



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 8GRN / pdb_00008grn
EMDB ID : EMD-34209
Title : AtOSCA1.1 extended state
Authors : Zhang, M.F.
Deposited on : 2022-09-02
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

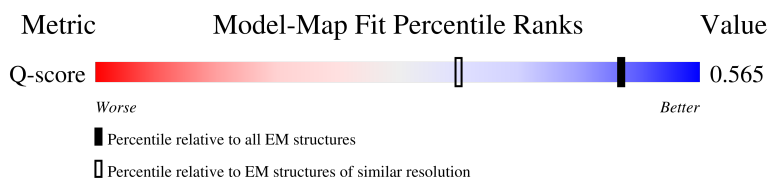
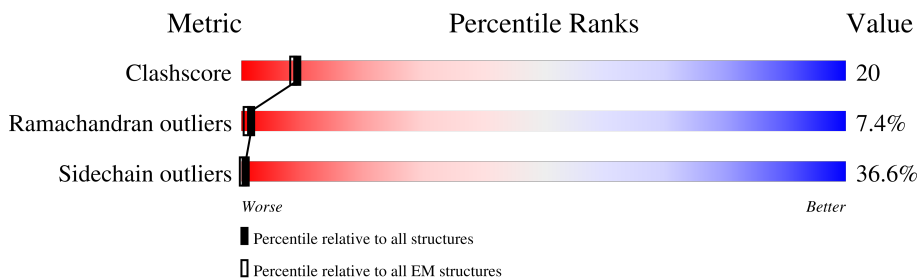
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	772	 10% 22% 36% 24% 11% 7%
1	B	772	 9% 24% 36% 23% 10% 7%

2 Entry composition [i](#)

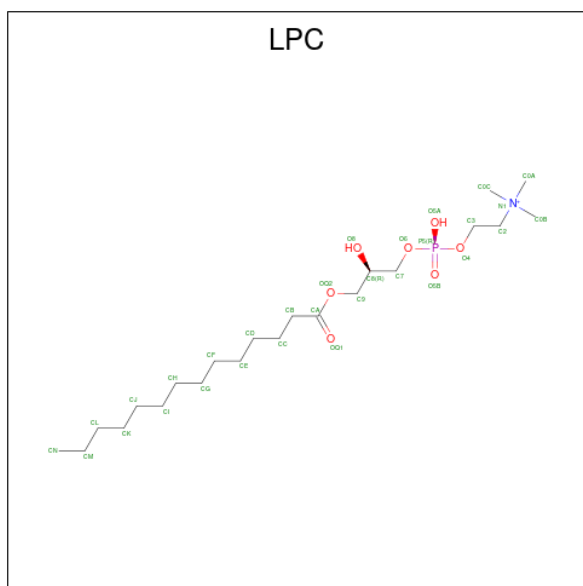
There are 2 unique types of molecules in this entry. The entry contains 11602 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein OSCA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	716	Total	C	N	O	S	0	0
			5770	3802	948	994	26		
1	B	716	Total	C	N	O	S	0	0
			5770	3802	948	994	26		

- Molecule 2 is [1-MYRISTOYL-GLYCEROL-3-YL]PHOSPHONYLCHOLINE (CCD ID: LPC) (formula: $C_{22}H_{47}NO_7P$) (labeled as "Ligand of Interest" by depositor).

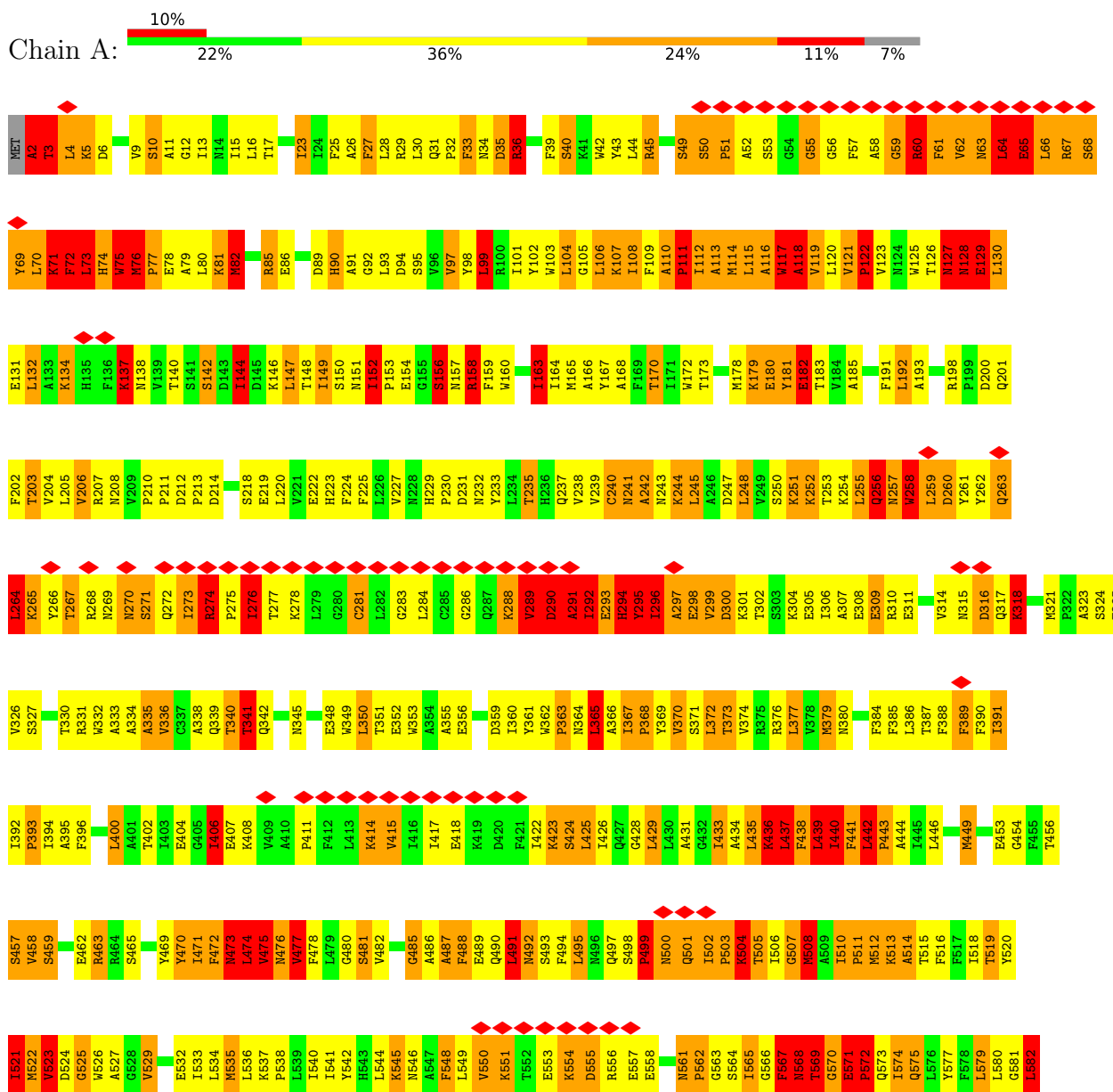


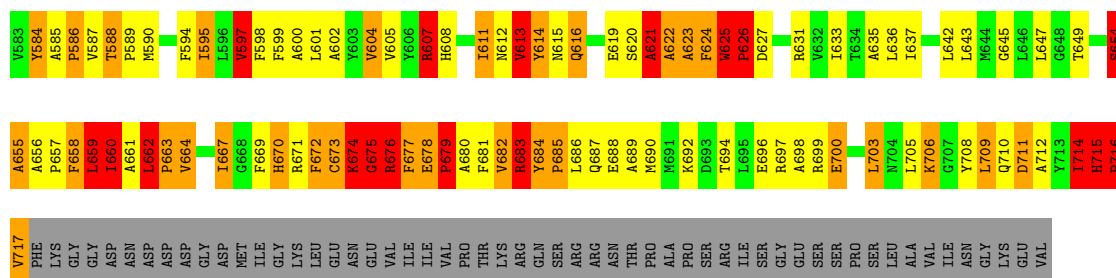
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	22	1	7	1	
2	B	1	Total	C	N	O	P	0
			31	22	1	7	1	

3 Residue-property plots

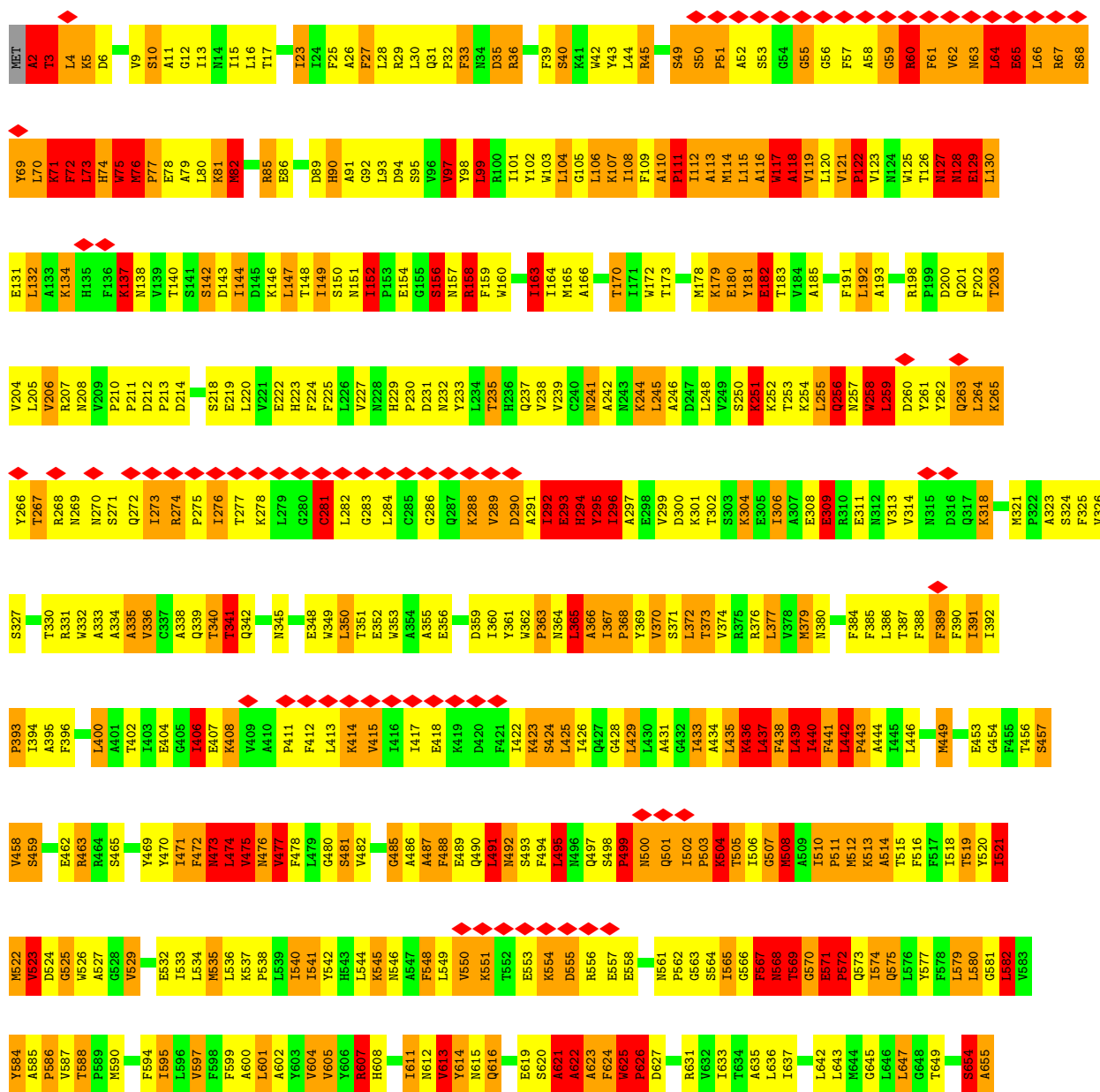
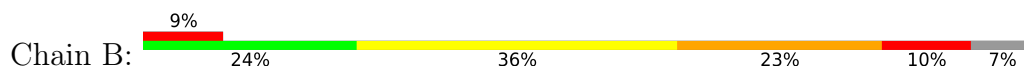
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Protein OSCA1





• Molecule 1: Protein OSCA1



A656	P657	F658	L659	A661	L662	P663	V664		I667	G668	F669	H670	R671	F672	C673	K674	G675	R676	F677	E678	P679	A680	F681	V682	R683	Y684	P685	L686	Q687	E688	A689	M690	M691	K692	D693	T694	L695	E696	R697	A698	R699	E700		L703	N704	L705	K706	G707	Y708	L709	Q710	D711	A712	Y713	I714	H715	P716	V717
PHE	LYS	GLY	GLY	ASP	ASN	ASP	ASP	GLY	ASP	MET	ILE	GLY	LYS	LEU	GLU	ASN	GLU	VAL	ILE	ILE	VAL	PRO	THR	LYS	ARG	GLN	SER	ARG	ARG	ASN	THR	PRO	PRO	SER	ARG	ILE	SER	GLY	GLU	SER	SER	PRO	SER	SER	LEU	ALA	VAL	ILE	ASN	GLY	LYS	GLU	VAL					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	838000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.375	Depositor
Minimum map value	-2.032	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	339.59998, 339.59998, 339.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8489999, 0.8489999, 0.8489999	Depositor

5 Model quality

5.1 Standard geometry

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

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	2.46	340/5928 (5.7%)	2.23	324/8061 (4.0%)
1	B	2.39	320/5928 (5.4%)	2.13	297/8061 (3.7%)
All	All	2.42	660/11856 (5.6%)	2.18	621/16122 (3.9%)

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	9
1	B	0	7
All	All	0	16

All (660) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	LEU	C-O	24.58	1.52	1.24
1	B	437	LEU	C-O	24.58	1.52	1.24
1	A	623	ALA	C-O	23.42	1.55	1.24
1	B	623	ALA	C-O	23.42	1.55	1.24
1	A	440	ILE	C-O	23.10	1.50	1.24
1	B	440	ILE	C-O	23.10	1.50	1.24
1	A	241	ASN	C-O	22.86	1.60	1.23
1	A	655	ALA	C-O	17.99	1.44	1.24
1	B	655	ALA	C-O	17.99	1.44	1.24
1	A	241	ASN	CA-C	17.13	1.73	1.53
1	A	676	ARG	C-O	16.82	1.43	1.24
1	B	676	ARG	C-O	16.82	1.43	1.24
1	A	369	TYR	C-O	14.66	1.43	1.24
1	B	369	TYR	C-O	14.66	1.43	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	PHE	C-O	13.35	1.39	1.24
1	B	438	PHE	C-O	13.35	1.39	1.24
1	A	511	PRO	C-O	13.10	1.41	1.24
1	B	511	PRO	C-O	13.10	1.41	1.24
1	A	655	ALA	CA-C	12.86	1.70	1.52
1	B	655	ALA	CA-C	12.86	1.70	1.52
1	A	241	ASN	N-CA	12.86	1.62	1.46
1	A	507	GLY	C-O	12.74	1.41	1.23
1	B	507	GLY	C-O	12.74	1.41	1.23
1	A	500	ASN	C-O	12.51	1.42	1.23
1	B	500	ASN	C-O	12.51	1.42	1.23
1	A	622	ALA	CA-C	-12.16	1.42	1.53
1	B	622	ALA	CA-C	-12.16	1.42	1.53
1	A	293	GLU	C-O	12.11	1.41	1.23
1	A	98	TYR	C-O	11.54	1.37	1.24
1	B	98	TYR	C-O	11.54	1.37	1.24
1	A	582	LEU	C-O	11.47	1.37	1.24
1	B	582	LEU	C-O	11.47	1.37	1.24
1	A	512	MET	C-O	11.32	1.38	1.24
1	B	512	MET	C-O	11.32	1.38	1.24
1	A	434	ALA	C-O	10.74	1.36	1.24
1	B	434	ALA	C-O	10.74	1.36	1.24
1	A	116	ALA	CA-C	-10.70	1.38	1.52
1	B	116	ALA	CA-C	-10.70	1.38	1.52
1	A	298	GLU	N-CA	-10.60	1.32	1.46
1	A	291	ALA	C-O	10.55	1.37	1.24
1	A	521	ILE	C-O	-10.50	1.11	1.24
1	B	521	ILE	C-O	-10.50	1.11	1.24
1	A	623	ALA	CA-C	10.40	1.66	1.52
1	B	623	ALA	CA-C	10.40	1.66	1.52
1	A	118	ALA	C-O	10.04	1.36	1.24
1	B	118	ALA	C-O	10.04	1.36	1.24
1	A	72	PHE	CA-C	-10.03	1.39	1.52
1	B	72	PHE	CA-C	-10.03	1.39	1.52
1	A	660	ILE	C-O	9.96	1.35	1.24
1	B	660	ILE	C-O	9.96	1.35	1.24
1	A	436	LYS	C-O	9.96	1.36	1.24
1	B	436	LYS	C-O	9.96	1.36	1.24
1	A	607	ARG	CA-C	-9.94	1.40	1.52
1	B	607	ARG	CA-C	-9.94	1.40	1.52
1	A	508	MET	C-O	9.90	1.35	1.24
1	B	508	MET	C-O	9.90	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	LEU	CA-C	-9.86	1.40	1.52
1	B	106	LEU	CA-C	-9.86	1.40	1.52
1	A	428	GLY	C-O	9.77	1.37	1.23
1	B	428	GLY	C-O	9.77	1.37	1.23
1	A	294	HIS	C-O	9.73	1.37	1.23
1	A	658	PHE	C-O	9.63	1.35	1.24
1	B	658	PHE	C-O	9.63	1.35	1.24
1	A	469	TYR	C-O	-9.59	1.12	1.24
1	B	469	TYR	C-O	-9.59	1.12	1.24
1	A	107	LYS	C-O	9.53	1.35	1.24
1	B	107	LYS	C-O	9.53	1.35	1.24
1	A	431	ALA	C-O	9.51	1.35	1.24
1	B	431	ALA	C-O	9.51	1.35	1.24
1	A	489	GLU	C-O	9.50	1.35	1.24
1	B	489	GLU	C-O	9.50	1.35	1.24
1	A	511	PRO	CA-C	9.43	1.68	1.52
1	B	511	PRO	CA-C	9.43	1.68	1.52
1	A	469	TYR	CA-C	-9.42	1.40	1.52
1	B	469	TYR	CA-C	-9.42	1.40	1.52
1	A	158	ARG	CA-C	-9.40	1.44	1.52
1	B	158	ARG	CA-C	-9.40	1.44	1.52
1	A	715	HIS	CA-C	9.26	1.64	1.52
1	B	715	HIS	CA-C	9.26	1.64	1.52
1	A	504	LYS	C-O	9.19	1.34	1.24
1	B	504	LYS	C-O	9.19	1.34	1.24
1	A	675	GLY	C-O	9.16	1.36	1.23
1	B	675	GLY	C-O	9.16	1.36	1.23
1	A	655	ALA	N-CA	9.13	1.58	1.46
1	B	655	ALA	N-CA	9.13	1.58	1.46
1	A	659	LEU	C-O	9.10	1.34	1.24
1	B	659	LEU	C-O	9.10	1.34	1.24
1	A	353	TRP	CA-C	-9.04	1.41	1.52
1	A	674	LYS	CA-C	-9.04	1.40	1.52
1	B	353	TRP	CA-C	-9.04	1.41	1.52
1	B	674	LYS	CA-C	-9.04	1.40	1.52
1	A	258	TRP	CA-C	-9.03	1.40	1.52
1	B	258	TRP	CA-C	-8.87	1.41	1.52
1	A	457	SER	CA-C	-8.82	1.42	1.52
1	B	457	SER	CA-C	-8.82	1.42	1.52
1	A	510	ILE	C-O	8.80	1.35	1.24
1	B	510	ILE	C-O	8.80	1.35	1.24
1	A	388	PHE	C-O	8.78	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	PHE	C-O	8.78	1.34	1.24
1	A	622	ALA	CA-CB	-8.78	1.41	1.53
1	B	622	ALA	CA-CB	-8.78	1.41	1.53
1	A	491	LEU	CA-C	-8.77	1.41	1.52
1	B	491	LEU	CA-C	-8.77	1.41	1.52
1	A	439	LEU	C-O	8.74	1.35	1.24
1	B	439	LEU	C-O	8.74	1.35	1.24
1	A	370	VAL	C-O	8.73	1.35	1.24
1	B	370	VAL	C-O	8.73	1.35	1.24
1	A	473	ASN	C-O	-8.71	1.13	1.24
1	B	473	ASN	C-O	-8.71	1.13	1.24
1	A	333	ALA	CA-C	-8.68	1.40	1.52
1	B	333	ALA	CA-C	-8.68	1.40	1.52
1	A	521	ILE	CA-C	-8.65	1.41	1.52
1	B	521	ILE	CA-C	-8.65	1.41	1.52
1	A	298	GLU	C-N	8.58	1.44	1.33
1	A	291	ALA	CA-C	8.55	1.64	1.52
1	A	43	TYR	CA-C	-8.49	1.41	1.52
1	B	43	TYR	CA-C	-8.49	1.41	1.52
1	A	627	ASP	N-CA	8.42	1.56	1.46
1	B	627	ASP	N-CA	8.42	1.56	1.46
1	A	110	ALA	N-CA	-8.41	1.39	1.46
1	B	110	ALA	N-CA	-8.41	1.39	1.46
1	A	81	LYS	N-CA	8.39	1.58	1.46
1	B	81	LYS	N-CA	8.39	1.58	1.46
1	A	298	GLU	C-O	8.30	1.34	1.24
1	A	473	ASN	CA-C	-8.30	1.41	1.52
1	B	473	ASN	CA-C	-8.30	1.41	1.52
1	A	437	LEU	CA-C	8.18	1.63	1.52
1	B	437	LEU	CA-C	8.18	1.63	1.52
1	A	672	PHE	C-O	8.03	1.33	1.24
1	B	672	PHE	C-O	8.03	1.33	1.24
1	A	470	TYR	CA-C	-7.99	1.42	1.52
1	B	470	TYR	CA-C	-7.99	1.42	1.52
1	A	601	LEU	CA-C	-7.98	1.42	1.52
1	B	601	LEU	CA-C	-7.98	1.42	1.52
1	A	488	PHE	C-O	7.95	1.33	1.24
1	B	488	PHE	C-O	7.95	1.33	1.24
1	A	624	PHE	N-CA	-7.91	1.35	1.46
1	B	624	PHE	N-CA	-7.91	1.35	1.46
1	A	349	TRP	CA-C	-7.82	1.46	1.53
1	B	349	TRP	CA-C	-7.82	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	GLU	CA-C	-7.78	1.42	1.52
1	B	222	GLU	CA-C	-7.78	1.42	1.52
1	A	444	ALA	N-CA	7.76	1.55	1.46
1	B	444	ALA	N-CA	7.76	1.55	1.46
1	A	567	PHE	CA-C	-7.69	1.42	1.52
1	B	567	PHE	CA-C	-7.69	1.42	1.52
1	A	296	ILE	C-N	-7.69	1.23	1.33
1	A	113	ALA	CA-C	-7.63	1.43	1.52
1	B	113	ALA	CA-C	-7.63	1.43	1.52
1	A	679	PRO	CA-CB	-7.57	1.43	1.53
1	B	679	PRO	CA-CB	-7.57	1.43	1.53
1	A	79	ALA	CA-C	-7.56	1.43	1.52
1	B	79	ALA	CA-C	-7.56	1.43	1.52
1	A	191	PHE	CA-C	-7.56	1.43	1.52
1	B	191	PHE	CA-C	-7.56	1.43	1.52
1	A	441	PHE	N-CA	7.55	1.55	1.46
1	B	441	PHE	N-CA	7.55	1.55	1.46
1	A	657	PRO	C-O	7.52	1.33	1.24
1	B	657	PRO	C-O	7.52	1.33	1.24
1	A	369	TYR	CA-C	7.51	1.62	1.52
1	B	369	TYR	CA-C	7.51	1.62	1.52
1	A	352	GLU	C-O	-7.46	1.16	1.24
1	B	352	GLU	C-O	-7.46	1.16	1.24
1	A	336	VAL	C-O	-7.41	1.16	1.24
1	B	336	VAL	C-O	-7.41	1.16	1.24
1	A	299	VAL	C-O	7.40	1.32	1.24
1	A	516	PHE	N-CA	7.38	1.55	1.46
1	B	516	PHE	N-CA	7.38	1.55	1.46
1	A	117	TRP	CA-C	-7.29	1.43	1.52
1	B	117	TRP	CA-C	-7.29	1.43	1.52
1	A	433	ILE	C-O	7.29	1.32	1.24
1	B	433	ILE	C-O	7.29	1.32	1.24
1	A	712	ALA	CA-C	-7.28	1.43	1.52
1	B	712	ALA	CA-C	-7.28	1.43	1.52
1	A	371	SER	N-CA	-7.27	1.37	1.46
1	B	371	SER	N-CA	-7.27	1.37	1.46
1	A	680	ALA	N-CA	7.25	1.55	1.46
1	B	680	ALA	N-CA	7.25	1.55	1.46
1	A	239	VAL	C-O	-7.25	1.16	1.24
1	B	239	VAL	C-O	-7.25	1.16	1.24
1	A	428	GLY	CA-C	7.25	1.62	1.51
1	A	515	THR	N-CA	7.25	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	428	GLY	CA-C	7.25	1.62	1.51
1	B	515	THR	N-CA	7.25	1.55	1.46
1	A	110	ALA	C-O	7.21	1.32	1.24
1	B	110	ALA	C-O	7.21	1.32	1.24
1	A	443	PRO	C-O	7.21	1.33	1.24
1	B	443	PRO	C-O	7.21	1.33	1.24
1	A	373	THR	N-CA	7.20	1.54	1.46
1	B	373	THR	N-CA	7.20	1.54	1.46
1	A	586	PRO	C-O	-7.17	1.16	1.23
1	B	586	PRO	C-O	-7.17	1.16	1.23
1	A	326	VAL	C-O	-7.17	1.15	1.24
1	B	326	VAL	C-O	-7.17	1.15	1.24
1	A	296	ILE	N-CA	7.17	1.55	1.46
1	A	373	THR	C-O	7.16	1.32	1.24
1	B	373	THR	C-O	7.16	1.32	1.24
1	A	515	THR	C-O	7.15	1.32	1.24
1	B	515	THR	C-O	7.15	1.32	1.24
1	A	202	PHE	C-O	-7.12	1.15	1.24
1	B	202	PHE	C-O	-7.12	1.15	1.24
1	A	389	PHE	C-O	7.11	1.32	1.24
1	B	389	PHE	C-O	7.11	1.32	1.24
1	A	425	LEU	C-O	7.10	1.32	1.24
1	B	425	LEU	C-O	7.10	1.32	1.24
1	A	620	SER	CA-C	-7.03	1.43	1.53
1	B	620	SER	CA-C	-7.03	1.43	1.53
1	A	362	TRP	CA-C	-7.00	1.44	1.52
1	B	362	TRP	CA-C	-7.00	1.44	1.52
1	A	299	VAL	N-CA	6.99	1.54	1.46
1	A	659	LEU	CA-C	6.94	1.62	1.52
1	B	659	LEU	CA-C	6.94	1.62	1.52
1	A	429	LEU	N-CA	6.93	1.54	1.46
1	B	429	LEU	N-CA	6.93	1.54	1.46
1	A	613	VAL	C-O	-6.92	1.15	1.24
1	B	613	VAL	C-O	-6.92	1.15	1.24
1	A	508	MET	CA-C	6.87	1.61	1.52
1	B	508	MET	CA-C	6.87	1.61	1.52
1	A	334	ALA	CA-C	-6.86	1.43	1.52
1	B	334	ALA	CA-C	-6.86	1.43	1.52
1	A	692	LYS	CA-C	-6.85	1.43	1.52
1	B	692	LYS	CA-C	-6.85	1.43	1.52
1	A	424	SER	C-O	6.85	1.32	1.24
1	B	424	SER	C-O	6.85	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	ASN	CA-C	-6.84	1.44	1.52
1	B	345	ASN	CA-C	-6.84	1.44	1.52
1	A	384	PHE	C-O	6.81	1.31	1.24
1	A	514	ALA	CA-C	-6.81	1.44	1.52
1	B	384	PHE	C-O	6.81	1.31	1.24
1	B	514	ALA	CA-C	-6.81	1.44	1.52
1	A	71	LYS	CA-C	-6.81	1.44	1.52
1	B	71	LYS	CA-C	-6.81	1.44	1.52
1	A	181	TYR	CA-C	-6.81	1.44	1.52
1	B	181	TYR	CA-C	-6.81	1.44	1.52
1	A	356	GLU	CA-C	-6.81	1.44	1.53
1	B	356	GLU	CA-C	-6.81	1.44	1.53
1	A	299	VAL	CA-C	6.79	1.61	1.52
1	A	526	TRP	N-CA	-6.78	1.38	1.46
1	B	526	TRP	N-CA	-6.78	1.38	1.46
1	A	333	ALA	CA-CB	-6.76	1.42	1.53
1	B	333	ALA	CA-CB	-6.76	1.42	1.53
1	A	204	VAL	C-O	-6.75	1.16	1.23
1	B	204	VAL	C-O	-6.75	1.16	1.23
1	A	474	LEU	CA-C	-6.73	1.43	1.52
1	B	474	LEU	CA-C	-6.73	1.43	1.52
1	A	525	GLY	CA-C	-6.71	1.42	1.51
1	B	525	GLY	CA-C	-6.71	1.42	1.51
1	A	116	ALA	C-O	-6.70	1.15	1.24
1	B	116	ALA	C-O	-6.70	1.15	1.24
1	A	415	VAL	CA-C	-6.70	1.47	1.52
1	B	415	VAL	CA-C	-6.70	1.47	1.52
1	A	680	ALA	C-O	-6.68	1.16	1.24
1	B	680	ALA	C-O	-6.68	1.16	1.24
1	A	623	ALA	N-CA	6.62	1.54	1.46
1	B	623	ALA	N-CA	6.62	1.54	1.46
1	A	602	ALA	CA-CB	-6.59	1.43	1.53
1	B	602	ALA	CA-CB	-6.59	1.43	1.53
1	A	158	ARG	C-O	-6.54	1.19	1.23
1	B	158	ARG	C-O	-6.54	1.19	1.23
1	A	687	GLN	CA-C	-6.53	1.43	1.52
1	B	687	GLN	CA-C	-6.53	1.43	1.52
1	A	257	ASN	C-O	6.52	1.31	1.24
1	A	335	ALA	C-O	-6.52	1.15	1.24
1	B	335	ALA	C-O	-6.52	1.15	1.24
1	A	39	PHE	C-O	-6.51	1.17	1.23
1	B	39	PHE	C-O	-6.51	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLU	CA-C	-6.50	1.44	1.52
1	B	154	GLU	CA-C	-6.50	1.44	1.52
1	A	366	ALA	CA-CB	-6.49	1.44	1.53
1	B	366	ALA	CA-CB	-6.49	1.44	1.53
1	A	158	ARG	N-CA	-6.48	1.41	1.47
1	B	158	ARG	N-CA	-6.48	1.41	1.47
1	A	673	CYS	CA-C	-6.44	1.44	1.52
1	B	673	CYS	CA-C	-6.44	1.44	1.52
1	A	616	GLN	CA-C	-6.42	1.44	1.52
1	B	616	GLN	CA-C	-6.42	1.44	1.52
1	A	151	ASN	CA-C	-6.41	1.44	1.52
1	B	151	ASN	CA-C	-6.41	1.44	1.52
1	A	98	TYR	CA-C	6.41	1.61	1.52
1	B	98	TYR	CA-C	6.41	1.61	1.52
1	A	229	HIS	CA-C	-6.41	1.44	1.52
1	B	229	HIS	CA-C	-6.41	1.44	1.52
1	B	242	ALA	CA-C	-6.40	1.44	1.52
1	A	355	ALA	CA-C	-6.37	1.44	1.53
1	B	355	ALA	CA-C	-6.37	1.44	1.53
1	A	335	ALA	CA-C	-6.34	1.44	1.52
1	B	335	ALA	CA-C	-6.34	1.44	1.52
1	A	626	PRO	C-O	6.33	1.32	1.24
1	B	626	PRO	C-O	6.33	1.32	1.24
1	A	237	GLN	C-O	-6.33	1.16	1.23
1	A	240	CYS	C-N	6.33	1.41	1.33
1	B	237	GLN	C-O	-6.33	1.16	1.23
1	A	90	HIS	CA-C	-6.31	1.44	1.53
1	B	90	HIS	CA-C	-6.31	1.44	1.53
1	A	207	ARG	C-O	-6.29	1.16	1.24
1	B	207	ARG	C-O	-6.29	1.16	1.24
1	A	459	SER	CA-C	-6.29	1.44	1.52
1	B	459	SER	CA-C	-6.29	1.44	1.52
1	A	685	PRO	C-O	-6.28	1.16	1.23
1	B	685	PRO	C-O	-6.28	1.16	1.23
1	A	514	ALA	N-CA	6.27	1.53	1.46
1	B	514	ALA	N-CA	6.27	1.53	1.46
1	A	472	PHE	C-O	-6.27	1.16	1.24
1	B	472	PHE	C-O	-6.27	1.16	1.24
1	A	149	ILE	CA-C	-6.24	1.44	1.52
1	B	149	ILE	CA-C	-6.24	1.44	1.52
1	A	388	PHE	CA-C	6.24	1.61	1.52
1	B	388	PHE	CA-C	6.24	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ASP	N-CA	-6.24	1.38	1.46
1	B	94	ASP	N-CA	-6.24	1.38	1.46
1	A	369	TYR	N-CA	6.23	1.54	1.46
1	B	369	TYR	N-CA	6.23	1.54	1.46
1	A	512	MET	N-CA	6.23	1.54	1.46
1	B	512	MET	N-CA	6.23	1.54	1.46
1	A	44	LEU	CA-C	-6.19	1.43	1.52
1	B	44	LEU	CA-C	-6.19	1.43	1.52
1	A	612	ASN	C-O	-6.19	1.16	1.24
1	A	676	ARG	CA-C	6.19	1.60	1.52
1	B	612	ASN	C-O	-6.19	1.16	1.24
1	B	676	ARG	CA-C	6.19	1.60	1.52
1	A	297	ALA	CA-C	-6.18	1.44	1.52
1	B	256	GLN	C-O	-6.17	1.17	1.24
1	A	111	PRO	C-O	6.15	1.31	1.24
1	B	111	PRO	C-O	6.15	1.31	1.24
1	A	27	PHE	CA-C	-6.14	1.45	1.52
1	B	27	PHE	CA-C	-6.14	1.45	1.52
1	A	607	ARG	N-CA	-6.14	1.38	1.46
1	A	656	ALA	CA-C	6.14	1.60	1.52
1	B	607	ARG	N-CA	-6.14	1.38	1.46
1	B	656	ALA	CA-C	6.14	1.60	1.52
1	A	478	PHE	CA-C	-6.12	1.45	1.52
1	B	478	PHE	CA-C	-6.12	1.45	1.52
1	A	207	ARG	CA-C	-6.12	1.45	1.52
1	B	207	ARG	CA-C	-6.12	1.45	1.52
1	A	654	SER	C-N	6.10	1.42	1.33
1	B	654	SER	C-N	6.10	1.42	1.33
1	A	670	HIS	CA-C	-6.08	1.45	1.52
1	B	670	HIS	CA-C	-6.08	1.45	1.52
1	A	514	ALA	CA-CB	-6.07	1.43	1.53
1	B	514	ALA	CA-CB	-6.07	1.43	1.53
1	A	361	TYR	CA-C	-6.07	1.45	1.53
1	B	361	TYR	CA-C	-6.07	1.45	1.53
1	A	119	VAL	C-O	6.06	1.30	1.24
1	B	119	VAL	C-O	6.06	1.30	1.24
1	A	76	MET	C-O	6.05	1.31	1.24
1	B	76	MET	C-O	6.05	1.31	1.24
1	A	709	LEU	CA-C	-6.05	1.44	1.52
1	B	709	LEU	CA-C	-6.05	1.44	1.52
1	A	263	GLN	CA-C	-6.04	1.46	1.52
1	A	586	PRO	CA-C	6.03	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	PRO	CA-C	6.03	1.58	1.52
1	A	458	VAL	C-O	-6.02	1.17	1.24
1	B	458	VAL	C-O	-6.02	1.17	1.24
1	A	111	PRO	CA-CB	-6.01	1.44	1.53
1	B	111	PRO	CA-CB	-6.01	1.44	1.53
1	A	604	VAL	CA-C	6.00	1.60	1.52
1	B	604	VAL	CA-C	6.00	1.60	1.52
1	A	440	ILE	N-CA	5.99	1.53	1.46
1	B	440	ILE	N-CA	5.99	1.53	1.46
1	A	245	LEU	N-CA	5.98	1.53	1.46
1	A	457	SER	C-O	-5.97	1.16	1.23
1	B	457	SER	C-O	-5.97	1.16	1.23
1	A	490	GLN	C-O	-5.97	1.15	1.24
1	B	490	GLN	C-O	-5.97	1.15	1.24
1	A	95	SER	C-O	5.96	1.31	1.24
1	B	95	SER	C-O	5.96	1.31	1.24
1	A	220	LEU	N-CA	-5.94	1.38	1.45
1	B	220	LEU	N-CA	-5.94	1.38	1.45
1	A	198	ARG	C-O	-5.91	1.18	1.24
1	B	198	ARG	C-O	-5.91	1.18	1.24
1	A	481	SER	N-CA	-5.91	1.39	1.46
1	B	481	SER	N-CA	-5.91	1.39	1.46
1	A	332	TRP	CA-C	-5.89	1.44	1.52
1	B	332	TRP	CA-C	-5.89	1.44	1.52
1	A	182	GLU	CA-C	-5.88	1.45	1.52
1	A	325	PHE	C-O	-5.88	1.17	1.24
1	B	182	GLU	CA-C	-5.88	1.45	1.52
1	B	325	PHE	C-O	-5.88	1.17	1.24
1	A	235	THR	C-O	-5.88	1.17	1.23
1	B	235	THR	C-O	-5.88	1.17	1.23
1	A	625	TRP	N-CA	-5.87	1.41	1.46
1	B	625	TRP	N-CA	-5.87	1.41	1.46
1	A	193	ALA	CA-CB	-5.86	1.43	1.53
1	B	193	ALA	CA-CB	-5.86	1.43	1.53
1	B	245	LEU	CA-C	-5.86	1.44	1.52
1	A	623	ALA	CA-CB	-5.84	1.44	1.53
1	B	623	ALA	CA-CB	-5.84	1.44	1.53
1	A	324	SER	C-O	-5.82	1.16	1.23
1	B	324	SER	C-O	-5.82	1.16	1.23
1	A	677	PHE	C-O	5.82	1.31	1.24
1	B	677	PHE	C-O	5.82	1.31	1.24
1	A	567	PHE	C-O	-5.82	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	567	PHE	C-O	-5.82	1.16	1.24
1	A	518	ILE	CA-C	-5.81	1.46	1.52
1	A	623	ALA	C-N	-5.81	1.25	1.33
1	B	518	ILE	CA-C	-5.81	1.46	1.52
1	B	623	ALA	C-N	-5.81	1.25	1.33
1	A	488	PHE	CA-C	5.81	1.60	1.52
1	B	488	PHE	CA-C	5.81	1.60	1.52
1	A	615	ASN	C-O	-5.81	1.17	1.23
1	B	615	ASN	C-O	-5.81	1.17	1.23
1	A	229	HIS	C-O	-5.80	1.17	1.24
1	A	660	ILE	N-CA	5.80	1.53	1.46
1	B	229	HIS	C-O	-5.80	1.17	1.24
1	B	660	ILE	N-CA	5.80	1.53	1.46
1	A	689	ALA	CA-CB	-5.80	1.43	1.53
1	B	689	ALA	CA-CB	-5.80	1.43	1.53
1	A	128	ASN	N-CA	5.79	1.53	1.46
1	B	128	ASN	N-CA	5.79	1.53	1.46
1	A	291	ALA	N-CA	5.78	1.53	1.46
1	A	608	HIS	C-O	-5.77	1.17	1.24
1	B	608	HIS	C-O	-5.77	1.17	1.24
1	A	475	VAL	CA-C	-5.77	1.45	1.52
1	B	475	VAL	CA-C	-5.77	1.45	1.52
1	A	520	TYR	C-O	-5.76	1.17	1.24
1	B	520	TYR	C-O	-5.76	1.17	1.24
1	A	495	LEU	C-O	-5.76	1.17	1.24
1	B	495	LEU	C-O	-5.76	1.17	1.24
1	A	237	GLN	CA-C	-5.75	1.45	1.52
1	B	237	GLN	CA-C	-5.75	1.45	1.52
1	A	444	ALA	CA-CB	-5.75	1.44	1.53
1	B	444	ALA	CA-CB	-5.75	1.44	1.53
1	A	146	LYS	N-CA	-5.74	1.39	1.46
1	B	146	LYS	N-CA	-5.74	1.39	1.46
1	A	476	ASN	C-O	-5.73	1.16	1.24
1	B	476	ASN	C-O	-5.73	1.16	1.24
1	A	571	GLU	N-CA	-5.73	1.41	1.46
1	B	571	GLU	N-CA	-5.73	1.41	1.46
1	A	656	ALA	C-O	5.72	1.31	1.24
1	B	656	ALA	C-O	5.72	1.31	1.24
1	A	99	LEU	C-O	5.72	1.31	1.24
1	B	99	LEU	C-O	5.72	1.31	1.24
1	A	348	GLU	CA-C	-5.71	1.45	1.52
1	B	348	GLU	CA-C	-5.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	ARG	CA-C	-5.71	1.45	1.52
1	B	85	ARG	CA-C	-5.71	1.45	1.52
1	A	74	HIS	N-CA	-5.70	1.39	1.46
1	B	74	HIS	N-CA	-5.70	1.39	1.46
1	A	678	GLU	CA-C	-5.69	1.45	1.52
1	B	678	GLU	CA-C	-5.69	1.45	1.52
1	A	321	MET	CA-C	-5.67	1.44	1.52
1	B	321	MET	CA-C	-5.67	1.44	1.52
1	A	323	ALA	CA-CB	-5.67	1.44	1.53
1	B	323	ALA	CA-CB	-5.67	1.44	1.53
1	A	527	ALA	CA-C	-5.66	1.44	1.52
1	B	527	ALA	CA-C	-5.66	1.44	1.52
1	A	515	THR	CA-C	5.65	1.60	1.52
1	B	515	THR	CA-C	5.65	1.60	1.52
1	A	102	TYR	N-CA	5.64	1.53	1.46
1	B	102	TYR	N-CA	5.64	1.53	1.46
1	A	435	LEU	C-O	5.63	1.30	1.24
1	B	435	LEU	C-O	5.63	1.30	1.24
1	A	569	THR	C-O	5.63	1.30	1.24
1	B	569	THR	C-O	5.63	1.30	1.24
1	A	185	ALA	CA-CB	-5.62	1.44	1.53
1	B	185	ALA	CA-CB	-5.62	1.44	1.53
1	A	502	ILE	CA-C	5.57	1.58	1.52
1	B	502	ILE	CA-C	5.57	1.58	1.52
1	A	225	PHE	C-O	-5.57	1.16	1.24
1	B	225	PHE	C-O	-5.57	1.16	1.24
1	A	350	LEU	C-O	-5.57	1.17	1.23
1	B	350	LEU	C-O	-5.57	1.17	1.23
1	A	207	ARG	N-CA	-5.57	1.39	1.46
1	B	207	ARG	N-CA	-5.57	1.39	1.46
1	A	180	GLU	CA-C	-5.56	1.45	1.52
1	B	180	GLU	CA-C	-5.56	1.45	1.52
1	A	251	LYS	CA-C	-5.55	1.45	1.52
1	A	290	ASP	C-N	5.55	1.41	1.33
1	A	477	VAL	CA-C	-5.54	1.46	1.52
1	B	477	VAL	CA-C	-5.54	1.46	1.52
1	A	572	PRO	CA-CB	-5.54	1.46	1.53
1	B	572	PRO	CA-CB	-5.54	1.46	1.53
1	A	206	VAL	C-O	-5.53	1.18	1.24
1	B	206	VAL	C-O	-5.53	1.18	1.24
1	A	198	ARG	CA-C	-5.53	1.47	1.52
1	B	198	ARG	CA-C	-5.53	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439	LEU	CA-C	5.53	1.60	1.52
1	B	439	LEU	CA-C	5.53	1.60	1.52
1	A	355	ALA	N-CA	-5.52	1.38	1.45
1	A	614	TYR	C-O	-5.52	1.17	1.24
1	B	355	ALA	N-CA	-5.52	1.38	1.45
1	B	614	TYR	C-O	-5.52	1.17	1.24
1	A	3	THR	C-O	5.51	1.30	1.24
1	A	360	ILE	C-O	-5.51	1.18	1.24
1	B	3	THR	C-O	5.51	1.30	1.24
1	B	360	ILE	C-O	-5.51	1.18	1.24
1	A	429	LEU	CA-C	5.50	1.60	1.52
1	B	429	LEU	CA-C	5.50	1.60	1.52
1	A	341	THR	CA-C	-5.50	1.45	1.52
1	B	341	THR	CA-C	-5.50	1.45	1.52
1	A	86	GLU	CA-C	-5.49	1.45	1.52
1	B	86	GLU	CA-C	-5.49	1.45	1.52
1	A	256	GLN	C-O	-5.47	1.17	1.24
1	A	573	GLN	CA-C	-5.46	1.45	1.52
1	B	573	GLN	CA-C	-5.46	1.45	1.52
1	A	621	ALA	CA-CB	-5.46	1.44	1.53
1	B	621	ALA	CA-CB	-5.46	1.44	1.53
1	A	449	MET	C-O	-5.45	1.17	1.24
1	B	251	LYS	CA-C	-5.45	1.45	1.52
1	B	449	MET	C-O	-5.45	1.17	1.24
1	A	242	ALA	C-O	-5.44	1.15	1.24
1	A	36	ARG	CA-C	-5.42	1.45	1.52
1	B	36	ARG	CA-C	-5.42	1.45	1.52
1	A	619	GLU	CA-C	-5.42	1.46	1.52
1	B	619	GLU	CA-C	-5.42	1.46	1.52
1	A	529	VAL	N-CA	-5.42	1.39	1.46
1	B	529	VAL	N-CA	-5.42	1.39	1.46
1	A	227	VAL	C-O	-5.40	1.17	1.24
1	B	227	VAL	C-O	-5.40	1.17	1.24
1	A	109	PHE	C-O	-5.38	1.17	1.24
1	B	109	PHE	C-O	-5.38	1.17	1.24
1	A	200	ASP	CA-C	-5.37	1.45	1.52
1	B	200	ASP	CA-C	-5.37	1.45	1.52
1	A	222	GLU	CA-CB	-5.36	1.45	1.53
1	B	222	GLU	CA-CB	-5.36	1.45	1.53
1	A	338	ALA	CA-CB	-5.35	1.44	1.53
1	A	470	TYR	C-O	-5.35	1.17	1.24
1	B	338	ALA	CA-CB	-5.35	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	470	TYR	C-O	-5.35	1.17	1.24
1	A	635	ALA	CA-CB	-5.34	1.45	1.53
1	B	635	ALA	CA-CB	-5.34	1.45	1.53
1	B	270	ASN	CA-C	-5.33	1.48	1.53
1	A	364	ASN	CA-C	-5.32	1.46	1.52
1	B	364	ASN	CA-C	-5.32	1.46	1.52
1	A	193	ALA	CA-C	-5.31	1.45	1.52
1	B	193	ALA	CA-C	-5.31	1.45	1.52
1	A	380	ASN	C-O	5.31	1.30	1.24
1	B	380	ASN	C-O	5.31	1.30	1.24
1	A	534	LEU	CA-C	-5.31	1.45	1.52
1	B	534	LEU	CA-C	-5.31	1.45	1.52
1	A	584	TYR	CA-C	-5.30	1.45	1.52
1	B	584	TYR	CA-C	-5.30	1.45	1.52
1	A	348	GLU	N-CA	-5.30	1.39	1.45
1	B	348	GLU	N-CA	-5.30	1.39	1.45
1	A	542	TYR	CA-C	-5.29	1.45	1.52
1	B	542	TYR	CA-C	-5.29	1.45	1.52
1	A	108	ILE	C-O	5.29	1.30	1.24
1	B	108	ILE	C-O	5.29	1.30	1.24
1	A	392	ILE	N-CA	5.28	1.53	1.46
1	B	392	ILE	N-CA	5.28	1.53	1.46
1	A	353	TRP	C-O	-5.28	1.17	1.23
1	B	353	TRP	C-O	-5.28	1.17	1.23
1	A	334	ALA	CA-CB	-5.27	1.45	1.53
1	B	334	ALA	CA-CB	-5.27	1.45	1.53
1	A	330	THR	C-O	-5.26	1.17	1.23
1	B	330	THR	C-O	-5.26	1.17	1.23
1	A	459	SER	CA-CB	-5.26	1.45	1.53
1	B	459	SER	CA-CB	-5.26	1.45	1.53
1	A	122	PRO	C-O	5.25	1.31	1.24
1	B	122	PRO	C-O	5.25	1.31	1.24
1	A	607	ARG	CA-CB	-5.25	1.45	1.53
1	B	607	ARG	CA-CB	-5.25	1.45	1.53
1	A	198	ARG	N-CA	-5.24	1.41	1.45
1	A	532	GLU	C-O	-5.24	1.17	1.24
1	B	198	ARG	N-CA	-5.24	1.41	1.45
1	B	532	GLU	C-O	-5.24	1.17	1.24
1	A	465	SER	CA-CB	-5.24	1.45	1.53
1	B	465	SER	CA-CB	-5.24	1.45	1.53
1	A	360	ILE	CA-C	-5.24	1.46	1.52
1	B	360	ILE	CA-C	-5.24	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	472	PHE	CA-C	-5.23	1.45	1.52
1	B	472	PHE	CA-C	-5.23	1.45	1.52
1	A	694	THR	CA-C	-5.23	1.45	1.52
1	B	694	THR	CA-C	-5.23	1.45	1.52
1	A	715	HIS	C-N	5.23	1.46	1.33
1	B	715	HIS	C-N	5.23	1.46	1.33
1	A	377	LEU	N-CA	5.23	1.52	1.46
1	B	377	LEU	N-CA	5.23	1.52	1.46
1	A	110	ALA	CA-CB	-5.22	1.46	1.53
1	B	110	ALA	CA-CB	-5.22	1.46	1.53
1	B	259	LEU	N-CA	-5.22	1.39	1.46
1	A	224	PHE	CA-C	-5.22	1.46	1.52
1	A	385	PHE	C-O	5.22	1.30	1.24
1	B	224	PHE	CA-C	-5.22	1.46	1.52
1	B	385	PHE	C-O	5.22	1.30	1.24
1	A	440	ILE	CA-C	5.22	1.58	1.52
1	B	440	ILE	CA-C	5.22	1.58	1.52
1	A	373	THR	CA-C	5.21	1.59	1.52
1	B	373	THR	CA-C	5.21	1.59	1.52
1	A	463	ARG	N-CA	-5.20	1.40	1.46
1	B	463	ARG	N-CA	-5.20	1.40	1.46
1	A	15	ILE	N-CA	-5.20	1.40	1.46
1	B	15	ILE	N-CA	-5.20	1.40	1.46
1	A	11	ALA	CA-C	-5.19	1.46	1.52
1	A	519	THR	N-CA	5.19	1.52	1.46
1	B	11	ALA	CA-C	-5.19	1.46	1.52
1	B	519	THR	N-CA	5.19	1.52	1.46
1	A	493	SER	N-CA	5.19	1.52	1.46
1	B	493	SER	N-CA	5.19	1.52	1.46
1	A	110	ALA	CA-C	-5.18	1.46	1.52
1	B	110	ALA	CA-C	-5.18	1.46	1.52
1	A	683	ARG	C-O	-5.18	1.17	1.23
1	B	683	ARG	C-O	-5.18	1.17	1.23
1	A	480	GLY	CA-C	-5.18	1.44	1.51
1	B	480	GLY	CA-C	-5.18	1.44	1.51
1	A	619	GLU	C-O	-5.16	1.18	1.24
1	B	619	GLU	C-O	-5.16	1.18	1.24
1	A	342	GLN	CA-C	-5.15	1.46	1.52
1	B	342	GLN	CA-C	-5.15	1.46	1.52
1	A	481	SER	CA-C	-5.14	1.46	1.52
1	B	481	SER	CA-C	-5.14	1.46	1.52
1	A	201	GLN	CA-C	-5.14	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	GLN	CA-C	-5.14	1.45	1.52
1	A	429	LEU	C-O	5.14	1.30	1.24
1	B	429	LEU	C-O	5.14	1.30	1.24
1	A	622	ALA	N-CA	-5.14	1.39	1.46
1	B	622	ALA	N-CA	-5.14	1.39	1.46
1	A	712	ALA	CA-CB	-5.13	1.45	1.53
1	B	712	ALA	CA-CB	-5.13	1.45	1.53
1	A	92	GLY	C-O	-5.13	1.17	1.23
1	A	165	MET	CA-C	-5.13	1.46	1.52
1	B	92	GLY	C-O	-5.13	1.17	1.23
1	B	165	MET	CA-C	-5.13	1.46	1.52
1	A	232	ASN	C-O	-5.13	1.18	1.23
1	B	232	ASN	C-O	-5.13	1.18	1.23
1	A	219	GLU	CA-C	-5.12	1.45	1.52
1	B	219	GLU	CA-C	-5.12	1.45	1.52
1	A	192	LEU	CA-C	-5.11	1.45	1.52
1	B	192	LEU	CA-C	-5.11	1.45	1.52
1	A	331	ARG	C-O	-5.11	1.17	1.24
1	B	331	ARG	C-O	-5.11	1.17	1.24
1	A	523	VAL	N-CA	5.10	1.52	1.46
1	B	523	VAL	N-CA	5.10	1.52	1.46
1	A	625	TRP	CA-CB	-5.10	1.46	1.53
1	B	625	TRP	CA-CB	-5.10	1.46	1.53
1	A	352	GLU	CA-C	-5.10	1.47	1.53
1	B	352	GLU	CA-C	-5.10	1.47	1.53
1	A	622	ALA	C-O	-5.09	1.15	1.23
1	B	622	ALA	C-O	-5.09	1.15	1.23
1	A	363	PRO	CA-CB	-5.09	1.46	1.53
1	B	363	PRO	CA-CB	-5.09	1.46	1.53
1	A	594	PHE	C-O	5.08	1.30	1.24
1	B	594	PHE	C-O	5.08	1.30	1.24
1	A	255	LEU	C-O	-5.08	1.18	1.24
1	A	316	ASP	CA-C	5.07	1.60	1.52
1	A	442	LEU	N-CA	5.06	1.53	1.46
1	B	442	LEU	N-CA	5.06	1.53	1.46
1	A	2	ALA	C-N	-5.06	1.26	1.33
1	B	2	ALA	C-N	-5.06	1.26	1.33
1	B	255	LEU	C-O	-5.05	1.18	1.24
1	A	166	ALA	CA-CB	-5.05	1.45	1.53
1	B	166	ALA	CA-CB	-5.05	1.45	1.53
1	A	684	TYR	CA-C	-5.05	1.46	1.52
1	B	684	TYR	CA-C	-5.05	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	ALA	C-N	5.04	1.38	1.33
1	B	585	ALA	C-N	5.04	1.38	1.33
1	A	94	ASP	CA-CB	-5.04	1.45	1.53
1	B	94	ASP	CA-CB	-5.04	1.45	1.53
1	A	223	HIS	C-O	-5.04	1.17	1.24
1	B	223	HIS	C-O	-5.04	1.17	1.24
1	A	510	ILE	CA-C	5.03	1.58	1.52
1	B	510	ILE	CA-C	5.03	1.58	1.52
1	A	469	TYR	CA-CB	-5.03	1.45	1.53
1	A	700	GLU	CA-C	-5.03	1.46	1.52
1	B	469	TYR	CA-CB	-5.03	1.45	1.53
1	B	700	GLU	CA-C	-5.03	1.46	1.52
1	A	182	GLU	CA-CB	-5.01	1.45	1.53
1	B	182	GLU	CA-CB	-5.01	1.45	1.53
1	A	540	ILE	CA-C	-5.01	1.47	1.52
1	B	540	ILE	CA-C	-5.01	1.47	1.52

All (621) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	GLU	N-CA-C	-33.46	70.54	111.69
1	A	585	ALA	CA-C-N	-21.14	99.27	120.83
1	A	585	ALA	C-N-CA	-21.14	99.27	120.83
1	B	585	ALA	CA-C-N	-21.14	99.27	120.83
1	B	585	ALA	C-N-CA	-21.14	99.27	120.83
1	A	316	ASP	N-CA-C	20.78	138.48	112.92
1	A	81	LYS	N-CA-C	19.10	135.17	113.21
1	B	81	LYS	N-CA-C	19.10	135.17	113.21
1	A	567	PHE	N-CA-C	-18.80	70.77	110.80
1	B	567	PHE	N-CA-C	-18.80	70.77	110.80
1	A	623	ALA	CA-C-O	17.26	139.47	119.27
1	B	623	ALA	CA-C-O	17.26	139.47	119.27
1	A	63	ASN	N-CA-C	-15.73	94.54	114.04
1	B	63	ASN	N-CA-C	-15.73	94.54	114.04
1	A	586	PRO	CA-C-N	14.96	148.90	121.97
1	A	586	PRO	C-N-CA	14.96	148.90	121.97
1	B	586	PRO	CA-C-N	14.96	148.90	121.97
1	B	586	PRO	C-N-CA	14.96	148.90	121.97
1	B	260	ASP	N-CA-C	-14.90	94.41	112.89
1	A	298	GLU	CA-C-N	-14.39	102.03	120.60
1	A	298	GLU	C-N-CA	-14.39	102.03	120.60
1	A	440	ILE	CA-C-N	-14.30	99.69	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	ILE	C-N-CA	-14.30	99.69	120.28
1	B	440	ILE	CA-C-N	-14.30	99.69	120.28
1	B	440	ILE	C-N-CA	-14.30	99.69	120.28
1	A	241	ASN	N-CA-C	14.20	130.41	110.68
1	A	510	ILE	CA-C-N	-13.80	103.46	119.47
1	A	510	ILE	C-N-CA	-13.80	103.46	119.47
1	B	510	ILE	CA-C-N	-13.80	103.46	119.47
1	B	510	ILE	C-N-CA	-13.80	103.46	119.47
1	B	309	GLU	N-CA-C	-13.71	97.02	113.88
1	A	260	ASP	N-CA-C	-13.62	95.92	112.54
1	A	241	ASN	CA-C-O	13.43	142.39	122.38
1	A	110	ALA	CA-C-N	-13.11	104.50	119.05
1	A	110	ALA	C-N-CA	-13.11	104.50	119.05
1	B	110	ALA	CA-C-N	-13.11	104.50	119.05
1	B	110	ALA	C-N-CA	-13.11	104.50	119.05
1	A	586	PRO	CA-C-O	-13.02	104.08	118.92
1	B	586	PRO	CA-C-O	-13.02	104.08	118.92
1	A	294	HIS	N-CA-C	-12.68	93.74	111.24
1	A	86	GLU	N-CA-C	-12.25	97.79	113.72
1	B	86	GLU	N-CA-C	-12.25	97.79	113.72
1	A	318	LYS	N-CA-C	-12.05	99.25	114.56
1	B	318	LYS	N-CA-C	-12.05	99.25	114.56
1	B	266	TYR	N-CA-C	-12.03	96.36	113.21
1	A	622	ALA	O-C-N	-11.68	109.09	123.33
1	B	622	ALA	O-C-N	-11.68	109.09	123.33
1	A	662	LEU	CA-C-N	-11.61	105.32	119.84
1	A	662	LEU	C-N-CA	-11.61	105.32	119.84
1	B	662	LEU	CA-C-N	-11.61	105.32	119.84
1	B	662	LEU	C-N-CA	-11.61	105.32	119.84
1	A	266	TYR	N-CA-C	-11.60	96.98	113.21
1	A	198	ARG	N-CA-C	-11.59	90.46	108.55
1	B	198	ARG	N-CA-C	-11.59	90.46	108.55
1	B	259	LEU	N-CA-C	11.45	127.01	112.92
1	A	128	ASN	N-CA-C	11.43	135.15	110.80
1	B	128	ASN	N-CA-C	11.43	135.15	110.80
1	A	500	ASN	CA-C-O	11.32	133.21	119.06
1	B	500	ASN	CA-C-O	11.32	133.21	119.06
1	A	151	ASN	N-CA-C	-11.24	98.88	112.59
1	B	151	ASN	N-CA-C	-11.24	98.88	112.59
1	A	69	TYR	N-CA-C	-11.23	99.02	113.17
1	B	69	TYR	N-CA-C	-11.23	99.02	113.17
1	A	244	LYS	CA-C-N	-11.16	104.22	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	LYS	C-N-CA	-11.16	104.22	120.28
1	A	296	ILE	O-C-N	-10.97	108.85	122.57
1	A	415	VAL	CB-CA-C	-10.82	101.10	113.22
1	B	415	VAL	CB-CA-C	-10.82	101.10	113.22
1	A	676	ARG	N-CA-C	10.63	123.99	111.02
1	B	676	ARG	N-CA-C	10.63	123.99	111.02
1	A	489	GLU	CA-C-O	10.54	131.76	120.90
1	B	489	GLU	CA-C-O	10.54	131.76	120.90
1	A	291	ALA	N-CA-C	10.53	133.23	110.80
1	A	233	TYR	N-CA-C	-10.24	91.96	108.55
1	B	233	TYR	N-CA-C	-10.24	91.96	108.55
1	A	655	ALA	CA-C-O	10.13	130.01	118.47
1	B	655	ALA	CA-C-O	10.13	130.01	118.47
1	A	443	PRO	CA-C-N	-10.11	106.73	120.28
1	A	443	PRO	C-N-CA	-10.11	106.73	120.28
1	B	443	PRO	CA-C-N	-10.11	106.73	120.28
1	B	443	PRO	C-N-CA	-10.11	106.73	120.28
1	A	45	ARG	N-CA-C	-10.04	99.30	114.16
1	B	45	ARG	N-CA-C	-10.04	99.30	114.16
1	A	40	SER	N-CA-C	9.96	123.38	111.82
1	B	40	SER	N-CA-C	9.96	123.38	111.82
1	A	682	VAL	N-CA-C	9.94	122.74	113.10
1	B	682	VAL	N-CA-C	9.94	122.74	113.10
1	A	454	GLY	N-CA-C	9.91	131.34	115.08
1	B	454	GLY	N-CA-C	9.91	131.34	115.08
1	A	491	LEU	N-CA-C	-9.90	99.32	111.40
1	B	491	LEU	N-CA-C	-9.90	99.32	111.40
1	A	265	LYS	N-CA-C	-9.86	100.79	113.12
1	A	440	ILE	CA-C-O	9.85	131.65	121.41
1	B	440	ILE	CA-C-O	9.85	131.65	121.41
1	A	716	PRO	CB-CA-C	-9.84	95.33	111.56
1	B	716	PRO	CB-CA-C	-9.84	95.33	111.56
1	A	373	THR	N-CA-C	9.75	121.50	111.07
1	B	373	THR	N-CA-C	9.75	121.50	111.07
1	A	201	GLN	N-CA-C	-9.61	101.56	113.38
1	B	201	GLN	N-CA-C	-9.61	101.56	113.38
1	A	698	ALA	N-CA-C	-9.47	102.81	114.75
1	B	698	ALA	N-CA-C	-9.47	102.81	114.75
1	B	265	LYS	N-CA-C	-9.47	101.04	111.36
1	B	244	LYS	N-CA-C	9.30	121.42	111.28
1	B	291	ALA	N-CA-C	9.22	130.43	110.80
1	A	129	GLU	N-CA-C	9.14	123.72	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ILE	N-CA-C	9.14	128.35	109.34
1	B	129	GLU	N-CA-C	9.14	123.72	113.21
1	A	369	TYR	CA-C-O	9.12	129.72	119.41
1	B	369	TYR	CA-C-O	9.12	129.72	119.41
1	A	715	HIS	CA-C-N	9.03	131.12	119.84
1	A	715	HIS	C-N-CA	9.03	131.12	119.84
1	B	715	HIS	CA-C-N	9.03	131.12	119.84
1	B	715	HIS	C-N-CA	9.03	131.12	119.84
1	A	241	ASN	CA-C-N	-8.99	104.29	122.55
1	A	241	ASN	C-N-CA	-8.99	104.29	122.55
1	A	147	LEU	N-CA-C	-8.98	99.69	113.89
1	B	147	LEU	N-CA-C	-8.98	99.69	113.89
1	A	70	LEU	N-CA-C	-8.88	98.34	110.68
1	B	70	LEU	N-CA-C	-8.88	98.34	110.68
1	A	43	TYR	N-CA-C	-8.85	103.00	113.88
1	B	43	TYR	N-CA-C	-8.85	103.00	113.88
1	A	121	VAL	CA-C-N	-8.82	110.07	119.24
1	A	121	VAL	C-N-CA	-8.82	110.07	119.24
1	B	121	VAL	CA-C-N	-8.82	110.07	119.24
1	B	121	VAL	C-N-CA	-8.82	110.07	119.24
1	A	406	ILE	N-CA-C	-8.81	100.44	113.39
1	B	406	ILE	N-CA-C	-8.81	100.44	113.39
1	A	620	SER	CB-CA-C	-8.76	96.97	111.51
1	B	620	SER	CB-CA-C	-8.76	96.97	111.51
1	A	220	LEU	N-CA-C	-8.74	103.04	114.31
1	B	220	LEU	N-CA-C	-8.74	103.04	114.31
1	A	444	ALA	N-CA-C	8.71	120.78	111.28
1	B	444	ALA	N-CA-C	8.71	120.78	111.28
1	A	681	PHE	N-CA-C	8.65	123.09	112.54
1	B	681	PHE	N-CA-C	8.65	123.09	112.54
1	A	443	PRO	CA-N-CD	-8.65	99.89	112.00
1	B	443	PRO	CA-N-CD	-8.65	99.89	112.00
1	A	679	PRO	CA-N-CD	-8.57	100.00	112.00
1	B	679	PRO	CA-N-CD	-8.57	100.00	112.00
1	A	676	ARG	CA-C-O	8.56	130.49	121.07
1	B	676	ARG	CA-C-O	8.56	130.49	121.07
1	A	158	ARG	N-CA-C	-8.54	101.25	113.21
1	B	158	ARG	N-CA-C	-8.54	101.25	113.21
1	B	270	ASN	N-CA-C	8.52	124.41	108.65
1	A	299	VAL	N-CA-C	8.49	119.27	110.36
1	A	163	ILE	N-CA-C	8.42	118.50	110.42
1	B	163	ILE	N-CA-C	8.42	118.50	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	PRO	CA-C-O	8.42	132.94	119.64
1	B	511	PRO	CA-C-O	8.42	132.94	119.64
1	A	56	GLY	N-CA-C	-8.36	104.06	114.92
1	B	56	GLY	N-CA-C	-8.36	104.06	114.92
1	A	144	ILE	N-CA-C	-8.26	101.75	113.07
1	B	144	ILE	N-CA-C	-8.26	101.75	113.07
1	A	241	ASN	O-C-N	-8.25	111.30	122.68
1	A	240	CYS	O-C-N	-8.25	111.10	122.81
1	A	658	PHE	CA-C-N	-8.25	109.08	120.38
1	A	658	PHE	C-N-CA	-8.25	109.08	120.38
1	B	658	PHE	CA-C-N	-8.25	109.08	120.38
1	B	658	PHE	C-N-CA	-8.25	109.08	120.38
1	A	507	GLY	CA-C-N	-8.24	109.24	120.28
1	A	507	GLY	C-N-CA	-8.24	109.24	120.28
1	B	507	GLY	CA-C-N	-8.24	109.24	120.28
1	B	507	GLY	C-N-CA	-8.24	109.24	120.28
1	A	90	HIS	N-CA-C	-8.15	100.30	112.04
1	A	566	GLY	N-CA-C	-8.15	93.85	113.18
1	B	90	HIS	N-CA-C	-8.15	100.30	112.04
1	B	566	GLY	N-CA-C	-8.15	93.85	113.18
1	A	627	ASP	N-CA-C	8.14	119.78	111.07
1	B	627	ASP	N-CA-C	8.14	119.78	111.07
1	A	442	LEU	CA-C-N	-8.12	109.69	119.84
1	A	442	LEU	C-N-CA	-8.12	109.69	119.84
1	B	442	LEU	CA-C-N	-8.12	109.69	119.84
1	B	442	LEU	C-N-CA	-8.12	109.69	119.84
1	A	678	GLU	CA-C-N	-8.11	109.70	119.84
1	A	678	GLU	C-N-CA	-8.11	109.70	119.84
1	B	678	GLU	CA-C-N	-8.11	109.70	119.84
1	B	678	GLU	C-N-CA	-8.11	109.70	119.84
1	A	660	ILE	N-CA-C	8.10	118.20	110.42
1	B	660	ILE	N-CA-C	8.10	118.20	110.42
1	A	392	ILE	CA-C-N	-8.03	110.16	119.47
1	A	392	ILE	C-N-CA	-8.03	110.16	119.47
1	B	392	ILE	CA-C-N	-8.03	110.16	119.47
1	B	392	ILE	C-N-CA	-8.03	110.16	119.47
1	A	586	PRO	N-CA-C	8.02	123.02	114.68
1	B	586	PRO	N-CA-C	8.02	123.02	114.68
1	A	604	VAL	N-CA-C	7.98	118.74	110.36
1	B	604	VAL	N-CA-C	7.98	118.74	110.36
1	A	242	ALA	N-CA-C	-7.97	104.04	113.21
1	A	371	SER	N-CA-C	-7.94	102.70	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	SER	N-CA-C	-7.94	102.70	111.36
1	A	388	PHE	N-CA-C	7.91	120.60	111.11
1	B	388	PHE	N-CA-C	7.91	120.60	111.11
1	A	203	THR	N-CA-C	7.84	122.27	109.72
1	B	203	THR	N-CA-C	7.84	122.27	109.72
1	A	571	GLU	CA-C-N	-7.83	110.05	119.84
1	A	571	GLU	C-N-CA	-7.83	110.05	119.84
1	B	571	GLU	CA-C-N	-7.83	110.05	119.84
1	B	571	GLU	C-N-CA	-7.83	110.05	119.84
1	A	655	ALA	N-CA-C	7.83	124.61	114.75
1	B	655	ALA	N-CA-C	7.83	124.61	114.75
1	A	514	ALA	CA-C-N	-7.79	109.13	120.82
1	A	514	ALA	C-N-CA	-7.79	109.13	120.82
1	B	514	ALA	CA-C-N	-7.79	109.13	120.82
1	B	514	ALA	C-N-CA	-7.79	109.13	120.82
1	A	437	LEU	CA-C-N	-7.72	110.11	120.54
1	A	437	LEU	C-N-CA	-7.72	110.11	120.54
1	B	437	LEU	CA-C-N	-7.72	110.11	120.54
1	B	437	LEU	C-N-CA	-7.72	110.11	120.54
1	A	65	GLU	N-CA-C	7.72	121.76	108.02
1	B	65	GLU	N-CA-C	7.72	121.76	108.02
1	B	258	TRP	CA-C-N	-7.71	110.31	122.65
1	B	258	TRP	C-N-CA	-7.71	110.31	122.65
1	A	299	VAL	N-CA-CB	7.70	119.06	110.51
1	A	540	ILE	N-CA-C	-7.70	102.83	110.30
1	B	540	ILE	N-CA-C	-7.70	102.83	110.30
1	A	567	PHE	N-CA-CB	7.67	123.45	110.49
1	B	567	PHE	N-CA-CB	7.67	123.45	110.49
1	A	42	TRP	N-CA-C	-7.66	103.03	113.30
1	B	42	TRP	N-CA-C	-7.66	103.03	113.30
1	A	365	LEU	N-CA-C	-7.60	104.03	113.38
1	B	365	LEU	N-CA-C	-7.60	104.03	113.38
1	A	499	PRO	O-C-N	-7.53	112.48	122.64
1	B	499	PRO	O-C-N	-7.53	112.48	122.64
1	A	622	ALA	N-CA-C	7.49	119.67	110.91
1	B	622	ALA	N-CA-C	7.49	119.67	110.91
1	A	437	LEU	N-CA-C	7.48	120.15	111.02
1	B	437	LEU	N-CA-C	7.48	120.15	111.02
1	A	600	ALA	N-CA-C	7.44	119.03	111.07
1	B	600	ALA	N-CA-C	7.44	119.03	111.07
1	A	156	SER	N-CA-C	7.42	126.60	110.80
1	B	156	SER	N-CA-C	7.42	126.60	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	PRO	O-C-N	-7.41	112.63	122.64
1	B	368	PRO	O-C-N	-7.41	112.63	122.64
1	A	91	ALA	N-CA-C	7.39	122.39	111.96
1	B	91	ALA	N-CA-C	7.39	122.39	111.96
1	A	230	PRO	N-CA-C	7.38	123.79	113.53
1	B	230	PRO	N-CA-C	7.38	123.79	113.53
1	A	437	LEU	CA-C-O	7.38	129.19	121.07
1	B	437	LEU	CA-C-O	7.38	129.19	121.07
1	A	372	LEU	CA-C-N	-7.36	110.87	120.44
1	A	372	LEU	C-N-CA	-7.36	110.87	120.44
1	B	372	LEU	CA-C-N	-7.36	110.87	120.44
1	B	372	LEU	C-N-CA	-7.36	110.87	120.44
1	A	438	PHE	CA-C-O	7.36	128.77	120.90
1	B	438	PHE	CA-C-O	7.36	128.77	120.90
1	A	103	TRP	N-CA-C	7.33	119.27	111.28
1	B	103	TRP	N-CA-C	7.33	119.27	111.28
1	A	637	ILE	N-CA-C	7.26	117.98	110.36
1	B	637	ILE	N-CA-C	7.26	117.98	110.36
1	A	440	ILE	N-CA-C	7.22	117.74	110.23
1	B	440	ILE	N-CA-C	7.22	117.74	110.23
1	A	79	ALA	N-CA-C	-7.20	103.43	111.28
1	B	79	ALA	N-CA-C	-7.20	103.43	111.28
1	A	511	PRO	O-C-N	-7.17	113.49	122.17
1	B	511	PRO	O-C-N	-7.17	113.49	122.17
1	A	512	MET	CA-C-O	7.16	128.20	119.97
1	B	512	MET	CA-C-O	7.16	128.20	119.97
1	A	385	PHE	N-CA-C	7.14	119.06	111.28
1	A	489	GLU	CA-C-N	-7.14	108.03	122.31
1	A	489	GLU	C-N-CA	-7.14	108.03	122.31
1	B	385	PHE	N-CA-C	7.14	119.06	111.28
1	B	489	GLU	CA-C-N	-7.14	108.03	122.31
1	B	489	GLU	C-N-CA	-7.14	108.03	122.31
1	A	457	SER	N-CA-C	-7.08	98.31	109.50
1	B	457	SER	N-CA-C	-7.08	98.31	109.50
1	A	98	TYR	CA-C-O	7.04	128.01	120.55
1	B	98	TYR	CA-C-O	7.04	128.01	120.55
1	A	519	THR	N-CA-C	7.02	119.53	111.11
1	B	519	THR	N-CA-C	7.02	119.53	111.11
1	A	714	ILE	CA-C-O	-6.98	112.05	120.78
1	B	714	ILE	CA-C-O	-6.98	112.05	120.78
1	A	675	GLY	CA-C-N	-6.96	111.12	120.79
1	A	675	GLY	C-N-CA	-6.96	111.12	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	GLY	CA-C-N	-6.96	111.12	120.79
1	B	675	GLY	C-N-CA	-6.96	111.12	120.79
1	A	3	THR	CA-C-O	6.93	130.42	120.51
1	B	3	THR	CA-C-O	6.93	130.42	120.51
1	A	130	LEU	N-CA-C	-6.90	105.39	113.88
1	B	130	LEU	N-CA-C	-6.90	105.39	113.88
1	A	433	ILE	N-CA-C	6.89	118.48	110.62
1	B	433	ILE	N-CA-C	6.89	118.48	110.62
1	A	511	PRO	N-CA-C	6.84	123.73	113.81
1	B	511	PRO	N-CA-C	6.84	123.73	113.81
1	A	570	GLY	N-CA-C	6.81	120.89	112.64
1	B	570	GLY	N-CA-C	6.81	120.89	112.64
1	A	503	PRO	N-CA-C	6.77	124.74	113.78
1	B	503	PRO	N-CA-C	6.77	124.74	113.78
1	A	518	ILE	CB-CA-C	-6.75	103.06	111.70
1	B	518	ILE	CB-CA-C	-6.75	103.06	111.70
1	A	400	LEU	N-CA-C	-6.75	104.86	113.23
1	B	400	LEU	N-CA-C	-6.75	104.86	113.23
1	A	80	LEU	N-CA-C	6.73	118.61	111.28
1	B	80	LEU	N-CA-C	6.73	118.61	111.28
1	A	663	PRO	CA-N-CD	-6.72	102.59	112.00
1	B	663	PRO	CA-N-CD	-6.72	102.59	112.00
1	A	481	SER	N-CA-C	-6.71	104.05	111.36
1	B	481	SER	N-CA-C	-6.71	104.05	111.36
1	A	276	ILE	N-CA-C	-6.69	100.94	109.30
1	A	500	ASN	N-CA-C	-6.66	105.78	114.04
1	B	500	ASN	N-CA-C	-6.66	105.78	114.04
1	A	626	PRO	CA-C-N	-6.65	111.79	120.44
1	A	626	PRO	C-N-CA	-6.65	111.79	120.44
1	B	626	PRO	CA-C-N	-6.65	111.79	120.44
1	B	626	PRO	C-N-CA	-6.65	111.79	120.44
1	A	389	PHE	CA-C-O	6.64	127.61	120.10
1	B	389	PHE	CA-C-O	6.64	127.61	120.10
1	A	89	ASP	N-CA-C	6.62	121.36	113.28
1	B	89	ASP	N-CA-C	6.62	121.36	113.28
1	B	246	ALA	N-CA-C	-6.61	104.00	111.14
1	A	658	PHE	N-CA-C	-6.60	104.01	111.14
1	B	658	PHE	N-CA-C	-6.60	104.01	111.14
1	A	316	ASP	CA-C-O	-6.57	111.87	119.56
1	A	152	ILE	CB-CA-C	6.57	117.39	110.37
1	B	152	ILE	CB-CA-C	6.57	117.39	110.37
1	A	353	TRP	N-CA-C	-6.56	99.23	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	TRP	N-CA-C	-6.56	99.23	109.72
1	A	97	VAL	CB-CA-C	6.53	122.28	112.16
1	B	97	VAL	CB-CA-C	6.53	122.28	112.16
1	A	193	ALA	N-CA-C	6.51	121.08	113.20
1	B	193	ALA	N-CA-C	6.51	121.08	113.20
1	A	703	LEU	N-CA-C	6.46	124.56	110.80
1	B	703	LEU	N-CA-C	6.46	124.56	110.80
1	A	72	PHE	CB-CA-C	-6.44	97.61	110.42
1	B	72	PHE	CB-CA-C	-6.44	97.61	110.42
1	A	711	ASP	N-CA-C	6.44	119.84	112.57
1	B	711	ASP	N-CA-C	6.44	119.84	112.57
1	A	555	ASP	N-CA-C	-6.43	97.09	110.80
1	B	555	ASP	N-CA-C	-6.43	97.09	110.80
1	B	263	GLN	CA-C-N	-6.38	112.50	122.08
1	B	263	GLN	C-N-CA	-6.38	112.50	122.08
1	A	134	LYS	N-CA-C	-6.35	105.36	113.23
1	B	134	LYS	N-CA-C	-6.35	105.36	113.23
1	A	708	TYR	N-CA-C	6.34	118.19	111.28
1	B	708	TYR	N-CA-C	6.34	118.19	111.28
1	A	182	GLU	N-CA-C	6.32	118.16	111.28
1	B	182	GLU	N-CA-C	6.32	118.16	111.28
1	A	623	ALA	CA-C-N	-6.30	109.50	121.54
1	A	623	ALA	C-N-CA	-6.30	109.50	121.54
1	B	623	ALA	CA-C-N	-6.30	109.50	121.54
1	B	623	ALA	C-N-CA	-6.30	109.50	121.54
1	A	614	TYR	N-CA-C	6.30	124.21	110.80
1	B	614	TYR	N-CA-C	6.30	124.21	110.80
1	A	597	VAL	CB-CA-C	6.29	120.63	112.14
1	B	597	VAL	CB-CA-C	6.29	120.63	112.14
1	B	286	GLY	N-CA-C	6.29	119.35	110.74
1	A	367	ILE	N-CA-C	-6.27	100.15	107.61
1	A	439	LEU	CB-CA-C	6.27	122.23	110.63
1	B	367	ILE	N-CA-C	-6.27	100.15	107.61
1	B	439	LEU	CB-CA-C	6.27	122.23	110.63
1	A	362	TRP	CA-C-N	-6.24	113.71	119.82
1	A	362	TRP	C-N-CA	-6.24	113.71	119.82
1	B	362	TRP	CA-C-N	-6.24	113.71	119.82
1	B	362	TRP	C-N-CA	-6.24	113.71	119.82
1	A	656	ALA	N-CA-C	6.22	123.56	109.81
1	B	656	ALA	N-CA-C	6.22	123.56	109.81
1	A	488	PHE	N-CA-C	6.21	124.03	110.80
1	B	488	PHE	N-CA-C	6.21	124.03	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	THR	N-CA-C	6.21	120.01	110.20
1	B	351	THR	N-CA-C	6.21	120.01	110.20
1	A	575	GLN	N-CA-C	6.19	118.11	111.36
1	B	575	GLN	N-CA-C	6.19	118.11	111.36
1	A	293	GLU	CB-CA-C	6.17	120.95	111.39
1	A	2	ALA	N-CA-C	-6.17	93.72	111.00
1	A	229	HIS	N-CA-C	-6.17	98.26	108.75
1	B	2	ALA	N-CA-C	-6.17	93.72	111.00
1	B	229	HIS	N-CA-C	-6.17	98.26	108.75
1	A	154	GLU	N-CA-C	-6.16	101.16	110.28
1	A	664	VAL	N-CA-C	6.16	116.33	110.42
1	B	154	GLU	N-CA-C	-6.16	101.16	110.28
1	B	664	VAL	N-CA-C	6.16	116.33	110.42
1	A	667	ILE	N-CA-C	6.15	116.89	110.62
1	B	667	ILE	N-CA-C	6.15	116.89	110.62
1	A	508	MET	CA-C-O	6.12	127.04	120.55
1	B	508	MET	CA-C-O	6.12	127.04	120.55
1	A	138	ASN	N-CA-C	6.08	119.81	111.54
1	B	138	ASN	N-CA-C	6.08	119.81	111.54
1	A	363	PRO	N-CA-C	6.07	121.81	113.98
1	B	363	PRO	N-CA-C	6.07	121.81	113.98
1	A	286	GLY	N-CA-C	6.06	119.05	110.74
1	A	393	PRO	CA-N-CD	-6.05	103.53	112.00
1	B	393	PRO	CA-N-CD	-6.05	103.53	112.00
1	A	23	ILE	N-CA-C	6.04	116.22	110.42
1	B	23	ILE	N-CA-C	6.04	116.22	110.42
1	A	350	LEU	N-CA-C	6.03	119.49	107.62
1	B	350	LEU	N-CA-C	6.03	119.49	107.62
1	A	572	PRO	CA-N-CD	-6.01	103.59	112.00
1	B	572	PRO	CA-N-CD	-6.01	103.59	112.00
1	A	219	GLU	N-CA-C	-6.00	105.15	112.88
1	B	219	GLU	N-CA-C	-6.00	105.15	112.88
1	A	473	ASN	CA-C-O	-5.98	111.96	120.51
1	B	473	ASN	CA-C-O	-5.98	111.96	120.51
1	B	273	ILE	CB-CA-C	-5.98	101.49	111.29
1	A	676	ARG	CA-C-N	-5.97	109.94	121.58
1	A	676	ARG	C-N-CA	-5.97	109.94	121.58
1	B	676	ARG	CA-C-N	-5.97	109.94	121.58
1	B	676	ARG	C-N-CA	-5.97	109.94	121.58
1	A	680	ALA	N-CA-C	5.96	121.21	111.37
1	B	680	ALA	N-CA-C	5.96	121.21	111.37
1	A	273	ILE	CB-CA-C	-5.96	101.53	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	TYR	N-CA-C	-5.95	98.12	110.80
1	A	369	TYR	N-CA-C	5.95	120.67	113.41
1	B	369	TYR	N-CA-C	5.95	120.67	113.41
1	A	94	ASP	N-CA-CB	-5.92	101.11	109.94
1	B	94	ASP	N-CA-CB	-5.92	101.11	109.94
1	A	74	HIS	CB-CA-C	5.92	120.26	110.90
1	B	74	HIS	CB-CA-C	5.92	120.26	110.90
1	A	581	GLY	N-CA-C	5.90	119.78	112.64
1	B	581	GLY	N-CA-C	5.90	119.78	112.64
1	A	294	HIS	CB-CA-C	5.90	121.17	112.09
1	A	716	PRO	CA-N-CD	-5.90	103.75	112.00
1	B	716	PRO	CA-N-CD	-5.90	103.75	112.00
1	A	73	LEU	CA-C-N	-5.89	112.43	120.44
1	A	73	LEU	C-N-CA	-5.89	112.43	120.44
1	B	73	LEU	CA-C-N	-5.89	112.43	120.44
1	B	73	LEU	C-N-CA	-5.89	112.43	120.44
1	A	491	LEU	CA-C-N	-5.89	111.82	121.19
1	A	491	LEU	C-N-CA	-5.89	111.82	121.19
1	B	491	LEU	CA-C-N	-5.89	111.82	121.19
1	B	491	LEU	C-N-CA	-5.89	111.82	121.19
1	A	95	SER	N-CA-CB	-5.89	101.47	110.12
1	B	95	SER	N-CA-CB	-5.89	101.47	110.12
1	B	276	ILE	N-CA-C	-5.86	101.97	109.30
1	A	210	PRO	N-CA-C	5.86	117.84	110.70
1	B	210	PRO	N-CA-C	5.86	117.84	110.70
1	A	377	LEU	N-CA-C	5.84	118.12	111.11
1	B	377	LEU	N-CA-C	5.84	118.12	111.11
1	A	570	GLY	CA-C-N	-5.83	112.55	119.78
1	A	570	GLY	C-N-CA	-5.83	112.55	119.78
1	B	570	GLY	CA-C-N	-5.83	112.55	119.78
1	B	570	GLY	C-N-CA	-5.83	112.55	119.78
1	A	294	HIS	O-C-N	5.82	130.02	122.86
1	A	66	LEU	N-CA-C	-5.80	102.32	110.50
1	B	66	LEU	N-CA-C	-5.80	102.32	110.50
1	A	77	PRO	CA-N-CD	-5.79	103.89	112.00
1	B	77	PRO	CA-N-CD	-5.79	103.89	112.00
1	B	281	CYS	CB-CA-C	-5.79	109.88	116.54
1	A	315	ASN	N-CA-C	5.79	120.50	113.38
1	A	529	VAL	CB-CA-C	5.79	120.21	112.22
1	A	677	PHE	CA-C-O	5.79	126.52	119.11
1	B	529	VAL	CB-CA-C	5.79	120.21	112.22
1	B	677	PHE	CA-C-O	5.79	126.52	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LEU	N-CA-C	5.79	118.37	111.71
1	B	28	LEU	N-CA-C	5.79	118.37	111.71
1	A	663	PRO	N-CA-C	5.78	124.38	112.47
1	B	663	PRO	N-CA-C	5.78	124.38	112.47
1	A	573	GLN	N-CA-C	5.76	117.23	111.07
1	B	573	GLN	N-CA-C	5.76	117.23	111.07
1	A	281	CYS	CB-CA-C	-5.75	109.93	116.54
1	A	514	ALA	CB-CA-C	-5.75	101.78	110.92
1	B	514	ALA	CB-CA-C	-5.75	101.78	110.92
1	A	296	ILE	CA-C-O	5.72	127.92	120.78
1	A	515	THR	N-CA-C	5.71	120.80	111.37
1	B	515	THR	N-CA-C	5.71	120.80	111.37
1	A	611	ILE	N-CA-C	5.71	117.22	111.00
1	B	611	ILE	N-CA-C	5.71	117.22	111.00
1	A	307	ALA	N-CA-C	5.69	117.94	111.11
1	A	577	TYR	N-CA-C	5.67	117.46	111.28
1	B	577	TYR	N-CA-C	5.67	117.46	111.28
1	A	676	ARG	O-C-N	-5.67	116.02	122.08
1	B	676	ARG	O-C-N	-5.67	116.02	122.08
1	A	485	GLY	N-CA-C	-5.64	105.55	112.77
1	B	485	GLY	N-CA-C	-5.64	105.55	112.77
1	A	125	TRP	CA-C-N	-5.64	113.55	122.23
1	A	125	TRP	C-N-CA	-5.64	113.55	122.23
1	B	125	TRP	CA-C-N	-5.64	113.55	122.23
1	B	125	TRP	C-N-CA	-5.64	113.55	122.23
1	A	119	VAL	N-CA-C	5.63	116.08	110.23
1	B	119	VAL	N-CA-C	5.63	116.08	110.23
1	A	77	PRO	N-CA-C	5.62	121.96	113.81
1	B	77	PRO	N-CA-C	5.62	121.96	113.81
1	A	565	ILE	N-CA-C	5.62	121.02	109.34
1	B	565	ILE	N-CA-C	5.62	121.02	109.34
1	A	109	PHE	N-CA-C	5.59	118.31	111.82
1	B	109	PHE	N-CA-C	5.59	118.31	111.82
1	A	434	ALA	CA-C-N	-5.59	113.18	120.44
1	A	434	ALA	C-N-CA	-5.59	113.18	120.44
1	B	434	ALA	CA-C-N	-5.59	113.18	120.44
1	B	434	ALA	C-N-CA	-5.59	113.18	120.44
1	A	291	ALA	CA-C-O	5.58	128.49	120.51
1	A	159	PHE	N-CA-C	-5.58	106.47	113.72
1	B	159	PHE	N-CA-C	-5.58	106.47	113.72
1	A	512	MET	N-CA-C	5.55	118.26	111.82
1	B	512	MET	N-CA-C	5.55	118.26	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	ARG	N-CA-C	-5.55	105.31	111.36
1	B	607	ARG	N-CA-C	-5.55	105.31	111.36
1	A	270	ASN	N-CA-C	5.54	122.60	110.80
1	A	518	ILE	N-CA-CB	5.53	116.43	110.62
1	B	518	ILE	N-CA-CB	5.53	116.43	110.62
1	A	437	LEU	N-CA-CB	-5.53	101.42	109.82
1	B	437	LEU	N-CA-CB	-5.53	101.42	109.82
1	B	290	ASP	N-CA-C	5.52	122.56	110.80
1	A	110	ALA	O-C-N	5.51	124.73	120.38
1	B	110	ALA	O-C-N	5.51	124.73	120.38
1	A	548	PHE	N-CA-C	-5.50	99.09	110.80
1	B	548	PHE	N-CA-C	-5.50	99.09	110.80
1	A	462	GLU	N-CA-C	5.48	117.25	111.28
1	B	462	GLU	N-CA-C	5.48	117.25	111.28
1	A	71	LYS	N-CA-C	-5.47	105.30	112.41
1	B	71	LYS	N-CA-C	-5.47	105.30	112.41
1	A	645	GLY	N-CA-C	5.46	119.25	112.64
1	B	645	GLY	N-CA-C	5.46	119.25	112.64
1	A	711	ASP	N-CA-CB	-5.46	102.28	110.91
1	B	711	ASP	N-CA-CB	-5.46	102.28	110.91
1	A	118	ALA	CA-C-N	-5.45	113.63	120.77
1	A	118	ALA	C-N-CA	-5.45	113.63	120.77
1	B	118	ALA	CA-C-N	-5.45	113.63	120.77
1	B	118	ALA	C-N-CA	-5.45	113.63	120.77
1	A	586	PRO	CA-N-CD	-5.45	104.37	112.00
1	B	586	PRO	CA-N-CD	-5.45	104.37	112.00
1	A	508	MET	N-CA-C	5.44	117.21	111.28
1	B	508	MET	N-CA-C	5.44	117.21	111.28
1	A	414	LYS	N-CA-C	5.43	122.37	110.80
1	B	414	LYS	N-CA-C	5.43	122.37	110.80
1	A	631	ARG	N-CA-C	5.42	117.88	111.33
1	B	631	ARG	N-CA-C	5.42	117.88	111.33
1	A	529	VAL	N-CA-C	-5.41	105.25	110.72
1	B	529	VAL	N-CA-C	-5.41	105.25	110.72
1	A	240	CYS	CA-C-N	5.41	130.20	122.08
1	A	240	CYS	C-N-CA	5.41	130.20	122.08
1	A	715	HIS	N-CA-C	5.41	121.75	109.81
1	B	715	HIS	N-CA-C	5.41	121.75	109.81
1	A	113	ALA	CA-C-N	-5.40	113.24	120.54
1	A	113	ALA	C-N-CA	-5.40	113.24	120.54
1	B	113	ALA	CA-C-N	-5.40	113.24	120.54
1	B	113	ALA	C-N-CA	-5.40	113.24	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	VAL	N-CA-C	-5.39	105.47	113.39
1	B	336	VAL	N-CA-C	-5.39	105.47	113.39
1	A	572	PRO	CB-CA-C	5.38	120.44	111.56
1	B	572	PRO	CB-CA-C	5.38	120.44	111.56
1	A	81	LYS	CB-CA-C	-5.38	101.20	110.72
1	B	81	LYS	CB-CA-C	-5.38	101.20	110.72
1	A	71	LYS	CB-CA-C	-5.36	102.33	111.02
1	B	71	LYS	CB-CA-C	-5.36	102.33	111.02
1	A	122	PRO	CA-N-CD	-5.35	104.51	112.00
1	A	415	VAL	CA-C-O	-5.35	117.97	122.63
1	B	122	PRO	CA-N-CD	-5.35	104.51	112.00
1	B	415	VAL	CA-C-O	-5.35	117.97	122.63
1	B	292	ILE	N-CA-C	5.35	120.46	109.34
1	A	494	PHE	CB-CA-C	-5.34	101.77	110.85
1	B	494	PHE	CB-CA-C	-5.34	101.77	110.85
1	A	211	PRO	N-CA-C	5.32	119.58	111.34
1	B	211	PRO	N-CA-C	5.32	119.58	111.34
1	A	127	ASN	N-CA-C	5.31	122.11	110.80
1	B	127	ASN	N-CA-C	5.31	122.11	110.80
1	A	296	ILE	CA-C-N	-5.30	111.42	121.54
1	A	296	ILE	C-N-CA	-5.30	111.42	121.54
1	A	2	ALA	O-C-N	-5.29	114.54	123.00
1	B	2	ALA	O-C-N	-5.29	114.54	123.00
1	A	356	GLU	N-CA-C	-5.28	102.53	110.24
1	A	558	GLU	N-CA-C	5.28	117.84	109.24
1	B	356	GLU	N-CA-C	-5.28	102.53	110.24
1	B	558	GLU	N-CA-C	5.28	117.84	109.24
1	A	59	GLY	N-CA-C	-5.26	100.72	113.18
1	B	59	GLY	N-CA-C	-5.26	100.72	113.18
1	B	259	LEU	CB-CA-C	5.25	119.43	110.56
1	A	373	THR	N-CA-CB	5.24	117.61	110.01
1	B	373	THR	N-CA-CB	5.24	117.61	110.01
1	A	429	LEU	N-CA-C	5.23	117.66	111.33
1	B	429	LEU	N-CA-C	5.23	117.66	111.33
1	A	75	TRP	CA-CB-CG	5.21	123.51	113.60
1	B	75	TRP	CA-CB-CG	5.21	123.51	113.60
1	A	655	ALA	O-C-N	-5.20	115.25	121.64
1	B	655	ALA	O-C-N	-5.20	115.25	121.64
1	A	518	ILE	CA-C-N	-5.20	113.53	120.54
1	A	518	ILE	C-N-CA	-5.20	113.53	120.54
1	B	518	ILE	CA-C-N	-5.20	113.53	120.54
1	B	518	ILE	C-N-CA	-5.20	113.53	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ASP	CA-C-N	-5.19	113.92	120.56
1	A	6	ASP	C-N-CA	-5.19	113.92	120.56
1	B	6	ASP	CA-C-N	-5.19	113.92	120.56
1	B	6	ASP	C-N-CA	-5.19	113.92	120.56
1	A	716	PRO	N-CA-C	-5.19	101.79	112.47
1	B	716	PRO	N-CA-C	-5.19	101.79	112.47
1	A	415	VAL	N-CA-C	-5.18	100.66	106.21
1	B	415	VAL	N-CA-C	-5.18	100.66	106.21
1	A	82	MET	N-CA-C	-5.18	102.11	109.62
1	B	82	MET	N-CA-C	-5.18	102.11	109.62
1	A	55	GLY	N-CA-C	5.17	121.69	112.22
1	B	55	GLY	N-CA-C	5.17	121.69	112.22
1	A	714	ILE	N-CA-C	5.16	120.08	109.34
1	B	714	ILE	N-CA-C	5.16	120.08	109.34
1	A	434	ALA	N-CA-C	5.15	116.58	111.07
1	A	623	ALA	N-CA-C	5.15	119.61	113.23
1	B	434	ALA	N-CA-C	5.15	116.58	111.07
1	B	623	ALA	N-CA-C	5.15	119.61	113.23
1	A	677	PHE	CB-CA-C	5.14	120.19	109.95
1	B	677	PHE	CB-CA-C	5.14	120.19	109.95
1	A	568	ASN	N-CA-C	5.13	121.72	110.80
1	B	568	ASN	N-CA-C	5.13	121.72	110.80
1	A	290	ASP	N-CA-C	5.12	121.72	110.80
1	A	352	GLU	N-CA-C	-5.12	101.00	108.07
1	B	352	GLU	N-CA-C	-5.12	101.00	108.07
1	A	677	PHE	N-CA-C	5.12	119.37	113.18
1	B	677	PHE	N-CA-C	5.12	119.37	113.18
1	A	36	ARG	N-CA-C	-5.11	106.73	113.17
1	B	36	ARG	N-CA-C	-5.11	106.73	113.17
1	A	247	ASP	CA-C-N	-5.11	113.44	120.28
1	A	247	ASP	C-N-CA	-5.11	113.44	120.28
1	A	370	VAL	CA-C-O	5.09	125.97	120.47
1	B	370	VAL	CA-C-O	5.09	125.97	120.47
1	A	302	THR	CA-C-N	-5.07	113.43	120.38
1	A	302	THR	C-N-CA	-5.07	113.43	120.38
1	A	49	SER	N-CA-C	5.07	121.60	110.80
1	B	49	SER	N-CA-C	5.07	121.60	110.80
1	A	289	VAL	N-CA-C	5.06	119.87	109.34
1	A	101	ILE	CA-C-N	-5.05	113.72	120.54
1	A	101	ILE	C-N-CA	-5.05	113.72	120.54
1	B	101	ILE	CA-C-N	-5.05	113.72	120.54
1	B	101	ILE	C-N-CA	-5.05	113.72	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	PRO	CA-N-CD	-5.04	104.94	112.00
1	B	111	PRO	CA-N-CD	-5.04	104.94	112.00
1	A	658	PHE	N-CA-CB	-5.04	102.77	110.07
1	B	658	PHE	N-CA-CB	-5.04	102.77	110.07
1	A	572	PRO	N-CA-CB	-5.02	97.98	103.25
1	B	572	PRO	N-CA-CB	-5.02	97.98	103.25
1	A	359	ASP	N-CA-C	-5.01	100.12	110.80
1	B	359	ASP	N-CA-C	-5.01	100.12	110.80
1	A	505	THR	CB-CA-C	5.00	118.81	110.90
1	B	505	THR	CB-CA-C	5.00	118.81	110.90
1	A	264	LEU	N-CA-C	-5.00	97.87	107.57

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	THR	Mainchain
1	A	2	ALA	Mainchain
1	A	240	CYS	Mainchain
1	A	296	ILE	Mainchain
1	A	477	VAL	Mainchain
1	A	499	PRO	Mainchain
1	A	501	GLN	Mainchain
1	A	622	ALA	Mainchain
1	A	654	SER	Mainchain
1	B	126	THR	Mainchain
1	B	2	ALA	Mainchain
1	B	477	VAL	Mainchain
1	B	499	PRO	Mainchain
1	B	501	GLN	Mainchain
1	B	622	ALA	Mainchain
1	B	654	SER	Mainchain

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	5770	0	5856	244	0
1	B	5770	0	5856	243	0
2	A	31	0	46	3	0
2	B	31	0	46	4	0
All	All	11602	0	11804	478	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 20.

All (478) 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:274:ARG:CD	1:B:289:VAL:HG13	1.92	1.00
1:A:295:TYR:O	1:A:297:ALA:N	1.96	0.99
1:A:414:LYS:HZ2	1:A:417:ILE:HG13	1.28	0.97
1:B:414:LYS:HZ2	1:B:417:ILE:HG13	1.28	0.94
1:B:293:GLU:OE2	1:B:296:ILE:HD12	1.68	0.93
1:B:407:GLU:HB3	1:B:414:LYS:HE2	1.52	0.92
1:A:407:GLU:HB3	1:A:414:LYS:HE2	1.52	0.92
1:A:686:LEU:HD22	1:B:340:THR:CG2	2.03	0.88
1:A:340:THR:CG2	1:B:686:LEU:HD22	2.03	0.87
1:B:259:LEU:HD23	1:B:294:HIS:CG	2.11	0.86
1:A:341:THR:HG21	1:B:683:ARG:HG2	1.58	0.85
1:B:659:LEU:O	1:B:663:PRO:HD2	1.77	0.85
1:B:439:LEU:O	1:B:443:PRO:HD2	1.77	0.85
1:B:258:TRP:HB3	1:B:259:LEU:HD22	1.59	0.85
1:A:341:THR:CG2	1:B:683:ARG:HG2	2.07	0.84
1:A:659:LEU:O	1:A:663:PRO:HD2	1.77	0.84
1:A:683:ARG:HG2	1:B:341:THR:HG21	1.58	0.84
1:A:439:LEU:O	1:A:443:PRO:HD2	1.77	0.84
1:A:683:ARG:HG2	1:B:341:THR:CG2	2.07	0.84
1:A:582:LEU:O	1:A:586:PRO:HD2	1.80	0.81
1:B:571:GLU:HG3	1:B:572:PRO:HD3	1.63	0.80
1:B:582:LEU:O	1:B:586:PRO:HD2	1.80	0.80
1:A:571:GLU:HG3	1:A:572:PRO:HD3	1.63	0.80
1:A:340:THR:HG21	1:B:686:LEU:HD22	1.64	0.79
1:A:340:THR:HG21	1:B:686:LEU:CD2	2.13	0.79
1:A:686:LEU:HD22	1:B:340:THR:HG21	1.64	0.79
1:A:686:LEU:CD2	1:B:340:THR:HG21	2.13	0.79
1:A:178:MET:HB2	1:A:669:PHE:HE2	1.48	0.78
1:B:178:MET:HB2	1:B:669:PHE:HE2	1.48	0.78
1:B:3:THR:O	1:B:4:LEU:C	2.23	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ARG:HD3	1:B:289:VAL:HG13	1.65	0.77
1:A:3:THR:O	1:A:4:LEU:C	2.23	0.76
1:A:297:ALA:HA	1:A:300:ASP:H	1.50	0.76
1:A:715:HIS:HB3	1:A:716:PRO:HD3	1.68	0.75
1:A:259:LEU:HD12	1:A:293:GLU:H	1.52	0.74
1:B:715:HIS:HB3	1:B:716:PRO:HD3	1.68	0.74
1:B:67:ARG:NH1	1:B:68:SER:O	2.22	0.73
1:B:274:ARG:NE	1:B:289:VAL:CG1	2.52	0.73
1:A:67:ARG:NH1	1:A:68:SER:O	2.22	0.73
1:B:67:ARG:HH11	1:B:68:SER:C	1.97	0.73
1:B:414:LYS:NZ	1:B:417:ILE:HG13	2.04	0.72
1:A:67:ARG:HH11	1:A:68:SER:C	1.97	0.71
1:A:715:HIS:CB	1:A:716:PRO:HD3	2.20	0.71
1:B:258:TRP:O	1:B:261:TYR:HB3	1.91	0.71
1:B:274:ARG:CD	1:B:289:VAL:CG1	2.66	0.70
1:A:297:ALA:N	1:A:299:VAL:H	1.90	0.70
1:A:107:LYS:O	1:A:111:PRO:HD2	1.91	0.69
1:B:715:HIS:CB	1:B:716:PRO:HD3	2.20	0.69
1:A:414:LYS:NZ	1:A:417:ILE:HG13	2.04	0.69
1:B:259:LEU:HB2	1:B:294:HIS:H	1.54	0.69
1:B:259:LEU:HD12	1:B:262:TYR:HB2	1.74	0.69
1:A:514:ALA:HB2	1:A:584:TYR:CE1	2.28	0.69
1:B:514:ALA:HB2	1:B:584:TYR:CE1	2.28	0.68
1:B:107:LYS:O	1:B:111:PRO:HD2	1.91	0.68
1:B:274:ARG:HD3	1:B:289:VAL:CG1	2.24	0.68
1:B:389:PHE:O	1:B:393:PRO:HD2	1.94	0.68
1:B:437:LEU:O	1:B:440:ILE:HG12	1.94	0.68
1:A:437:LEU:O	1:A:440:ILE:HG12	1.94	0.67
1:B:51:PRO:HB2	1:B:55:GLY:HA2	1.75	0.67
1:A:389:PHE:O	1:A:393:PRO:HD2	1.94	0.67
1:A:51:PRO:HB2	1:A:55:GLY:HA2	1.75	0.67
1:A:297:ALA:H	1:A:299:VAL:H	1.42	0.66
1:B:274:ARG:NE	1:B:289:VAL:HG13	2.11	0.66
1:A:550:VAL:HG13	1:A:551:LYS:H	1.61	0.65
1:B:295:TYR:O	1:B:297:ALA:N	2.29	0.65
1:A:259:LEU:HD12	1:A:293:GLU:N	2.11	0.65
1:A:297:ALA:N	1:A:299:VAL:N	2.44	0.65
1:B:550:VAL:HG13	1:B:551:LYS:H	1.61	0.65
1:A:294:HIS:O	1:A:295:TYR:O	2.15	0.65
1:B:259:LEU:CB	1:B:294:HIS:H	2.10	0.65
1:A:623:ALA:O	1:A:624:PHE:C	2.40	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HG	1:A:294:HIS:N	2.11	0.64
1:B:715:HIS:CG	1:B:716:PRO:HD3	2.33	0.64
1:B:584:TYR:HD1	1:B:588:THR:HG23	1.63	0.64
1:A:241:ASN:O	1:A:242:ALA:C	2.37	0.63
1:A:715:HIS:CG	1:A:716:PRO:HD3	2.33	0.63
1:A:584:TYR:HD1	1:A:588:THR:HG23	1.63	0.63
1:B:117:TRP:O	1:B:118:ALA:C	2.41	0.62
1:B:414:LYS:HB3	1:B:417:ILE:HA	1.81	0.62
1:B:390:PHE:HE1	1:B:438:PHE:HB3	1.63	0.62
1:B:58:ALA:HB1	1:B:60:ARG:HG3	1.82	0.61
1:B:293:GLU:O	1:B:294:HIS:C	2.41	0.61
1:A:390:PHE:HE1	1:A:438:PHE:HB3	1.63	0.61
1:A:414:LYS:HB3	1:A:417:ILE:HA	1.81	0.61
1:A:537:LYS:HB3	1:A:538:PRO:HD3	1.83	0.61
1:A:58:ALA:HB1	1:A:60:ARG:HG3	1.82	0.61
1:B:170:THR:HG21	1:B:662:LEU:HG	1.83	0.61
1:B:714:ILE:O	1:B:715:HIS:HB2	2.00	0.61
1:A:507:GLY:O	1:A:511:PRO:HD2	2.00	0.61
1:B:259:LEU:HB2	1:B:294:HIS:N	2.15	0.61
1:B:507:GLY:O	1:B:511:PRO:HD2	2.00	0.61
1:A:521:ILE:O	1:A:522:MET:C	2.42	0.61
1:B:414:LYS:HZ2	1:B:417:ILE:CG1	2.10	0.60
1:B:258:TRP:O	1:B:259:LEU:HD13	2.01	0.60
1:A:117:TRP:O	1:A:118:ALA:C	2.41	0.60
1:B:537:LYS:HB3	1:B:538:PRO:HD3	1.83	0.60
1:A:568:ASN:O	1:A:572:PRO:HD2	2.02	0.60
1:A:440:ILE:O	1:A:441:PHE:C	2.45	0.59
1:A:675:GLY:O	1:A:679:PRO:HD2	2.03	0.59
1:B:623:ALA:O	1:B:624:PHE:C	2.40	0.59
1:A:714:ILE:O	1:A:715:HIS:HB2	2.00	0.59
1:B:568:ASN:O	1:B:572:PRO:HD2	2.02	0.59
1:B:2:ALA:O	1:B:3:THR:C	2.43	0.59
1:B:414:LYS:NZ	1:B:417:ILE:HA	2.17	0.59
1:A:170:THR:HG21	1:A:662:LEU:HG	1.83	0.59
1:A:414:LYS:NZ	1:A:417:ILE:HA	2.17	0.59
1:A:241:ASN:C	1:A:243:ASN:H	2.10	0.59
1:A:2:ALA:O	1:A:3:THR:O	2.21	0.58
1:B:440:ILE:O	1:B:441:PHE:C	2.45	0.58
1:B:675:GLY:O	1:B:679:PRO:HD2	2.03	0.58
1:A:340:THR:HG23	1:B:686:LEU:HD22	1.83	0.58
1:B:116:ALA:O	1:B:117:TRP:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HG23	1:A:142:SER:HB2	1.86	0.58
1:A:116:ALA:O	1:A:117:TRP:C	2.45	0.58
1:A:298:GLU:O	1:A:299:VAL:C	2.46	0.58
1:B:3:THR:HG23	1:B:142:SER:HB2	1.86	0.58
1:B:293:GLU:OE2	1:B:296:ILE:CD1	2.47	0.58
1:B:2:ALA:O	1:B:3:THR:O	2.21	0.57
1:A:414:LYS:HZ2	1:A:417:ILE:CG1	2.10	0.57
1:B:521:ILE:O	1:B:522:MET:C	2.42	0.57
1:B:571:GLU:HG3	1:B:572:PRO:CD	2.32	0.57
1:A:571:GLU:HG3	1:A:572:PRO:CD	2.32	0.57
1:B:74:HIS:O	1:B:75:TRP:C	2.47	0.57
1:B:108:ILE:O	1:B:112:ILE:HG23	2.05	0.57
1:A:74:HIS:O	1:A:75:TRP:C	2.47	0.56
1:A:336:VAL:O	1:A:340:THR:HB	2.05	0.56
1:A:108:ILE:O	1:A:112:ILE:HG23	2.05	0.56
1:A:118:ALA:O	1:A:119:VAL:C	2.47	0.56
1:A:293:GLU:O	1:A:294:HIS:C	2.46	0.56
1:B:336:VAL:O	1:B:340:THR:HB	2.05	0.56
1:B:475:VAL:O	1:B:476:ASN:C	2.48	0.56
1:B:275:PRO:HB3	1:B:283:GLY:HA2	1.87	0.56
1:B:365:LEU:HD13	1:B:456:THR:HG21	1.88	0.56
1:A:584:TYR:CD1	1:A:588:THR:HG23	2.40	0.56
1:B:294:HIS:O	1:B:295:TYR:C	2.49	0.56
1:A:255:LEU:HD13	1:A:298:GLU:HB3	1.87	0.55
1:B:584:TYR:CD1	1:B:588:THR:HG23	2.40	0.55
1:A:261:TYR:C	1:A:263:GLN:H	2.13	0.55
1:A:473:ASN:O	1:A:474:LEU:C	2.49	0.55
1:B:497:GLN:NE2	1:B:501:GLN:HE22	2.05	0.55
1:A:2:ALA:O	1:A:3:THR:C	2.43	0.55
1:A:99:LEU:HD21	1:A:607:ARG:HG3	1.88	0.55
1:B:99:LEU:HD21	1:B:607:ARG:HG3	1.88	0.55
1:A:365:LEU:HD13	1:A:456:THR:HG21	1.88	0.55
1:A:686:LEU:HD22	1:B:340:THR:HG23	1.83	0.54
1:A:474:LEU:HD12	1:A:579:LEU:HD11	1.89	0.54
1:A:259:LEU:HG	1:A:294:HIS:H	1.71	0.54
1:A:316:ASP:O	1:A:318:LYS:N	2.41	0.54
1:A:674:LYS:O	1:A:675:GLY:C	2.49	0.54
1:B:118:ALA:O	1:B:119:VAL:C	2.47	0.54
1:A:241:ASN:C	1:A:243:ASN:N	2.59	0.54
1:B:674:LYS:O	1:B:675:GLY:C	2.49	0.54
1:A:72:PHE:O	1:A:74:HIS:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLN:NE2	1:A:501:GLN:HE22	2.05	0.54
1:B:72:PHE:O	1:B:74:HIS:N	2.40	0.54
1:B:474:LEU:HD12	1:B:579:LEU:HD11	1.89	0.54
1:B:76:MET:HB3	1:B:77:PRO:CD	2.39	0.53
1:A:23:ILE:HD11	1:A:71:LYS:HD2	1.90	0.53
1:B:31:GLN:HB3	1:B:33:PHE:CZ	2.43	0.53
1:A:76:MET:HB3	1:A:77:PRO:CD	2.39	0.53
1:B:474:LEU:O	1:B:475:VAL:C	2.52	0.53
1:A:476:ASN:O	1:A:477:VAL:C	2.48	0.53
1:A:31:GLN:HB3	1:A:33:PHE:CZ	2.43	0.53
1:B:473:ASN:O	1:B:474:LEU:C	2.49	0.53
1:B:488:PHE:O	1:B:491:LEU:HB3	2.09	0.53
1:A:340:THR:HG21	1:B:686:LEU:HD21	1.91	0.53
1:A:475:VAL:O	1:A:476:ASN:C	2.48	0.53
1:A:488:PHE:O	1:A:491:LEU:HB3	2.09	0.53
1:B:23:ILE:HD11	1:B:71:LYS:HD2	1.90	0.53
1:A:522:MET:O	1:A:523:VAL:C	2.52	0.52
1:B:258:TRP:C	1:B:259:LEU:HD13	2.34	0.52
1:A:686:LEU:HD21	1:B:340:THR:HG21	1.91	0.52
1:A:491:LEU:O	1:A:492:ASN:C	2.52	0.52
1:B:568:ASN:N	1:B:568:ASN:HD22	2.06	0.52
1:A:241:ASN:O	1:A:243:ASN:N	2.43	0.52
1:A:293:GLU:HA	1:A:293:GLU:OE1	2.10	0.52
1:B:476:ASN:O	1:B:477:VAL:C	2.48	0.52
1:B:491:LEU:O	1:B:492:ASN:C	2.52	0.52
1:B:522:MET:O	1:B:523:VAL:C	2.52	0.52
1:A:73:LEU:O	1:A:77:PRO:HD2	2.10	0.51
1:A:64:LEU:HD22	1:A:65:GLU:H	1.75	0.51
1:A:568:ASN:HD22	1:A:568:ASN:N	2.06	0.51
1:B:64:LEU:HD22	1:B:65:GLU:H	1.75	0.51
1:A:295:TYR:C	1:A:297:ALA:N	2.66	0.51
1:A:3:THR:O	1:A:5:LYS:N	2.43	0.51
1:B:73:LEU:O	1:B:77:PRO:HD2	2.10	0.51
1:A:563:GLY:O	1:A:564:SER:HB2	2.10	0.51
1:B:76:MET:HB3	1:B:77:PRO:HD2	1.93	0.51
1:B:258:TRP:CB	1:B:259:LEU:HD22	2.36	0.51
1:B:274:ARG:HD2	1:B:289:VAL:HG13	1.89	0.51
1:B:414:LYS:HZ2	1:B:417:ILE:HA	1.75	0.51
1:A:178:MET:HB2	1:A:669:PHE:CE2	2.38	0.51
1:A:259:LEU:C	1:A:261:TYR:N	2.59	0.51
1:B:61:PHE:HA	1:B:64:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:O	1:A:114:MET:C	2.51	0.51
1:A:244:LYS:O	1:A:245:LEU:C	2.52	0.51
1:A:411:PRO:C	1:A:414:LYS:HD2	2.36	0.50
1:A:414:LYS:HZ2	1:A:417:ILE:HA	1.75	0.50
1:B:411:PRO:C	1:B:414:LYS:HD2	2.36	0.50
1:B:563:GLY:O	1:B:564:SER:HB2	2.10	0.50
1:A:474:LEU:O	1:A:475:VAL:C	2.52	0.50
1:B:118:ALA:O	1:B:122:PRO:HD2	2.12	0.50
1:B:3:THR:O	1:B:5:LYS:N	2.43	0.50
1:A:76:MET:HB3	1:A:77:PRO:HD2	1.93	0.50
1:A:297:ALA:CA	1:A:299:VAL:N	2.75	0.50
1:B:501:GLN:O	1:B:502:ILE:C	2.53	0.50
1:A:275:PRO:HB3	1:A:283:GLY:HA2	1.93	0.50
1:B:137:LYS:HG2	1:B:501:GLN:NE2	2.27	0.49
1:B:414:LYS:HZ2	1:B:417:ILE:CA	2.25	0.49
1:A:61:PHE:HA	1:A:64:LEU:HB3	1.92	0.49
1:B:113:ALA:O	1:B:114:MET:C	2.51	0.49
1:A:662:LEU:O	1:A:663:PRO:C	2.54	0.49
1:B:259:LEU:HB3	1:B:293:GLU:HA	1.93	0.49
1:B:595:ILE:HG23	1:B:599:PHE:CE2	2.48	0.49
1:B:678:GLU:O	1:B:679:PRO:C	2.52	0.49
1:A:118:ALA:O	1:A:122:PRO:HD2	2.12	0.49
1:A:248:LEU:HD22	1:A:305:GLU:HG2	1.94	0.49
1:A:379:MET:HE3	1:A:449:MET:HG2	1.95	0.49
1:A:623:ALA:C	1:A:625:TRP:N	2.70	0.49
1:A:137:LYS:HG2	1:A:501:GLN:NE2	2.27	0.49
1:A:407:GLU:HB3	1:A:414:LYS:CE	2.36	0.49
1:A:595:ILE:HG23	1:A:599:PHE:CE2	2.48	0.49
1:A:523:VAL:O	1:A:524:ASP:C	2.55	0.49
1:B:107:LYS:O	1:B:108:ILE:C	2.55	0.49
1:B:259:LEU:CD1	1:B:262:TYR:CD2	2.96	0.49
1:B:633:ILE:HD11	1:B:669:PHE:HE1	1.78	0.49
1:A:107:LYS:O	1:A:108:ILE:C	2.55	0.49
1:A:571:GLU:O	1:A:572:PRO:C	2.51	0.49
1:B:523:VAL:O	1:B:524:ASP:C	2.55	0.48
1:A:414:LYS:HZ2	1:A:417:ILE:CA	2.26	0.48
1:A:633:ILE:HD11	1:A:669:PHE:HE1	1.78	0.48
1:B:121:VAL:O	1:B:122:PRO:C	2.55	0.48
1:B:486:ALA:O	1:B:487:ALA:C	2.56	0.48
1:B:33:PHE:HE1	1:B:60:ARG:HB3	1.78	0.48
1:B:395:ALA:O	1:B:396:PHE:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:O	1:A:26:ALA:C	2.55	0.48
1:A:683:ARG:HG2	1:B:341:THR:HG22	1.94	0.48
1:B:245:LEU:HD13	1:B:309:GLU:HB3	1.95	0.48
1:B:276:ILE:HB	1:B:282:LEU:HG	1.96	0.48
1:B:259:LEU:CB	1:B:293:GLU:HA	2.43	0.48
1:B:25:PHE:O	1:B:26:ALA:C	2.55	0.48
1:B:716:PRO:HD2	1:B:717:VAL:HG22	1.96	0.48
1:A:258:TRP:HA	1:A:258:TRP:CE3	2.48	0.48
1:A:535:MET:HB3	1:A:535:MET:HE3	1.52	0.48
1:B:379:MET:HE3	1:B:449:MET:HG2	1.95	0.48
1:B:675:GLY:O	1:B:676:ARG:C	2.56	0.48
1:B:258:TRP:HA	1:B:258:TRP:CE3	2.48	0.47
1:A:93:LEU:HD23	1:A:621:ALA:HB1	1.97	0.47
1:A:395:ALA:O	1:A:396:PHE:C	2.55	0.47
1:A:675:GLY:O	1:A:676:ARG:C	2.56	0.47
1:A:678:GLU:O	1:A:679:PRO:C	2.52	0.47
1:B:473:ASN:O	1:B:474:LEU:O	2.32	0.47
1:B:673:CYS:O	1:B:674:LYS:C	2.57	0.47
1:B:261:TYR:C	1:B:263:GLN:H	2.22	0.47
1:B:571:GLU:O	1:B:572:PRO:C	2.51	0.47
1:A:129:GLU:HG2	1:A:132:LEU:HD22	1.96	0.47
1:A:473:ASN:O	1:A:474:LEU:O	2.32	0.47
1:A:716:PRO:HD2	1:A:717:VAL:HG22	1.96	0.47
1:A:33:PHE:HE1	1:A:60:ARG:HB3	1.78	0.47
1:A:274:ARG:HA	1:A:288:LYS:HE2	1.97	0.47
1:A:486:ALA:O	1:A:487:ALA:C	2.56	0.47
1:B:545:LYS:HB2	1:B:545:LYS:HE2	1.40	0.47
1:A:90:HIS:HE1	1:A:611:ILE:O	1.97	0.47
1:A:149:ILE:O	1:A:152:ILE:HG22	2.15	0.47
1:A:341:THR:HG22	1:B:683:ARG:HG2	1.94	0.47
1:A:672:PHE:O	1:A:673:CYS:C	2.58	0.47
1:A:121:VAL:O	1:A:122:PRO:C	2.55	0.47
1:A:673:CYS:O	1:A:674:LYS:C	2.57	0.47
1:B:32:PRO:HG3	1:B:58:ALA:C	2.40	0.47
1:B:514:ALA:CB	1:B:588:THR:HG21	2.45	0.47
1:B:662:LEU:O	1:B:663:PRO:C	2.54	0.47
1:B:655:ALA:O	1:B:658:PHE:HB2	2.15	0.46
1:B:672:PHE:O	1:B:673:CYS:C	2.58	0.46
1:A:390:PHE:CE1	1:A:438:PHE:HB3	2.49	0.46
1:B:90:HIS:HE1	1:B:611:ILE:O	1.97	0.46
1:A:625:TRP:O	1:A:626:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ALA:O	1:A:658:PHE:HB2	2.15	0.46
1:B:129:GLU:HG2	1:B:132:LEU:HD22	1.96	0.46
1:A:442:LEU:HD22	1:A:442:LEU:HA	1.59	0.46
1:B:93:LEU:HD23	1:B:621:ALA:HB1	1.97	0.46
1:A:120:LEU:O	1:A:121:VAL:C	2.55	0.46
1:A:514:ALA:CB	1:A:588:THR:HG21	2.45	0.46
1:A:500:ASN:C	1:A:502:ILE:N	2.68	0.46
1:A:568:ASN:O	1:A:569:THR:C	2.57	0.46
1:A:660:ILE:O	1:A:661:ALA:C	2.58	0.46
1:B:63:ASN:O	1:B:65:GLU:N	2.48	0.46
1:B:149:ILE:O	1:B:152:ILE:HG22	2.15	0.46
1:B:623:ALA:C	1:B:625:TRP:N	2.70	0.46
1:A:270:ASN:HB3	1:A:271:SER:H	1.54	0.46
1:B:110:ALA:HB3	1:B:111:PRO:CD	2.46	0.46
1:B:669:PHE:O	1:B:670:HIS:C	2.57	0.46
1:A:501:GLN:O	1:A:502:ILE:C	2.53	0.46
1:A:669:PHE:O	1:A:670:HIS:C	2.57	0.46
1:B:259:LEU:HD11	1:B:262:TYR:CD2	2.51	0.46
1:B:535:MET:HB3	1:B:535:MET:HE3	1.52	0.46
1:B:684:TYR:HA	1:B:685:PRO:HD2	1.83	0.46
2:B:801:LPC:H32	2:B:801:LPC:H0A2	1.56	0.46
1:A:63:ASN:O	1:A:65:GLU:N	2.48	0.45
1:A:437:LEU:O	1:A:438:PHE:C	2.59	0.45
1:B:178:MET:HB2	1:B:669:PHE:CE2	2.38	0.45
1:B:500:ASN:C	1:B:502:ILE:N	2.68	0.45
1:B:633:ILE:HD11	1:B:669:PHE:CE1	2.51	0.45
1:A:390:PHE:O	1:A:391:ILE:C	2.60	0.45
1:B:263:GLN:HG3	1:B:264:LEU:HD23	1.98	0.45
1:B:281:CYS:HB3	1:B:282:LEU:H	1.51	0.45
1:A:137:LYS:HG2	1:A:501:GLN:CD	2.41	0.45
1:A:259:LEU:HD13	1:A:262:TYR:HB2	1.97	0.45
1:A:276:ILE:HA	1:A:276:ILE:HD13	1.71	0.45
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.78	0.45
1:A:633:ILE:HD11	1:A:669:PHE:CE1	2.51	0.45
1:B:120:LEU:O	1:B:121:VAL:C	2.55	0.45
1:B:137:LYS:HG2	1:B:501:GLN:CD	2.41	0.45
1:B:568:ASN:O	1:B:569:THR:C	2.57	0.45
1:B:156:SER:HB2	1:B:157:ASN:H	1.26	0.45
1:B:259:LEU:HD23	1:B:294:HIS:ND1	2.29	0.45
1:A:32:PRO:HG3	1:A:58:ALA:C	2.40	0.45
1:A:110:ALA:HB3	1:A:111:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LEU:O	1:B:438:PHE:C	2.59	0.45
1:B:442:LEU:O	1:B:443:PRO:C	2.59	0.45
1:B:658:PHE:O	1:B:659:LEU:C	2.58	0.45
1:B:714:ILE:H	1:B:714:ILE:HG13	1.60	0.45
1:A:163:ILE:HG13	1:A:164:ILE:N	2.32	0.45
1:A:442:LEU:O	1:A:443:PRO:C	2.59	0.45
1:A:481:SER:O	1:A:482:VAL:C	2.59	0.45
1:B:335:ALA:O	1:B:339:GLN:HG2	2.17	0.45
1:A:714:ILE:O	1:A:715:HIS:CB	2.64	0.45
1:B:508:MET:H	1:B:508:MET:HG2	1.54	0.45
2:B:801:LPC:HD1	2:B:801:LPC:HG1	1.71	0.45
1:B:660:ILE:O	1:B:661:ALA:C	2.58	0.45
1:B:9:VAL:O	1:B:10:SER:C	2.57	0.44
1:B:408:LYS:HA	1:B:408:LYS:HD3	1.49	0.44
1:A:471:ILE:O	1:A:472:PHE:C	2.59	0.44
1:A:675:GLY:O	1:A:679:PRO:CD	2.65	0.44
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.78	0.44
1:A:474:LEU:O	1:A:475:VAL:O	2.36	0.44
2:A:801:LPC:H32	2:A:801:LPC:H0A2	1.56	0.44
1:A:662:LEU:HB3	1:A:663:PRO:CD	2.47	0.44
1:B:259:LEU:HD12	1:B:262:TYR:CB	2.43	0.44
1:B:471:ILE:O	1:B:472:PHE:C	2.59	0.44
1:B:662:LEU:HB3	1:B:663:PRO:CD	2.47	0.44
1:B:72:PHE:O	1:B:73:LEU:C	2.60	0.44
1:B:407:GLU:HB3	1:B:414:LYS:CE	2.36	0.44
1:A:179:LYS:O	1:A:182:GLU:HG3	2.18	0.44
2:A:801:LPC:HD1	2:A:801:LPC:HG1	1.71	0.44
1:B:172:TRP:O	1:B:173:THR:C	2.60	0.44
2:B:801:LPC:HE1	2:B:801:LPC:HB1	1.53	0.44
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.78	0.44
1:A:152:ILE:HA	1:A:153:PRO:HD3	1.90	0.44
1:B:114:MET:HB2	1:B:114:MET:HE2	1.70	0.44
1:B:544:LEU:O	1:B:545:LYS:C	2.60	0.44
1:A:104:LEU:O	1:A:105:GLY:C	2.60	0.44
1:A:335:ALA:O	1:A:339:GLN:HG2	2.17	0.44
1:B:474:LEU:HB3	1:B:475:VAL:H	1.71	0.44
1:A:52:ALA:HB3	1:A:57:PHE:HD2	1.83	0.43
1:A:72:PHE:O	1:A:73:LEU:C	2.60	0.43
1:A:252:LYS:O	1:A:253:THR:C	2.60	0.43
1:A:259:LEU:HD12	1:A:292:ILE:HA	2.00	0.43
1:B:625:TRP:O	1:B:626:PRO:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:HD3	1:A:417:ILE:HA	2.01	0.43
1:A:544:LEU:O	1:A:545:LYS:C	2.60	0.43
1:B:179:LYS:O	1:B:182:GLU:HG3	2.18	0.43
1:B:274:ARG:HA	1:B:288:LYS:HE2	2.00	0.43
1:B:474:LEU:O	1:B:475:VAL:O	2.36	0.43
1:B:485:GLY:O	1:B:486:ALA:C	2.61	0.43
1:A:34:ASN:O	1:A:36:ARG:N	2.45	0.43
1:B:163:ILE:HG13	1:B:164:ILE:N	2.32	0.43
1:B:304:LYS:HD2	1:B:304:LYS:HA	1.43	0.43
1:A:156:SER:HB2	1:A:157:ASN:H	1.26	0.43
1:B:302:THR:O	1:B:306:ILE:HB	2.19	0.43
1:B:567:PHE:CZ	1:B:624:PHE:HB2	2.54	0.43
1:B:714:ILE:O	1:B:715:HIS:CB	2.64	0.43
1:A:148:THR:C	1:A:150:SER:H	2.26	0.43
1:A:290:ASP:O	1:A:291:ALA:HB2	2.18	0.43
1:A:658:PHE:O	1:A:659:LEU:C	2.58	0.43
2:A:801:LPC:H0B3	2:A:801:LPC:H31	0.77	0.43
1:B:675:GLY:O	1:B:679:PRO:CD	2.65	0.43
1:A:567:PHE:CZ	1:A:624:PHE:HB2	2.54	0.43
1:B:51:PRO:HB2	1:B:52:ALA:H	1.62	0.43
1:B:471:ILE:H	1:B:471:ILE:HG12	1.62	0.43
1:B:510:ILE:O	1:B:511:PRO:C	2.62	0.43
1:B:123:VAL:HG13	1:B:158:ARG:HD3	2.01	0.43
1:B:522:MET:O	1:B:523:VAL:O	2.37	0.43
1:B:568:ASN:O	1:B:572:PRO:CD	2.67	0.43
1:A:545:LYS:HE2	1:A:545:LYS:HB2	1.40	0.43
1:B:148:THR:C	1:B:150:SER:H	2.26	0.43
1:B:390:PHE:O	1:B:391:ILE:C	2.60	0.43
1:B:575:GLN:HE21	1:B:575:GLN:HB3	1.59	0.43
2:B:801:LPC:HM2	2:B:801:LPC:HJ1	1.66	0.43
1:A:485:GLY:O	1:A:486:ALA:C	2.61	0.42
1:B:251:LYS:O	1:B:255:LEU:HG	2.18	0.42
1:B:414:LYS:HD3	1:B:417:ILE:HA	2.01	0.42
1:A:522:MET:O	1:A:523:VAL:O	2.37	0.42
1:A:568:ASN:O	1:A:572:PRO:CD	2.67	0.42
1:B:406:ILE:CG1	1:B:488:PHE:HB3	2.49	0.42
1:A:82:MET:O	1:A:607:ARG:NH2	2.51	0.42
1:A:406:ILE:CG1	1:A:488:PHE:HB3	2.49	0.42
1:A:9:VAL:O	1:A:10:SER:C	2.57	0.42
1:A:26:ALA:O	1:A:27:PHE:C	2.61	0.42
1:A:575:GLN:HE21	1:A:575:GLN:HB3	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLY:HA3	1:B:513:LYS:HD3	2.01	0.42
1:B:504:LYS:O	1:B:508:MET:HG2	2.20	0.42
1:A:74:HIS:O	1:A:78:GLU:HG2	2.20	0.42
1:A:504:LYS:O	1:A:508:MET:HG2	2.20	0.42
1:B:104:LEU:O	1:B:105:GLY:C	2.60	0.42
1:B:115:LEU:O	1:B:116:ALA:C	2.61	0.42
1:A:82:MET:HE2	1:A:82:MET:HB3	1.52	0.42
1:A:144:ILE:HD12	1:A:144:ILE:HA	1.71	0.42
1:B:662:LEU:HD12	1:B:662:LEU:HA	1.69	0.42
1:A:115:LEU:O	1:A:116:ALA:C	2.61	0.42
1:A:258:TRP:O	1:A:259:LEU:HD22	2.20	0.42
1:B:67:ARG:HH11	1:B:69:TYR:N	2.17	0.42
1:A:114:MET:HB2	1:A:114:MET:HE2	1.70	0.42
1:A:474:LEU:HB3	1:A:475:VAL:H	1.71	0.42
1:A:510:ILE:O	1:A:511:PRO:C	2.62	0.42
1:A:588:THR:HA	1:A:589:PRO:HD3	1.90	0.42
1:B:26:ALA:O	1:B:27:PHE:C	2.61	0.42
1:B:435:LEU:O	1:B:436:LYS:C	2.63	0.42
1:A:172:TRP:O	1:A:173:THR:C	2.60	0.42
1:A:179:LYS:O	1:A:183:THR:HG23	2.20	0.42
1:A:423:LYS:HA	1:A:423:LYS:HD2	1.75	0.42
1:A:435:LEU:O	1:A:436:LYS:C	2.63	0.42
1:A:485:GLY:HA3	1:A:513:LYS:HD3	2.01	0.42
1:B:74:HIS:O	1:B:78:GLU:HG2	2.20	0.42
1:A:123:VAL:HG13	1:A:158:ARG:HD3	2.01	0.41
1:A:561:ASN:HA	1:A:562:PRO:HD3	1.85	0.41
1:B:52:ALA:HB3	1:B:57:PHE:HD2	1.83	0.41
1:B:257:ASN:O	1:B:258:TRP:C	2.62	0.41
1:B:481:SER:O	1:B:482:VAL:C	2.59	0.41
1:B:525:GLY:O	1:B:529:VAL:HG22	2.20	0.41
1:B:435:LEU:HG	1:B:439:LEU:HD22	2.01	0.41
1:A:258:TRP:HA	1:A:258:TRP:HE3	1.83	0.41
1:A:570:GLY:O	1:A:574:ILE:HG13	2.20	0.41
1:A:598:PHE:O	1:A:599:PHE:C	2.63	0.41
1:A:684:TYR:HA	1:A:685:PRO:HD2	1.83	0.41
1:B:241:ASN:OD1	1:B:366:ALA:HB1	2.21	0.41
1:B:647:LEU:HD12	1:B:647:LEU:HA	1.86	0.41
1:A:60:ARG:HG3	1:A:60:ARG:H	1.46	0.41
1:A:259:LEU:HD23	1:A:294:HIS:ND1	2.36	0.41
1:A:288:LYS:H	1:A:288:LYS:HG3	1.61	0.41
1:A:435:LEU:HG	1:A:439:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LYS:O	1:B:183:THR:HG23	2.20	0.41
1:B:256:GLN:O	1:B:257:ASN:C	2.61	0.41
1:B:390:PHE:CE1	1:B:438:PHE:HB3	2.49	0.41
1:B:412:PHE:HB3	1:B:413:LEU:H	1.61	0.41
1:A:12:GLY:O	1:A:13:ILE:C	2.61	0.41
1:A:36:ARG:H	1:A:36:ARG:HG3	1.68	0.41
1:A:67:ARG:HH11	1:A:69:TYR:N	2.17	0.41
1:A:72:PHE:HB3	1:A:73:LEU:H	0.98	0.41
1:B:540:ILE:O	1:B:541:ILE:C	2.64	0.41
1:A:105:GLY:O	1:A:106:LEU:C	2.60	0.41
1:B:50:SER:CB	1:B:51:PRO:HD2	2.51	0.41
1:B:295:TYR:C	1:B:297:ALA:N	2.79	0.41
1:B:367:ILE:HG21	1:B:367:ILE:HD13	1.83	0.41
1:B:579:LEU:O	1:B:580:LEU:C	2.64	0.41
1:A:137:LYS:HB2	1:A:137:LYS:HE2	1.60	0.41
1:B:97:VAL:HG21	1:B:622:ALA:HB2	2.03	0.41
1:B:601:LEU:O	1:B:605:VAL:HG13	2.21	0.41
1:A:167:TYR:O	1:A:168:ALA:C	2.64	0.41
1:A:706:LYS:HZ2	1:A:706:LYS:HG3	1.67	0.41
1:B:105:GLY:O	1:B:106:LEU:C	2.60	0.41
1:A:367:ILE:HD13	1:A:367:ILE:HG21	1.83	0.41
1:A:525:GLY:O	1:A:529:VAL:HG22	2.20	0.41
1:A:597:VAL:O	1:A:598:PHE:C	2.64	0.41
1:B:12:GLY:O	1:B:13:ILE:C	2.61	0.41
1:A:50:SER:CB	1:A:51:PRO:HD2	2.51	0.40
1:B:292:ILE:O	1:B:293:GLU:C	2.63	0.40
1:B:423:LYS:HA	1:B:423:LYS:HD2	1.75	0.40
1:A:137:LYS:HE2	1:A:137:LYS:HB3	1.84	0.40
1:A:264:LEU:HD22	1:A:264:LEU:HA	1.76	0.40
1:A:309:GLU:O	1:A:310:ARG:C	2.64	0.40
1:B:82:MET:O	1:B:607:ARG:NH2	2.51	0.40
1:B:142:SER:HB2	1:B:143:ASP:H	1.74	0.40
1:B:570:GLY:O	1:B:574:ILE:HG13	2.20	0.40
1:A:256:GLN:O	1:A:257:ASN:C	2.61	0.40
1:A:470:TYR:O	1:A:471:ILE:C	2.63	0.40
1:A:60:ARG:HB2	1:A:61:PHE:H	1.27	0.40
1:A:114:MET:O	1:A:115:LEU:C	2.63	0.40
1:B:500:ASN:C	1:B:502:ILE:H	2.29	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	714/772 (92%)	555 (78%)	106 (15%)	53 (7%)	1	1
1	B	714/772 (92%)	556 (78%)	105 (15%)	53 (7%)	1	1
All	All	1428/1544 (92%)	1111 (78%)	211 (15%)	106 (7%)	1	1

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	51	PRO
1	A	128	ASN
1	A	156	SER
1	A	289	VAL
1	A	291	ALA
1	A	296	ILE
1	A	317	GLN
1	A	418	GLU
1	A	474	LEU
1	A	523	VAL
1	A	567	PHE
1	A	568	ASN
1	A	614	TYR
1	A	621	ALA
1	A	703	LEU
1	A	715	HIS
1	A	716	PRO
1	B	3	THR
1	B	51	PRO
1	B	128	ASN
1	B	156	SER
1	B	289	VAL
1	B	293	GLU
1	B	296	ILE

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Mol	Chain	Res	Type
1	B	418	GLU
1	B	474	LEU
1	B	523	VAL
1	B	567	PHE
1	B	568	ASN
1	B	614	TYR
1	B	621	ALA
1	B	703	LEU
1	B	715	HIS
1	B	716	PRO
1	A	62	VAL
1	A	64	LEU
1	A	72	PHE
1	A	137	LYS
1	A	208	ASN
1	A	213	PRO
1	A	295	TYR
1	A	368	PRO
1	A	475	VAL
1	A	487	ALA
1	A	562	PRO
1	A	674	LYS
1	A	675	GLY
1	B	62	VAL
1	B	64	LEU
1	B	72	PHE
1	B	137	LYS
1	B	208	ASN
1	B	213	PRO
1	B	368	PRO
1	B	475	VAL
1	B	487	ALA
1	B	562	PRO
1	B	674	LYS
1	B	675	GLY
1	A	35	ASP
1	A	73	LEU
1	A	118	ALA
1	A	267	THR
1	B	35	ASP
1	B	73	LEU
1	B	118	ALA

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Mol	Chain	Res	Type
1	B	295	TYR
1	A	60	ARG
1	A	117	TRP
1	A	522	MET
1	A	554	LYS
1	A	555	ASP
1	A	561	ASN
1	A	565	ILE
1	A	613	VAL
1	B	60	ARG
1	B	117	TRP
1	B	267	THR
1	B	292	ILE
1	B	522	MET
1	B	554	LYS
1	B	555	ASP
1	B	561	ASN
1	B	565	ILE
1	B	613	VAL
1	A	127	ASN
1	A	453	GLU
1	B	127	ASN
1	B	294	HIS
1	B	453	GLU
1	A	4	LEU
1	A	59	GLY
1	A	76	MET
1	A	473	ASN
1	A	499	PRO
1	A	548	PHE
1	B	4	LEU
1	B	59	GLY
1	B	76	MET
1	B	473	ASN
1	B	499	PRO
1	B	548	PHE
1	A	587	VAL
1	B	587	VAL
1	A	274	ARG

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	618/666 (93%)	394 (64%)	224 (36%)	0	0
1	B	618/666 (93%)	390 (63%)	228 (37%)	0	0
All	All	1236/1332 (93%)	784 (63%)	452 (37%)	1	0

All (452) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	LYS
1	A	10	SER
1	A	16	LEU
1	A	17	THR
1	A	29	ARG
1	A	30	LEU
1	A	33	PHE
1	A	35	ASP
1	A	36	ARG
1	A	40	SER
1	A	45	ARG
1	A	49	SER
1	A	50	SER
1	A	53	SER
1	A	60	ARG
1	A	61	PHE
1	A	62	VAL
1	A	64	LEU
1	A	65	GLU
1	A	66	LEU
1	A	67	ARG
1	A	68	SER
1	A	70	LEU
1	A	71	LYS
1	A	73	LEU
1	A	75	TRP

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Mol	Chain	Res	Type
1	A	76	MET
1	A	81	LYS
1	A	82	MET
1	A	85	ARG
1	A	97	VAL
1	A	99	LEU
1	A	104	LEU
1	A	111	PRO
1	A	112	ILE
1	A	114	MET
1	A	115	LEU
1	A	122	PRO
1	A	127	ASN
1	A	128	ASN
1	A	129	GLU
1	A	131	GLU
1	A	132	LEU
1	A	134	LYS
1	A	137	LYS
1	A	140	THR
1	A	142	SER
1	A	144	ILE
1	A	147	LEU
1	A	152	ILE
1	A	156	SER
1	A	158	ARG
1	A	160	TRP
1	A	163	ILE
1	A	170	THR
1	A	179	LYS
1	A	180	GLU
1	A	181	TYR
1	A	182	GLU
1	A	192	LEU
1	A	203	THR
1	A	205	LEU
1	A	206	VAL
1	A	212	ASP
1	A	214	ASP
1	A	218	SER
1	A	231	ASP
1	A	235	THR

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Mol	Chain	Res	Type
1	A	238	VAL
1	A	248	LEU
1	A	250	SER
1	A	251	LYS
1	A	252	LYS
1	A	254	LYS
1	A	256	GLN
1	A	258	TRP
1	A	259	LEU
1	A	260	ASP
1	A	264	LEU
1	A	265	LYS
1	A	267	THR
1	A	268	ARG
1	A	269	ASN
1	A	271	SER
1	A	272	GLN
1	A	273	ILE
1	A	274	ARG
1	A	276	ILE
1	A	277	THR
1	A	278	LYS
1	A	281	CYS
1	A	284	LEU
1	A	288	LYS
1	A	289	VAL
1	A	290	ASP
1	A	292	ILE
1	A	294	HIS
1	A	295	TYR
1	A	300	ASP
1	A	301	LYS
1	A	304	LYS
1	A	306	ILE
1	A	308	GLU
1	A	309	GLU
1	A	311	GLU
1	A	314	VAL
1	A	318	LYS
1	A	327	SER
1	A	340	THR
1	A	341	THR

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Mol	Chain	Res	Type
1	A	350	LEU
1	A	363	PRO
1	A	365	LEU
1	A	370	VAL
1	A	372	LEU
1	A	373	THR
1	A	374	VAL
1	A	376	ARG
1	A	377	LEU
1	A	379	MET
1	A	386	LEU
1	A	387	THR
1	A	391	ILE
1	A	394	ILE
1	A	400	LEU
1	A	402	THR
1	A	404	GLU
1	A	406	ILE
1	A	408	LYS
1	A	415	VAL
1	A	422	ILE
1	A	423	LYS
1	A	424	SER
1	A	425	LEU
1	A	426	ILE
1	A	429	LEU
1	A	433	ILE
1	A	436	LYS
1	A	437	LEU
1	A	439	LEU
1	A	440	ILE
1	A	442	LEU
1	A	446	LEU
1	A	457	SER
1	A	458	VAL
1	A	459	SER
1	A	463	ARG
1	A	471	ILE
1	A	491	LEU
1	A	492	ASN
1	A	495	LEU
1	A	498	SER

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Mol	Chain	Res	Type
1	A	503	PRO
1	A	504	LYS
1	A	505	THR
1	A	506	ILE
1	A	508	MET
1	A	512	MET
1	A	513	LYS
1	A	519	THR
1	A	521	ILE
1	A	533	ILE
1	A	535	MET
1	A	536	LEU
1	A	541	ILE
1	A	545	LYS
1	A	546	ASN
1	A	549	LEU
1	A	550	VAL
1	A	551	LYS
1	A	553	GLU
1	A	554	LYS
1	A	556	ARG
1	A	557	GLU
1	A	568	ASN
1	A	569	THR
1	A	571	GLU
1	A	572	PRO
1	A	574	ILE
1	A	579	LEU
1	A	580	LEU
1	A	582	LEU
1	A	588	THR
1	A	590	MET
1	A	595	ILE
1	A	597	VAL
1	A	604	VAL
1	A	605	VAL
1	A	607	ARG
1	A	613	VAL
1	A	616	GLN
1	A	625	TRP
1	A	626	PRO
1	A	636	LEU

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Mol	Chain	Res	Type
1	A	642	LEU
1	A	643	LEU
1	A	647	LEU
1	A	649	THR
1	A	654	SER
1	A	659	LEU
1	A	660	ILE
1	A	662	LEU
1	A	664	VAL
1	A	667	ILE
1	A	671	ARG
1	A	676	ARG
1	A	677	PHE
1	A	679	PRO
1	A	682	VAL
1	A	683	ARG
1	A	688	GLU
1	A	690	MET
1	A	696	GLU
1	A	697	ARG
1	A	699	ARG
1	A	700	GLU
1	A	705	LEU
1	A	706	LYS
1	A	709	LEU
1	A	710	GLN
1	A	711	ASP
1	A	714	ILE
1	A	717	VAL
1	B	3	THR
1	B	5	LYS
1	B	10	SER
1	B	16	LEU
1	B	17	THR
1	B	29	ARG
1	B	30	LEU
1	B	33	PHE
1	B	35	ASP
1	B	36	ARG
1	B	40	SER
1	B	45	ARG
1	B	49	SER

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Mol	Chain	Res	Type
1	B	50	SER
1	B	53	SER
1	B	60	ARG
1	B	61	PHE
1	B	62	VAL
1	B	64	LEU
1	B	65	GLU
1	B	66	LEU
1	B	67	ARG
1	B	68	SER
1	B	70	LEU
1	B	71	LYS
1	B	73	LEU
1	B	75	TRP
1	B	76	MET
1	B	81	LYS
1	B	82	MET
1	B	85	ARG
1	B	97	VAL
1	B	99	LEU
1	B	104	LEU
1	B	111	PRO
1	B	112	ILE
1	B	114	MET
1	B	115	LEU
1	B	122	PRO
1	B	127	ASN
1	B	128	ASN
1	B	129	GLU
1	B	131	GLU
1	B	132	LEU
1	B	134	LYS
1	B	137	LYS
1	B	140	THR
1	B	142	SER
1	B	144	ILE
1	B	147	LEU
1	B	152	ILE
1	B	156	SER
1	B	158	ARG
1	B	160	TRP
1	B	163	ILE

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Mol	Chain	Res	Type
1	B	170	THR
1	B	179	LYS
1	B	180	GLU
1	B	181	TYR
1	B	182	GLU
1	B	192	LEU
1	B	203	THR
1	B	205	LEU
1	B	206	VAL
1	B	212	ASP
1	B	214	ASP
1	B	218	SER
1	B	231	ASP
1	B	235	THR
1	B	238	VAL
1	B	241	ASN
1	B	244	LYS
1	B	248	LEU
1	B	250	SER
1	B	251	LYS
1	B	252	LYS
1	B	253	THR
1	B	254	LYS
1	B	256	GLN
1	B	258	TRP
1	B	259	LEU
1	B	264	LEU
1	B	265	LYS
1	B	267	THR
1	B	268	ARG
1	B	269	ASN
1	B	271	SER
1	B	272	GLN
1	B	273	ILE
1	B	274	ARG
1	B	277	THR
1	B	278	LYS
1	B	281	CYS
1	B	284	LEU
1	B	288	LYS
1	B	290	ASP
1	B	292	ILE

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Mol	Chain	Res	Type
1	B	293	GLU
1	B	294	HIS
1	B	295	TYR
1	B	296	ILE
1	B	299	VAL
1	B	300	ASP
1	B	301	LYS
1	B	304	LYS
1	B	306	ILE
1	B	308	GLU
1	B	309	GLU
1	B	311	GLU
1	B	313	VAL
1	B	314	VAL
1	B	318	LYS
1	B	327	SER
1	B	340	THR
1	B	341	THR
1	B	350	LEU
1	B	363	PRO
1	B	365	LEU
1	B	370	VAL
1	B	372	LEU
1	B	373	THR
1	B	374	VAL
1	B	376	ARG
1	B	377	LEU
1	B	379	MET
1	B	386	LEU
1	B	387	THR
1	B	391	ILE
1	B	394	ILE
1	B	400	LEU
1	B	402	THR
1	B	404	GLU
1	B	406	ILE
1	B	408	LYS
1	B	415	VAL
1	B	422	ILE
1	B	423	LYS
1	B	424	SER
1	B	425	LEU

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Mol	Chain	Res	Type
1	B	426	ILE
1	B	429	LEU
1	B	433	ILE
1	B	436	LYS
1	B	437	LEU
1	B	439	LEU
1	B	440	ILE
1	B	442	LEU
1	B	446	LEU
1	B	457	SER
1	B	458	VAL
1	B	459	SER
1	B	463	ARG
1	B	471	ILE
1	B	491	LEU
1	B	492	ASN
1	B	495	LEU
1	B	498	SER
1	B	503	PRO
1	B	504	LYS
1	B	505	THR
1	B	506	ILE
1	B	508	MET
1	B	512	MET
1	B	513	LYS
1	B	519	THR
1	B	521	ILE
1	B	533	ILE
1	B	535	MET
1	B	536	LEU
1	B	541	ILE
1	B	545	LYS
1	B	546	ASN
1	B	549	LEU
1	B	550	VAL
1	B	551	LYS
1	B	553	GLU
1	B	554	LYS
1	B	556	ARG
1	B	557	GLU
1	B	568	ASN
1	B	569	THR

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Mol	Chain	Res	Type
1	B	571	GLU
1	B	572	PRO
1	B	574	ILE
1	B	579	LEU
1	B	580	LEU
1	B	582	LEU
1	B	588	THR
1	B	590	MET
1	B	595	ILE
1	B	597	VAL
1	B	604	VAL
1	B	605	VAL
1	B	607	ARG
1	B	613	VAL
1	B	616	GLN
1	B	625	TRP
1	B	626	PRO
1	B	636	LEU
1	B	642	LEU
1	B	643	LEU
1	B	647	LEU
1	B	649	THR
1	B	654	SER
1	B	659	LEU
1	B	660	ILE
1	B	662	LEU
1	B	664	VAL
1	B	667	ILE
1	B	671	ARG
1	B	676	ARG
1	B	677	PHE
1	B	679	PRO
1	B	682	VAL
1	B	683	ARG
1	B	688	GLU
1	B	690	MET
1	B	696	GLU
1	B	697	ARG
1	B	699	ARG
1	B	700	GLU
1	B	705	LEU
1	B	706	LYS

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Mol	Chain	Res	Type
1	B	709	LEU
1	B	710	GLN
1	B	711	ASP
1	B	714	ILE
1	B	717	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	63	ASN
1	A	90	HIS
1	A	124	ASN
1	A	237	GLN
1	A	256	GLN
1	A	270	ASN
1	A	476	ASN
1	A	490	GLN
1	A	497	GLN
1	A	500	ASN
1	A	501	GLN
1	A	543	HIS
1	A	568	ASN
1	A	573	GLN
1	A	575	GLN
1	A	608	HIS
1	A	687	GLN
1	A	710	GLN
1	B	63	ASN
1	B	90	HIS
1	B	124	ASN
1	B	237	GLN
1	B	270	ASN
1	B	272	GLN
1	B	315	ASN
1	B	476	ASN
1	B	490	GLN
1	B	497	GLN
1	B	500	ASN
1	B	501	GLN
1	B	543	HIS
1	B	568	ASN

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Mol	Chain	Res	Type
1	B	573	GLN
1	B	575	GLN
1	B	608	HIS
1	B	687	GLN
1	B	710	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	LPC	B	801	-	30,30,30	0.88	1 (3%)	35,37,37	2.38	9 (25%)
2	LPC	A	801	-	30,30,30	0.88	1 (3%)	35,37,37	2.38	9 (25%)

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
2	LPC	B	801	-	-	17/32/32/32	-
2	LPC	A	801	-	-	17/32/32/32	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	LPC	OQ2-CA	4.03	1.45	1.33
2	B	801	LPC	OQ2-CA	4.03	1.45	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	LPC	C0B-N1-C2	-6.50	84.05	109.91
2	B	801	LPC	C0B-N1-C2	-6.50	84.05	109.91
2	A	801	LPC	C0A-N1-C2	-6.33	84.75	109.91
2	B	801	LPC	C0A-N1-C2	-6.33	84.75	109.91
2	A	801	LPC	C0C-N1-C2	-6.31	84.81	109.91
2	B	801	LPC	C0C-N1-C2	-6.31	84.81	109.91
2	A	801	LPC	C0C-N1-C0B	4.00	119.48	108.98
2	B	801	LPC	C0C-N1-C0B	4.00	119.48	108.98
2	A	801	LPC	C0B-N1-C0A	3.95	119.35	108.98
2	B	801	LPC	C0B-N1-C0A	3.95	119.35	108.98
2	A	801	LPC	C0C-N1-C0A	3.62	118.48	108.98
2	B	801	LPC	C0C-N1-C0A	3.62	118.48	108.98
2	A	801	LPC	OQ2-CA-CB	2.47	119.36	111.83
2	B	801	LPC	OQ2-CA-CB	2.47	119.36	111.83
2	A	801	LPC	OQ2-CA-OQ1	-2.03	118.55	123.63
2	B	801	LPC	OQ2-CA-OQ1	-2.03	118.55	123.63
2	A	801	LPC	O5A-P5-O5B	2.02	121.86	112.44
2	B	801	LPC	O5A-P5-O5B	2.02	121.86	112.44

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	LPC	C3-O4-P5-O6
2	A	801	LPC	C7-O6-P5-O4
2	A	801	LPC	C7-O6-P5-O5A
2	A	801	LPC	C7-O6-P5-O5B
2	A	801	LPC	C7-C8-C9-OQ2
2	B	801	LPC	C3-O4-P5-O6
2	B	801	LPC	C7-O6-P5-O4

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Mol	Chain	Res	Type	Atoms
2	B	801	LPC	C7-O6-P5-O5A
2	B	801	LPC	C7-O6-P5-O5B
2	B	801	LPC	C7-C8-C9-OQ2
2	A	801	LPC	CJ-CK-CL-CM
2	B	801	LPC	CJ-CK-CL-CM
2	A	801	LPC	O8-C8-C9-OQ2
2	B	801	LPC	O8-C8-C9-OQ2
2	A	801	LPC	CB-CC-CD-CE
2	B	801	LPC	CB-CC-CD-CE
2	A	801	LPC	CB-CA-OQ2-C9
2	B	801	LPC	CB-CA-OQ2-C9
2	A	801	LPC	CD-CE-CF-CG
2	B	801	LPC	CD-CE-CF-CG
2	A	801	LPC	CG-CH-CI-CJ
2	B	801	LPC	CG-CH-CI-CJ
2	A	801	LPC	CI-CJ-CK-CL
2	B	801	LPC	CI-CJ-CK-CL
2	A	801	LPC	CH-CI-CJ-CK
2	B	801	LPC	CH-CI-CJ-CK
2	A	801	LPC	CE-CF-CG-CH
2	B	801	LPC	CE-CF-CG-CH
2	A	801	LPC	OQ1-CA-OQ2-C9
2	B	801	LPC	OQ1-CA-OQ2-C9
2	A	801	LPC	N1-C2-C3-O4
2	B	801	LPC	N1-C2-C3-O4
2	A	801	LPC	C3-O4-P5-O5B
2	B	801	LPC	C3-O4-P5-O5B

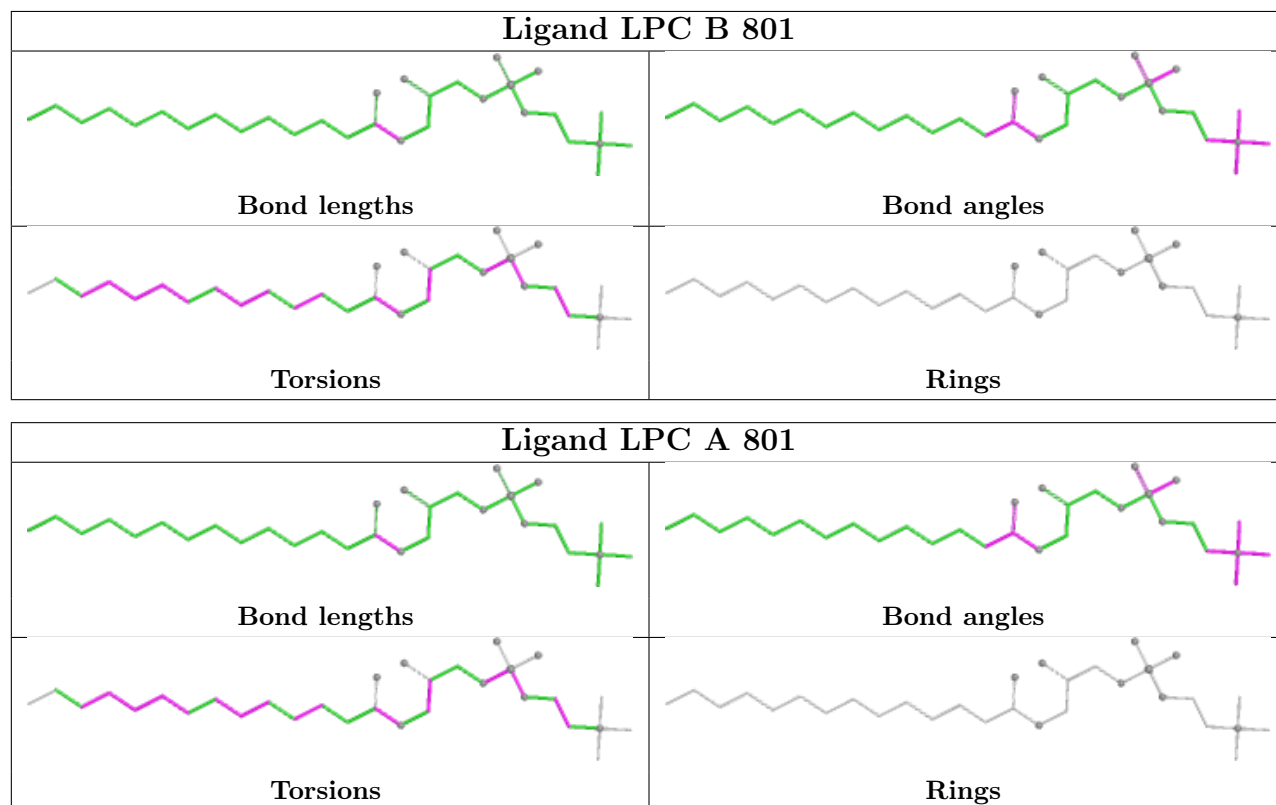
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	LPC	4	0
2	A	801	LPC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

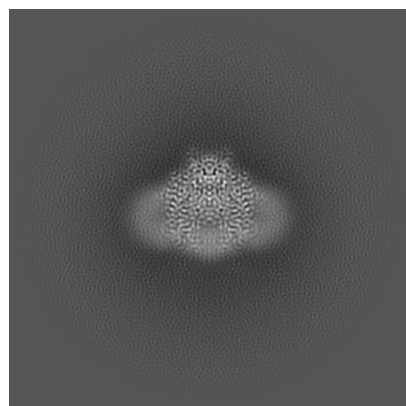
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34209. These allow visual inspection of the internal detail of the map and identification of artifacts.

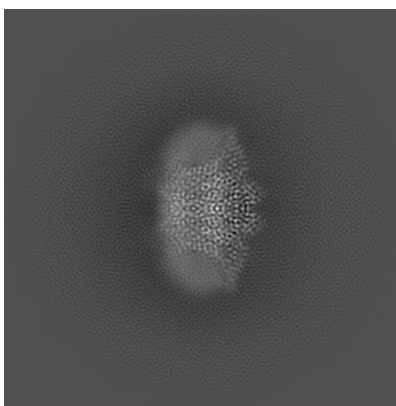
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

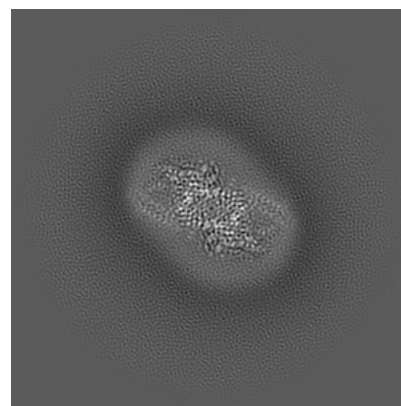
6.1.1 Primary map



X

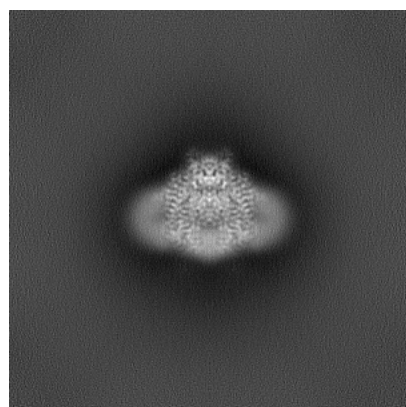


Y

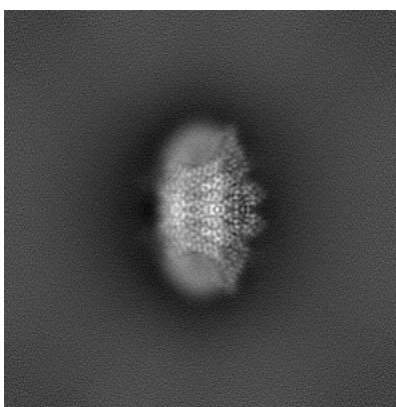


Z

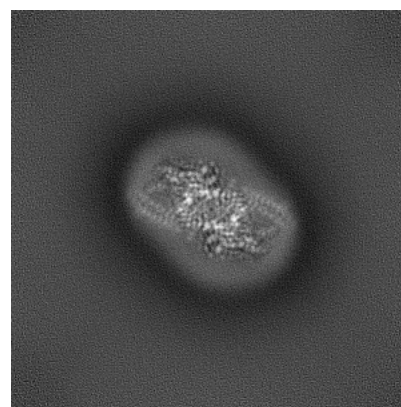
6.1.2 Raw map



X



Y

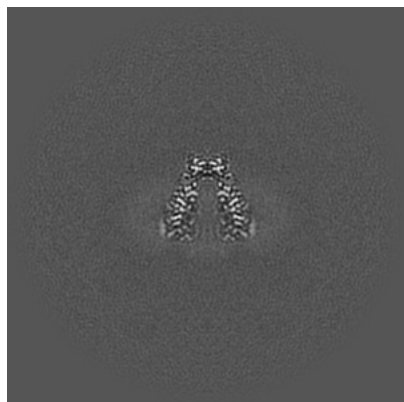


Z

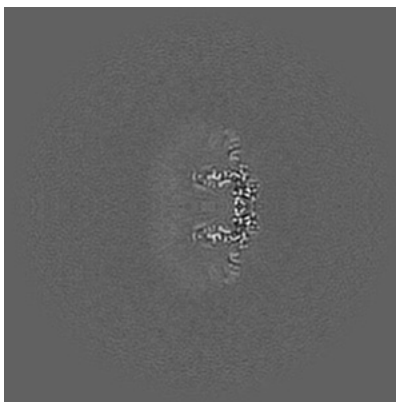
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

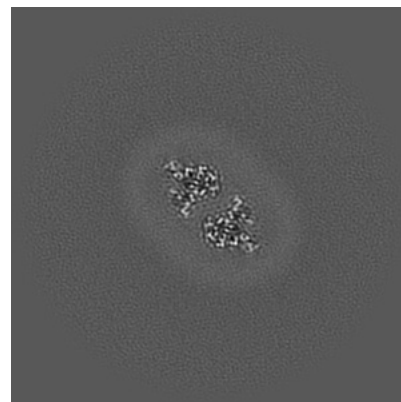
6.2.1 Primary map



X Index: 200

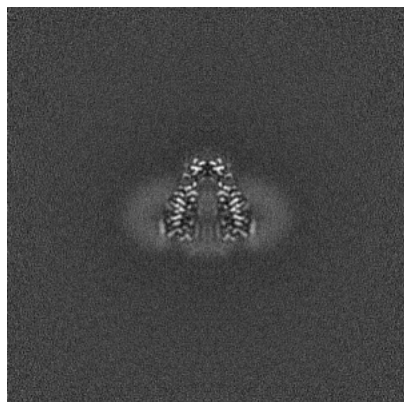


Y Index: 200

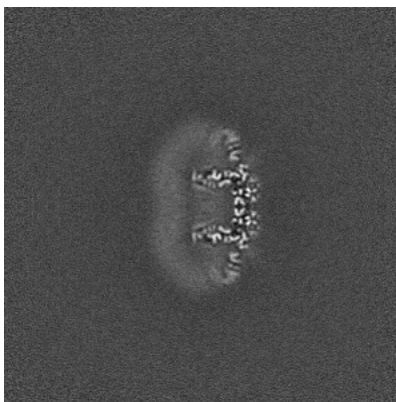


Z Index: 200

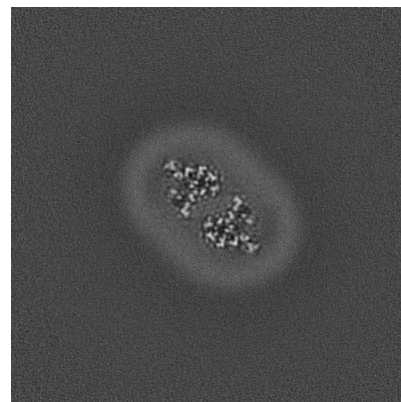
6.2.2 Raw map



X Index: 200



Y Index: 200

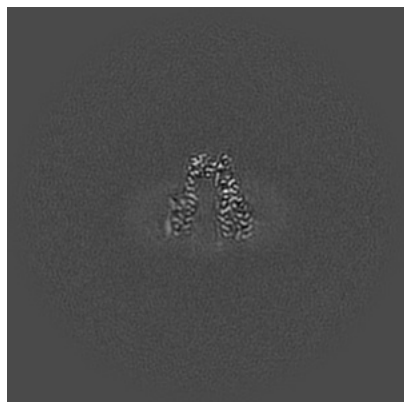


Z Index: 200

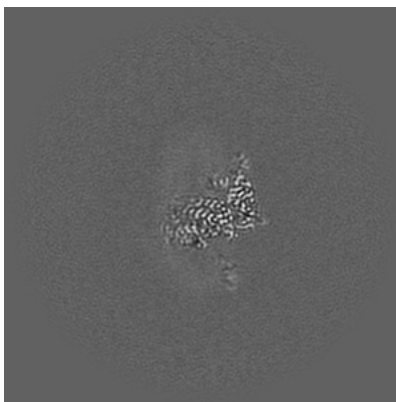
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

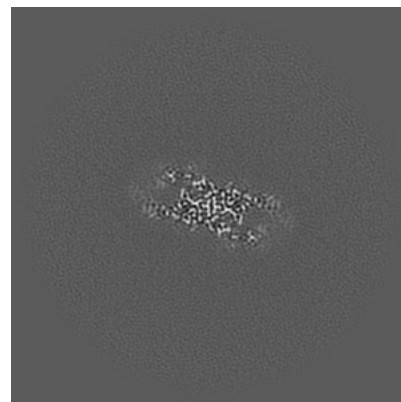
6.3.1 Primary map



X Index: 195

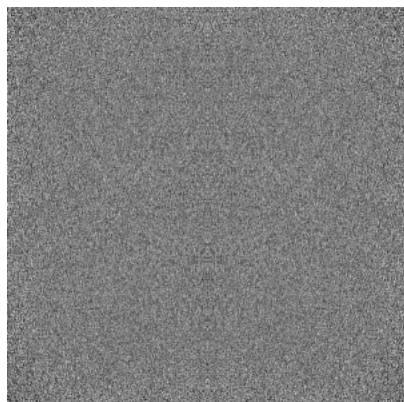


Y Index: 215

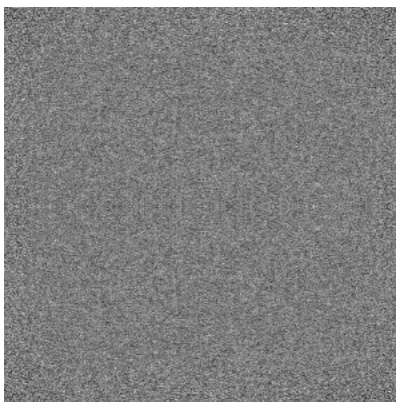


Z Index: 232

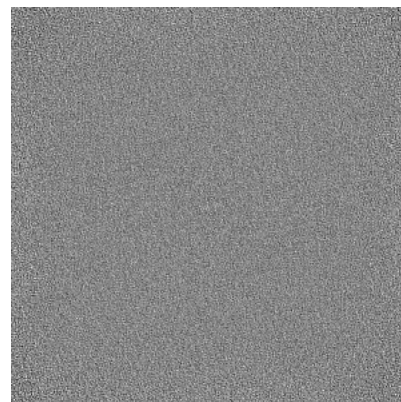
6.3.2 Raw map



X Index: 0



Y Index: 0

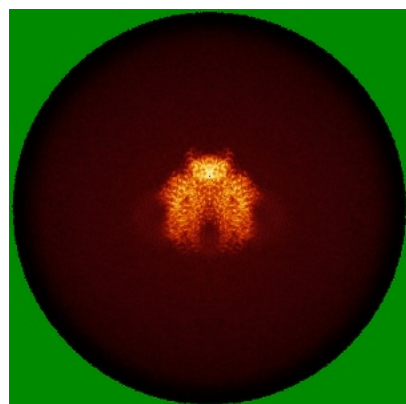


Z Index: 0

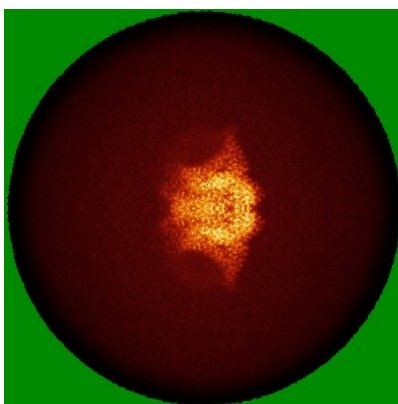
The images above show the largest variance slices of the map in three orthogonal directions.

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

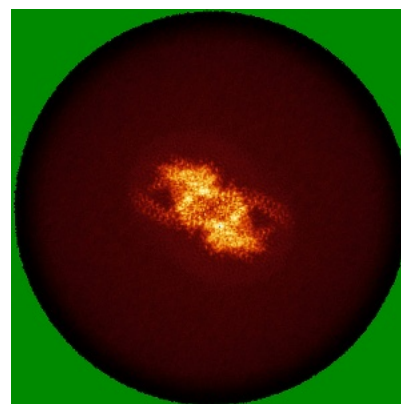
6.4.1 Primary map



X

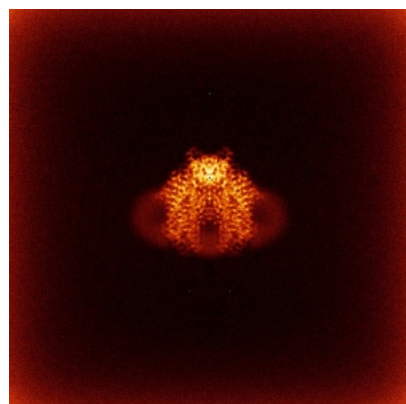


Y

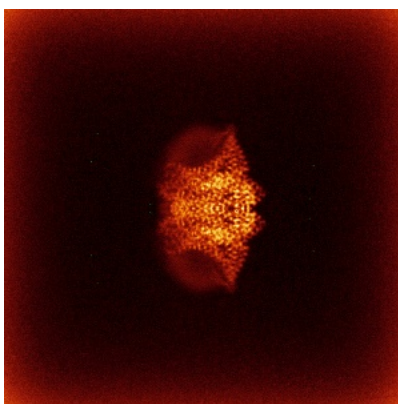


Z

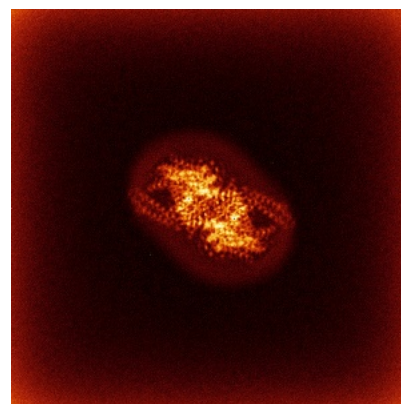
6.4.2 Raw map



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.

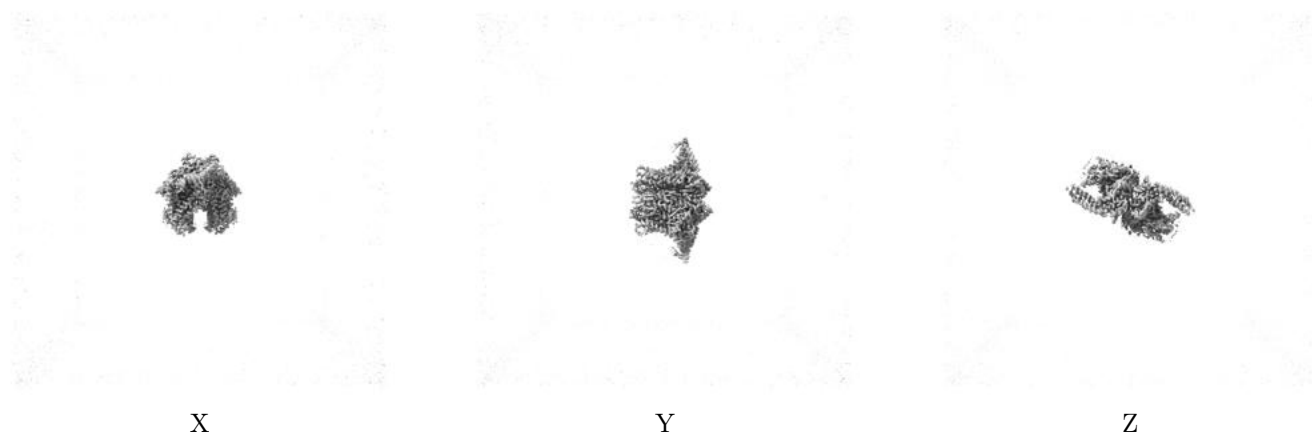
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

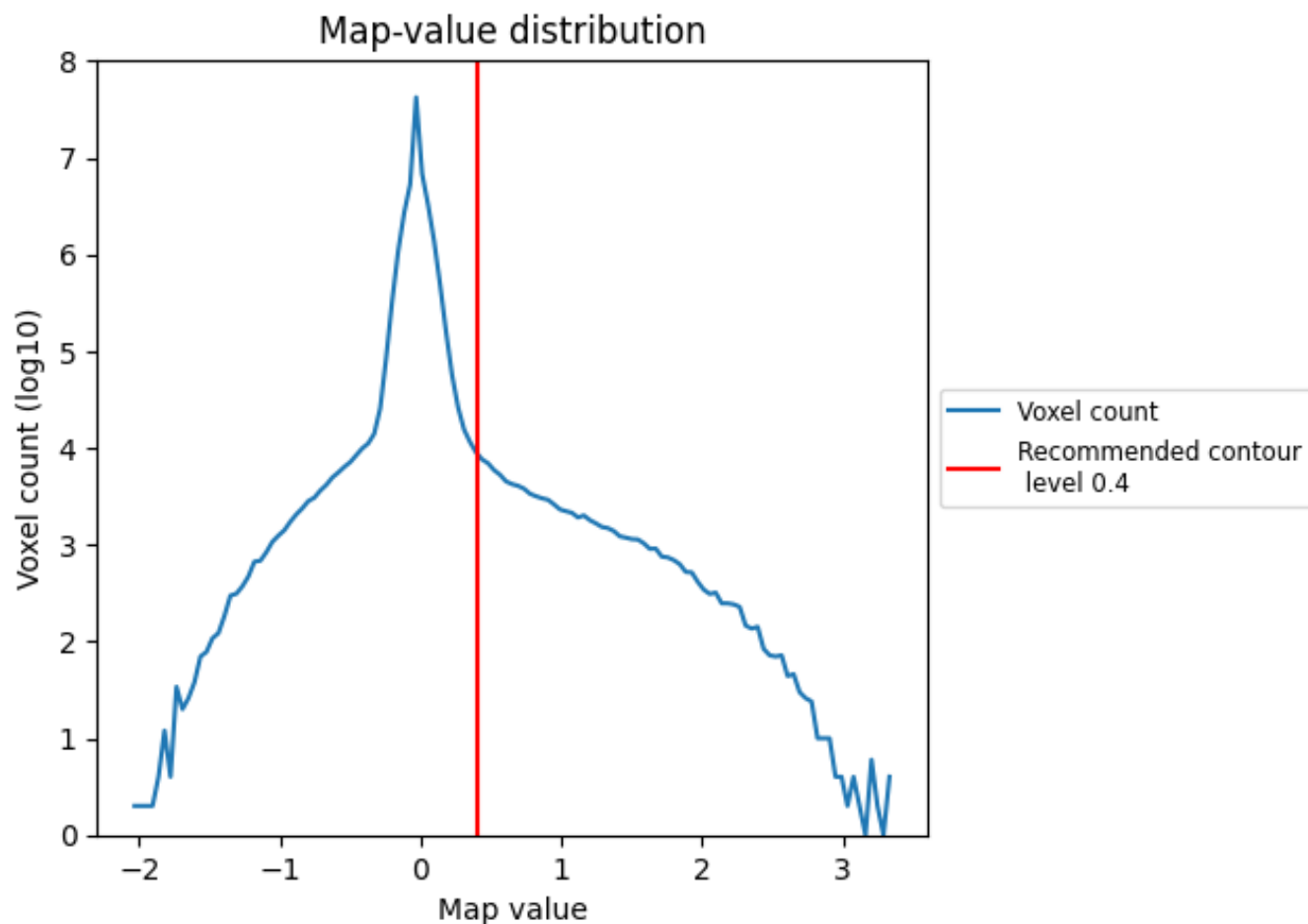
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

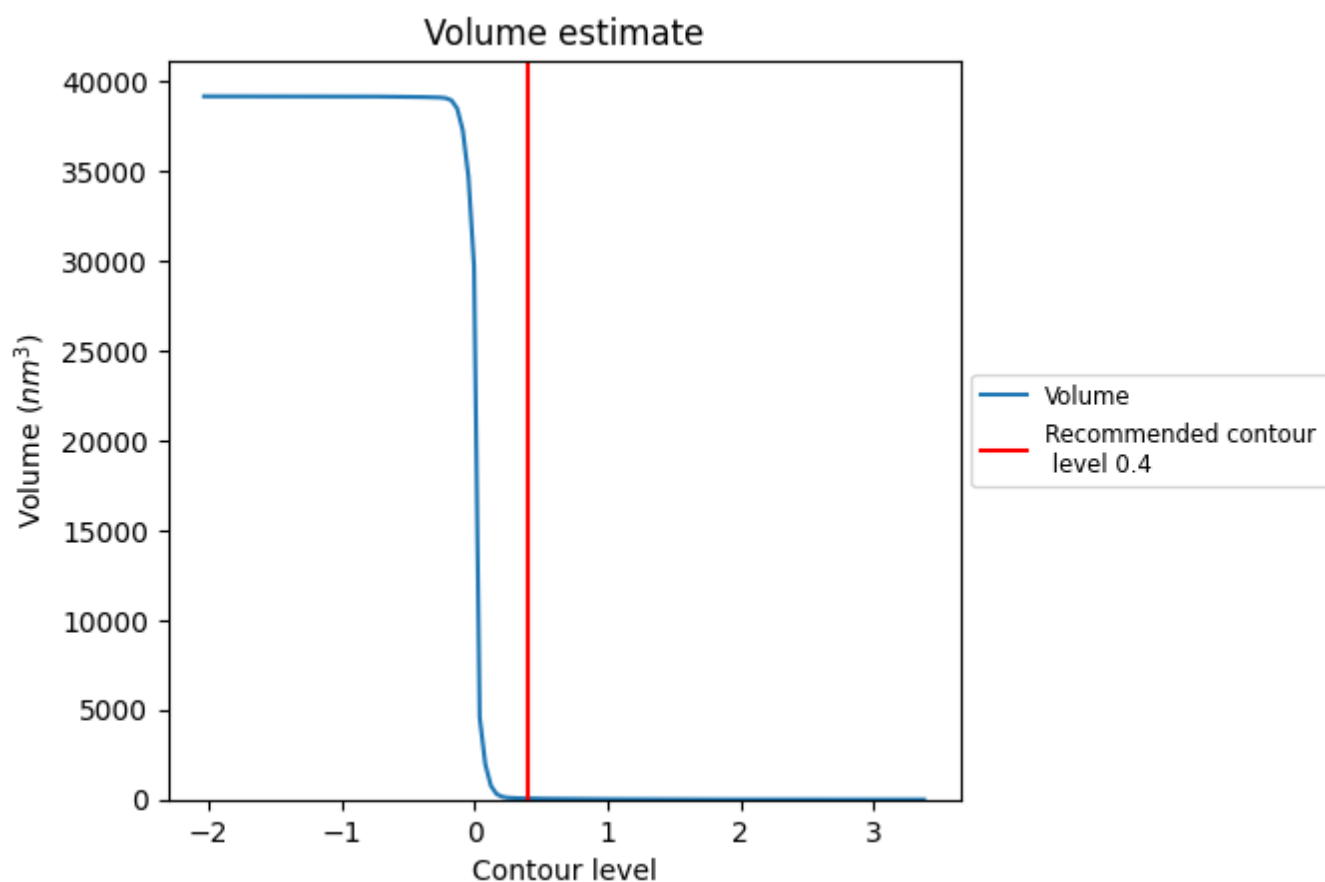
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

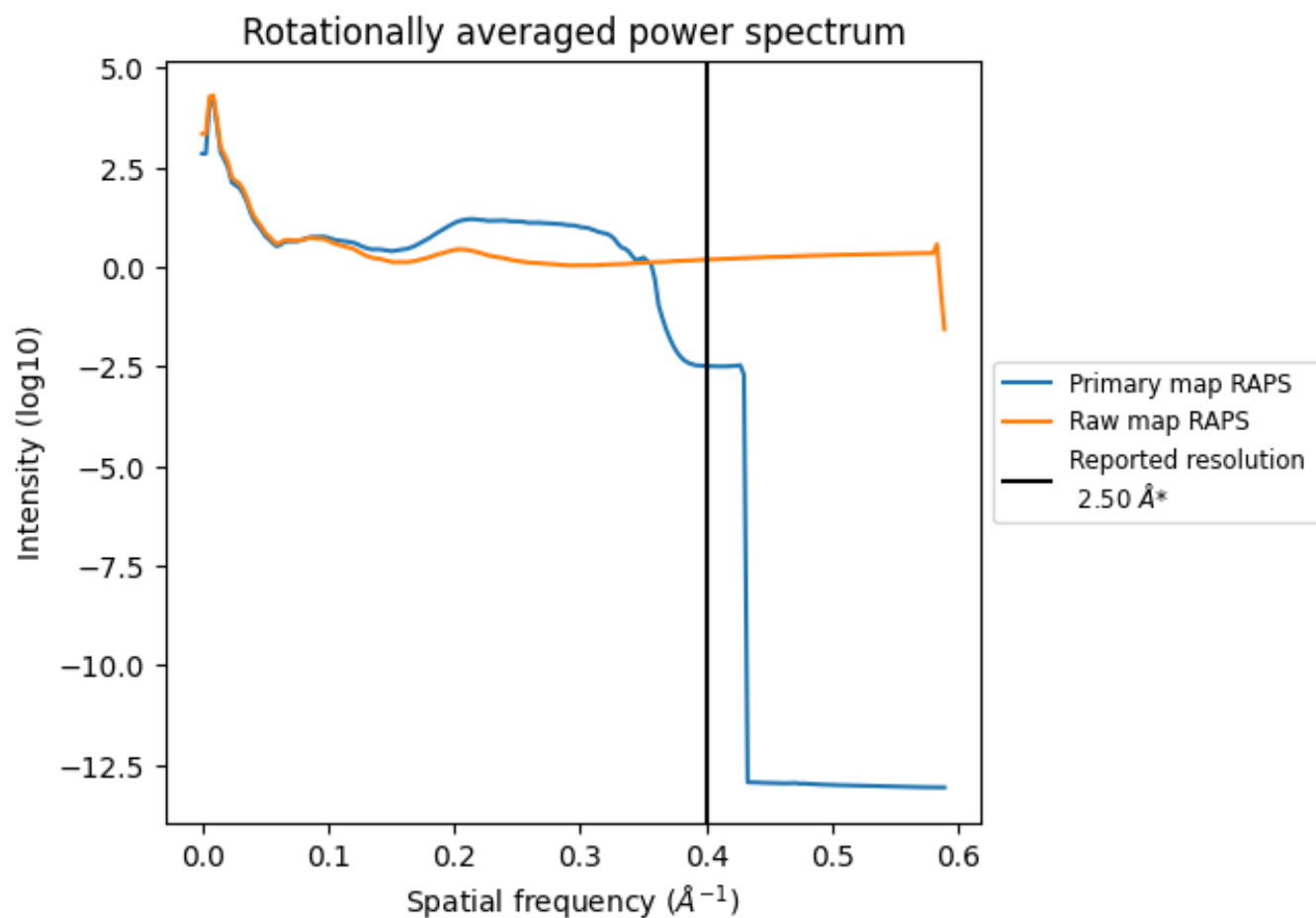
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 55 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 ⓘ

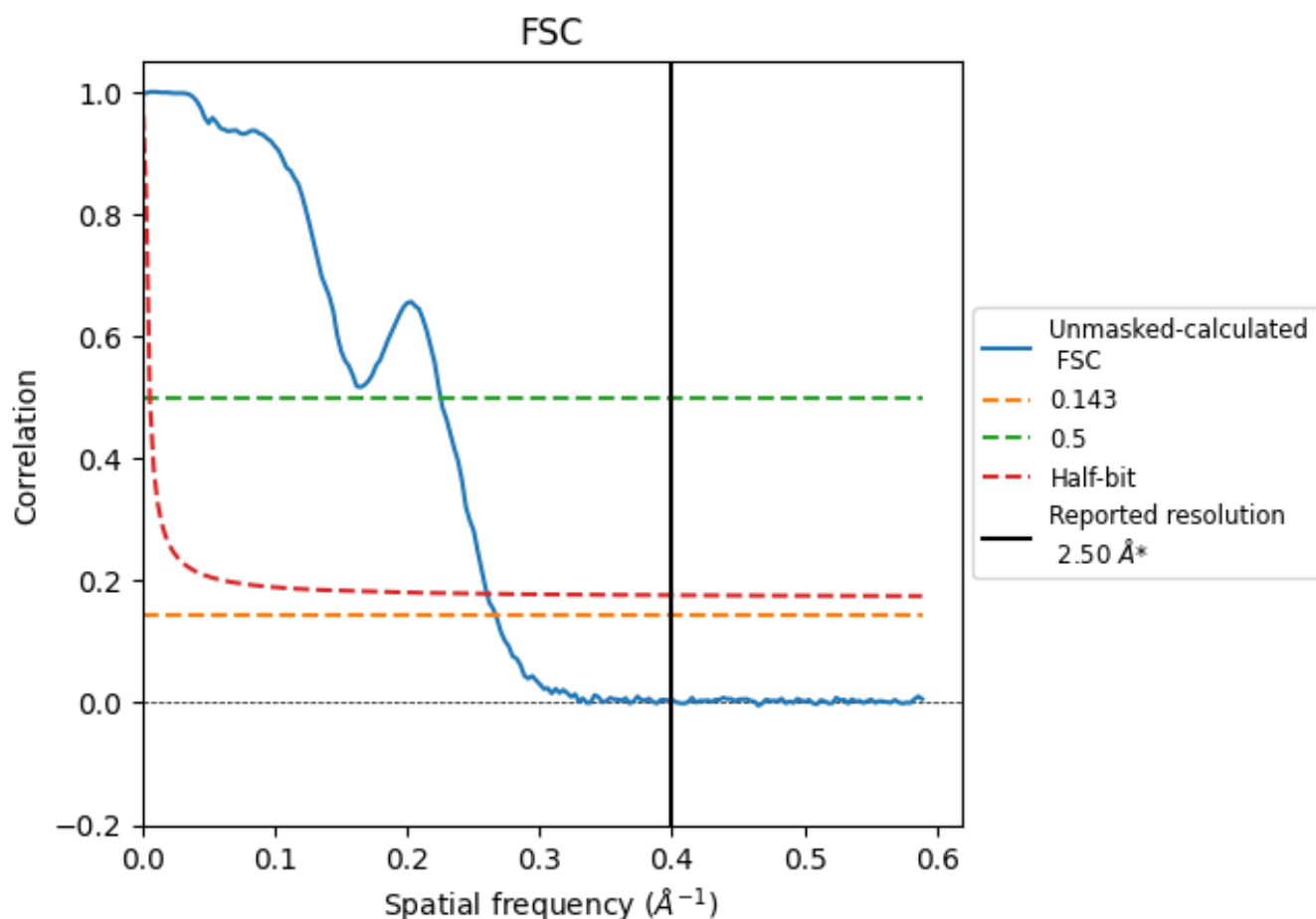


*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.400 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

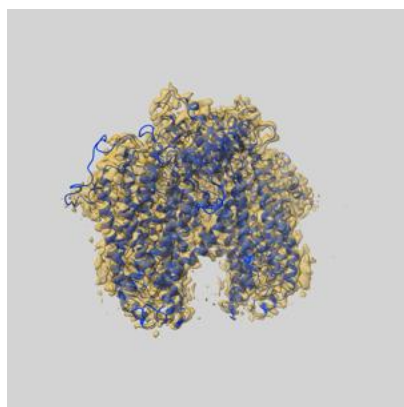
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	4.44	3.84

*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 3.75 differs from the reported value 2.5 by more than 10 %

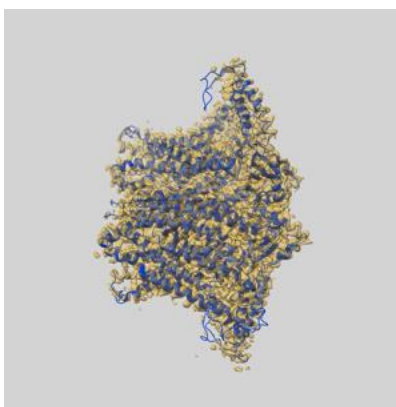
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34209 and PDB model 8GRN. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

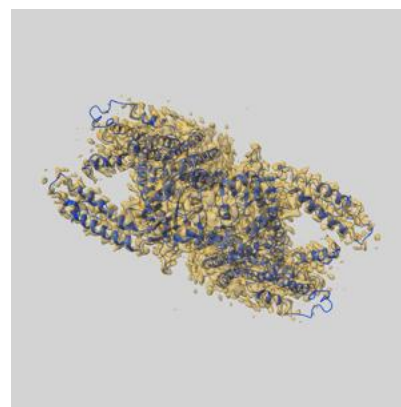
9.1 Map-model overlay [i](#)



X



Y



Z

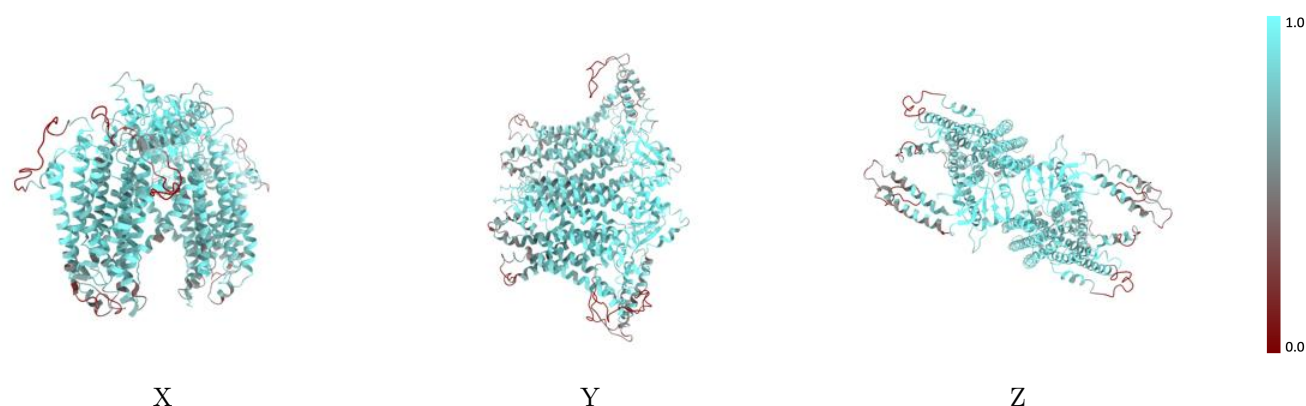
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



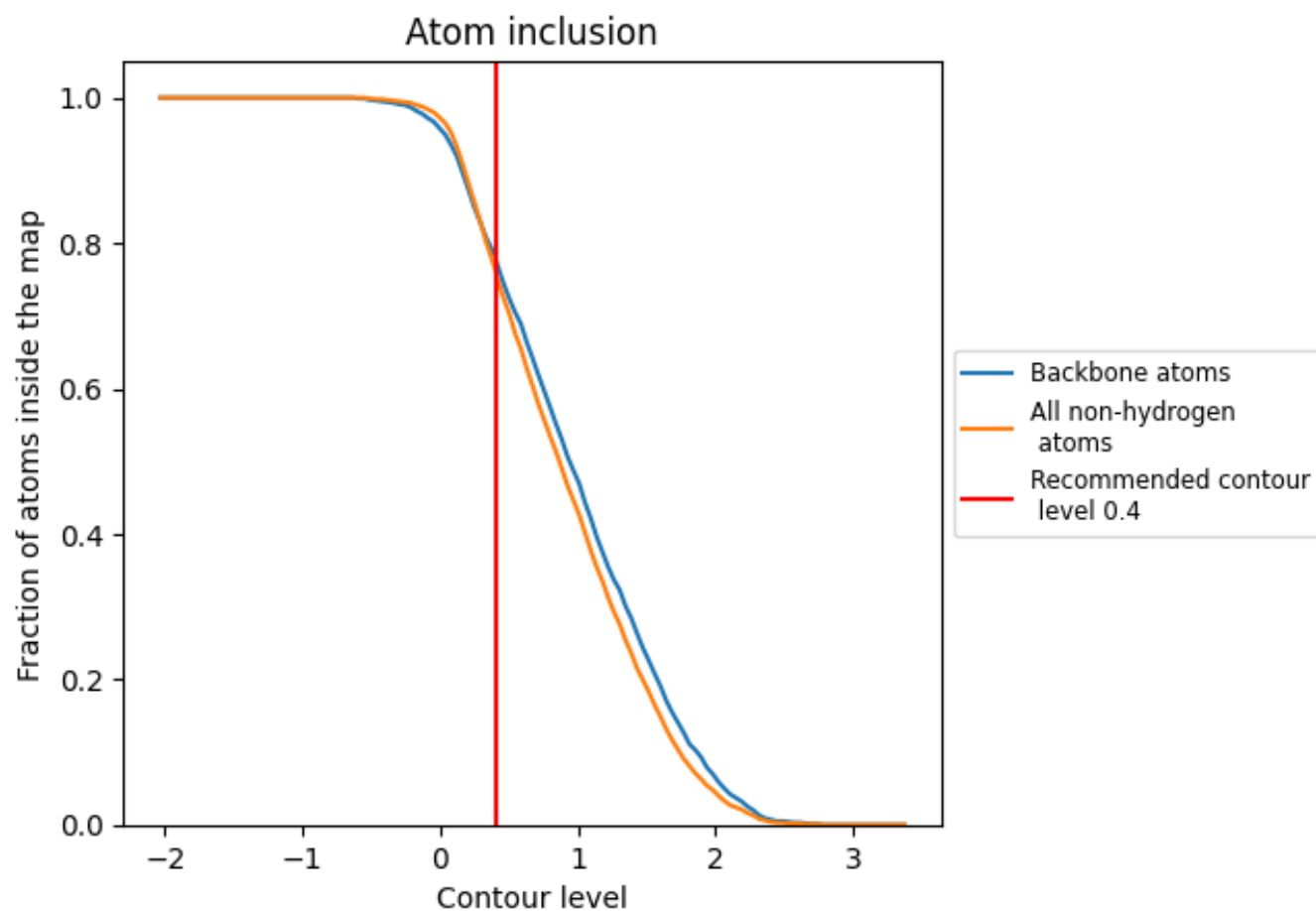
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.5650
A	0.7630	0.5640
B	0.7640	0.5660

