:PHE:CD2	2.35	0.62
1:A:207:VAL:HG13	1:A:211:PHE:CZ	2.34	0.62
1:A:226:HIS:CD2	1:A:370:ASP:O	2.53	0.62
1:B:423:GLY:C	1:B:425:MET:H	2.02	0.62
1:A:223:LEU:H	1:A:229:ARG:NH1	1.98	0.62
1:B:483:PHE:CD1	1:B:484:PRO:HD3	2.34	0.61
1:A:154:LEU:HA	1:A:157:TYR:CZ	2.34	0.61
1:A:261:LYS:O	1:A:262:LEU:HD23	2.01	0.61
1:B:24:ILE:HB	1:B:25:TRP:CE2	2.36	0.61
1:B:443:ARG:HA	1:B:443:ARG:HH11	1.65	0.61
1:B:460:PHE:HA	1:B:463:PHE:CE2	2.36	0.61
1:A:487:LEU:O	1:A:491:VAL:HG22	2.01	0.61
1:A:134:TRP:CE2	1:A:292:VAL:HA	2.36	0.61
1:A:216:LYS:HD2	1:A:219:HIS:CE1	2.36	0.61
1:A:135:ILE:HA	1:A:138:TRP:CD1	2.36	0.60
1:B:107:THR:HG23	1:B:110:ILE:N	2.15	0.60
1:B:53:ASP:HA	1:B:56:PHE:CZ	2.36	0.60
1:A:391:MET:HG2	1:A:394:GLY:H	1.67	0.60
1:B:135:ILE:HG23	1:B:295:ALA:HB1	1.84	0.60
1:B:138:TRP:HZ2	1:B:295:ALA:HB3	1.67	0.60
1:B:80:ASN:HA	1:B:83:LEU:HD12	1.84	0.60
1:B:305:LEU:HA	1:B:308:PHE:CD2	2.36	0.60
1:A:24:ILE:HG12	1:A:331:HIS:CE1	2.37	0.59
1:A:432:ARG:HA	1:A:435:PHE:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:SER:HA	1:B:499:TYR:CE2	2.36	0.59
1:A:150:ASN:HA	1:A:152:VAL:HG22	1.84	0.59
1:A:224:PHE:H	1:A:229:ARG:NH1	2.00	0.59
1:B:432:ARG:HH21	1:B:449:LEU:HD13	1.66	0.59
1:A:26:LEU:HD23	1:A:26:LEU:H	1.68	0.59
1:A:455:ARG:HE	1:A:456:SER:H	1.49	0.59
1:B:154:LEU:O	1:B:157:TYR:CD2	2.56	0.59
1:A:307:TYR:CD1	1:A:307:TYR:C	2.75	0.59
1:B:38:ASP:HA	1:B:41:ASP:OD2	2.03	0.59
1:B:161:PHE:CE2	1:B:491:VAL:HG12	2.38	0.59
1:B:493:VAL:HA	1:B:495:PHE:CE2	2.36	0.59
1:A:169:PHE:HD2	1:A:170:ILE:HD13	1.67	0.58
1:B:38:ASP:HB3	1:B:382:ARG:H	1.67	0.58
1:B:38:ASP:HB2	1:B:39:TRP:CE3	2.37	0.58
1:B:319:ARG:HD3	1:B:322:TYR:CE2	2.38	0.58
1:A:416:PHE:HA	1:A:419:MET:SD	2.44	0.58
1:B:45:TYR:O	1:B:49:PRO:HD2	2.03	0.58
1:A:427:ASN:O	1:A:431:HIS:CE1	2.56	0.58
1:B:24:ILE:HB	1:B:25:TRP:CZ2	2.38	0.58
1:B:72:ARG:HH22	1:B:111:SER:CB	2.16	0.58
1:B:331:HIS:O	1:B:331:HIS:CD2	2.57	0.58
1:A:169:PHE:CZ	1:A:483:PHE:CE2	2.92	0.58
1:B:462:CYS:HA	1:B:465:LEU:HD12	1.85	0.58
1:A:149:THR:HG23	1:A:151:VAL:H	1.69	0.58
1:A:175:ILE:HA	1:A:416:PHE:CD1	2.39	0.57
1:B:307:TYR:CD2	1:B:308:PHE:CD1	2.93	0.57
1:B:497:PHE:O	1:B:497:PHE:CD1	2.57	0.57
1:A:174:TYR:HB3	1:A:416:PHE:CZ	2.39	0.57
1:A:367:LEU:HD13	1:A:368:VAL:H	1.69	0.57
1:A:140:MET:HA	1:A:143:HIS:NE2	2.19	0.57
1:A:429:ILE:HA	1:A:432:ARG:HB2	1.86	0.57
1:A:430:ILE:HB	1:A:431:HIS:CD2	2.40	0.57
1:A:427:ASN:H	1:A:431:HIS:CE1	2.22	0.57
1:A:24:ILE:HB	1:A:25:TRP:CZ3	2.40	0.57
1:A:135:ILE:HA	1:A:138:TRP:NE1	2.18	0.57
1:A:186:PHE:CE1	1:A:197:ASP:HB3	2.39	0.56
1:B:174:TYR:HB3	1:B:416:PHE:CZ	2.40	0.56
1:A:98:GLY:HA3	1:A:333:ASP:HB3	1.88	0.56
1:A:203:VAL:CG2	1:B:203:VAL:HG22	2.34	0.56
1:A:226:HIS:O	1:A:230:THR:HB	2.04	0.56
1:A:460:PHE:HA	1:A:463:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:VAL:HB	1:A:259:PHE:CE1	2.40	0.56
1:B:126:THR:HG22	1:B:127:SER:N	2.21	0.56
1:A:211:PHE:HA	1:A:214:PHE:CD2	2.41	0.56
1:A:457:MET:HA	1:A:460:PHE:CD2	2.41	0.56
1:A:31:ARG:HE	1:A:98:GLY:HA2	1.71	0.56
1:B:154:LEU:HD22	1:B:307:TYR:OH	2.05	0.56
1:A:26:LEU:H	1:A:26:LEU:CD2	2.17	0.56
1:B:321:GLN:C	1:B:323:LYS:H	2.09	0.56
1:B:331:HIS:O	1:B:331:HIS:CG	2.58	0.56
1:A:39:TRP:CZ2	1:A:382:ARG:NH1	2.74	0.55
1:A:104:VAL:HA	1:A:353:ASN:O	2.06	0.55
1:B:282:LEU:HD12	1:B:283:ALA:H	1.70	0.55
1:B:485:LEU:O	1:B:489:LEU:HD23	2.05	0.55
1:A:78:GLY:HA3	1:A:269:PHE:CD2	2.41	0.55
1:A:135:ILE:HG12	1:A:295:ALA:HB1	1.88	0.55
1:A:369:ARG:O	1:A:373:GLN:HA	2.07	0.55
1:B:324:LEU:HD13	1:B:326:LYS:H	1.71	0.55
1:B:287:ILE:HD12	1:B:288:PRO:HD2	1.89	0.55
1:A:68:ASP:HA	1:A:71:ASP:OD2	2.06	0.55
1:A:263:PRO:O	1:A:404:LEU:HD11	2.05	0.55
1:B:38:ASP:HB2	1:B:39:TRP:CZ3	2.41	0.55
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.89	0.55
1:A:99:GLN:HG3	1:A:101:LEU:H	1.72	0.55
1:B:170:ILE:CG2	1:B:174:TYR:CZ	2.90	0.55
1:A:99:GLN:HA	1:A:99:GLN:OE1	2.06	0.54
1:A:319:ARG:HD2	1:A:321:GLN:HG3	1.87	0.54
1:B:38:ASP:HB2	1:B:39:TRP:CD2	2.43	0.54
1:A:455:ARG:NE	1:A:456:SER:H	2.05	0.54
1:B:156:GLN:HB2	1:B:157:TYR:CD1	2.43	0.54
1:A:258:LYS:HD3	1:A:260:LYS:HZ3	1.73	0.54
1:B:36:LYS:O	1:B:39:TRP:CD1	2.60	0.54
1:B:68:ASP:HA	1:B:71:ASP:OD2	2.07	0.54
1:B:87:ALA:HB1	1:B:395:THR:HA	1.88	0.54
1:A:153:CYS:O	1:A:157:TYR:CE1	2.61	0.54
1:B:218:PHE:O	1:B:222:PRO:HA	2.08	0.54
1:B:319:ARG:HD3	1:B:322:TYR:CZ	2.42	0.54
1:B:104:VAL:HG13	1:B:353:ASN:O	2.07	0.54
1:B:170:ILE:HG22	1:B:174:TYR:CE2	2.43	0.54
1:B:104:VAL:HA	1:B:353:ASN:O	2.07	0.54
1:A:421:ILE:O	1:A:425:MET:SD	2.66	0.54
1:B:307:TYR:CD1	1:B:307:TYR:C	2.78	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD12	1:A:60:LEU:O	2.07	0.53
1:B:421:ILE:O	1:B:425:MET:SD	2.66	0.53
1:B:161:PHE:CD2	1:B:491:VAL:HG12	2.43	0.53
1:B:170:ILE:HG23	1:B:174:TYR:CZ	2.44	0.53
1:A:105:GLY:O	1:A:355:LEU:HD21	2.08	0.53
1:A:408:PRO:HG2	1:A:411:VAL:HG23	1.91	0.53
1:A:139:SER:O	1:A:143:HIS:CD2	2.60	0.53
1:B:260:LYS:HB3	1:B:409:GLN:HB2	1.91	0.53
1:A:436:LEU:HD23	1:A:437:PHE:CZ	2.43	0.53
1:B:34:TYR:CE2	1:B:327:PRO:HB3	2.43	0.53
1:A:421:ILE:O	1:A:424:LEU:HD13	2.08	0.53
1:B:205:ALA:O	1:B:208:MET:SD	2.67	0.53
1:A:138:TRP:NE1	1:A:295:ALA:HB3	2.23	0.53
1:A:38:ASP:HA	1:A:41:ASP:OD2	2.08	0.53
1:B:138:TRP:CZ2	1:B:295:ALA:HB3	2.43	0.53
1:B:186:PHE:CE2	1:B:197:ASP:HB3	2.44	0.53
1:B:495:PHE:O	1:B:499:TYR:CZ	2.62	0.53
1:B:129:PHE:CE1	1:B:273:LYS:HB3	2.44	0.52
1:B:359:ALA:O	1:B:362:HIS:CD2	2.61	0.52
1:B:81:GLU:HB3	1:B:350:PRO:HD3	1.91	0.52
1:B:169:PHE:CZ	1:B:483:PHE:CE1	2.98	0.52
1:A:280:THR:HA	1:A:347:LEU:HA	1.91	0.52
1:A:280:THR:HA	1:A:347:LEU:O	2.08	0.52
1:B:226:HIS:CE1	1:B:370:ASP:C	2.83	0.52
1:B:455:ARG:HA	1:B:455:ARG:NE	2.25	0.52
1:A:162:PRO:HB3	1:A:491:VAL:HG11	1.91	0.52
1:B:39:TRP:CD2	1:B:39:TRP:N	2.75	0.52
1:B:223:LEU:HG	1:B:224:PHE:CZ	2.44	0.52
1:B:463:PHE:N	1:B:463:PHE:CD1	2.73	0.52
1:A:304:ILE:O	1:A:307:TYR:CD2	2.63	0.52
1:A:319:ARG:HD2	1:A:322:TYR:CG	2.44	0.52
1:A:138:TRP:CD1	1:A:296:LEU:HA	2.45	0.52
1:B:432:ARG:HH21	1:B:449:LEU:HD22	1.75	0.52
1:A:483:PHE:O	1:A:486:VAL:HB	2.10	0.52
1:B:99:GLN:HG3	1:B:101:LEU:H	1.75	0.51
1:A:134:TRP:CD2	1:A:292:VAL:HA	2.45	0.51
1:A:432:ARG:HA	1:A:435:PHE:CE2	2.46	0.51
1:A:197:ASP:HB2	1:A:199:PHE:CD1	2.44	0.51
1:B:51:THR:HG23	1:B:384:THR:OG1	2.11	0.51
1:A:368:VAL:HG21	1:A:376:VAL:H	1.75	0.51
1:A:457:MET:HA	1:A:460:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:PHE:O	1:A:499:TYR:CE1	2.64	0.51
1:B:106:VAL:HA	1:B:353:ASN:OD1	2.10	0.51
1:B:241:VAL:O	1:B:245:SER:HB2	2.10	0.51
1:B:324:LEU:HD13	1:B:326:LYS:N	2.26	0.51
1:B:153:CYS:O	1:B:157:TYR:CE1	2.63	0.51
1:B:439:ASP:HB3	1:B:442:ARG:HG2	1.92	0.51
1:A:232:ILE:HA	1:A:235:TYR:CD2	2.46	0.51
1:A:320:HIS:CE1	1:A:325:ARG:HB2	2.46	0.51
1:A:463:PHE:O	1:A:466:ALA:HB3	2.11	0.51
1:B:77:TYR:CZ	1:B:269:PHE:CZ	2.98	0.51
1:A:324:LEU:HD13	1:A:377:ARG:HH21	1.76	0.51
1:B:118:TYR:CZ	1:B:128:TYR:CZ	2.98	0.51
1:B:135:ILE:HG22	1:B:295:ALA:O	2.10	0.51
1:A:50:SER:OG	1:A:365:THR:HG21	2.11	0.51
1:A:258:LYS:HZ2	1:A:260:LYS:HD3	1.75	0.51
1:B:138:TRP:CE2	1:B:296:LEU:HA	2.46	0.51
1:A:31:ARG:HH22	1:A:100:PRO:CD	2.23	0.50
1:A:485:LEU:O	1:A:488:LEU:HB3	2.11	0.50
1:B:468:PHE:HA	1:B:471:GLU:OE2	2.10	0.50
1:B:356:ILE:HB	1:B:357:PRO:CD	2.41	0.50
1:B:460:PHE:HA	1:B:463:PHE:CD2	2.46	0.50
1:A:416:PHE:CD1	1:A:416:PHE:C	2.84	0.50
1:B:62:ALA:HA	1:B:65:PHE:CE2	2.46	0.50
1:B:128:TYR:CE1	1:B:132:MET:SD	3.05	0.50
1:A:131:PHE:HA	1:A:134:TRP:CZ2	2.46	0.50
1:A:87:ALA:CB	1:A:395:THR:HA	2.42	0.50
1:A:280:THR:HB	1:A:347:LEU:HA	1.94	0.50
1:A:358:GLN:H	1:A:358:GLN:NE2	2.09	0.50
1:A:484:PRO:HA	1:A:487:LEU:HB2	1.94	0.50
1:B:260:LYS:C	1:B:409:GLN:H	2.15	0.50
1:B:443:ARG:CZ	1:B:447:SER:HB2	2.41	0.50
1:A:289:VAL:O	1:A:292:VAL:HG22	2.11	0.50
1:A:493:VAL:C	1:A:495:PHE:H	2.15	0.50
1:B:44:ASN:CG	1:B:45:TYR:H	2.15	0.50
1:B:436:LEU:HB3	1:B:437:PHE:CZ	2.47	0.50
1:A:175:ILE:HA	1:A:416:PHE:CE1	2.46	0.50
1:A:382:ARG:HA	1:A:385:ASN:HD21	1.76	0.50
1:A:488:LEU:HD13	1:A:489:LEU:N	2.25	0.50
1:B:81:GLU:HB3	1:B:350:PRO:CD	2.42	0.50
1:B:136:CYS:SG	1:B:345:GLY:HA3	2.52	0.50
1:B:289:VAL:O	1:B:292:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:CG	1:A:498:THR:N	2.80	0.49
1:B:255:ASN:HA	1:B:259:PHE:CE2	2.47	0.49
1:B:497:PHE:O	1:B:497:PHE:CG	2.65	0.49
1:A:134:TRP:CD1	1:A:295:ALA:CB	2.94	0.49
1:A:435:PHE:N	1:A:435:PHE:CD1	2.75	0.49
1:B:319:ARG:HG2	1:B:322:TYR:CD2	2.48	0.49
1:A:307:TYR:CG	1:A:308:PHE:N	2.80	0.49
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.93	0.49
1:B:319:ARG:CG	1:B:322:TYR:CG	2.95	0.49
1:A:154:LEU:O	1:A:157:TYR:CD2	2.65	0.49
1:A:440:PRO:C	1:A:442:ARG:H	2.15	0.49
1:A:262:LEU:HD11	1:A:407:ILE:HB	1.93	0.49
1:A:359:ALA:O	1:A:362:HIS:CG	2.66	0.49
1:B:175:ILE:HA	1:B:416:PHE:CE1	2.48	0.49
1:A:244:TRP:CZ3	1:A:247:PHE:CE1	3.00	0.49
1:B:432:ARG:NH2	1:B:449:LEU:HD22	2.28	0.49
1:B:484:PRO:HA	1:B:487:LEU:HB3	1.95	0.49
1:A:166:PHE:O	1:A:169:PHE:HB3	2.13	0.49
1:A:25:TRP:CE3	1:A:25:TRP:N	2.80	0.49
1:B:397:THR:HA	1:B:400:LEU:HB2	1.94	0.49
1:A:131:PHE:HA	1:A:134:TRP:CE2	2.48	0.49
1:A:218:PHE:HA	1:A:222:PRO:HA	1.94	0.49
1:B:443:ARG:HH22	1:B:451:LYS:HB2	1.78	0.49
1:A:114:ASN:O	1:A:117:VAL:HB	2.13	0.48
1:B:32:ILE:N	1:B:33:PRO:HD2	2.28	0.48
1:B:104:VAL:HG22	1:B:354:GLY:HA2	1.93	0.48
1:B:290:LYS:HA	1:B:293:PHE:CE2	2.48	0.48
1:B:426:THR:O	1:B:428:VAL:HG23	2.14	0.48
1:B:483:PHE:CE1	1:B:484:PRO:HG3	2.49	0.48
1:A:359:ALA:HA	1:A:362:HIS:NE2	2.28	0.48
1:A:364:GLU:HA	1:A:367:LEU:HB2	1.95	0.48
1:B:455:ARG:HA	1:B:455:ARG:CZ	2.43	0.48
1:A:432:ARG:HH21	1:A:449:LEU:HG	1.77	0.48
1:B:428:VAL:O	1:B:432:ARG:N	2.43	0.48
1:A:140:MET:HA	1:A:143:HIS:CE1	2.48	0.48
1:B:416:PHE:CD1	1:B:416:PHE:C	2.85	0.48
1:A:368:VAL:CG2	1:A:376:VAL:H	2.27	0.48
1:B:161:PHE:O	1:B:165:ILE:HG13	2.14	0.48
1:B:377:ARG:CZ	1:B:378:CYS:O	2.62	0.48
1:A:498:THR:HG23	1:A:499:TYR:CD1	2.49	0.48
1:B:157:TYR:CD1	1:B:157:TYR:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:HIS:CE1	1:A:372:ASN:O	2.67	0.48
1:B:283:ALA:C	1:B:284:TYR:CD1	2.87	0.48
1:B:431:HIS:O	1:B:434:VAL:HB	2.13	0.48
1:A:161:PHE:CE2	1:A:491:VAL:HG12	2.49	0.48
1:B:155:LEU:CD1	1:B:155:LEU:H	2.27	0.48
1:A:105:GLY:C	1:A:355:LEU:HD21	2.34	0.48
1:A:274:PHE:CD1	1:A:276:ARG:HB2	2.48	0.48
1:A:447:SER:HB3	1:A:448:PRO:HD3	1.96	0.48
1:A:468:PHE:CE1	1:A:472:PHE:HB2	2.49	0.48
1:B:199:PHE:O	1:B:202:VAL:HB	2.13	0.48
1:A:119:GLU:OE2	1:A:120:ILE:HG23	2.13	0.47
1:A:143:HIS:CE1	1:A:335:ALA:O	2.67	0.47
1:A:300:ILE:HG13	1:A:301:ILE:HG23	1.96	0.47
1:A:424:LEU:HB2	1:A:425:MET:SD	2.54	0.47
1:B:356:ILE:CB	1:B:357:PRO:HD3	2.44	0.47
1:B:153:CYS:SG	1:B:154:LEU:HD13	2.53	0.47
1:B:42:ALA:O	1:B:47:VAL:HG21	2.14	0.47
1:B:153:CYS:SG	1:B:154:LEU:CD1	3.02	0.47
1:B:38:ASP:HB2	1:B:39:TRP:CH2	2.49	0.47
1:B:262:LEU:HD11	1:B:404:LEU:C	2.35	0.47
1:A:47:VAL:O	1:A:51:THR:HG23	2.15	0.47
1:A:223:LEU:N	1:A:229:ARG:HH12	2.09	0.47
1:B:114:ASN:HA	1:B:117:VAL:HB	1.95	0.47
1:B:169:PHE:CZ	1:B:483:PHE:CD1	3.03	0.47
1:B:261:LYS:HA	1:B:408:PRO:HA	1.96	0.47
1:A:369:ARG:O	1:A:369:ARG:HG2	2.14	0.47
1:B:226:HIS:HA	1:B:229:ARG:HE	1.79	0.47
1:B:241:VAL:HG23	1:B:242:LEU:HG	1.95	0.47
1:B:485:LEU:HG	1:B:486:VAL:N	2.29	0.47
1:A:430:ILE:O	1:A:433:ILE:HB	2.15	0.47
1:A:459:ILE:O	1:A:463:PHE:CD1	2.68	0.47
1:B:38:ASP:CB	1:B:382:ARG:H	2.27	0.47
1:B:61:PRO:O	1:B:64:ALA:HB3	2.15	0.47
1:B:157:TYR:CD2	1:B:492:ILE:HG22	2.49	0.47
1:B:307:TYR:CG	1:B:308:PHE:N	2.83	0.47
1:B:356:ILE:H	1:B:356:ILE:HD12	1.78	0.47
1:A:431:HIS:O	1:A:435:PHE:CD1	2.67	0.47
1:A:485:LEU:HD22	1:A:488:LEU:HD12	1.97	0.47
1:B:110:ILE:O	1:B:113:PHE:HB3	2.15	0.47
1:B:118:TYR:CE1	1:B:128:TYR:CE1	3.02	0.47
1:A:31:ARG:NH1	1:A:328:SER:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG13	1:B:353:ASN:N	2.30	0.47
1:B:209:THR:HG21	1:B:417:PHE:HB3	1.97	0.47
1:B:316:MET:SD	1:B:319:ARG:HD2	2.55	0.47
1:A:312:VAL:HG23	1:A:313:SER:N	2.29	0.46
1:A:364:GLU:O	1:A:367:LEU:HB2	2.14	0.46
1:B:38:ASP:HB2	1:B:39:TRP:CE2	2.51	0.46
1:B:451:LYS:HG3	1:B:454:LYS:HZ3	1.80	0.46
1:A:226:HIS:CG	1:A:371:SER:HA	2.50	0.46
1:A:244:TRP:CE2	1:A:247:PHE:HB2	2.50	0.46
1:B:439:ASP:OD2	1:B:441:LYS:HG2	2.15	0.46
1:A:24:ILE:HA	1:A:27:ASP:CG	2.36	0.46
1:B:68:ASP:HB2	1:B:72:ARG:HE	1.81	0.46
1:B:140:MET:HB2	1:B:342:CYS:SG	2.55	0.46
1:B:391:MET:SD	1:B:391:MET:N	2.89	0.46
1:A:218:PHE:CD1	1:A:222:PRO:C	2.89	0.46
1:B:51:THR:HG23	1:B:384:THR:HA	1.97	0.46
1:B:54:THR:HB	1:B:388:GLN:HE22	1.81	0.46
1:B:140:MET:SD	1:B:338:GLY:O	2.74	0.46
1:B:443:ARG:HH22	1:B:451:LYS:CD	2.29	0.46
1:B:128:TYR:CZ	1:B:132:MET:SD	3.08	0.46
1:B:218:PHE:CD1	1:B:223:LEU:CB	2.96	0.46
1:B:223:LEU:HB3	1:B:224:PHE:CE2	2.51	0.46
1:B:443:ARG:NH2	1:B:451:LYS:HD3	2.30	0.46
1:A:297:PRO:HA	1:A:300:ILE:HG23	1.97	0.46
1:A:431:HIS:O	1:A:434:VAL:HB	2.16	0.46
1:B:277:PRO:CD	1:B:278:GLN:H	2.29	0.46
1:B:395:THR:O	1:B:397:THR:HG23	2.16	0.46
1:A:105:GLY:C	1:A:353:ASN:H	2.19	0.46
1:A:132:MET:SD	1:A:132:MET:C	2.94	0.46
1:B:128:TYR:O	1:B:132:MET:SD	2.74	0.46
1:B:323:LYS:HE2	1:B:375:VAL:HG11	1.98	0.46
1:B:367:LEU:HD21	1:B:375:VAL:HG13	1.98	0.46
1:A:147:ALA:HB2	1:A:335:ALA:HB2	1.98	0.46
1:A:186:PHE:CD1	1:A:197:ASP:HA	2.51	0.46
1:A:483:PHE:CD2	1:A:484:PRO:HD3	2.50	0.46
1:B:38:ASP:HB2	1:B:39:TRP:CZ2	2.51	0.46
1:B:72:ARG:C	1:B:74:ASP:H	2.18	0.46
1:B:175:ILE:O	1:B:179:ILE:HG13	2.16	0.46
1:B:377:ARG:HH11	1:B:377:ARG:HB2	1.80	0.46
1:B:459:ILE:O	1:B:463:PHE:CE1	2.69	0.46
1:A:77:TYR:HA	1:A:81:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:CE2	1:A:491:VAL:HA	2.51	0.46
1:A:199:PHE:CE2	1:B:195:VAL:HB	2.51	0.46
1:A:227:LYS:HA	1:A:230:THR:HG22	1.98	0.46
1:B:273:LYS:O	1:B:274:PHE:CG	2.68	0.46
1:B:366:LEU:HD22	1:B:381:GLN:HE22	1.81	0.46
1:A:304:ILE:HA	1:A:307:TYR:HD2	1.81	0.45
1:B:36:LYS:HA	1:B:39:TRP:HE1	1.81	0.45
1:B:60:LEU:O	1:B:63:ILE:HB	2.16	0.45
1:B:129:PHE:CD1	1:B:273:LYS:HB3	2.51	0.45
1:B:170:ILE:O	1:B:174:TYR:CG	2.69	0.45
1:B:175:ILE:HG22	1:B:416:PHE:HE1	1.81	0.45
1:B:492:ILE:HG13	1:B:493:VAL:HG13	1.98	0.45
1:A:27:ASP:OD2	1:A:331:HIS:CD2	2.70	0.45
1:A:481:ILE:O	1:A:484:PRO:HD3	2.16	0.45
1:B:35:TYR:O	1:B:39:TRP:CZ2	2.70	0.45
1:A:330:PHE:CD1	1:A:330:PHE:N	2.81	0.45
1:B:59:LEU:O	1:B:62:ALA:HB3	2.16	0.45
1:A:113:PHE:CD1	1:A:113:PHE:C	2.89	0.45
1:A:165:ILE:O	1:A:168:LEU:HB3	2.17	0.45
1:A:431:HIS:O	1:A:435:PHE:CE1	2.69	0.45
1:B:38:ASP:OD2	1:B:382:ARG:HB2	2.16	0.45
1:B:319:ARG:HD3	1:B:322:TYR:CD2	2.52	0.45
1:A:280:THR:CA	1:A:347:LEU:HA	2.46	0.45
1:A:324:LEU:HD13	1:A:377:ARG:NH2	2.32	0.45
1:B:257:VAL:O	1:B:259:PHE:CD2	2.70	0.45
1:B:283:ALA:O	1:B:284:TYR:CD1	2.70	0.45
1:A:157:TYR:N	1:A:157:TYR:CD1	2.78	0.45
1:A:323:LYS:O	1:A:324:LEU:HG	2.16	0.45
1:A:356:ILE:O	1:A:359:ALA:HB3	2.17	0.45
1:B:126:THR:CG2	1:B:127:SER:H	2.27	0.45
1:B:443:ARG:HH21	1:B:448:PRO:HG3	1.82	0.45
1:A:141:ILE:HG13	1:A:142:PHE:CG	2.52	0.45
1:A:349:ILE:HG23	1:A:350:PRO:HD2	1.99	0.45
1:B:55:TYR:CE2	1:B:393:LEU:HB3	2.52	0.45
1:B:103:ILE:HB	1:B:355:LEU:HD12	1.99	0.45
1:B:443:ARG:HH22	1:B:451:LYS:HD3	1.81	0.45
1:B:490:SER:O	1:B:493:VAL:HG22	2.17	0.45
1:A:218:PHE:CE1	1:A:223:LEU:HB2	2.52	0.45
1:A:144:LEU:HG	1:A:145:LEU:N	2.30	0.45
1:A:455:ARG:NE	1:A:455:ARG:H	2.14	0.45
1:B:114:ASN:O	1:B:117:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LYS:CE	1:B:375:VAL:HG11	2.47	0.45
1:A:34:TYR:CZ	1:A:327:PRO:HG2	2.52	0.44
1:A:186:PHE:CD1	1:A:186:PHE:N	2.77	0.44
1:B:208:MET:SD	1:B:414:GLY:HA3	2.57	0.44
1:B:310:HIS:CG	1:B:337:LEU:HD22	2.51	0.44
1:A:25:TRP:HA	1:A:25:TRP:CZ2	2.52	0.44
1:A:425:MET:O	1:A:431:HIS:CE1	2.70	0.44
1:B:155:LEU:CD1	1:B:155:LEU:N	2.81	0.44
1:A:59:LEU:O	1:A:62:ALA:HB3	2.18	0.44
1:A:224:PHE:CD1	1:A:225:THR:HG23	2.52	0.44
1:A:234:ASP:OD2	1:A:235:TYR:CD1	2.69	0.44
1:A:436:LEU:CD2	1:A:437:PHE:CZ	3.00	0.44
1:A:493:VAL:HA	1:A:495:PHE:CZ	2.53	0.44
1:B:77:TYR:CE1	1:B:269:PHE:CE2	3.06	0.44
1:B:81:GLU:O	1:B:85:SER:HB2	2.18	0.44
1:B:166:PHE:CZ	1:B:312:VAL:HG21	2.52	0.44
1:B:432:ARG:HH21	1:B:449:LEU:CD1	2.30	0.44
1:A:319:ARG:CZ	1:A:322:TYR:CE2	3.01	0.44
1:B:257:VAL:H	1:B:259:PHE:HE2	1.65	0.44
1:B:274:PHE:CZ	1:B:285:GLU:OE2	2.71	0.44
1:B:460:PHE:O	1:B:460:PHE:CD1	2.70	0.44
1:B:489:LEU:O	1:B:492:ILE:HG12	2.18	0.44
1:A:60:LEU:O	1:A:63:ILE:HB	2.18	0.44
1:A:463:PHE:CD1	1:A:463:PHE:N	2.83	0.44
1:B:24:ILE:HD12	1:B:148:PHE:CE1	2.53	0.44
1:A:147:ALA:O	1:A:331:HIS:CE1	2.71	0.44
1:A:288:PRO:HB2	1:A:290:LYS:HB3	2.00	0.44
1:A:326:LYS:HB3	1:A:327:PRO:HD3	1.99	0.44
1:B:55:TYR:HA	1:B:58:ASN:HD21	1.82	0.44
1:B:138:TRP:O	1:B:142:PHE:CD2	2.70	0.44
1:B:198:GLY:O	1:B:202:VAL:N	2.50	0.44
1:B:402:VAL:O	1:B:406:GLU:HG3	2.17	0.44
1:B:57:ASN:O	1:B:61:PRO:HD2	2.18	0.44
1:B:161:PHE:CD2	1:B:491:VAL:HA	2.53	0.44
1:B:211:PHE:CD1	1:B:211:PHE:N	2.85	0.44
1:B:487:LEU:O	1:B:491:VAL:HG22	2.18	0.44
1:A:150:ASN:HD22	1:A:152:VAL:HG22	1.82	0.44
1:A:166:PHE:CE1	1:A:312:VAL:HG21	2.53	0.44
1:A:319:ARG:HB3	1:A:322:TYR:HB2	2.00	0.44
1:B:55:TYR:HA	1:B:58:ASN:ND2	2.33	0.44
1:B:289:VAL:HG23	1:B:290:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:PHE:CD2	1:B:463:PHE:CE2	3.06	0.44
1:A:171:ASN:O	1:A:174:TYR:HB2	2.18	0.43
1:A:280:THR:CB	1:A:347:LEU:HA	2.48	0.43
1:B:225:THR:O	1:B:229:ARG:HB3	2.18	0.43
1:B:468:PHE:O	1:B:471:GLU:OE1	2.36	0.43
1:A:211:PHE:CD1	1:A:211:PHE:N	2.82	0.43
1:A:224:PHE:CD1	1:B:437:PHE:O	2.71	0.43
1:A:298:PHE:CD1	1:A:298:PHE:N	2.85	0.43
1:A:483:PHE:CD1	1:A:484:PRO:N	2.86	0.43
1:B:140:MET:O	1:B:143:HIS:HB3	2.17	0.43
1:B:322:TYR:N	1:B:322:TYR:CD1	2.79	0.43
1:B:105:GLY:H	1:B:355:LEU:HG	1.82	0.43
1:B:208:MET:SD	1:B:414:GLY:CA	3.07	0.43
1:B:484:PRO:HA	1:B:487:LEU:CB	2.49	0.43
1:A:305:LEU:O	1:A:308:PHE:HB2	2.19	0.43
1:A:459:ILE:HG22	1:A:463:PHE:CZ	2.54	0.43
1:B:105:GLY:N	1:B:353:ASN:O	2.51	0.43
1:B:151:VAL:O	1:B:154:LEU:HB2	2.18	0.43
1:B:170:ILE:O	1:B:174:TYR:CD1	2.71	0.43
1:B:183:THR:O	1:B:187:HIS:CG	2.71	0.43
1:B:280:THR:HG22	1:B:281:TRP:N	2.32	0.43
1:B:293:PHE:O	1:B:296:LEU:HB3	2.19	0.43
1:B:304:ILE:O	1:B:308:PHE:CG	2.71	0.43
1:B:181:ILE:HG23	1:B:184:ARG:HH12	1.83	0.43
1:B:229:ARG:HG2	1:B:229:ARG:HH11	1.84	0.43
1:B:356:ILE:CB	1:B:357:PRO:CD	2.95	0.43
1:A:107:THR:HG23	1:A:110:ILE:H	1.83	0.43
1:A:285:GLU:N	1:A:286:PRO:HD3	2.32	0.43
1:B:68:ASP:C	1:B:72:ARG:HE	2.22	0.43
1:B:260:LYS:O	1:B:408:PRO:HA	2.18	0.43
1:B:324:LEU:HD21	1:B:380:GLU:OE2	2.19	0.43
1:B:134:TRP:HA	1:B:134:TRP:CE3	2.53	0.43
1:B:161:PHE:CE2	1:B:491:VAL:HA	2.54	0.43
1:B:163:CYS:SG	1:B:316:MET:HB2	2.58	0.43
1:B:39:TRP:CH2	1:B:382:ARG:HB2	2.53	0.43
1:B:91:ILE:HG12	1:B:390:LEU:HA	2.01	0.43
1:B:134:TRP:HB3	1:B:138:TRP:CE2	2.54	0.43
1:B:267:SER:HA	1:B:398:ARG:HH21	1.84	0.43
1:B:287:ILE:HG23	1:B:288:PRO:HD2	2.01	0.43
1:B:297:PRO:HD2	1:B:298:PHE:CD2	2.53	0.43
1:B:374:ASN:O	1:B:376:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:GLY:H	1:B:425:MET:HB2	1.83	0.43
1:A:169:PHE:CD1	1:A:483:PHE:CD1	3.07	0.43
1:A:216:LYS:O	1:A:219:HIS:CG	2.72	0.43
1:A:224:PHE:CG	1:B:437:PHE:HB3	2.53	0.43
1:A:326:LYS:HZ1	1:A:377:ARG:HH11	1.65	0.43
1:B:135:ILE:HA	1:B:138:TRP:NE1	2.33	0.43
1:B:154:LEU:O	1:B:157:TYR:CG	2.72	0.43
1:B:207:VAL:HG13	1:B:211:PHE:CE2	2.54	0.43
1:A:32:ILE:HA	1:A:35:TYR:HB2	2.01	0.43
1:A:139:SER:O	1:A:143:HIS:CG	2.72	0.43
1:A:319:ARG:HB3	1:A:322:TYR:H	1.83	0.43
1:A:324:LEU:HD21	1:A:377:ARG:NE	2.34	0.43
1:B:290:LYS:HA	1:B:293:PHE:CD2	2.53	0.43
1:A:132:MET:SD	1:A:136:CYS:SG	3.17	0.42
1:A:368:VAL:HG21	1:A:376:VAL:N	2.34	0.42
1:A:391:MET:N	1:A:391:MET:SD	2.91	0.42
1:A:482:GLY:C	1:A:484:PRO:HD2	2.38	0.42
1:A:493:VAL:O	1:A:495:PHE:CD1	2.72	0.42
1:B:106:VAL:HG12	1:B:107:THR:H	1.83	0.42
1:B:391:MET:SD	1:B:391:MET:O	2.77	0.42
1:B:483:PHE:CG	1:B:484:PRO:N	2.87	0.42
1:A:120:ILE:HD11	1:A:298:PHE:CZ	2.54	0.42
1:A:150:ASN:O	1:A:153:CYS:HB2	2.19	0.42
1:B:248:THR:HA	1:B:255:ASN:CG	2.39	0.42
1:A:238:ALA:HA	1:A:241:VAL:HG22	2.01	0.42
1:A:324:LEU:CD1	1:A:377:ARG:HH21	2.32	0.42
1:A:384:THR:HG23	1:A:385:ASN:N	2.34	0.42
1:A:453:SER:HA	1:A:455:ARG:CZ	2.49	0.42
1:B:211:PHE:HA	1:B:214:PHE:CE2	2.54	0.42
1:A:46:ARG:NH1	1:A:368:VAL:HG22	2.34	0.42
1:A:324:LEU:HD22	1:A:326:LYS:HB2	2.00	0.42
1:B:118:TYR:CE2	1:B:128:TYR:CZ	3.07	0.42
1:B:262:LEU:HG	1:B:405:GLY:HA2	2.01	0.42
1:A:36:LYS:C	1:A:39:TRP:HE1	2.23	0.42
1:A:133:PHE:CE2	1:A:285:GLU:OE2	2.72	0.42
1:B:180:GLN:HA	1:B:183:THR:OG1	2.19	0.42
1:B:200:ALA:O	1:B:204:VAL:HG23	2.20	0.42
1:A:168:LEU:C	1:A:168:LEU:HD13	2.40	0.42
1:A:218:PHE:HD1	1:A:222:PRO:C	2.23	0.42
1:A:244:TRP:CE3	1:A:244:TRP:HA	2.55	0.42
1:B:46:ARG:C	1:B:49:PRO:HD2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TRP:HE3	1:B:26:LEU:HD21	1.84	0.42
1:B:25:TRP:CE3	1:B:26:LEU:HD21	2.54	0.42
1:B:226:HIS:O	1:B:229:ARG:CZ	2.67	0.42
1:A:321:GLN:CD	1:A:322:TYR:CE1	2.93	0.42
1:A:359:ALA:N	1:A:360:PRO:HD2	2.34	0.42
1:A:459:ILE:HG22	1:A:463:PHE:HE1	1.78	0.42
1:B:30:ASP:HB2	1:B:31:ARG:HH11	1.85	0.42
1:B:79:VAL:HB	1:B:264:ILE:HD13	2.01	0.42
1:B:152:VAL:CA	1:B:155:LEU:HD13	2.50	0.42
1:B:396:MET:SD	1:B:399:PRO:HD2	2.60	0.42
1:A:143:HIS:NE2	1:A:338:GLY:C	2.72	0.42
1:A:168:LEU:O	1:A:172:VAL:HG23	2.20	0.42
1:B:204:VAL:O	1:B:208:MET:HB3	2.19	0.42
1:B:260:LYS:HB3	1:B:409:GLN:CB	2.49	0.42
1:A:33:PRO:HA	1:A:36:LYS:HD2	2.02	0.42
1:A:369:ARG:O	1:A:370:ASP:CG	2.58	0.42
1:B:25:TRP:O	1:B:29:LYS:HG3	2.20	0.42
1:B:186:PHE:CD1	1:B:186:PHE:C	2.93	0.42
1:B:226:HIS:CG	1:B:229:ARG:HH21	2.37	0.42
1:B:244:TRP:O	1:B:244:TRP:CD1	2.72	0.42
1:A:169:PHE:CE2	1:A:483:PHE:CZ	3.08	0.41
1:A:208:MET:HA	1:A:211:PHE:CD2	2.55	0.41
1:A:397:THR:HA	1:A:400:LEU:HB3	2.02	0.41
1:B:287:ILE:HG23	1:B:288:PRO:N	2.35	0.41
1:B:401:LEU:HA	1:B:404:LEU:HD12	2.01	0.41
1:B:447:SER:N	1:B:448:PRO:CD	2.83	0.41
1:A:200:ALA:O	1:A:203:VAL:HB	2.20	0.41
1:A:428:VAL:O	1:A:431:HIS:HB2	2.20	0.41
1:A:431:HIS:CD2	1:A:431:HIS:H	2.28	0.41
1:B:97:ALA:HB1	1:B:382:ARG:HE	1.85	0.41
1:B:319:ARG:O	1:B:322:TYR:C	2.59	0.41
1:A:31:ARG:HH22	1:A:100:PRO:HG3	1.85	0.41
1:A:213:LEU:HG	1:A:214:PHE:CE1	2.55	0.41
1:A:262:LEU:HG	1:A:407:ILE:O	2.20	0.41
1:A:311:ASN:N	1:A:311:ASN:HD22	2.17	0.41
1:B:68:ASP:OD2	1:B:72:ARG:NH2	2.54	0.41
1:A:80:ASN:HA	1:A:83:LEU:HB3	2.02	0.41
1:A:226:HIS:CE1	1:A:372:ASN:N	2.89	0.41
1:B:27:ASP:OD1	1:B:27:ASP:N	2.52	0.41
1:B:107:THR:O	1:B:110:ILE:HG22	2.20	0.41
1:B:402:VAL:HG13	1:B:403:CYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLY:HA2	1:A:352:PRO:HA	2.02	0.41
1:A:164:ASP:HA	1:A:316:MET:SD	2.60	0.41
1:B:277:PRO:HB2	1:B:278:GLN:OE1	2.21	0.41
1:B:356:ILE:O	1:B:360:PRO:HD2	2.21	0.41
1:B:364:GLU:C	1:B:364:GLU:CD	2.79	0.41
1:A:101:LEU:HD21	1:A:380:GLU:HB2	2.02	0.41
1:A:274:PHE:CG	1:A:276:ARG:HB2	2.56	0.41
1:A:324:LEU:HD22	1:A:326:LYS:CG	2.51	0.41
1:A:416:PHE:CE1	1:A:416:PHE:O	2.74	0.41
1:A:428:VAL:O	1:A:432:ARG:N	2.51	0.41
1:A:499:TYR:CD1	1:A:499:TYR:N	2.86	0.41
1:B:64:ALA:O	1:B:68:ASP:OD1	2.38	0.41
1:B:292:VAL:HG22	1:B:293:PHE:CE1	2.55	0.41
1:B:326:LYS:HD2	1:B:378:CYS:HB3	2.02	0.41
1:B:481:ILE:O	1:B:484:PRO:HD3	2.20	0.41
1:A:34:TYR:O	1:A:38:ASP:OD1	2.39	0.41
1:A:169:PHE:CE1	1:A:483:PHE:CG	3.09	0.41
1:A:390:LEU:O	1:A:391:MET:C	2.58	0.41
1:B:118:TYR:CZ	1:B:128:TYR:CE1	3.08	0.41
1:B:143:HIS:ND1	1:B:338:GLY:HA3	2.34	0.41
1:B:339:LEU:O	1:B:342:CYS:HB3	2.21	0.41
1:B:425:MET:SD	1:B:425:MET:N	2.94	0.41
1:B:427:ASN:O	1:B:430:ILE:HB	2.21	0.41
1:A:180:GLN:O	1:A:180:GLN:CD	2.59	0.41
1:A:321:GLN:HG3	1:A:322:TYR:CD1	2.55	0.41
1:A:323:LYS:O	1:A:324:LEU:HD23	2.21	0.41
1:A:358:GLN:CD	1:A:359:ALA:N	2.74	0.41
1:B:55:TYR:CZ	1:B:393:LEU:HB3	2.56	0.41
1:B:141:ILE:O	1:B:144:LEU:HB3	2.20	0.41
1:B:324:LEU:HD22	1:B:324:LEU:HA	1.91	0.41
1:B:430:ILE:HG22	1:B:434:VAL:HG23	2.02	0.41
1:A:270:PRO:HB3	1:A:274:PHE:HB3	2.03	0.41
1:A:492:ILE:O	1:A:495:PHE:CD2	2.74	0.41
1:A:493:VAL:HA	1:A:495:PHE:CE1	2.56	0.41
1:B:33:PRO:HG2	1:B:34:TYR:CD1	2.55	0.41
1:B:297:PRO:HB2	1:B:298:PHE:CD1	2.56	0.41
1:B:457:MET:O	1:B:461:LEU:HG	2.21	0.41
1:A:88:MET:O	1:A:92:VAL:HG22	2.21	0.40
1:A:296:LEU:HB3	1:A:297:PRO:HD3	2.03	0.40
1:B:115:TYR:O	1:B:119:GLU:CD	2.60	0.40
1:B:155:LEU:C	1:B:157:TYR:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PHE:CE1	1:B:483:PHE:CE1	3.09	0.40
1:B:358:GLN:OE1	1:B:358:GLN:CA	2.69	0.40
1:B:487:LEU:O	1:B:491:VAL:HG13	2.21	0.40
1:A:199:PHE:CD2	1:B:195:VAL:HB	2.56	0.40
1:A:307:TYR:O	1:A:310:HIS:HB3	2.20	0.40
1:A:368:VAL:HG21	1:A:376:VAL:O	2.21	0.40
1:A:483:PHE:CG	1:A:484:PRO:HD3	2.56	0.40
1:A:483:PHE:HA	1:A:486:VAL:HB	2.03	0.40
1:B:263:PRO:O	1:B:264:ILE:HB	2.21	0.40
1:B:369:ARG:HA	1:B:374:ASN:O	2.21	0.40
1:B:70:PHE:O	1:B:75:ASN:HA	2.21	0.40
1:B:140:MET:CE	1:B:143:HIS:CD2	3.05	0.40
1:B:183:THR:O	1:B:187:HIS:CD2	2.74	0.40
1:B:289:VAL:O	1:B:293:PHE:CE2	2.75	0.40
1:B:304:ILE:O	1:B:307:TYR:HB3	2.21	0.40
1:A:37:SER:HB2	1:A:41:ASP:OD2	2.21	0.40
1:A:54:THR:HA	1:A:57:ASN:ND2	2.36	0.40
1:A:203:VAL:O	1:A:207:VAL:HB	2.21	0.40
1:B:247:PHE:CZ	1:B:252:GLY:HA2	2.56	0.40
1:A:82:VAL:HA	1:A:350:PRO:HG2	2.04	0.40
1:B:110:ILE:HG12	1:B:351:ALA:HB3	2.02	0.40
1:B:122:LYS:N	1:B:123:PRO:HD2	2.36	0.40
1:B:166:PHE:CD2	1:B:487:LEU:HD23	2.56	0.40
1:B:294:ILE:O	1:B:298:PHE:CE2	2.75	0.40
1:B:440:PRO:HA	1:B:451:LYS:NZ	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	474/476 (100%)	408 (86%)	45 (10%)	21 (4%)	2 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/476 (100%)	392 (83%)	47 (10%)	35 (7%)	1	13
All	All	948/952 (100%)	800 (84%)	92 (10%)	56 (6%)	3	17

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ALA
1	A	100	PRO
1	A	102	CYS
1	A	106	VAL
1	A	190	SER
1	A	256	ASP
1	A	263	PRO
1	A	279	ASN
1	A	286	PRO
1	A	319	ARG
1	A	323	LYS
1	A	368	VAL
1	A	395	THR
1	A	444	ASP
1	B	77	TYR
1	B	106	VAL
1	B	190	SER
1	B	193	LYS
1	B	194	SER
1	B	264	ILE
1	B	319	ARG
1	B	327	PRO
1	B	371	SER
1	B	395	THR
1	B	439	ASP
1	B	478	ILE
1	A	149	THR
1	A	223	LEU
1	B	127	SER
1	B	223	LEU
1	B	257	VAL
1	B	277	PRO
1	B	376	VAL
1	B	391	MET
1	B	445	ASN
1	B	251	GLY

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Mol	Chain	Res	Type
1	B	255	ASN
1	B	261	LYS
1	B	282	LEU
1	B	323	LYS
1	B	422	ASN
1	A	127	SER
1	B	159	THR
1	B	286	PRO
1	B	381	GLN
1	A	356	ILE
1	A	478	ILE
1	B	222	PRO
1	B	276	ARG
1	B	350	PRO
1	B	356	ILE
1	B	494	SER
1	A	76	SER
1	A	222	PRO
1	B	392	ILE
1	B	349	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/424 (100%)	352 (83%)	72 (17%)	2	12
1	B	424/424 (100%)	342 (81%)	82 (19%)	1	8
All	All	848/848 (100%)	694 (82%)	154 (18%)	4	10

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	25	TRP
1	A	26	LEU

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Mol	Chain	Res	Type
1	A	28	LEU
1	A	32	ILE
1	A	39	TRP
1	A	44	ASN
1	A	50	SER
1	A	68	ASP
1	A	75	ASN
1	A	111	SER
1	A	113	PHE
1	A	115	TYR
1	A	119	GLU
1	A	128	TYR
1	A	132	MET
1	A	134	TRP
1	A	136	CYS
1	A	144	LEU
1	A	148	PHE
1	A	149	THR
1	A	152	VAL
1	A	207	VAL
1	A	208	MET
1	A	213	LEU
1	A	222	PRO
1	A	224	PHE
1	A	226	HIS
1	A	229	ARG
1	A	230	THR
1	A	237	THR
1	A	248	THR
1	A	256	ASP
1	A	263	PRO
1	A	269	PHE
1	A	272	SER
1	A	274	PHE
1	A	292	VAL
1	A	300	ILE
1	A	307	TYR
1	A	308	PHE
1	A	318	GLN
1	A	321	GLN
1	A	328	SER
1	A	331	HIS

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Mol	Chain	Res	Type
1	A	334	PHE
1	A	339	LEU
1	A	353	ASN
1	A	356	ILE
1	A	358	GLN
1	A	363	THR
1	A	364	GLU
1	A	367	LEU
1	A	368	VAL
1	A	371	SER
1	A	380	GLU
1	A	391	MET
1	A	403	CYS
1	A	422	ASN
1	A	424	LEU
1	A	425	MET
1	A	426	THR
1	A	431	HIS
1	A	441	LYS
1	A	444	ASP
1	A	454	LYS
1	A	455	ARG
1	A	461	LEU
1	A	468	PHE
1	A	488	LEU
1	A	495	PHE
1	A	498	THR
1	B	24	ILE
1	B	26	LEU
1	B	27	ASP
1	B	30	ASP
1	B	51	THR
1	B	55	TYR
1	B	65	PHE
1	B	68	ASP
1	B	71	ASP
1	B	74	ASP
1	B	75	ASN
1	B	80	ASN
1	B	96	LEU
1	B	102	CYS
1	B	103	ILE

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Mol	Chain	Res	Type
1	B	109	PRO
1	B	111	SER
1	B	115	TYR
1	B	116	THR
1	B	119	GLU
1	B	131	PHE
1	B	134	TRP
1	B	138	TRP
1	B	145	LEU
1	B	150	ASN
1	B	151	VAL
1	B	155	LEU
1	B	163	CYS
1	B	165	ILE
1	B	197	ASP
1	B	201	SER
1	B	207	VAL
1	B	208	MET
1	B	213	LEU
1	B	222	PRO
1	B	223	LEU
1	B	225	THR
1	B	256	ASP
1	B	280	THR
1	B	284	TYR
1	B	287	ILE
1	B	288	PRO
1	B	290	LYS
1	B	296	LEU
1	B	302	LEU
1	B	304	ILE
1	B	305	LEU
1	B	307	TYR
1	B	316	MET
1	B	324	LEU
1	B	327	PRO
1	B	333	ASP
1	B	358	GLN
1	B	362	HIS
1	B	363	THR
1	B	364	GLU
1	B	377	ARG

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Mol	Chain	Res	Type
1	B	381	GLN
1	B	382	ARG
1	B	385	ASN
1	B	388	GLN
1	B	391	MET
1	B	392	ILE
1	B	395	THR
1	B	396	MET
1	B	411	VAL
1	B	424	LEU
1	B	425	MET
1	B	429	ILE
1	B	438	SER
1	B	441	LYS
1	B	442	ARG
1	B	443	ARG
1	B	449	LEU
1	B	456	SER
1	B	459	ILE
1	B	464	SER
1	B	471	GLU
1	B	478	ILE
1	B	485	LEU
1	B	488	LEU
1	B	489	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	187	HIS
1	A	219	HIS
1	A	311	ASN
1	A	318	GLN
1	A	358	GLN
1	A	431	HIS
1	B	156	GLN
1	B	171	ASN
1	B	196	GLN
1	B	219	HIS
1	B	226	HIS
1	B	310	HIS

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Mol	Chain	Res	Type
1	B	331	HIS
1	B	381	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8313. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

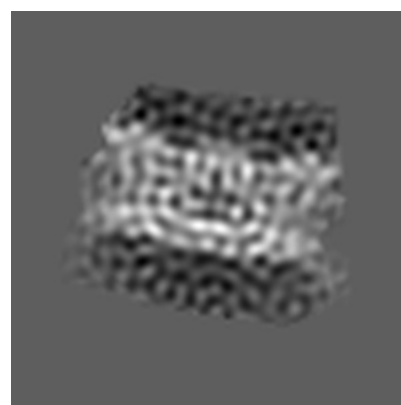
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 50



Y Index: 50



Z Index: 50

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

6.3 Largest variance slices [i](#)

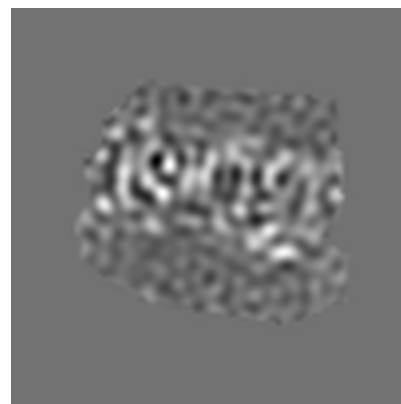
6.3.1 Primary map



X Index: 39



Y Index: 46

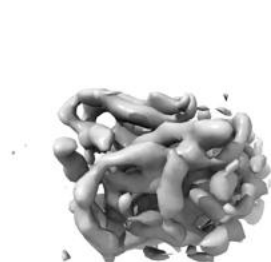


Z Index: 50

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

6.4 Orthogonal surface views [i](#)

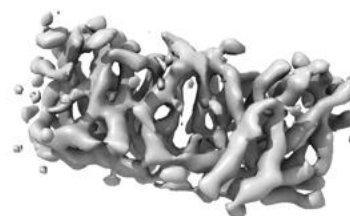
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 130.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

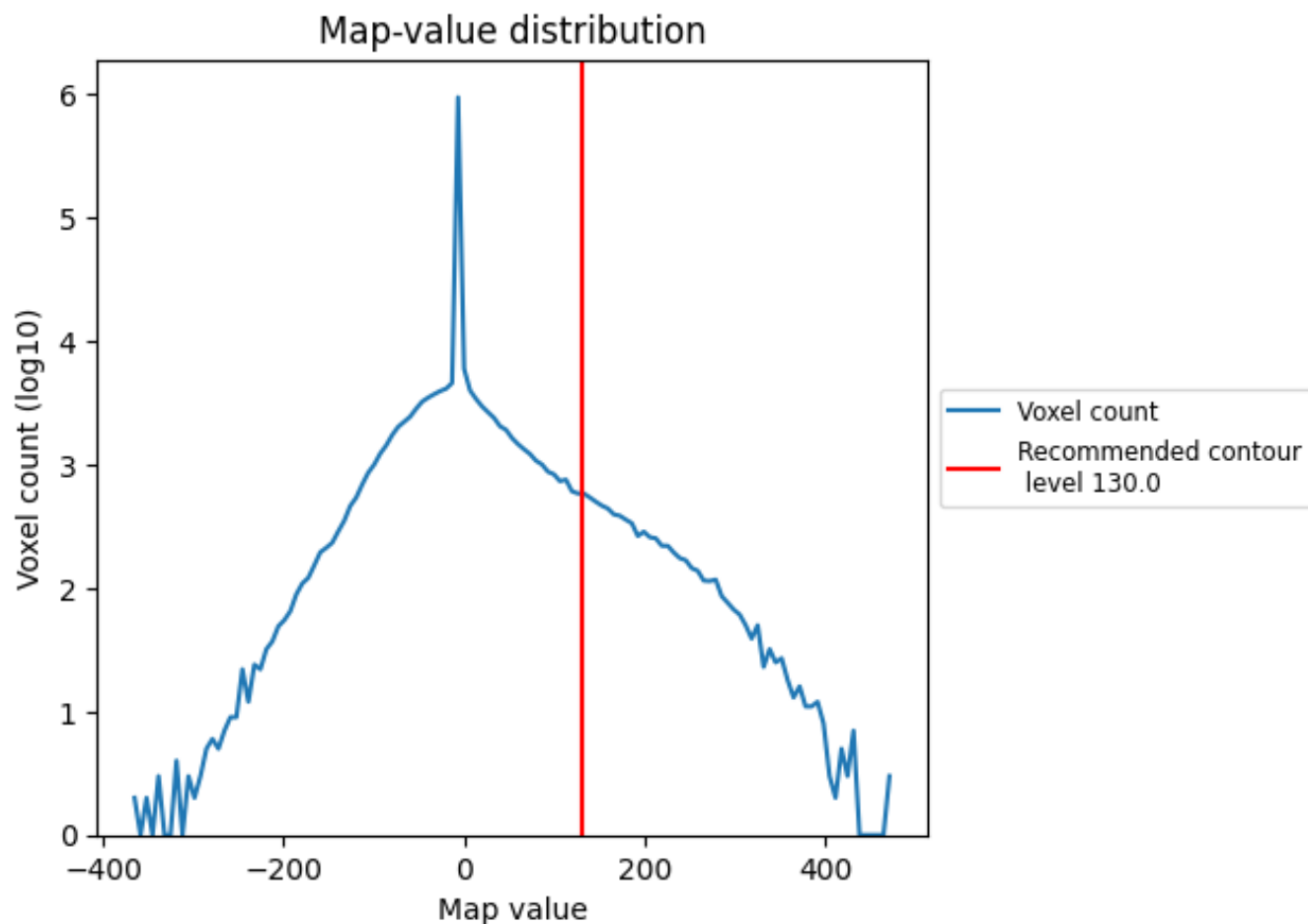
6.5 Mask visualisation

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

7 Map analysis [i](#)

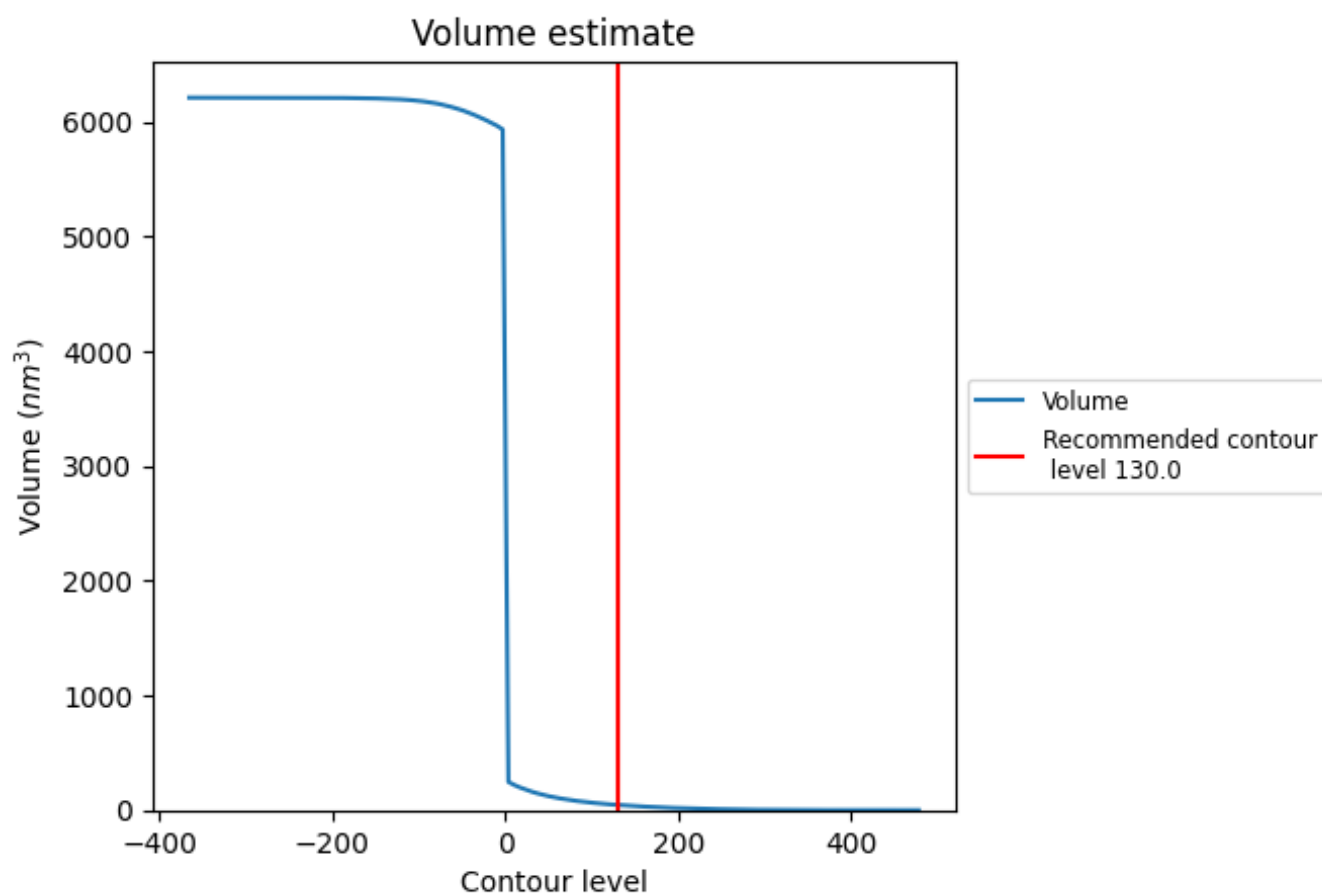
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

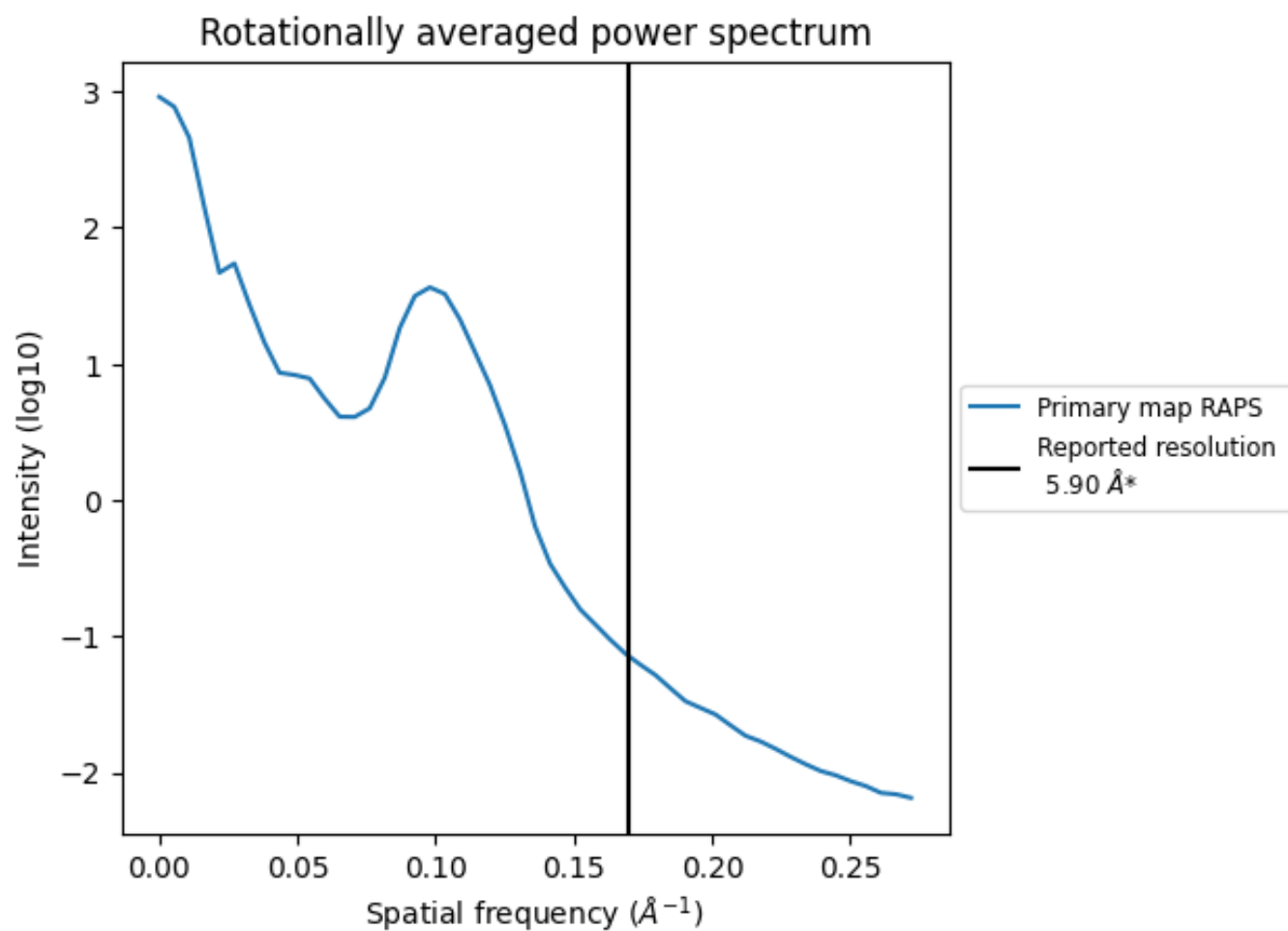
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm^3 ; this corresponds to an approximate mass of 41 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

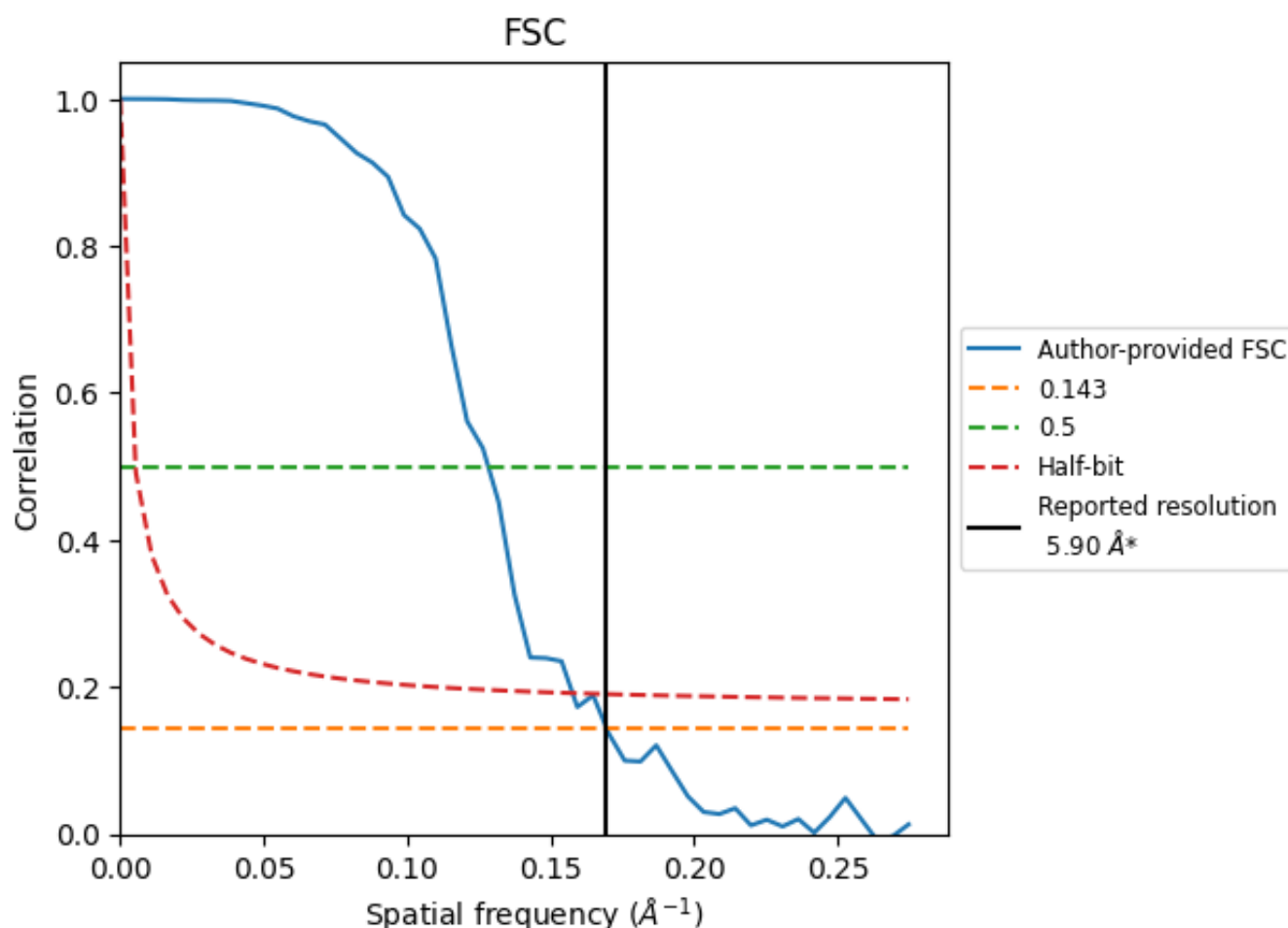


*Reported resolution corresponds to spatial frequency of 0.169 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.169 \AA^{-1}

8.2 Resolution estimates [i](#)

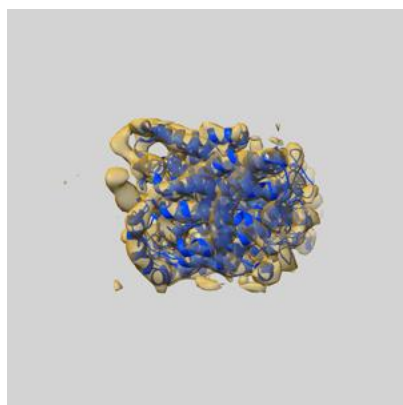
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.90	7.80	6.34
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

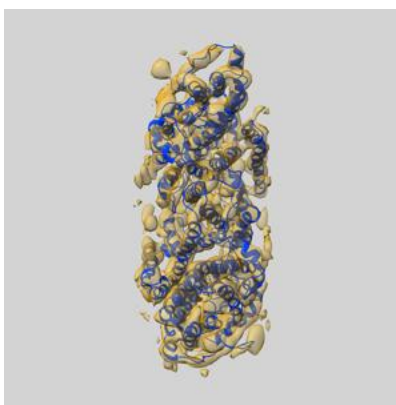
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8313 and PDB model 5SV9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

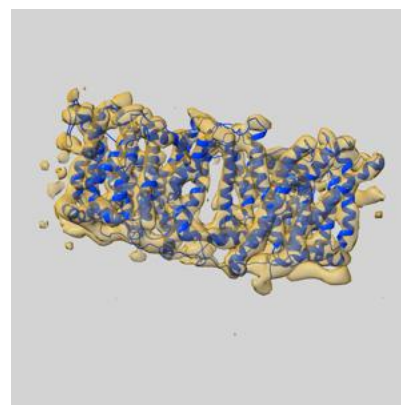
9.1 Map-model overlay [i](#)



X



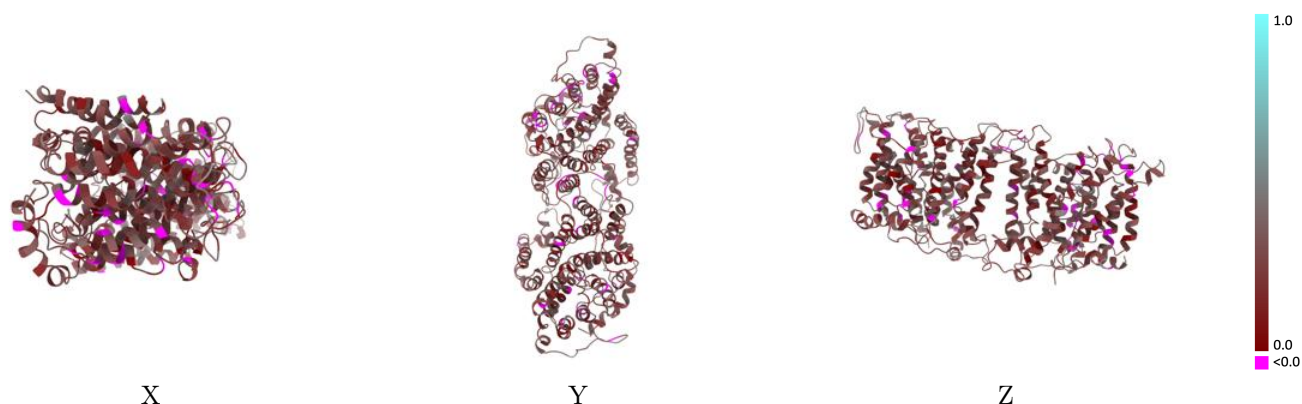
Y



Z

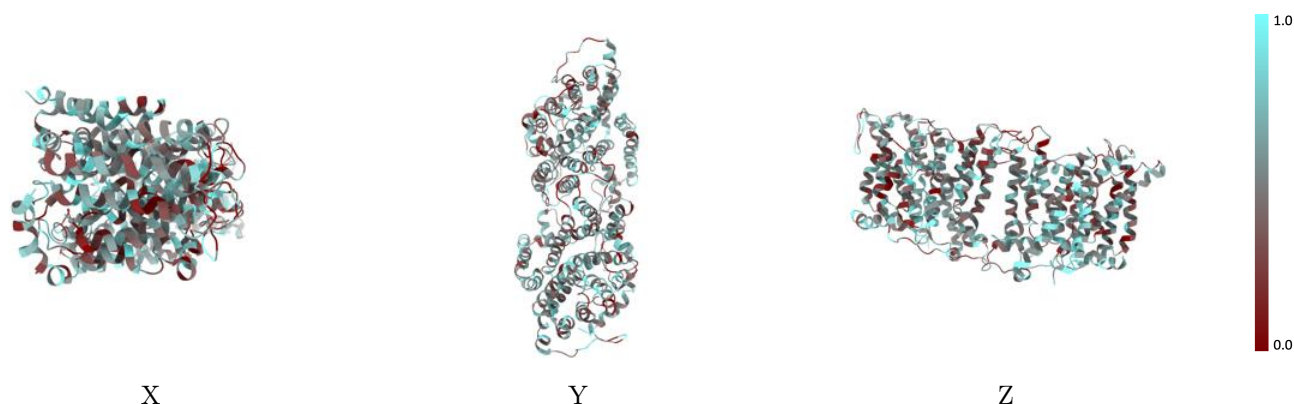
The images above show the 3D surface view of the map at the recommended contour level 130.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



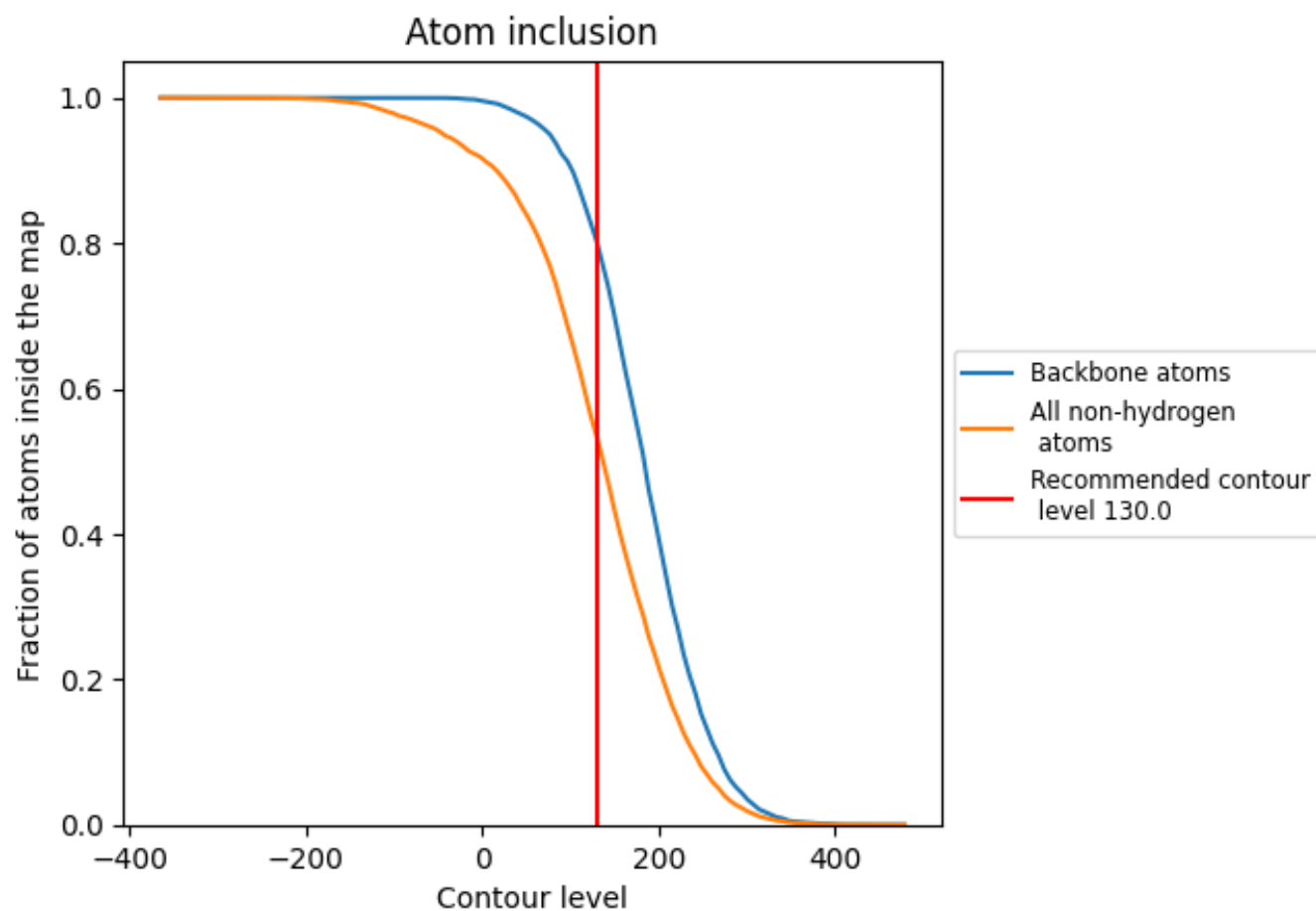
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (130.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 53% 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 (130.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5316	<div></div> 0.2490
A	<div></div> 0.5264	<div></div> 0.2440
B	<div></div> 0.5368	<div></div> 0.2540

