



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:30 PM UTC

PDB ID : 6SUF / pdb_00006suf
EMDB ID : EMD-10313
Title : Structure of Photorhabdus luminescens Tc holotoxin pore
Authors : Roderer, D.; Raunser, S.
Deposited on : 2019-09-13
Resolution : 3.40 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:

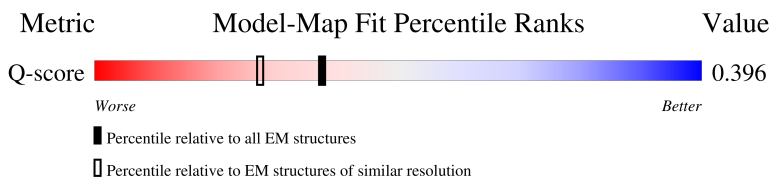
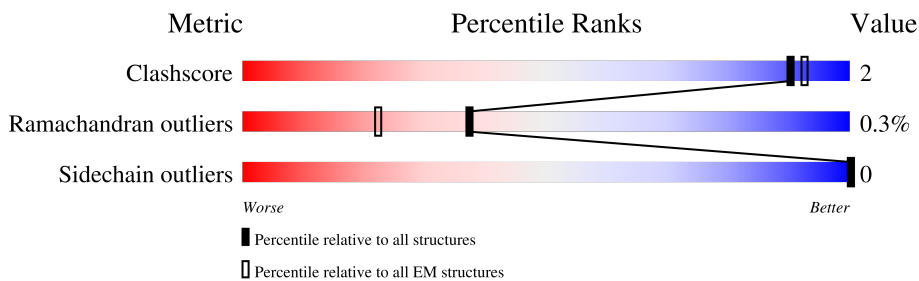
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



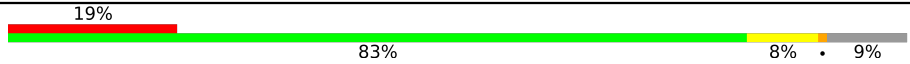

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	2516	
1	B	2516	
1	C	2516	
1	D	2516	

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Mol	Chain	Length	Quality of chain
1	E	2516	 <p>19% 83% 8% 9%</p>
2	F	2439	 <p>5% 80% 8% 12%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 108112 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 TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2292	18197	11530	3083	3525	59	0	0
1	B	2292	18197	11530	3083	3525	59	0	0
1	C	2292	18197	11530	3083	3525	59	0	0
1	D	2292	18197	11530	3083	3525	59	0	0
1	E	2292	18197	11530	3083	3525	59	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	904	GLU	GLN	conflict	UNP Q9RN43
B	904	GLU	GLN	conflict	UNP Q9RN43
C	904	GLU	GLN	conflict	UNP Q9RN43
D	904	GLU	GLN	conflict	UNP Q9RN43
E	904	GLU	GLN	conflict	UNP Q9RN43

- Molecule 2 is a protein called TcdB2,TccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	2147	17127	10729	3040	3323	35	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	543	GLU	ASP	conflict	UNP Q8GF99
F	1475	PRO	-	linker	UNP Q8GF99
F	1476	GLY	-	linker	UNP Q8GF99
F	1477	SER	-	linker	UNP Q8GF99

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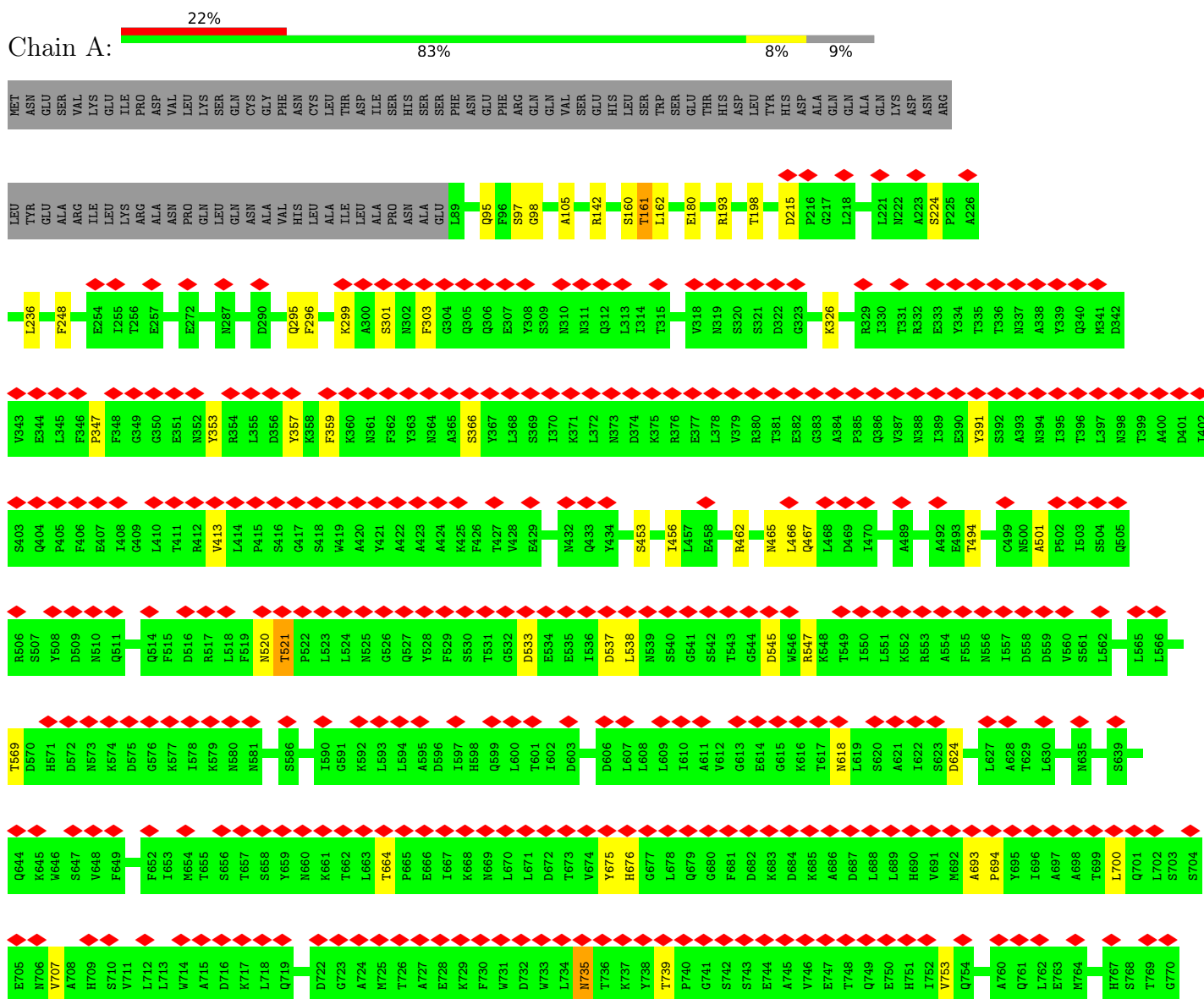
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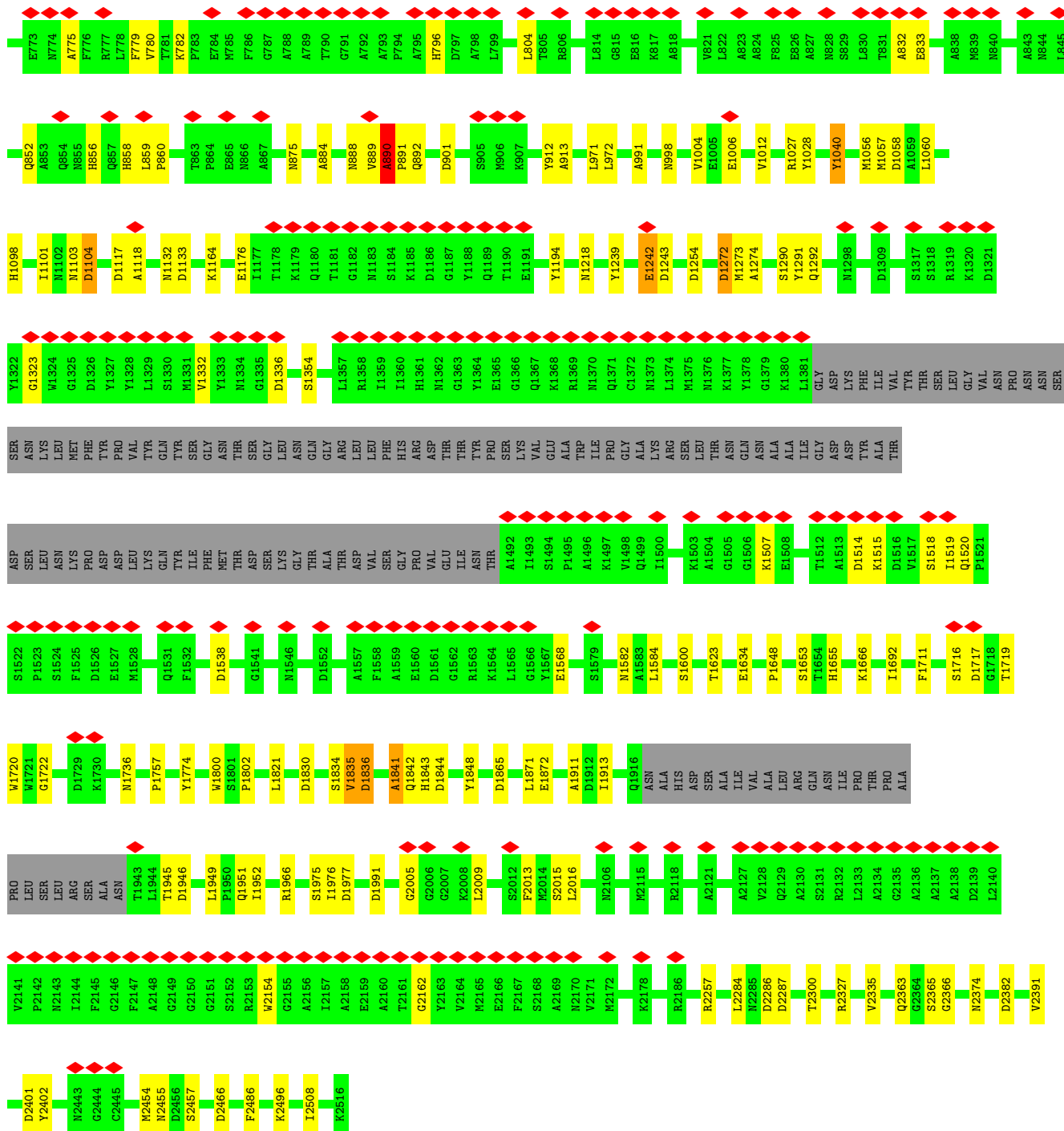
Chain	Residue	Modelled	Actual	Comment	Reference
F	1478	ARG	-	linker	UNP Q8GF99
F	1479	PRO	-	linker	UNP Q8GF99

3 Residue-property plots

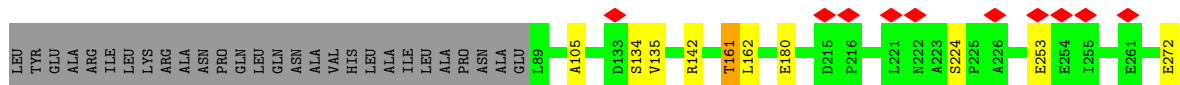
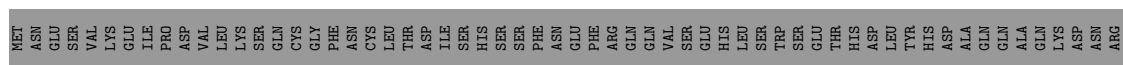
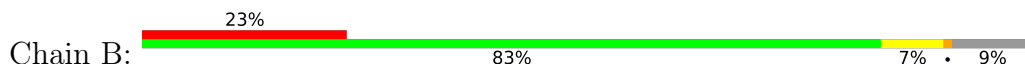
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: TcdA1

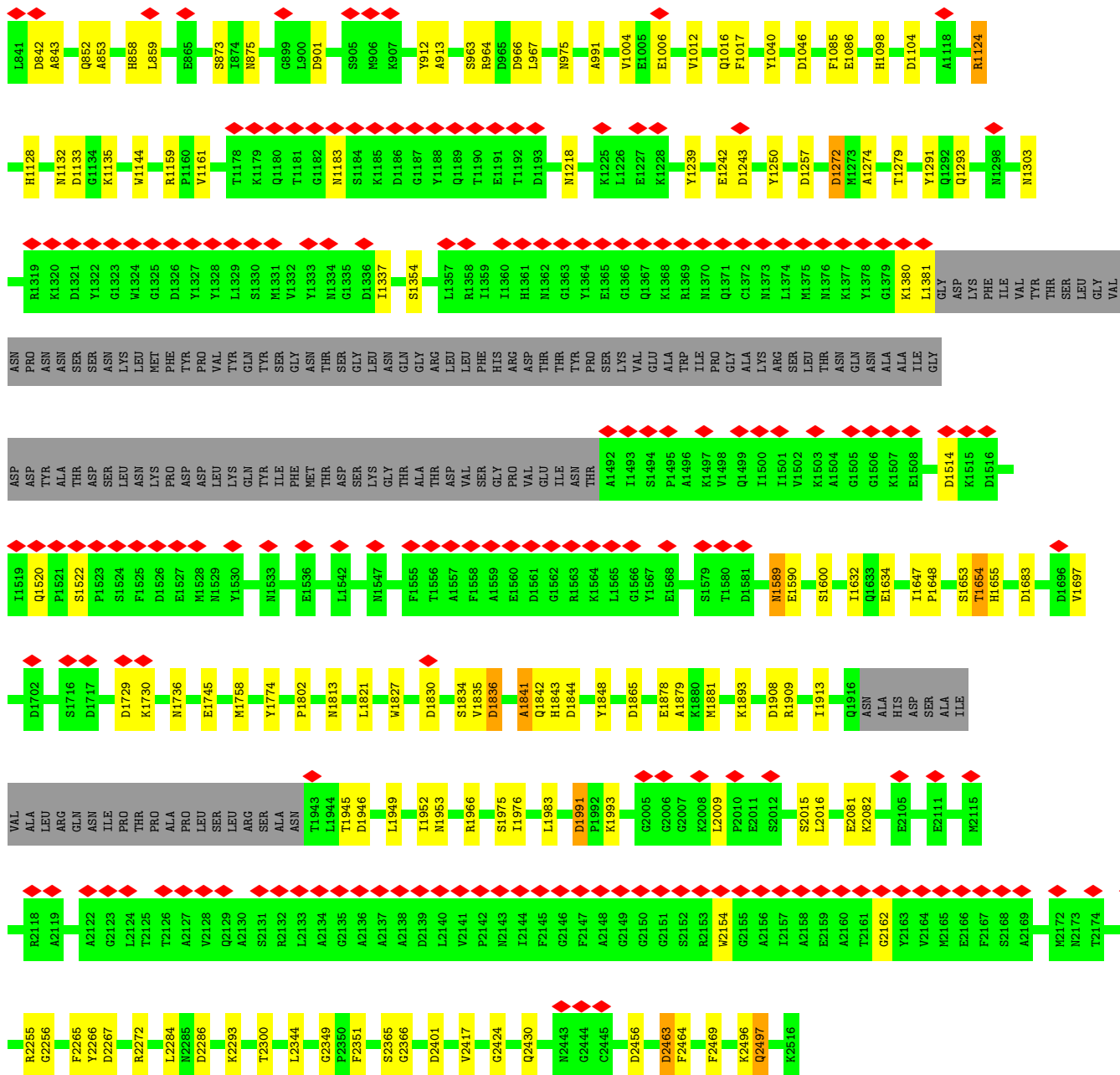




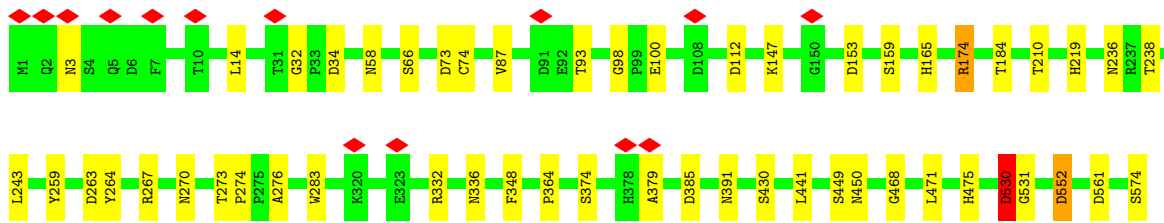
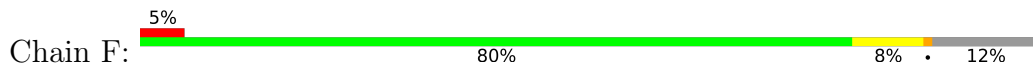
• Molecule 1: TcdA1



PHE	A1492	I330	D469	W546	I610	G680	F740	L801	M906	G1182	K1343	GLY	A1503
MET	I1493	T331	I470	K547	A611	F681	G741	I802	K907	M1183	S1354	THR	A1504
ASP	S1494	R332	I486	K548	V612	D682	S742	R803	E908	S1184	S1354	THR	G1505
SER	S1495	E333	Q486	T949	G616	K683	S743	R806	T909	K1185	L1357	LEU	G1506
LYS	P1496	R334	R487	N950	T617	D684	E744	D809	H935	D1186	R1358	LEU	G1507
GLY	A1497	Y335	Y488	N951	L619	K685	A745	R936	A936	G1187	I1359	ALA	G1508
THR	K1498	T336	I489	K552	L619	A686	V746	D937	Y936	Y1188	H1360	ARG	G1509
ALA	A1499	T337	I490	R553	L619	D687	E747	R812	K962	Q1189	H1361	ARG	G1510
ARG	K1500	G238	I491	R554	S620	L688	T748	A813	S963	S963	H1362	LEU	G1511
LEU	A1501	I239	H491	F555	A621	L689	Q749	L814	R964	F1190	N1362	VAL	G1512
ASP	A1502	I239	H492	F556	A621	L689	Q749	L814	R964	F1191	N1362	VAL	G1513
VAL	A1503	I239	H493	F557	L622	H690	E750	G815	Y968	T1192	G1363	PHE	G1514
PHE	A1504	I239	H494	F558	S623	H691	H751	E816	A991	D1193	G1364	HIS	G1515
HIS	A1505	I239	T494	D558	D624	V691	I752	F817	A991	D1194	Y1366	ARG	G1516
PRO	A1506	I239	A495	D559	L627	A693	V753	K817	V1004	H1202	G1366	ASP	G1517
ASP	A1507	I239	A495	D560	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1518
THR	A1508	I239	A495	V560	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1519
THR	A1509	I239	A495	V561	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1520
THR	A1510	I239	A495	V562	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1521
THR	A1511	I239	A495	V563	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1522
THR	A1512	I239	A495	V564	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1523
THR	A1513	I239	A495	V565	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1524
THR	A1514	I239	A495	V566	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1525
THR	A1515	I239	A495	V567	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1526
THR	A1516	I239	A495	V568	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1527
THR	A1517	I239	A495	V569	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1528
THR	A1518	I239	A495	V570	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1529
THR	A1519	I239	A495	V571	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1530
THR	A1520	I239	A495	V572	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1531
THR	A1521	I239	A495	V573	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1532
THR	A1522	I239	A495	V574	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1533
THR	A1523	I239	A495	V575	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1534
THR	A1524	I239	A495	V576	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1535
THR	A1525	I239	A495	V577	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1536
THR	A1526	I239	A495	V578	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1537
THR	A1527	I239	A495	V579	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1538
THR	A1528	I239	A495	V580	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1539
THR	A1529	I239	A495	V581	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1540
THR	A1530	I239	A495	V582	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1541
THR	A1531	I239	A495	V583	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1542
THR	A1532	I239	A495	V584	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1543
THR	A1533	I239	A495	V585	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1544
THR	A1534	I239	A495	V586	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1545
THR	A1535	I239	A495	V587	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1546
THR	A1536	I239	A495	V588	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1547
THR	A1537	I239	A495	V589	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1548
THR	A1538	I239	A495	V590	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1549
THR	A1539	I239	A495	V591	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1550
THR	A1540	I239	A495	V592	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1551
THR	A1541	I239	A495	V593	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1552
THR	A1542	I239	A495	V594	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1553
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THR	A1545	I239	A495	V597	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1556
THR	A1546	I239	A495	V598	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1557
THR	A1547	I239	A495	V599	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1558
THR	A1548	I239	A495	V600	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1559
THR	A1549	I239	A495	V601	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1560
THR	A1550	I239	A495	V602	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1561
THR	A1551	I239	A495	V603	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1562
THR	A1552	I239	A495	V604	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1563
THR	A1553	I239	A495	V605	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1564
THR	A1554	I239	A495	V606	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1565
THR	A1555	I239	A495	V607	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1566
THR	A1556	I239	A495	V608	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1567
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THR	A1558	I239	A495	V610	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1569
THR	A1559	I239	A495	V611	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1570
THR	A1560	I239	A495	V612	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1571
THR	A1561	I239	A495	V613	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1572
THR	A1562	I239	A495	V614	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1573
THR	A1563	I239	A495	V615	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1574
THR	A1564	I239	A495	V616	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1575
THR	A1565	I239	A495	V617	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1576
THR	A1566	I239	A495	V618	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1577
THR	A1567	I239	A495	V619	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1578
THR	A1568	I239	A495	V620	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1579
THR	A1569	I239	A495	V621	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1580
THR	A1570	I239	A495	V622	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1581
THR	A1571	I239	A495	V623	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1582
THR	A1572	I239	A495	V624	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1583
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THR	A1581	I239	A495	V633	A628	P694	Q754	A818	E1005	H1202	G1366	THR	G1592
THR	A1582	I239	A495	V634	A628	P694	Q754	A818	E				



• Molecule 2: TcdB2,TccC3



A575	D878	D1193	K1304	I1483	S1766	S1990	ILE	SER	THR	ILE
L595	D879	D1201	A1305	D1484	A1757	N1991	ALA	GLY	THR	GLU
Q600	S880	S1224	I1306	T1491	H1766	M1992	ALA	SER	VAL	PHE
T603	T881	S1231	P1307	P1492	D1769	A2007	LYS	ALA	VAL	THR
M606	S904	S1233	L1308	T1493	D1790	S2012	ASN	PRO	THR	THR
D616	R905	P1232	L1309	D1498	R1790	T2013	LYS	LEU	PRO	ALA
G617	Y906	S1234	I1310	H1510	K1795	A2014	VAL	LEU	ASP	ALA
S618	R923	D1285	S1311	R1511	E1818	E2038	ASP	THR	THR	HIS
G619	R927	V1236	L1312	R1514	M1829	E2043	GLY	GLY	GLU	GLY
D622	Y952	K1244	L1313	A1514	P1830	D2044	ALA	ASN	ALA	GLY
R630	Q956	A1255	M1314	D1517	E1831	N2056	LYS	LYS	GLY	GLY
L631	T966	W1259	M1315	R1521	D1837	D2066	ASN	ARG	GLN	ASN
D632	L967	M1260	G1316	I1522	F1860	I2072	PRO	THR	GLN	ASP
I633	P968	P1261	R1317	D1528	S1867	Y2078	VAL	LEU	GLY	THR
V646	D969	V1262	L1318	I1537	Y1872	R2106	ALA	SER	GLN	ILE
V679	W992	S1264	M1319	M1549	D1882	D2107	ASN	ILE	ASN	ASP
G707	H993	Q1265	P1320	K1562	S1894	W2119	ARG	PRO	THR	LEU
T734	N1020	Q1266	D1329	D1560	P1895	Q2120	PRO	ASN	LEU	ASN
L739	V1021	F1268	D1334	T1562	A1896	W2121	VAL	SER	LEU	VAL
H744	K1034	N1269	R1340	T1566	T1897	I2123	ALA	PRO	GLU	PRO
E754	T1055	R1270	D1347	L1566	Q1898	R2124	PRO	THR	PHE	ALA
I755	D1056	L1271	D1370	R1585	M1909	R2125	LYS	THR	ILE	ALA
V761	T1065	E1273	T1390	L1606	E1921	W2126	ASN	THR	GLY	GLY
A770	N1089	Q1274	Q1403	E1619	D1922	A2132	LEU	ASN	LEU	LYS
S789	D1095	W1276	W1410	T1626	D1931	G2133	ALA	LYS	THR	ASN
H790	Q1108	Q1277	D1416	S1673	D1941	T2134	THR	LYS	TRP	PRO
G795	F1113	L1278	D1432	E1681	I1940	I2135	SER	ALA	ALA	PRO
N796	D1119	Y1280	I1438	G1686	S1941	G1942	GLN	THR	LYS	GLY
A797	H126	N1281	T1442	D1687	R1950	K1960	PRO	THR	ARG	THR
P798	Q1136	A1282	A1443	D1688	R1961	D1962	ILE	ALA	ALA	THR
E799	F1137	R1283	F1447	T1710	R1963	K1963	GLY	THR	ALA	THR
R800	W1138	I1284	K1470	D1718	G1964	A1965	ALA	ASN	THR	THR
P802	R1139	E1287	K1471	I1723	A1965	D1968	ASN	PRO	THR	THR
R827	T1146	D1288	VAL	D1729	Y1972	MET	LYS	GLY	THR	THR
V848	Q1147	G1289	K1470	K1751	Q1986	PRO	THR	THR	THR	THR
E853	L1148	R1290	K1471	S1752	A1989	THR	ILE	ILE	ILE	THR
D854	L1148	I1291	ARG			ALA	ALA	ALA	ALA	GLU
D855	D1157	A1295	SER			GLU	GLU	GLU	GLU	ARG
	A1169	W1298	ARG			ARG	ARG	ARG	ARG	
		R1299	PRO							
		W1299	MET							
		V1300	LYS							
		Q1301	LYS							
		S1302	LYS							
		Q1303	LYS							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.16	12/18587 (0.1%)	1.26	118/25239 (0.5%)
1	B	1.15	14/18587 (0.1%)	1.27	129/25239 (0.5%)
1	C	1.16	15/18587 (0.1%)	1.27	133/25239 (0.5%)
1	D	1.15	10/18587 (0.1%)	1.28	130/25239 (0.5%)
1	E	1.15	10/18587 (0.1%)	1.27	129/25239 (0.5%)
2	F	1.17	16/17548 (0.1%)	1.33	164/23921 (0.7%)
All	All	1.16	77/110483 (0.1%)	1.28	803/150116 (0.5%)

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1098	HIS	CB-CG	-11.34	1.34	1.50
1	D	1098	HIS	CB-CG	-9.71	1.36	1.50
1	B	1843	HIS	CB-CG	-9.41	1.36	1.50
1	E	1843	HIS	CB-CG	-9.33	1.37	1.50
2	F	744	HIS	CB-CG	-9.24	1.37	1.50
1	A	1843	HIS	CB-CG	-9.20	1.37	1.50
1	D	1843	HIS	CB-CG	-8.68	1.38	1.50
1	C	1202	HIS	CB-CG	-8.55	1.38	1.50
1	C	1843	HIS	CB-CG	-8.17	1.38	1.50
1	D	1202	HIS	CB-CG	-7.88	1.39	1.50
1	B	1124	ARG	CD-NE	-7.74	1.35	1.46
2	F	993	HIS	CB-CG	-7.34	1.39	1.50
1	A	675	TYR	CB-CG	-7.26	1.35	1.51
1	C	1124	ARG	CD-NE	-7.00	1.36	1.46
2	F	174	ARG	CZ-NH2	-6.92	1.24	1.33
1	A	779	PHE	CB-CG	-6.76	1.35	1.50
1	A	1098	HIS	CB-CG	-6.69	1.40	1.50
2	F	391	ASN	CB-CG	-6.46	1.35	1.52
1	D	1145	HIS	CB-CG	-6.46	1.41	1.50
1	C	1800	TRP	NE1-CE2	-6.46	1.30	1.37
1	C	858	HIS	CB-CG	-6.35	1.41	1.50
1	E	762	LEU	CB-CG	-6.34	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1124	ARG	CD-NE	-6.29	1.37	1.46
1	A	1242	GLU	CG-CD	-6.21	1.36	1.52
1	D	1218	ASN	CB-CG	-6.21	1.36	1.52
1	C	2272	ARG	CD-NE	-6.21	1.37	1.46
1	B	1372	CYS	CB-SG	-6.20	1.60	1.81
1	B	2452	HIS	CB-CG	-6.20	1.41	1.50
2	F	992	TRP	NE1-CE2	-6.18	1.30	1.37
2	F	790	HIS	CB-CG	-6.18	1.41	1.50
1	A	804	LEU	CB-CG	6.16	1.65	1.53
1	C	1163	TYR	CB-CG	-5.97	1.38	1.51
1	B	1218	ASN	CB-CG	-5.89	1.37	1.52
1	B	1128	HIS	CB-CG	-5.88	1.42	1.50
1	C	1242	GLU	CG-CD	-5.84	1.37	1.52
1	E	875	ASN	CB-CG	-5.79	1.37	1.52
1	B	2272	ARG	CD-NE	-5.69	1.38	1.46
1	E	1218	ASN	CB-CG	-5.68	1.37	1.52
1	A	1800	TRP	NE1-CE2	-5.64	1.31	1.37
2	F	165	HIS	CB-CG	-5.63	1.42	1.50
2	F	475	HIS	CB-CG	-5.59	1.42	1.50
2	F	2119	TYR	CB-CG	-5.59	1.39	1.51
1	C	585	LEU	CB-CG	-5.58	1.42	1.53
1	C	2272	ARG	CG-CD	-5.56	1.35	1.52
1	D	1800	TRP	NE1-CE2	-5.52	1.31	1.37
1	D	1587	HIS	CB-CG	-5.43	1.42	1.50
1	C	1169	LEU	CB-CG	-5.41	1.42	1.53
2	F	1511	ARG	CD-NE	-5.40	1.38	1.46
1	B	1587	HIS	CB-CG	-5.39	1.42	1.50
1	C	578	ILE	CB-CG1	5.37	1.64	1.53
1	E	2272	ARG	CG-CD	-5.37	1.36	1.52
1	D	1242	GLU	CG-CD	-5.37	1.38	1.52
2	F	259	TYR	CB-CG	-5.35	1.39	1.51
1	D	858	HIS	CB-CG	-5.33	1.42	1.50
1	B	1848	TYR	CB-CG	-5.30	1.40	1.51
1	A	462	ARG	CD-NE	5.30	1.53	1.46
1	B	1163	TYR	CB-CG	-5.30	1.40	1.51
1	B	359	PHE	CB-CG	-5.28	1.38	1.50
1	A	875	ASN	CB-CG	-5.25	1.39	1.52
1	A	796	HIS	CB-CG	-5.25	1.42	1.50
1	B	1800	TRP	NE1-CE2	-5.24	1.31	1.37
1	C	1765	SER	CA-CB	-5.22	1.44	1.53
2	F	1766	HIS	CB-CG	-5.22	1.42	1.50
1	D	1827	TRP	NE1-CE2	-5.21	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2122	TRP	NE1-CE2	-5.19	1.31	1.37
1	A	1218	ASN	CB-CG	-5.19	1.39	1.52
2	F	2106	ARG	NE-CZ	5.17	1.38	1.33
2	F	219	HIS	CB-CG	-5.17	1.43	1.50
1	E	1881	MET	CG-SD	-5.16	1.67	1.80
2	F	2126	TRP	NE1-CE2	-5.11	1.31	1.37
1	C	1169	LEU	CA-C	-5.08	1.46	1.52
1	A	1568	GLU	CG-CD	-5.08	1.39	1.52
1	E	1128	HIS	CB-CG	-5.07	1.43	1.50
1	B	431	TYR	CB-CG	-5.05	1.40	1.51
1	C	1587	HIS	CB-CG	-5.02	1.43	1.50
1	B	1139	ASN	CB-CG	-5.02	1.39	1.52
1	E	2272	ARG	CD-NE	-5.02	1.39	1.46

All (803) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1843	HIS	N-CA-C	-10.90	100.53	114.04
1	C	1860	LEU	N-CA-C	-10.77	97.17	110.41
1	D	436	PHE	N-CA-C	-10.74	100.72	114.04
1	A	1600	SER	N-CA-C	-10.62	100.38	113.97
1	E	1952	ILE	N-CA-C	10.22	121.04	110.62
1	C	1843	HIS	N-CA-C	-10.04	99.87	112.72
1	D	1952	ILE	N-CA-C	9.79	120.61	110.62
1	D	696	ILE	N-CA-C	-9.68	103.49	111.81
1	A	303	PHE	N-CA-C	-9.65	101.62	113.97
1	C	1952	ILE	N-CA-C	9.61	120.42	110.62
1	C	161	THR	N-CA-C	-9.50	98.73	110.41
1	A	1952	ILE	N-CA-C	9.38	120.19	110.62
1	C	1004	VAL	N-CA-C	-9.38	101.25	110.72
1	B	1354	SER	CA-C-N	9.25	129.19	120.03
1	B	1354	SER	C-N-CA	9.25	129.19	120.03
1	C	619	LEU	N-CA-C	-9.23	102.59	114.04
2	F	603	THR	N-CA-C	-9.23	102.60	114.04
1	C	1841	ALA	N-CA-C	-9.21	98.38	110.53
2	F	1894	SER	CA-C-N	9.12	128.86	119.56
2	F	1894	SER	C-N-CA	9.12	128.86	119.56
1	E	161	THR	N-CA-C	-9.05	99.27	110.41
1	C	1354	SER	CA-C-N	8.99	128.93	120.03
1	C	1354	SER	C-N-CA	8.99	128.93	120.03
1	A	1655	HIS	CA-CB-CG	8.97	122.77	113.80
1	B	1840	VAL	N-CA-C	-8.90	103.18	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	872	THR	N-CA-C	-8.87	98.82	110.53
1	E	1354	SER	CA-C-N	8.82	128.77	120.03
1	E	1354	SER	C-N-CA	8.82	128.77	120.03
1	E	198	THR	N-CA-C	8.82	119.49	108.11
1	D	161	THR	N-CA-C	-8.78	99.61	110.41
1	D	1354	SER	CA-C-N	8.78	128.72	120.03
1	D	1354	SER	C-N-CA	8.78	128.72	120.03
1	B	1006	GLU	N-CA-C	8.77	120.92	111.36
2	F	1829	MET	CA-C-N	8.43	128.57	120.31
2	F	1829	MET	C-N-CA	8.43	128.57	120.31
1	B	782	LYS	CA-C-N	8.37	128.58	119.87
1	B	782	LYS	C-N-CA	8.37	128.58	119.87
1	E	436	PHE	N-CA-C	-8.32	103.64	113.88
1	B	161	THR	N-CA-C	-8.31	99.81	110.53
1	E	1006	GLU	N-CA-C	8.30	121.26	111.71
1	E	2497	GLN	N-CA-C	-8.26	102.99	113.23
1	C	1669	VAL	N-CA-C	-8.24	105.45	113.53
1	B	801	LEU	N-CA-C	-8.22	99.93	110.53
1	C	791	GLY	N-CA-C	-8.13	104.35	114.92
1	E	1844	ASP	CA-C-N	8.10	127.82	119.56
1	E	1844	ASP	C-N-CA	8.10	127.82	119.56
1	E	664	THR	CA-C-N	8.05	128.81	119.47
1	E	664	THR	C-N-CA	8.05	128.81	119.47
1	B	303	PHE	N-CA-C	-8.04	103.67	113.97
1	A	1101	ILE	N-CA-C	-8.04	104.67	113.43
1	A	1006	GLU	N-CA-C	8.04	120.95	111.71
1	A	1802	PRO	N-CA-C	-8.01	98.64	111.38
1	D	1004	VAL	N-CA-C	-8.01	102.27	111.00
1	A	1272	ASP	N-CA-C	-8.00	96.28	108.67
1	D	699	THR	N-CA-C	-7.98	103.75	113.97
1	C	1272	ASP	N-CA-C	-7.97	97.05	109.25
1	E	735	ASN	CA-CB-CG	-7.95	104.65	112.60
1	C	1844	ASP	CA-C-N	7.95	127.66	119.56
1	C	1844	ASP	C-N-CA	7.95	127.66	119.56
1	E	402	ILE	N-CA-C	7.94	118.74	110.72
1	D	340	GLN	N-CA-C	-7.94	102.12	112.68
1	A	1354	SER	CA-C-N	7.92	127.85	119.85
1	A	1354	SER	C-N-CA	7.92	127.85	119.85
1	C	303	PHE	N-CA-C	-7.92	103.11	114.12
1	C	796	HIS	CA-CB-CG	7.91	121.71	113.80
1	E	1830	ASP	CA-C-N	7.88	127.90	119.78
1	E	1830	ASP	C-N-CA	7.88	127.90	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2013	PHE	CA-CB-CG	-7.87	105.93	113.80
1	D	1272	ASP	N-CA-C	-7.86	96.50	108.67
1	B	664	THR	CA-C-N	7.84	128.56	119.47
1	B	664	THR	C-N-CA	7.84	128.56	119.47
1	E	207	VAL	N-CA-C	-7.82	98.76	109.55
1	D	1101	ILE	N-CA-C	-7.81	105.10	111.81
1	D	2009	LEU	CA-C-N	7.76	127.66	120.21
1	D	2009	LEU	C-N-CA	7.76	127.66	120.21
1	D	664	THR	CA-C-N	7.75	128.46	119.47
1	D	664	THR	C-N-CA	7.75	128.46	119.47
1	D	224	SER	CA-C-N	7.74	127.45	119.56
1	D	224	SER	C-N-CA	7.74	127.45	119.56
1	B	1841	ALA	N-CA-C	-7.73	99.60	110.50
1	B	1844	ASP	CA-C-N	7.70	127.37	119.82
1	B	1844	ASP	C-N-CA	7.70	127.37	119.82
1	E	1736	ASN	CA-C-N	7.67	127.33	119.82
1	E	1736	ASN	C-N-CA	7.67	127.33	119.82
2	F	1566	LEU	N-CA-C	-7.65	104.47	113.88
1	A	456	ILE	N-CA-C	-7.65	103.40	110.82
1	D	1841	ALA	N-CA-C	-7.62	101.03	110.41
2	F	58	ASN	N-CA-C	7.61	120.81	108.41
1	A	161	THR	N-CA-C	-7.56	100.82	110.19
1	B	1233	GLY	N-CA-C	-7.54	102.41	112.14
1	D	1233	GLY	N-CA-C	-7.53	102.43	112.14
1	B	348	PHE	CA-CB-CG	7.52	121.32	113.80
1	B	800	SER	N-CA-C	-7.48	103.10	112.90
2	F	1395	LYS	N-CA-C	-7.47	104.69	113.88
1	D	1844	ASP	CA-C-N	7.45	127.15	119.56
1	D	1844	ASP	C-N-CA	7.45	127.15	119.56
1	C	185	VAL	N-CA-C	-7.43	104.61	111.67
2	F	1284	ILE	N-CA-C	-7.42	104.55	111.45
2	F	906	TYR	CA-C-N	7.41	127.58	120.31
2	F	906	TYR	C-N-CA	7.41	127.58	120.31
2	F	2120	GLN	CA-C-N	7.39	127.56	119.87
2	F	2120	GLN	C-N-CA	7.39	127.56	119.87
1	C	2424	GLY	CA-C-N	7.38	127.01	119.56
1	C	2424	GLY	C-N-CA	7.38	127.01	119.56
1	A	142	ARG	CA-C-N	7.36	127.07	119.56
1	A	142	ARG	C-N-CA	7.36	127.07	119.56
1	D	1736	ASN	CA-C-N	7.36	127.04	119.82
1	D	1736	ASN	C-N-CA	7.36	127.04	119.82
1	A	1844	ASP	CA-C-N	7.36	127.07	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1844	ASP	C-N-CA	7.36	127.07	119.56
1	A	1841	ALA	N-CA-C	-7.36	100.82	110.53
1	A	1004	VAL	N-CA-C	-7.36	103.29	110.72
2	F	1410	TRP	N-CA-C	-7.35	104.82	114.31
1	A	2009	LEU	CA-C-N	7.34	127.77	119.92
1	A	2009	LEU	C-N-CA	7.34	127.77	119.92
2	F	100	GLU	N-CA-C	-7.33	97.78	109.59
2	F	552	ASP	CA-C-N	7.28	126.96	119.82
2	F	552	ASP	C-N-CA	7.28	126.96	119.82
1	D	782	LYS	CA-C-N	7.27	126.97	119.56
1	D	782	LYS	C-N-CA	7.27	126.97	119.56
1	A	1648	PRO	CA-C-N	7.26	127.22	120.03
1	A	1648	PRO	C-N-CA	7.26	127.22	120.03
1	C	1736	ASN	CA-C-N	7.25	126.93	119.82
1	C	1736	ASN	C-N-CA	7.25	126.93	119.82
1	B	521	THR	N-CA-C	-7.25	103.83	113.25
1	B	1736	ASN	CA-C-N	7.21	126.89	119.82
1	B	1736	ASN	C-N-CA	7.21	126.89	119.82
2	F	1723	ILE	N-CA-C	7.21	118.28	107.75
1	B	577	LYS	N-CA-C	7.21	119.52	108.42
1	C	359	PHE	CA-CB-CG	7.20	121.00	113.80
2	F	1438	ILE	CB-CA-C	-7.18	104.62	111.44
1	B	479	PHE	CA-CB-CG	7.17	120.97	113.80
1	E	1841	ALA	N-CA-C	-7.15	101.09	110.53
1	B	1004	VAL	N-CA-C	-7.15	103.21	111.00
1	E	2009	LEU	CA-C-N	7.15	127.57	119.92
1	E	2009	LEU	C-N-CA	7.15	127.57	119.92
1	C	776	PHE	CA-CB-CG	7.13	120.94	113.80
1	D	1716	SER	N-CA-C	7.11	121.18	112.23
2	F	98	GLY	CA-C-N	7.08	127.39	119.32
2	F	98	GLY	C-N-CA	7.08	127.39	119.32
1	D	1293	GLN	N-CA-C	-7.07	104.13	114.39
1	D	303	PHE	N-CA-C	-7.05	104.81	113.41
1	B	431	TYR	N-CA-C	7.04	120.66	108.76
1	E	193	ARG	CA-C-N	7.04	126.67	119.56
1	E	193	ARG	C-N-CA	7.04	126.67	119.56
1	D	598	HIS	N-CA-C	-7.02	100.06	110.46
1	A	1655	HIS	CB-CA-C	-7.02	100.42	111.51
1	C	360	LYS	N-CA-C	-7.02	105.25	113.88
2	F	904	SER	N-CA-C	-7.01	101.50	110.19
2	F	1922	ASP	CA-C-N	7.01	126.71	119.56
2	F	1922	ASP	C-N-CA	7.01	126.71	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	32	GLY	CA-C-N	7.01	126.71	119.56
2	F	32	GLY	C-N-CA	7.01	126.71	119.56
2	F	1484	ASP	CA-C-N	6.98	127.13	119.87
2	F	1484	ASP	C-N-CA	6.98	127.13	119.87
1	B	1648	PRO	CA-C-N	6.98	126.94	120.03
1	B	1648	PRO	C-N-CA	6.98	126.94	120.03
1	E	1589	ASN	CA-CB-CG	6.98	119.58	112.60
1	A	224	SER	CA-C-N	6.97	126.67	119.56
1	A	224	SER	C-N-CA	6.97	126.67	119.56
1	A	707	VAL	N-CA-C	-6.96	104.06	110.82
2	F	1137	PHE	N-CA-C	-6.96	99.98	110.28
1	C	1291	TYR	N-CA-C	-6.94	100.71	110.50
1	A	1132	ASN	CA-CB-CG	6.94	119.54	112.60
1	E	2300	THR	N-CA-C	-6.94	100.02	110.28
1	E	2293	LYS	CA-C-N	6.92	127.07	119.87
1	E	2293	LYS	C-N-CA	6.92	127.07	119.87
2	F	739	LEU	CA-C-N	6.92	126.55	119.56
2	F	739	LEU	C-N-CA	6.92	126.55	119.56
1	E	501	ALA	CA-C-N	6.91	126.87	120.03
1	E	501	ALA	C-N-CA	6.91	126.87	120.03
1	E	1654	THR	N-CA-C	-6.90	98.92	109.41
1	A	295	GLN	N-CA-C	-6.88	103.88	112.90
2	F	66	SER	CA-C-N	6.88	126.56	119.82
2	F	66	SER	C-N-CA	6.88	126.56	119.82
1	C	479	PHE	CA-CB-CG	6.87	120.67	113.80
2	F	966	THR	N-CA-C	-6.87	103.31	113.61
1	E	479	PHE	CA-CB-CG	6.85	120.65	113.80
2	F	1113	PHE	CA-C-N	6.84	126.81	120.03
2	F	1113	PHE	C-N-CA	6.84	126.81	120.03
2	F	374	SER	CA-C-N	6.83	126.53	119.56
2	F	374	SER	C-N-CA	6.83	126.53	119.56
1	A	1736	ASN	CA-C-N	6.83	126.51	119.82
1	A	1736	ASN	C-N-CA	6.83	126.51	119.82
1	B	890	ALA	CA-C-N	6.82	128.36	119.84
1	B	890	ALA	C-N-CA	6.82	128.36	119.84
2	F	1224	SER	CA-C-N	6.81	126.50	119.56
2	F	1224	SER	C-N-CA	6.81	126.50	119.56
2	F	1510	HIS	N-CA-C	6.80	119.50	108.34
1	A	780	VAL	N-CA-C	-6.79	105.97	111.81
1	C	2293	LYS	CA-C-N	6.79	126.93	119.87
1	C	2293	LYS	C-N-CA	6.79	126.93	119.87
1	B	2293	LYS	CA-C-N	6.78	126.41	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2293	LYS	C-N-CA	6.78	126.41	119.56
1	D	890	ALA	CA-C-N	6.75	128.27	119.84
1	D	890	ALA	C-N-CA	6.75	128.27	119.84
1	B	2424	GLY	CA-C-N	6.70	128.21	119.84
1	B	2424	GLY	C-N-CA	6.70	128.21	119.84
1	C	2009	LEU	CA-C-N	6.69	126.65	120.03
1	C	2009	LEU	C-N-CA	6.69	126.65	120.03
1	B	990	ILE	N-CA-C	-6.69	95.43	109.34
1	D	193	ARG	CA-C-N	6.69	126.31	119.56
1	D	193	ARG	C-N-CA	6.69	126.31	119.56
1	D	431	TYR	N-CA-C	6.69	119.80	108.90
1	D	572	ASP	N-CA-C	-6.67	104.16	112.90
1	D	105	ALA	CA-C-N	6.66	126.34	119.82
1	D	105	ALA	C-N-CA	6.66	126.34	119.82
1	E	1040	TYR	CA-C-N	6.64	126.27	119.56
1	E	1040	TYR	C-N-CA	6.64	126.27	119.56
1	A	359	PHE	CA-CB-CG	-6.63	107.17	113.80
1	C	224	SER	CA-C-N	6.62	126.32	119.56
1	C	224	SER	C-N-CA	6.62	126.32	119.56
2	F	1972	TYR	N-CA-C	6.62	119.78	109.52
1	A	2013	PHE	CA-CB-CG	-6.62	107.18	113.80
1	A	1911	ALA	CA-C-N	6.60	131.42	122.84
1	A	1911	ALA	C-N-CA	6.60	131.42	122.84
1	C	889	VAL	N-CA-C	6.59	119.49	113.10
1	A	501	ALA	CA-C-N	6.59	126.55	120.03
1	A	501	ALA	C-N-CA	6.59	126.55	120.03
1	E	414	LEU	CA-C-N	6.58	126.28	119.56
1	E	414	LEU	C-N-CA	6.58	126.28	119.56
1	C	742	SER	N-CA-C	6.58	119.18	108.26
1	C	664	THR	CA-C-N	6.57	126.26	119.56
1	C	664	THR	C-N-CA	6.57	126.26	119.56
1	D	414	LEU	CA-C-N	6.56	126.69	119.87
1	D	414	LEU	C-N-CA	6.56	126.69	119.87
1	C	1648	PRO	CA-C-N	6.56	126.47	119.85
1	C	1648	PRO	C-N-CA	6.56	126.47	119.85
2	F	595	LEU	CA-C-N	6.53	126.49	120.03
2	F	595	LEU	C-N-CA	6.53	126.49	120.03
1	A	236	LEU	N-CA-C	-6.52	105.46	113.41
1	B	2300	THR	N-CA-C	-6.51	100.64	110.28
1	A	1835	VAL	N-CA-C	-6.50	106.90	113.47
1	A	700	LEU	N-CA-C	-6.50	101.17	110.59
1	E	521	THR	N-CA-C	-6.50	103.92	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	754	GLU	N-CA-C	-6.49	102.16	110.53
1	E	1648	PRO	CA-C-N	6.48	126.40	119.85
1	E	1648	PRO	C-N-CA	6.48	126.40	119.85
1	D	1692	ILE	CA-C-N	6.48	126.40	119.85
1	D	1692	ILE	C-N-CA	6.48	126.40	119.85
2	F	14	LEU	CA-C-N	6.47	126.44	120.03
2	F	14	LEU	C-N-CA	6.47	126.44	120.03
1	C	1335	GLY	N-CA-C	-6.46	103.36	112.60
1	C	414	LEU	CA-C-N	6.46	126.15	119.56
1	C	414	LEU	C-N-CA	6.46	126.15	119.56
2	F	364	PRO	CA-C-N	6.46	126.42	120.03
2	F	364	PRO	C-N-CA	6.46	126.42	120.03
1	C	105	ALA	CA-C-N	6.42	126.11	119.56
1	C	105	ALA	C-N-CA	6.42	126.11	119.56
1	B	1802	PRO	N-CA-C	-6.41	101.01	111.21
1	B	402	ILE	N-CA-C	6.40	119.04	112.90
1	A	521	THR	N-CA-C	-6.40	104.05	112.75
1	B	2374	ASN	N-CA-C	6.40	117.02	108.38
1	B	1835	VAL	N-CA-C	-6.39	107.01	113.47
1	E	1893	LYS	CA-C-N	6.39	126.31	119.85
1	E	1893	LYS	C-N-CA	6.39	126.31	119.85
2	F	967	LEU	CA-C-N	6.39	126.36	119.78
2	F	967	LEU	C-N-CA	6.39	126.36	119.78
1	B	105	ALA	CA-C-N	6.38	126.07	119.56
1	B	105	ALA	C-N-CA	6.38	126.07	119.56
1	C	1239	TYR	N-CA-C	-6.36	100.86	110.28
1	D	1648	PRO	CA-C-N	6.36	126.33	119.78
1	D	1648	PRO	C-N-CA	6.36	126.33	119.78
1	B	224	SER	CA-C-N	6.36	126.84	119.47
1	B	224	SER	C-N-CA	6.36	126.84	119.47
2	F	1491	THR	CA-C-N	6.35	126.53	120.31
2	F	1491	THR	C-N-CA	6.35	126.53	120.31
1	C	1101	ILE	N-CA-C	-6.34	106.36	111.81
2	F	1432	ASP	CA-C-N	6.33	126.46	119.87
2	F	1432	ASP	C-N-CA	6.33	126.46	119.87
2	F	159	SER	CA-C-N	6.33	126.02	119.56
2	F	159	SER	C-N-CA	6.33	126.02	119.56
1	C	750	GLU	N-CA-C	-6.31	104.50	111.82
1	A	901	ASP	N-CA-C	6.30	120.19	110.42
1	E	2162	GLY	N-CA-C	-6.30	105.20	112.50
2	F	952	TYR	CA-C-N	6.29	126.20	119.85
2	F	952	TYR	C-N-CA	6.29	126.20	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ARG	CA-C-N	6.29	125.97	119.56
1	D	142	ARG	C-N-CA	6.29	125.97	119.56
2	F	927	ASP	CA-CB-CG	6.28	118.88	112.60
1	E	224	SER	CA-C-N	6.27	125.95	119.56
1	E	224	SER	C-N-CA	6.27	125.95	119.56
1	E	1004	VAL	N-CA-C	-6.27	104.17	111.00
2	F	1020	ASN	CA-C-N	-6.25	118.35	122.60
2	F	1020	ASN	C-N-CA	-6.25	118.35	122.60
2	F	606	ASN	CA-C-N	6.24	127.64	119.84
2	F	606	ASN	C-N-CA	6.24	127.64	119.84
1	A	782	LYS	CA-C-N	6.23	126.69	119.47
1	A	782	LYS	C-N-CA	6.23	126.69	119.47
2	F	2147	ASN	CA-C-N	6.23	126.34	119.87
2	F	2147	ASN	C-N-CA	6.23	126.34	119.87
1	C	2486	PHE	CA-C-N	6.21	126.18	120.03
1	C	2486	PHE	C-N-CA	6.21	126.18	120.03
1	C	773	GLU	N-CA-C	6.21	118.05	111.28
2	F	1136	GLN	N-CA-C	-6.21	101.33	110.52
1	A	753	VAL	CB-CA-C	-6.20	103.76	112.14
2	F	1790	ARG	CA-C-N	6.20	125.82	119.56
2	F	1790	ARG	C-N-CA	6.20	125.82	119.56
1	C	542	SER	N-CA-C	6.20	116.26	108.45
1	D	2402	TYR	CA-C-N	6.20	126.17	119.78
1	D	2402	TYR	C-N-CA	6.20	126.17	119.78
2	F	927	ASP	CB-CA-C	-6.20	104.89	110.71
1	E	1600	SER	N-CA-C	-6.19	105.48	113.16
2	F	430	SER	N-CA-C	-6.19	102.80	110.41
1	C	142	ARG	CA-C-N	6.18	125.87	119.56
1	C	142	ARG	C-N-CA	6.18	125.87	119.56
2	F	2072	ILE	N-CA-C	-6.18	105.80	111.67
2	F	600	GLN	CA-C-N	6.17	125.87	119.82
2	F	600	GLN	C-N-CA	6.17	125.87	119.82
1	A	890	ALA	CA-C-N	6.17	127.55	119.84
1	A	890	ALA	C-N-CA	6.17	127.55	119.84
1	D	2335	VAL	N-CA-C	6.17	116.75	107.75
1	E	873	SER	N-CA-C	-6.15	104.65	111.36
1	E	1653	SER	N-CA-C	-6.15	104.84	112.90
1	E	335	THR	N-CA-C	-6.14	106.11	113.97
1	E	2349	GLY	CA-C-N	6.13	126.05	119.85
1	E	2349	GLY	C-N-CA	6.13	126.05	119.85
1	D	2300	THR	N-CA-C	-6.13	100.51	110.20
1	B	1949	LEU	CA-C-N	6.13	126.10	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1949	LEU	C-N-CA	6.13	126.10	120.21
1	D	1949	LEU	CA-C-N	6.12	126.09	120.03
1	D	1949	LEU	C-N-CA	6.12	126.09	120.03
1	D	1525	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	384	ALA	CA-C-N	6.11	126.08	120.03
1	B	384	ALA	C-N-CA	6.11	126.08	120.03
2	F	274	PRO	CA-C-N	6.11	126.02	119.85
2	F	274	PRO	C-N-CA	6.11	126.02	119.85
1	E	1132	ASN	CA-CB-CG	6.10	118.70	112.60
1	E	966	ASP	N-CA-C	-6.09	104.92	112.90
1	C	1653	SER	N-CA-C	-6.09	103.98	112.45
1	C	1040	TYR	CA-C-N	6.08	125.70	119.56
1	C	1040	TYR	C-N-CA	6.08	125.70	119.56
2	F	632	ASP	CA-CB-CG	6.08	118.67	112.60
1	B	1972	HIS	CA-CB-CG	-6.06	107.74	113.80
1	B	421	TYR	N-CA-C	6.05	118.27	109.07
1	A	1653	SER	N-CA-C	-6.04	104.77	111.36
1	A	453	SER	N-CA-C	-6.04	101.97	109.64
1	B	2402	TYR	CA-C-N	6.04	125.95	119.85
1	B	2402	TYR	C-N-CA	6.04	125.95	119.85
1	E	1983	LEU	CA-C-N	6.02	125.99	120.03
1	E	1983	LEU	C-N-CA	6.02	125.99	120.03
1	D	1291	TYR	N-CA-C	-6.00	102.75	110.19
1	C	1233	GLY	N-CA-C	-6.00	104.41	112.14
1	E	1279	THR	N-CA-C	-5.99	101.40	110.39
1	D	2012	SER	CA-C-N	-5.99	113.04	121.72
1	D	2012	SER	C-N-CA	-5.99	113.04	121.72
1	A	1584	LEU	N-CA-C	-5.98	101.63	110.48
2	F	1860	PHE	CA-C-N	5.98	125.95	120.03
2	F	1860	PHE	C-N-CA	5.98	125.95	120.03
1	E	140	THR	N-CA-C	-5.97	105.66	113.12
1	E	619	LEU	N-CA-C	-5.96	106.14	113.41
1	C	1731	GLY	CA-C-N	-5.96	114.92	122.37
1	C	1731	GLY	C-N-CA	-5.96	114.92	122.37
1	D	2424	GLY	CA-C-N	5.94	125.62	119.56
1	D	2424	GLY	C-N-CA	5.94	125.62	119.56
2	F	619	GLY	CA-C-N	5.93	125.84	119.85
2	F	619	GLY	C-N-CA	5.93	125.84	119.85
2	F	761	VAL	N-CA-C	5.93	116.41	107.75
1	E	2456	ASP	CA-CB-CG	5.92	118.53	112.60
2	F	1231	SER	CA-C-N	5.92	123.99	119.66
2	F	1231	SER	C-N-CA	5.92	123.99	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	956	GLN	N-CA-C	5.92	123.41	110.80
1	E	2424	GLY	CA-C-N	5.90	125.77	119.28
1	E	2424	GLY	C-N-CA	5.90	125.77	119.28
1	C	1632	ILE	N-CA-C	-5.90	101.93	109.30
2	F	1606	LEU	CA-C-N	5.89	125.59	119.82
2	F	1606	LEU	C-N-CA	5.89	125.59	119.82
2	F	1065	THR	CA-C-N	5.88	125.85	120.03
2	F	1065	THR	C-N-CA	5.88	125.85	120.03
1	C	1600	SER	N-CA-C	-5.88	106.11	113.28
1	B	386	GLN	N-CA-C	5.86	119.23	110.14
1	C	402	ILE	N-CA-C	5.86	118.79	113.10
1	E	1291	TYR	N-CA-C	-5.86	102.38	110.35
1	D	1494	SER	CA-C-N	5.86	127.17	119.84
1	D	1494	SER	C-N-CA	5.86	127.17	119.84
1	D	1745	GLU	N-CA-C	-5.85	104.98	111.36
1	A	193	ARG	CA-C-N	5.85	125.55	119.64
1	A	193	ARG	C-N-CA	5.85	125.55	119.64
1	E	1949	LEU	CA-C-N	5.84	125.82	120.03
1	E	1949	LEU	C-N-CA	5.84	125.82	120.03
1	B	1279	THR	CA-C-N	5.84	125.52	119.56
1	B	1279	THR	C-N-CA	5.84	125.52	119.56
1	B	1012	VAL	N-CA-C	-5.84	106.79	111.81
1	E	1821	LEU	N-CA-C	-5.83	106.30	113.41
1	B	2009	LEU	N-CA-C	-5.83	101.34	110.14
2	F	531	GLY	N-CA-C	-5.81	102.96	110.69
1	A	2005	GLY	N-CA-C	-5.81	99.41	113.18
1	C	722	ASP	CA-CB-CG	5.81	118.41	112.60
1	E	1239	TYR	N-CA-C	-5.79	101.71	110.28
2	F	1126	HIS	N-CA-C	5.79	117.05	108.60
2	F	1447	PHE	N-CA-C	5.79	117.98	109.24
1	A	1332	VAL	N-CA-C	-5.79	100.25	108.58
1	B	1124	ARG	CB-CA-C	-5.78	99.38	110.24
1	D	1250	TYR	N-CA-C	5.78	117.85	109.07
1	C	409	GLY	N-CA-C	-5.77	103.70	111.54
1	B	142	ARG	CA-C-N	5.75	125.85	119.87
1	B	142	ARG	C-N-CA	5.75	125.85	119.87
1	A	2363	GLN	N-CA-C	-5.75	102.79	110.55
1	D	302	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	1949	LEU	CA-C-N	5.74	125.71	120.03
1	A	1949	LEU	C-N-CA	5.74	125.71	120.03
1	A	2402	TYR	CA-C-N	5.73	125.75	119.90
1	A	2402	TYR	C-N-CA	5.73	125.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2344	LEU	CA-C-N	5.73	125.69	119.78
1	E	2344	LEU	C-N-CA	5.73	125.69	119.78
1	D	1006	GLU	N-CA-C	5.73	119.53	112.54
1	A	1991	ASP	CA-C-N	5.73	125.40	119.56
1	A	1991	ASP	C-N-CA	5.73	125.40	119.56
1	B	2508	ILE	N-CA-C	5.73	116.13	108.11
1	E	1802	PRO	N-CA-C	-5.72	102.21	111.14
1	E	142	ARG	CA-C-N	5.72	125.82	119.87
1	E	142	ARG	C-N-CA	5.72	125.82	119.87
2	F	243	LEU	CA-C-N	5.72	125.81	119.87
2	F	243	LEU	C-N-CA	5.72	125.81	119.87
1	E	1836	ASP	CA-C-N	5.71	125.39	119.56
1	E	1836	ASP	C-N-CA	5.71	125.39	119.56
2	F	770	ALA	N-CA-C	5.71	117.96	108.99
2	F	1334	ASP	CA-C-N	5.71	126.21	120.04
2	F	1334	ASP	C-N-CA	5.71	126.21	120.04
1	B	272	GLU	CA-C-N	5.71	125.39	119.56
1	B	272	GLU	C-N-CA	5.71	125.39	119.56
1	A	1623	THR	N-CA-C	-5.71	105.42	112.90
1	C	793	ALA	CA-C-N	5.71	125.66	119.78
1	C	793	ALA	C-N-CA	5.71	125.66	119.78
1	D	776	PHE	CA-CB-CG	5.71	119.51	113.80
2	F	1244	LYS	N-CA-C	5.71	120.67	113.25
1	E	1520	GLN	CA-C-N	5.70	125.60	119.85
1	E	1520	GLN	C-N-CA	5.70	125.60	119.85
1	D	348	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	1634	GLU	CA-C-N	5.69	125.59	119.85
1	A	1634	GLU	C-N-CA	5.69	125.59	119.85
1	B	501	ALA	CA-C-N	5.68	125.66	120.03
1	B	501	ALA	C-N-CA	5.68	125.66	120.03
1	C	1949	LEU	CA-C-N	5.68	125.67	120.21
1	C	1949	LEU	C-N-CA	5.68	125.67	120.21
2	F	1255	ALA	CA-C-N	5.68	125.78	119.87
2	F	1255	ALA	C-N-CA	5.68	125.78	119.87
1	B	1823	GLU	N-CA-C	-5.68	102.12	110.52
1	C	460	ILE	N-CA-C	-5.67	106.18	111.45
2	F	1585	ARG	NE-CZ-NH2	-5.66	114.10	119.20
1	B	1697	VAL	CA-C-N	5.66	125.64	120.03
1	B	1697	VAL	C-N-CA	5.66	125.64	120.03
1	E	272	GLU	CA-C-N	5.66	125.33	119.56
1	E	272	GLU	C-N-CA	5.66	125.33	119.56
1	A	2335	VAL	N-CA-C	5.64	115.98	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1159	ARG	CA-C-N	5.64	125.62	120.03
1	E	1159	ARG	C-N-CA	5.64	125.62	120.03
1	C	1250	TYR	N-CA-C	5.63	117.63	109.07
1	C	1821	LEU	N-CA-C	-5.63	106.54	113.41
1	D	322	ASP	N-CA-C	-5.63	107.66	114.75
1	E	1337	ILE	CA-C-N	5.63	125.25	119.56
1	E	1337	ILE	C-N-CA	5.63	125.25	119.56
1	B	1745	GLU	N-CA-C	-5.63	105.23	111.36
2	F	1235	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	1239	TYR	N-CA-C	-5.62	101.96	110.28
1	B	529	PHE	N-CA-C	5.62	121.03	113.72
1	C	1337	ILE	CA-C-N	5.62	125.24	119.56
1	C	1337	ILE	C-N-CA	5.62	125.24	119.56
2	F	2078	TYR	N-CA-C	-5.62	102.33	110.08
1	E	359	PHE	CA-CB-CG	-5.61	108.19	113.80
1	E	730	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	953	GLN	N-CA-C	5.61	120.78	113.88
1	A	533	ASP	N-CA-C	5.61	120.13	113.12
1	B	312	GLN	N-CA-C	5.61	115.95	108.38
2	F	1522	ILE	N-CA-C	5.60	115.92	107.80
2	F	622	ASP	CA-CB-CG	5.60	118.20	112.60
2	F	707	GLY	CA-C-N	-5.60	115.84	123.12
2	F	707	GLY	C-N-CA	-5.60	115.84	123.12
1	B	734	LEU	N-CA-C	-5.59	107.00	113.88
2	F	802	PRO	CA-C-N	5.59	125.57	120.03
2	F	802	PRO	C-N-CA	5.59	125.57	120.03
1	A	1836	ASP	CA-C-N	5.59	125.21	119.56
1	A	1836	ASP	C-N-CA	5.59	125.21	119.56
1	C	1759	ASP	N-CA-C	5.59	117.82	107.99
2	F	441	LEU	N-CA-C	-5.58	102.02	110.28
1	C	2456	ASP	CA-CB-CG	5.58	118.18	112.60
2	F	1136	GLN	CA-C-N	-5.58	112.95	120.87
2	F	1136	GLN	C-N-CA	-5.58	112.95	120.87
1	A	1012	VAL	N-CA-C	-5.57	107.02	111.81
1	A	2457	SER	N-CA-C	-5.57	100.73	109.25
1	A	1716	SER	N-CA-C	5.57	120.14	113.23
1	B	315	THR	CA-C-N	5.56	125.32	119.76
1	B	315	THR	C-N-CA	5.56	125.32	119.76
1	D	771	ILE	N-CA-C	5.56	118.12	108.95
1	A	889	VAL	N-CA-C	5.56	118.49	113.10
1	A	2300	THR	N-CA-C	-5.56	102.06	110.28
1	B	1871	LEU	N-CA-C	5.56	119.24	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1654	THR	N-CA-C	-5.55	100.97	109.41
1	C	511	GLN	CA-C-N	5.55	125.46	119.85
1	C	511	GLN	C-N-CA	5.55	125.46	119.85
1	D	2456	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	1148	ASP	CA-CB-CG	-5.54	107.06	112.60
1	D	359	PHE	CA-CB-CG	-5.53	108.27	113.80
1	B	1336	ASP	N-CA-C	5.53	115.85	108.38
1	B	1600	SER	N-CA-C	-5.53	105.89	113.30
1	D	511	GLN	CA-C-N	5.52	125.43	119.85
1	D	511	GLN	C-N-CA	5.52	125.43	119.85
1	C	140	THR	N-CA-C	-5.52	105.67	112.90
1	A	860	PRO	N-CA-C	-5.52	103.97	110.70
1	A	1722	GLY	CA-C-N	5.52	125.46	119.78
1	A	1722	GLY	C-N-CA	5.52	125.46	119.78
1	A	95	GLN	N-CA-C	-5.51	100.79	109.50
1	A	1056	MET	N-CA-C	-5.51	105.27	111.28
1	C	966	ASP	N-CA-C	-5.51	105.29	112.23
1	C	1584	LEU	N-CA-C	-5.50	102.15	110.28
2	F	1021	VAL	CB-CA-C	-5.49	104.58	110.95
1	E	572	ASP	N-CA-C	-5.49	105.71	112.90
1	C	2335	VAL	N-CA-C	5.49	115.76	107.75
1	A	1757	PRO	N-CA-C	5.48	122.58	112.33
1	E	1272	ASP	N-CA-C	-5.48	100.87	109.25
1	D	374	ASP	CA-CB-CG	-5.47	107.13	112.60
1	E	2265	PHE	N-CA-C	-5.47	105.39	111.36
1	D	1756	GLU	CA-C-N	5.46	125.44	120.03
1	D	1756	GLU	C-N-CA	5.46	125.44	120.03
2	F	969	ASP	CA-CB-CG	-5.46	107.14	112.60
1	D	300	ALA	N-CA-C	-5.46	103.51	108.75
2	F	1261	PRO	CB-CA-C	5.45	118.12	110.98
1	D	520	ASN	CA-CB-CG	-5.45	107.16	112.60
1	C	1913	ILE	N-CA-C	5.44	117.48	108.99
1	B	2335	VAL	N-CA-C	5.44	115.69	107.75
1	C	1836	ASP	CA-C-N	5.44	125.05	119.56
1	C	1836	ASP	C-N-CA	5.44	125.05	119.56
1	C	503	ILE	N-CA-C	-5.43	102.57	109.58
1	C	714	TRP	N-CA-C	-5.43	105.26	111.07
1	D	521	THR	N-CA-C	-5.42	105.38	112.75
1	D	909	THR	CA-C-N	5.42	125.18	119.76
1	D	909	THR	C-N-CA	5.42	125.18	119.76
1	E	318	VAL	N-CA-C	5.42	115.76	108.17
2	F	1752	SER	N-CA-C	5.42	117.32	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1745	GLU	N-CA-C	-5.41	105.46	111.36
1	E	1632	ILE	N-CA-C	-5.41	102.54	109.30
2	F	87	VAL	CA-C-N	5.41	125.35	119.78
2	F	87	VAL	C-N-CA	5.41	125.35	119.78
1	A	664	THR	CA-C-N	5.41	125.74	119.47
1	A	664	THR	C-N-CA	5.41	125.74	119.47
1	C	1865	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	1991	ASP	CA-C-N	5.40	125.22	119.28
1	B	1991	ASP	C-N-CA	5.40	125.22	119.28
1	D	1634	GLU	CA-C-N	5.40	125.31	119.85
1	D	1634	GLU	C-N-CA	5.40	125.31	119.85
2	F	848	VAL	N-CA-C	5.40	113.27	108.63
1	B	318	VAL	N-CA-C	5.39	116.07	108.36
1	B	1692	ILE	CA-C-N	5.39	125.30	119.85
1	B	1692	ILE	C-N-CA	5.39	125.30	119.85
1	D	1584	LEU	N-CA-C	-5.39	102.90	110.50
1	A	998	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	1520	GLN	CA-C-N	5.38	125.29	119.85
1	A	1520	GLN	C-N-CA	5.38	125.29	119.85
1	C	894	VAL	N-CA-C	-5.38	105.13	111.00
1	D	1702	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	682	ASP	CA-CB-CG	5.37	117.97	112.60
2	F	633	ILE	N-CA-C	5.37	115.83	107.99
1	C	436	PHE	N-CA-C	-5.37	105.87	112.90
1	C	1991	ASP	CA-C-N	5.37	125.03	119.56
1	C	1991	ASP	C-N-CA	5.37	125.03	119.56
1	B	1498	VAL	N-CA-C	-5.36	101.81	108.89
1	D	1911	ALA	CA-C-N	5.36	129.81	122.84
1	D	1911	ALA	C-N-CA	5.36	129.81	122.84
1	E	967	LEU	N-CA-C	-5.36	105.44	111.28
1	E	1913	ILE	N-CA-C	5.35	117.33	108.99
1	D	239	ILE	N-CA-C	-5.34	105.92	111.58
1	B	810	TRP	N-CA-C	-5.34	105.46	111.28
2	F	1537	ILE	N-CA-C	5.33	115.80	108.12
1	A	775	ALA	CA-C-N	5.33	127.69	120.44
1	A	775	ALA	C-N-CA	5.33	127.69	120.44
1	D	793	ALA	CA-C-N	5.33	125.27	119.78
1	D	793	ALA	C-N-CA	5.33	125.27	119.78
1	B	453	SER	CA-C-N	5.32	125.65	119.47
1	B	453	SER	C-N-CA	5.32	125.65	119.47
1	E	1827	TRP	N-CA-C	-5.32	102.41	110.28
1	A	2162	GLY	N-CA-C	-5.31	106.34	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	GLU	N-CA-C	5.31	117.06	111.28
1	B	1250	TYR	N-CA-C	5.31	117.14	109.07
1	C	100	ALA	N-CA-C	5.31	119.34	112.86
1	B	660	ASN	CA-C-N	5.30	128.24	120.71
1	B	660	ASN	C-N-CA	5.30	128.24	120.71
1	D	326	LYS	CA-C-N	-5.30	116.61	123.19
1	D	326	LYS	C-N-CA	-5.30	116.61	123.19
1	B	366	SER	N-CA-C	-5.30	105.55	112.23
1	B	1520	GLN	CA-C-N	5.30	125.20	119.85
1	B	1520	GLN	C-N-CA	5.30	125.20	119.85
1	C	1972	HIS	CA-CB-CG	-5.30	108.50	113.80
1	D	100	ALA	N-CA-C	5.30	117.57	109.62
1	A	1104	ASP	CA-CB-CG	-5.30	107.30	112.60
1	B	796	HIS	CA-C-N	5.29	128.36	120.90
1	B	796	HIS	C-N-CA	5.29	128.36	120.90
1	C	1369	ARG	N-CA-C	-5.29	105.59	111.36
1	D	1821	LEU	N-CA-C	-5.29	106.99	113.50
2	F	1201	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	1830	ASP	CA-C-N	5.29	125.19	119.85
1	A	1830	ASP	C-N-CA	5.29	125.19	119.85
1	A	1871	LEU	N-CA-C	5.29	118.88	111.74
1	B	1525	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	2391	VAL	N-CA-C	5.29	115.60	107.77
1	C	2457	SER	N-CA-C	-5.29	101.08	109.96
1	D	1632	ILE	N-CA-C	-5.29	102.69	109.30
1	B	831	THR	N-CA-C	5.29	116.03	108.74
1	E	2351	PHE	N-CA-C	5.29	116.32	108.60
1	E	1012	VAL	N-CA-C	-5.28	107.62	111.90
1	B	2363	GLN	N-CA-C	-5.28	102.71	110.52
2	F	1968	ASP	N-CA-C	-5.28	103.06	110.50
2	F	93	THR	N-CA-C	-5.27	106.90	113.38
2	F	2038	GLU	N-CA-C	-5.27	107.02	113.50
1	C	2015	SER	N-CA-C	5.27	117.87	110.23
1	E	824	ALA	CA-C-N	5.27	127.61	120.44
1	E	824	ALA	C-N-CA	5.27	127.61	120.44
1	A	1040	TYR	CA-C-N	5.27	124.93	119.56
1	A	1040	TYR	C-N-CA	5.27	124.93	119.56
1	D	1104	ASP	CA-CB-CG	-5.26	107.34	112.60
1	D	1157	THR	CB-CA-C	-5.26	103.53	112.00
1	E	1647	ILE	CA-C-N	5.25	125.79	120.38
1	E	1647	ILE	C-N-CA	5.25	125.79	120.38
1	D	1520	GLN	CA-C-N	5.25	125.16	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1520	GLN	C-N-CA	5.25	125.16	119.85
2	F	1493	THR	CA-C-N	-5.25	116.30	123.12
2	F	1493	THR	C-N-CA	-5.25	116.30	123.12
1	D	739	THR	N-CA-C	-5.25	99.96	109.09
1	C	1050	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	B	535	GLU	CA-C-N	5.24	128.20	120.91
1	B	535	GLU	C-N-CA	5.24	128.20	120.91
1	D	1951	GLN	CA-C-N	5.24	127.64	120.46
1	D	1951	GLN	C-N-CA	5.24	127.64	120.46
2	F	853	GLU	N-CA-C	5.24	116.99	111.28
1	D	392	SER	N-CA-C	5.24	116.76	108.96
1	E	786	PHE	CA-CB-CG	-5.24	108.56	113.80
2	F	1403	GLN	CA-C-N	5.24	125.14	119.85
2	F	1403	GLN	C-N-CA	5.24	125.14	119.85
2	F	379	ALA	CA-C-N	-5.24	116.03	122.84
2	F	379	ALA	C-N-CA	-5.24	116.03	122.84
1	E	590	ILE	CB-CA-C	-5.24	105.27	111.97
1	C	1620	GLY	N-CA-C	5.23	117.19	110.96
1	E	834	GLN	CB-CG-CD	-5.23	103.71	112.60
2	F	2056	ASN	CA-CB-CG	5.23	117.83	112.60
1	D	401	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	1991	ASP	CA-C-N	5.23	125.03	119.28
1	D	1991	ASP	C-N-CA	5.23	125.03	119.28
1	E	1250	TYR	N-CA-C	5.22	117.01	109.07
1	D	2374	ASN	N-CA-C	5.22	115.94	108.74
1	A	735	ASN	CA-CB-CG	-5.21	107.39	112.60
1	C	612	VAL	N-CA-C	-5.21	107.33	111.81
1	D	2267	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	1060	LEU	N-CA-C	-5.21	105.50	111.07
1	E	1991	ASP	CA-C-N	5.21	125.01	119.28
1	E	1991	ASP	C-N-CA	5.21	125.01	119.28
1	E	615	GLY	N-CA-C	-5.20	105.94	111.93
1	A	105	ALA	CA-C-N	5.20	125.28	119.87
1	A	105	ALA	C-N-CA	5.20	125.28	119.87
1	C	1634	GLU	CA-C-N	5.20	125.14	119.78
1	C	1634	GLU	C-N-CA	5.20	125.14	119.78
1	D	547	ARG	N-CA-C	-5.20	105.68	112.23
1	C	2363	GLN	N-CA-C	-5.20	103.53	110.55
1	E	1634	GLU	CA-C-N	5.20	125.10	119.85
1	E	1634	GLU	C-N-CA	5.20	125.10	119.85
1	B	696	ILE	N-CA-C	-5.19	104.60	111.09
1	C	1107	LEU	N-CA-C	5.19	117.86	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	782	LYS	CA-C-N	5.19	125.49	119.47
1	E	782	LYS	C-N-CA	5.19	125.49	119.47
1	A	248	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	1821	LEU	N-CA-C	-5.18	107.09	113.41
2	F	1562	THR	N-CA-C	-5.18	106.36	113.30
1	C	1688	ILE	N-CA-C	5.17	115.30	107.75
1	C	379	VAL	N-CA-C	5.17	115.72	108.17
2	F	1390	THR	N-CA-C	5.17	117.85	109.06
2	F	1552	LYS	CA-C-N	5.17	125.45	119.92
2	F	1552	LYS	C-N-CA	5.17	125.45	119.92
2	F	1837	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	529	PHE	N-CA-C	5.17	120.44	113.72
1	A	2508	ILE	N-CA-C	5.17	115.34	108.11
1	B	1717	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	180	GLU	N-CA-C	5.17	117.65	111.71
1	B	1159	ARG	CA-C-N	5.16	125.07	119.85
1	B	1159	ARG	C-N-CA	5.16	125.07	119.85
1	C	889	VAL	CB-CA-C	-5.16	105.25	110.93
1	C	2402	TYR	CA-C-N	5.16	125.06	119.85
1	C	2402	TYR	C-N-CA	5.16	125.06	119.85
1	D	1166	ARG	CA-C-N	-5.16	115.56	122.42
1	D	1166	ARG	C-N-CA	-5.16	115.56	122.42
1	A	2486	PHE	CA-C-N	5.16	125.14	120.03
1	A	2486	PHE	C-N-CA	5.16	125.14	120.03
1	C	1124	ARG	CB-CA-C	-5.16	99.22	109.79
1	C	1181	THR	CA-C-N	5.16	125.81	120.03
1	C	1181	THR	C-N-CA	5.16	125.81	120.03
1	B	1821	LEU	N-CA-C	-5.16	107.12	113.41
2	F	1232	PRO	CA-C-N	5.15	125.13	120.03
2	F	1232	PRO	C-N-CA	5.15	125.13	120.03
1	A	676	HIS	N-CA-C	-5.15	105.75	111.36
1	E	695	TYR	N-CA-C	-5.15	106.16	112.90
2	F	679	VAL	N-CA-C	5.14	113.24	108.15
1	A	1692	ILE	CA-C-N	5.14	125.04	119.85
1	A	1692	ILE	C-N-CA	5.14	125.04	119.85
2	F	468	GLY	CA-C-N	5.14	126.26	119.84
2	F	468	GLY	C-N-CA	5.14	126.26	119.84
1	D	501	ALA	CA-C-N	5.13	125.11	120.03
1	D	501	ALA	C-N-CA	5.13	125.11	120.03
1	A	326	LYS	CA-C-N	-5.13	116.28	123.10
1	A	326	LYS	C-N-CA	-5.13	116.28	123.10
2	F	789	SER	N-CA-C	5.13	117.75	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ILE	CB-CA-C	-5.12	105.12	111.32
1	A	198	THR	N-CA-C	5.12	118.91	107.95
1	E	577	LYS	N-CA-C	5.12	116.31	108.42
2	F	646	VAL	CA-C-N	-5.12	115.95	122.77
2	F	646	VAL	C-N-CA	-5.12	115.95	122.77
1	B	1911	ALA	CA-C-N	5.12	130.38	123.11
1	B	1911	ALA	C-N-CA	5.12	130.38	123.11
1	D	1835	VAL	N-CA-C	-5.12	108.30	113.47
1	E	1522	SER	CA-C-N	5.12	126.24	119.84
1	E	1522	SER	C-N-CA	5.12	126.24	119.84
1	C	1692	ILE	CA-C-N	5.12	125.02	119.85
1	C	1692	ILE	C-N-CA	5.12	125.02	119.85
1	C	1983	LEU	CA-C-N	5.12	125.10	120.03
1	C	1983	LEU	C-N-CA	5.12	125.10	120.03
1	C	1911	ALA	CA-C-N	5.12	129.22	122.42
1	C	1911	ALA	C-N-CA	5.12	129.22	122.42
1	D	272	GLU	CA-C-N	5.12	124.78	119.56
1	D	272	GLU	C-N-CA	5.12	124.78	119.56
1	A	1323	GLY	N-CA-C	5.11	118.04	110.42
1	B	1272	ASP	N-CA-C	-5.11	101.43	109.25
1	E	2463	ASP	CA-CB-CG	-5.11	107.49	112.60
1	D	693	ALA	CA-C-N	5.11	124.77	119.56
1	D	693	ALA	C-N-CA	5.11	124.77	119.56
1	E	812	ASN	CA-CB-CG	-5.11	107.49	112.60
1	C	572	ASP	N-CA-C	-5.10	106.21	112.90
1	E	2417	VAL	N-CA-C	5.10	115.25	108.11
1	A	1872	GLU	N-CA-C	-5.10	101.84	109.95
1	C	1006	GLU	N-CA-C	5.10	116.83	111.28
1	B	479	PHE	CB-CA-C	-5.10	102.19	110.85
1	C	2331	VAL	N-CA-C	5.10	115.25	108.11
1	B	299	LYS	CA-C-N	5.09	130.51	122.36
1	B	299	LYS	C-N-CA	5.09	130.51	122.36
1	D	1667	HIS	CA-C-N	-5.09	117.93	123.08
1	D	1667	HIS	C-N-CA	-5.09	117.93	123.08
1	B	468	LEU	CB-CA-C	-5.09	102.76	111.26
1	E	236	LEU	N-CA-C	-5.08	105.83	112.23
2	F	1320	PRO	CA-C-N	5.08	124.99	119.76
2	F	1320	PRO	C-N-CA	5.08	124.99	119.76
2	F	1585	ARG	CA-C-N	5.08	124.83	119.76
2	F	1585	ARG	C-N-CA	5.08	124.83	119.76
1	C	2265	PHE	N-CA-C	-5.07	105.83	111.36
1	E	901	ASP	N-CA-C	5.07	117.40	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1040	TYR	CA-C-N	5.07	124.73	119.56
1	B	1040	TYR	C-N-CA	5.07	124.73	119.56
1	D	350	GLY	N-CA-C	-5.07	105.43	111.36
1	C	782	LYS	CA-C-N	5.07	124.73	119.56
1	C	782	LYS	C-N-CA	5.07	124.73	119.56
1	C	2141	VAL	CA-C-N	5.06	124.72	119.56
1	C	2141	VAL	C-N-CA	5.06	124.72	119.56
1	B	1634	GLU	CA-C-N	5.06	124.96	119.85
1	B	1634	GLU	C-N-CA	5.06	124.96	119.85
1	A	494	THR	N-CA-C	-5.06	104.76	112.04
1	D	962	LYS	N-CA-C	-5.05	107.66	113.88
1	E	350	GLY	N-CA-C	-5.05	105.45	111.36
2	F	827	ARG	N-CA-C	5.05	117.85	109.46
1	B	889	VAL	N-CA-C	5.05	117.75	112.90
1	D	1983	LEU	CA-C-N	5.05	125.03	120.03
1	D	1983	LEU	C-N-CA	5.05	125.03	120.03
1	D	2293	LYS	CA-C-N	5.05	126.06	120.45
1	D	2293	LYS	C-N-CA	5.05	126.06	120.45
2	F	471	LEU	N-CA-C	5.05	116.81	108.13
1	B	295	GLN	N-CA-C	-5.05	105.87	112.23
1	E	1697	VAL	CA-C-N	5.04	124.94	119.85
1	E	1697	VAL	C-N-CA	5.04	124.94	119.85
2	F	391	ASN	N-CA-C	5.04	117.19	109.07
2	F	630	ARG	N-CA-C	5.04	116.18	108.52
2	F	1108	GLN	N-CA-C	5.04	116.97	108.96
1	D	248	PHE	CA-CB-CG	5.04	118.83	113.80
2	F	904	SER	CA-C-N	-5.04	113.48	120.38
2	F	904	SER	C-N-CA	-5.04	113.48	120.38
1	A	1060	LEU	N-CA-C	-5.03	105.68	111.07
1	B	1291	TYR	N-CA-C	-5.03	100.08	110.80
1	C	2478	ASP	CA-CB-CG	-5.03	107.57	112.60
2	F	1673	SER	N-CA-C	5.03	116.48	108.79
1	B	353	TYR	N-CA-C	5.03	117.44	109.50
1	C	272	GLU	CA-C-N	5.02	124.68	119.56
1	C	272	GLU	C-N-CA	5.02	124.68	119.56
1	E	312	GLN	N-CA-C	5.02	116.70	109.07
2	F	273	THR	CA-C-N	5.02	123.28	119.66
2	F	273	THR	C-N-CA	5.02	123.28	119.66
2	F	734	THR	CA-C-N	5.02	125.23	120.31
2	F	734	THR	C-N-CA	5.02	125.23	120.31
1	B	1983	LEU	CA-C-N	5.02	124.92	119.85
1	B	1983	LEU	C-N-CA	5.02	124.92	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	PRO	CB-CA-C	5.02	117.56	110.98
1	E	1046	ASP	CA-C-N	5.02	124.68	119.56
1	E	1046	ASP	C-N-CA	5.02	124.68	119.56
1	B	793	ALA	CA-C-N	5.02	125.29	119.92
1	B	793	ALA	C-N-CA	5.02	125.29	119.92
1	E	348	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	1913	ILE	N-CA-C	5.01	117.22	108.95
1	A	1336	ASP	N-CA-C	5.01	115.14	108.38
1	E	1161	VAL	CA-C-N	-5.01	116.62	122.93
1	E	1161	VAL	C-N-CA	-5.01	116.62	122.93
1	A	856	HIS	CA-C-N	-5.01	115.76	122.42
1	A	856	HIS	C-N-CA	-5.01	115.76	122.42
1	A	1239	TYR	N-CA-C	-5.01	102.87	110.28
1	D	1040	TYR	CA-C-N	5.01	124.67	119.56
1	D	1040	TYR	C-N-CA	5.01	124.67	119.56
1	E	373	ASN	N-CA-C	-5.01	105.83	112.24
1	C	2479	GLN	N-CA-C	5.00	117.56	109.40
1	B	1051	ILE	N-CA-C	5.00	115.51	108.36
1	C	156	ASP	N-CA-C	5.00	117.84	111.69
1	E	649	PHE	CA-CB-CG	-5.00	108.80	113.80
2	F	530	ASP	CA-C-N	5.00	127.81	120.91
2	F	530	ASP	C-N-CA	5.00	127.81	120.91

There are no chirality outliers.

There are no planarity outliers.

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	18197	0	17794	64	0
1	B	18197	0	17794	65	0
1	C	18197	0	17794	56	0
1	D	18197	0	17794	62	0
1	E	18197	0	17794	68	0
2	F	17127	0	16494	63	0
All	All	108112	0	105464	372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (372) 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:D:290:ASP:N	1:D:290:ASP:OD1	2.35	0.59
2:F:153:ASP:O	2:F:174:ARG:NH2	2.37	0.58
1:D:100:ALA:O	1:D:101:SER:C	2.47	0.58
1:B:624:ASP:OD1	1:B:624:ASP:N	2.37	0.58
1:C:575:ASP:OD2	1:C:577:LYS:NZ	2.35	0.57
1:B:2319:ASP:OD2	1:B:2323:LYS:NZ	2.37	0.57
1:E:1774:TYR:HH	1:E:1848:TYR:HH	1.53	0.57
1:C:624:ASP:N	1:C:624:ASP:OD1	2.37	0.57
1:E:624:ASP:OD1	1:E:624:ASP:N	2.37	0.57
1:A:624:ASP:N	1:A:624:ASP:OD1	2.35	0.57
1:C:250:ILE:O	1:C:442:LYS:NZ	2.38	0.57
1:E:817:LYS:NZ	1:E:837:ASP:OD2	2.38	0.57
2:F:1095:ASP:N	2:F:1095:ASP:OD1	2.37	0.56
1:A:1719:THR:HG1	1:A:1720:TRP:CD1	2.23	0.56
1:D:817:LYS:NZ	1:D:837:ASP:OD2	2.38	0.56
1:C:1683:ASP:OD1	1:C:1683:ASP:N	2.38	0.56
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.33	0.56
1:E:207:VAL:O	1:E:208:ARG:CB	2.54	0.55
1:A:1164:LYS:NZ	1:B:1622:ASP:OD2	2.32	0.55
1:B:890:ALA:O	1:B:892:GLN:N	2.40	0.55
1:D:963:SER:OG	1:D:964:ARG:N	2.38	0.55
1:D:1124:ARG:NE	1:D:1142:SER:O	2.39	0.55
1:E:2015:SER:OG	1:E:2016:LEU:N	2.39	0.55
1:B:1290:SER:C	1:B:1291:TYR:O	2.45	0.55
1:D:624:ASP:OD1	1:D:624:ASP:N	2.36	0.55
1:A:1841:ALA:O	1:A:1842:GLN:HB2	2.06	0.55
1:B:336:THR:OG1	1:B:423:ALA:N	2.40	0.54
1:C:1514:ASP:OD2	1:C:1515:LYS:NZ	2.39	0.54
1:B:2207:ASP:OD2	1:B:2211:LYS:NZ	2.41	0.54
2:F:878:ASP:OD2	2:F:923:ARG:NH1	2.40	0.54
1:D:533:ASP:OD1	1:D:533:ASP:N	2.37	0.54
2:F:263:ASP:OD1	2:F:264:TYR:N	2.41	0.53
1:B:253:GLU:O	1:B:442:LYS:NZ	2.41	0.53
1:D:322:ASP:OD1	1:D:323:GLY:N	2.42	0.53
1:E:193:ARG:NH1	1:E:195:SER:O	2.42	0.53
1:E:257:GLU:OE2	1:E:439:LYS:NZ	2.41	0.53
1:A:1291:TYR:O	1:A:1292:GLN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1104:ASP:OD1	1:D:1104:ASP:N	2.38	0.53
2:F:174:ARG:NH1	2:F:184:THR:OG1	2.42	0.53
2:F:1416:ASP:N	2:F:1416:ASP:OD1	2.37	0.53
1:D:890:ALA:O	1:D:892:GLN:N	2.42	0.53
1:D:1841:ALA:O	1:D:1842:GLN:HB2	2.09	0.53
1:E:1133:ASP:OD1	1:E:1133:ASP:N	2.41	0.53
1:A:1133:ASP:OD1	1:A:1133:ASP:N	2.39	0.53
1:D:253:GLU:O	1:D:442:LYS:NZ	2.42	0.53
1:C:1616:ARG:NE	1:C:1629:THR:OG1	2.42	0.53
1:A:1290:SER:C	1:A:1291:TYR:O	2.50	0.52
1:A:1774:TYR:HH	1:A:1848:TYR:HH	1.53	0.52
1:C:1774:TYR:HH	1:C:1848:TYR:HH	1.57	0.52
2:F:263:ASP:OD2	2:F:267:ARG:HD2	2.10	0.52
1:A:2257:ARG:NH2	1:B:2309:THR:OG1	2.43	0.52
1:B:1758:MET:O	1:B:1819:ARG:NH2	2.43	0.52
1:E:1841:ALA:O	1:E:1842:GLN:HB2	2.10	0.52
1:C:592:LYS:NZ	1:C:596:ASP:OD2	2.43	0.52
1:A:2327:ARG:NH2	1:E:2469:PHE:O	2.42	0.52
2:F:449:SER:OG	2:F:450:ASN:N	2.41	0.52
1:B:990:ILE:O	1:B:991:ALA:HB3	2.10	0.51
1:B:817:LYS:NZ	1:B:837:ASP:OD2	2.44	0.51
1:D:575:ASP:OD2	1:D:577:LYS:NZ	2.40	0.51
1:D:1514:ASP:OD2	1:D:1515:LYS:NZ	2.39	0.51
1:D:1975:SER:OG	1:D:1976:ILE:N	2.43	0.51
1:E:1257:ASP:OD1	1:E:1257:ASP:N	2.41	0.51
1:A:1254:ASP:OD1	1:A:1254:ASP:N	2.42	0.51
2:F:2143:MET:O	2:F:2145:ARG:N	2.44	0.51
2:F:385:ASP:N	2:F:385:ASP:OD1	2.42	0.51
1:E:852:GLN:O	1:E:853:ALA:C	2.53	0.50
1:A:1103:ASN:ND2	1:A:1582:ASN:O	2.44	0.50
1:B:1291:TYR:O	1:B:1292:GLN:HB2	2.12	0.50
1:E:540:SER:OG	1:E:541:GLY:N	2.44	0.50
1:A:735:ASN:N	1:A:735:ASN:OD1	2.34	0.50
1:A:1272:ASP:O	1:A:1274:ALA:N	2.44	0.50
2:F:754:GLU:O	2:F:755:ILE:HB	2.11	0.50
1:D:1683:ASP:N	1:D:1683:ASP:OD1	2.41	0.50
1:D:2008:LYS:NZ	1:D:2267:ASP:OD2	2.40	0.50
1:B:299:LYS:NZ	1:B:458:GLU:OE2	2.44	0.49
1:A:160:SER:C	1:A:161:THR:O	2.50	0.49
1:E:842:ASP:OD1	1:E:843:ALA:N	2.45	0.49
2:F:263:ASP:OD1	2:F:263:ASP:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:OG	1:B:135:VAL:N	2.45	0.49
2:F:880:SER:OG	2:F:881:THR:N	2.44	0.49
2:F:1340:ARG:NH2	2:F:1710:THR:OG1	2.45	0.49
2:F:3:ASN:HA	2:F:1126:HIS:CG	2.46	0.49
2:F:270:ASN:O	2:F:332:ARG:NH2	2.45	0.49
1:B:1774:TYR:HH	1:B:1848:TYR:HH	1.61	0.49
1:C:1291:TYR:O	1:C:1292:GLN:CB	2.60	0.49
1:D:1380:LYS:O	1:D:1381:LEU:C	2.56	0.49
1:C:1975:SER:OG	1:C:1976:ILE:N	2.44	0.49
1:C:2284:LEU:O	1:C:2286:ASP:N	2.45	0.49
2:F:1234:SER:OG	2:F:1235:ASP:N	2.44	0.49
1:B:1975:SER:OG	1:B:1976:ILE:N	2.46	0.49
1:E:1865:ASP:OD1	1:E:1966:ARG:NH1	2.46	0.49
1:A:2382:ASP:OD1	1:A:2382:ASP:N	2.45	0.48
1:A:2496:LYS:NZ	1:B:2401:ASP:OD1	2.35	0.48
1:C:160:SER:C	1:C:161:THR:O	2.53	0.48
1:C:322:ASP:OD1	1:C:323:GLY:N	2.46	0.48
2:F:561:ASP:C	2:F:561:ASP:OD1	2.51	0.48
2:F:854:ASP:C	2:F:854:ASP:OD1	2.54	0.48
1:B:548:LYS:NZ	1:B:559:ASP:OD2	2.45	0.48
2:F:1756:SER:OG	2:F:1757:ALA:N	2.47	0.48
1:B:329:ARG:HB3	1:B:431:TYR:CE1	2.49	0.48
1:E:2463:ASP:OD1	1:E:2464:PHE:N	2.47	0.48
1:A:1666:LYS:NZ	1:A:1717:ASP:OD2	2.37	0.48
1:D:1119:GLY:O	1:D:1120:GLU:HB2	2.13	0.48
1:D:1006:GLU:OE1	1:D:1343:LYS:NZ	2.46	0.48
2:F:616:ASP:OD1	2:F:616:ASP:N	2.45	0.48
1:B:1526:ASP:N	1:B:1526:ASP:OD1	2.45	0.48
2:F:1146:THR:HG23	2:F:1148:LEU:H	1.79	0.48
1:A:1518:SER:OG	1:A:1519:ILE:N	2.46	0.48
1:B:1320:LYS:NZ	1:B:1552:ASP:OD1	2.38	0.48
1:D:1133:ASP:OD1	1:D:1133:ASP:N	2.46	0.48
1:A:161:THR:O	1:A:162:LEU:HB3	2.14	0.47
1:A:2401:ASP:OD1	1:E:2496:LYS:NZ	2.42	0.47
1:C:329:ARG:HB3	1:C:431:TYR:CE1	2.49	0.47
1:C:571:HIS:O	1:C:574:LYS:NZ	2.46	0.47
1:C:161:THR:O	1:C:162:LEU:HB2	2.14	0.47
1:D:1220:LYS:NZ	1:D:1277:ASP:OD1	2.44	0.47
1:E:2365:SER:OG	1:E:2366:GLY:N	2.48	0.47
1:A:912:TYR:CG	1:A:913:ALA:N	2.82	0.47
1:B:2380:GLY:N	1:B:2383:THR:OG1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1975:SER:OG	1:E:1976:ILE:N	2.47	0.47
2:F:1329:ASP:OD1	2:F:1329:ASP:N	2.46	0.47
1:E:171:GLU:OE1	1:E:182:TYR:OH	2.32	0.47
1:B:359:PHE:CD1	1:B:359:PHE:N	2.83	0.47
1:C:1834:SER:OG	1:C:1835:VAL:N	2.48	0.47
1:D:797:ASP:OD1	1:D:798:ALA:N	2.48	0.47
2:F:1687:ASP:OD1	2:F:1687:ASP:N	2.38	0.47
1:A:1117:ASP:OD1	1:A:1118:ALA:N	2.48	0.47
1:C:477:LYS:NZ	1:C:624:ASP:OD2	2.37	0.47
1:C:1124:ARG:HD3	1:C:1144:TRP:CD2	2.49	0.47
1:E:1834:SER:OG	1:E:1835:VAL:N	2.48	0.47
1:C:304:GLY:O	1:C:354:ARG:NH2	2.47	0.47
1:D:359:PHE:CE1	1:D:385:PRO:HB2	2.50	0.47
1:E:1991:ASP:OD2	1:E:1993:LYS:NZ	2.48	0.47
1:A:296:PHE:O	1:A:299:LYS:NZ	2.46	0.47
1:A:1841:ALA:O	1:A:1842:GLN:CB	2.63	0.47
1:A:537:ASP:OD1	1:A:538:LEU:N	2.48	0.47
1:B:540:SER:OG	1:B:541:GLY:N	2.48	0.47
1:E:1683:ASP:OD1	1:E:1683:ASP:N	2.43	0.47
1:B:1514:ASP:OD1	1:B:1514:ASP:N	2.47	0.46
1:D:359:PHE:N	1:D:359:PHE:CD1	2.83	0.46
1:E:1293:GLN:O	1:E:1303:ASN:ND2	2.48	0.46
1:B:1774:TYR:OH	1:B:1848:TYR:OH	2.29	0.46
1:D:1834:SER:OG	1:D:1835:VAL:N	2.48	0.46
2:F:1795:LYS:NZ	2:F:1818:GLU:OE1	2.47	0.46
1:A:1865:ASP:OD1	1:A:1966:ARG:NH1	2.48	0.46
1:A:832:ALA:O	1:A:833:GLU:HB2	2.15	0.46
1:D:545:ASP:OD1	1:D:545:ASP:C	2.57	0.46
1:E:357:TYR:OH	1:E:381:THR:OG1	2.28	0.46
1:E:1945:THR:OG1	1:E:1946:ASP:N	2.49	0.46
1:A:1834:SER:OG	1:A:1835:VAL:N	2.48	0.46
1:B:290:ASP:OD1	1:B:290:ASP:N	2.47	0.46
1:A:890:ALA:O	1:A:892:GLN:N	2.49	0.46
1:D:133:ASP:OD1	1:D:133:ASP:N	2.43	0.46
1:E:1183:ASN:OD1	1:E:1183:ASN:N	2.48	0.46
1:E:1908:ASP:OD1	1:E:1909:ARG:N	2.48	0.46
2:F:1235:ASP:OD1	2:F:1236:VAL:N	2.49	0.46
2:F:1626:THR:OG1	2:F:1950:ARG:NH2	2.49	0.46
1:C:2287:ASP:N	1:C:2287:ASP:OD1	2.47	0.46
1:D:2284:LEU:O	1:D:2286:ASP:N	2.49	0.46
1:B:935:HIS:O	1:B:936:ALA:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1220:LYS:NZ	1:B:1277:ASP:OD1	2.45	0.46
1:C:329:ARG:NH1	1:C:434:TYR:OH	2.49	0.46
1:D:161:THR:O	1:D:162:LEU:HB2	2.16	0.46
1:D:2365:SER:OG	1:D:2366:GLY:N	2.49	0.46
1:B:2082:LYS:NZ	1:B:2086:GLU:OE2	2.44	0.46
1:A:1514:ASP:OD2	1:A:1515:LYS:NZ	2.43	0.45
2:F:1510:HIS:ND1	2:F:1521:ARG:NH2	2.64	0.45
1:B:714:TRP:CG	1:B:762:LEU:HD22	2.51	0.45
1:C:578:ILE:HG12	1:C:580:ASN:H	1.80	0.45
1:A:2284:LEU:O	1:A:2286:ASP:N	2.49	0.45
1:B:1507:LYS:NZ	1:B:1538:ASP:OD2	2.40	0.45
1:C:1133:ASP:OD1	1:C:1133:ASP:N	2.43	0.45
1:E:2284:LEU:O	1:E:2286:ASP:N	2.50	0.45
2:F:34:ASP:OD1	2:F:34:ASP:N	2.49	0.45
1:E:1124:ARG:HD3	1:E:1144:TRP:CD2	2.50	0.45
2:F:1432:ASP:OD1	2:F:1432:ASP:C	2.58	0.45
1:B:1022:ASP:OD2	1:B:1023:LYS:NZ	2.49	0.45
1:C:1130:LYS:NZ	1:C:1836:ASP:OD2	2.43	0.45
2:F:112:ASP:OD2	2:F:147:LYS:NZ	2.39	0.45
2:F:552:ASP:OD1	2:F:552:ASP:C	2.60	0.45
2:F:1498:ASP:OD1	2:F:1498:ASP:C	2.60	0.45
1:A:1291:TYR:O	1:A:1292:GLN:CB	2.64	0.45
1:A:1977:ASP:OD1	1:A:1977:ASP:N	2.41	0.45
1:E:2430:GLN:OE1	1:E:2497:GLN:NE2	2.50	0.45
2:F:283:TRP:H	2:F:283:TRP:CD1	2.33	0.45
2:F:1055:THR:OG1	2:F:1056:ASP:N	2.50	0.45
1:C:693:ALA:HB3	1:C:694:PRO:HD3	1.99	0.45
1:C:2024:GLU:OE2	1:C:2027:ARG:NH1	2.50	0.45
1:E:1514:ASP:OD1	1:E:1514:ASP:N	2.50	0.45
1:A:1176:GLU:HG2	1:A:1194:TYR:CE2	2.52	0.45
1:B:161:THR:O	1:B:162:LEU:HB2	2.17	0.45
1:D:1124:ARG:HG2	1:D:1144:TRP:CE3	2.52	0.45
1:E:1841:ALA:O	1:E:1842:GLN:CB	2.65	0.45
1:E:161:THR:O	1:E:162:LEU:HB2	2.16	0.45
1:E:975:ASN:OD1	1:E:975:ASN:N	2.40	0.45
2:F:1560:ASP:C	2:F:1560:ASP:OD1	2.59	0.45
1:A:569:THR:O	1:A:618:ASN:HB2	2.17	0.45
1:A:2365:SER:OG	1:A:2366:GLY:N	2.48	0.45
1:E:1380:LYS:O	1:E:1381:LEU:C	2.60	0.45
1:A:1975:SER:OG	1:A:1976:ILE:N	2.49	0.44
1:A:2015:SER:OG	1:A:2016:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:912:TYR:CG	1:C:913:ALA:N	2.83	0.44
1:E:207:VAL:O	1:E:208:ARG:HB3	2.15	0.44
2:F:1882:ASP:OD1	2:F:1882:ASP:C	2.59	0.44
1:C:1859:LEU:C	1:C:1860:LEU:O	2.54	0.44
2:F:1729:ASP:OD1	2:F:1729:ASP:C	2.59	0.44
1:A:301:SER:HB2	1:A:467:GLN:HB2	2.00	0.44
1:A:366:SER:N	1:A:413:VAL:O	2.50	0.44
1:C:191:THR:HG22	1:C:201:HIS:HA	2.00	0.44
1:D:935:HIS:O	1:D:936:ALA:C	2.60	0.44
1:D:204:TYR:OH	1:D:238:GLY:O	2.34	0.44
1:D:2496:LYS:NZ	1:E:2401:ASP:OD1	2.43	0.44
1:A:97:SER:OG	1:A:98:GLY:N	2.50	0.44
1:B:520:ASN:O	1:B:521:THR:C	2.58	0.44
1:A:520:ASN:O	1:A:521:THR:C	2.60	0.44
1:D:968:TYR:CD1	1:D:968:TYR:C	2.94	0.44
1:B:1139:ASN:ND2	1:B:1838:ASP:O	2.50	0.44
1:B:801:LEU:O	1:B:802:ILE:HB	2.17	0.44
1:E:963:SER:OG	1:E:964:ARG:N	2.49	0.44
2:F:236:ASN:ND2	2:F:238:THR:O	2.50	0.44
2:F:267:ARG:NH1	2:F:276:ALA:O	2.51	0.44
1:A:347:PRO:HB3	1:A:353:TYR:CE2	2.53	0.44
1:A:545:ASP:OD2	1:A:547:ARG:NH1	2.50	0.44
1:A:1040:TYR:OH	1:A:1951:GLN:O	2.35	0.44
1:B:2466:ASP:N	1:B:2466:ASP:OD1	2.47	0.44
1:D:329:ARG:HB3	1:D:431:TYR:CE1	2.53	0.44
1:D:1176:GLU:HG2	1:D:1194:TYR:CE2	2.53	0.44
1:E:336:THR:OG1	1:E:337:ASN:N	2.50	0.43
2:F:2119:TYR:HB2	2:F:2126:TRP:CZ3	2.53	0.43
1:A:2287:ASP:N	1:A:2287:ASP:OD1	2.40	0.43
1:D:649:PHE:O	1:D:650:GLN:C	2.58	0.43
1:B:545:ASP:C	1:B:545:ASP:OD1	2.60	0.43
1:B:2284:LEU:O	1:B:2286:ASP:N	2.51	0.43
1:C:975:ASN:OD1	1:C:975:ASN:N	2.48	0.43
2:F:210:THR:OG1	2:F:283:TRP:NE1	2.52	0.43
1:A:357:TYR:CZ	1:A:391:TYR:HB2	2.54	0.43
1:B:1178:THR:OG1	1:B:1179:LYS:N	2.51	0.43
1:B:2365:SER:OG	1:B:2366:GLY:N	2.49	0.43
2:F:73:ASP:OD1	2:F:74:CYS:N	2.50	0.43
2:F:1370:ASP:OD1	2:F:1370:ASP:N	2.46	0.43
1:B:2478:ASP:OD1	1:B:2478:ASP:N	2.51	0.43
1:B:1056:MET:HE1	1:B:1085:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1834:SER:OG	1:B:1835:VAL:N	2.51	0.43
1:E:436:PHE:O	1:E:437:LEU:C	2.62	0.43
1:E:1813:ASN:OD1	1:E:1813:ASN:N	2.45	0.43
1:A:852:GLN:NE2	1:A:892:GLN:OE1	2.52	0.43
1:E:228:ALA:O	1:E:233:GLN:NE2	2.51	0.43
2:F:2066:ASP:OD1	2:F:2066:ASP:C	2.60	0.43
1:B:1137:ALA:O	1:B:1138:ALA:HB3	2.19	0.43
1:D:193:ARG:NH1	1:D:195:SER:O	2.52	0.43
2:F:1931:ASP:C	2:F:1931:ASP:OD1	2.61	0.43
1:C:1380:LYS:O	1:C:1381:LEU:C	2.61	0.43
1:D:884:ALA:O	1:D:888:ASN:N	2.51	0.43
1:C:1774:TYR:OH	1:C:1848:TYR:OH	2.29	0.43
1:E:1836:ASP:OD1	1:E:1836:ASP:C	2.61	0.43
2:F:530:ASP:OD1	2:F:530:ASP:N	2.50	0.43
1:B:831:THR:OG1	1:B:832:ALA:N	2.52	0.42
1:A:1945:THR:OG1	1:A:1946:ASP:N	2.49	0.42
1:D:552:LYS:O	1:D:556:ASN:N	2.52	0.42
1:E:133:ASP:OD1	1:E:133:ASP:N	2.44	0.42
1:E:734:LEU:O	1:E:738:TYR:HB3	2.19	0.42
2:F:1718:ASP:OD1	2:F:1718:ASP:C	2.62	0.42
1:C:1684:THR:OG1	1:C:1685:ASN:N	2.52	0.42
1:C:912:TYR:CD2	1:C:912:TYR:C	2.96	0.42
1:D:1759:ASP:OD1	1:D:1759:ASP:C	2.62	0.42
1:E:93:ASN:OD1	1:E:93:ASN:N	2.48	0.42
1:D:1137:ALA:O	1:D:1139:ASN:N	2.52	0.42
1:E:271:ILE:O	1:E:272:GLU:C	2.61	0.42
2:F:336:ASN:HB2	2:F:348:PHE:HB3	2.02	0.42
1:E:533:ASP:OD1	1:E:533:ASP:N	2.47	0.42
2:F:1137:PHE:O	2:F:1139:ARG:N	2.52	0.42
2:F:1940:ILE:O	2:F:1941:SER:C	2.62	0.42
1:A:465:ASN:O	1:A:466:LEU:C	2.62	0.42
1:B:467:GLN:H	1:B:467:GLN:CD	2.27	0.42
1:B:1813:ASN:OD1	1:B:1813:ASN:N	2.48	0.42
1:E:858:HIS:O	1:E:859:LEU:C	2.58	0.42
2:F:1157:ASP:OD1	2:F:1157:ASP:C	2.63	0.42
1:D:2015:SER:OG	1:D:2016:LEU:N	2.49	0.42
1:E:1272:ASP:O	1:E:1274:ALA:N	2.52	0.42
1:A:884:ALA:O	1:A:888:ASN:N	2.52	0.42
1:C:1991:ASP:OD2	1:C:1993:LYS:NZ	2.47	0.42
1:D:1290:SER:C	1:D:1291:TYR:O	2.62	0.42
1:D:1333:TYR:CG	1:D:1334:ASN:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:ILE:HG23	1:E:428:VAL:HB	2.02	0.42
1:E:1589:ASN:OD1	1:E:1590:GLU:N	2.52	0.42
2:F:1751:LYS:NZ	2:F:1769:ASP:OD1	2.47	0.42
1:A:1104:ASP:N	1:A:1104:ASP:OD1	2.40	0.42
1:A:1242:GLU:O	1:A:1243:ASP:C	2.63	0.42
1:C:1257:ASP:N	1:C:1257:ASP:OD1	2.45	0.42
1:A:2454:MET:O	1:A:2455:ASN:C	2.62	0.41
1:C:503:ILE:HB	1:C:515:PHE:CZ	2.54	0.41
1:C:658:SER:O	1:C:659:TYR:C	2.61	0.41
1:D:196:GLY:O	1:D:445:ARG:NH2	2.52	0.41
1:D:1841:ALA:O	1:D:1842:GLN:CB	2.69	0.41
1:A:1057:MET:O	1:A:1058:ASP:C	2.61	0.41
1:A:2466:ASP:OD1	1:A:2466:ASP:N	2.51	0.41
1:B:2015:SER:OG	1:B:2016:LEU:N	2.52	0.41
1:D:658:SER:O	1:D:659:TYR:C	2.63	0.41
1:E:548:LYS:NZ	1:E:559:ASP:OD1	2.50	0.41
1:E:1133:ASP:OD2	1:E:1135:LYS:NZ	2.53	0.41
1:B:533:ASP:OD1	1:B:533:ASP:N	2.44	0.41
1:C:319:ASN:OD1	1:C:320:SER:N	2.53	0.41
1:D:241:ALA:O	1:D:243:ILE:N	2.54	0.41
1:E:1085:PHE:O	1:E:1086:GLU:C	2.64	0.41
1:B:614:GLU:OE2	1:B:633:LYS:NZ	2.42	0.41
1:B:1270:PHE:O	1:B:1271:ALA:C	2.60	0.41
1:B:2279:ALA:O	1:B:2280:TYR:C	2.63	0.41
1:D:2286:ASP:C	1:D:2286:ASP:OD1	2.64	0.41
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.42	0.41
1:D:2491:MET:HB3	1:D:2492:PRO:HD3	2.03	0.41
2:F:1528:ASP:OD1	2:F:1528:ASP:C	2.62	0.41
1:B:1683:ASP:N	1:B:1683:ASP:OD1	2.43	0.41
1:C:2266:TYR:O	1:C:2267:ASP:C	2.62	0.41
1:E:1654:THR:O	1:E:1655:HIS:C	2.60	0.41
1:E:1729:ASP:OD1	1:E:1730:LYS:N	2.53	0.41
1:E:2266:TYR:O	1:E:2267:ASP:C	2.61	0.41
1:C:1333:TYR:O	1:C:1335:GLY:N	2.53	0.41
1:D:1016:GLN:O	1:D:1017:PHE:C	2.62	0.41
1:E:1016:GLN:O	1:E:1017:PHE:C	2.62	0.41
2:F:574:SER:OG	2:F:575:ALA:N	2.53	0.41
2:F:1259:TRP:O	2:F:1318:ARG:HG2	2.21	0.41
1:B:1016:GLN:O	1:B:1017:PHE:C	2.62	0.41
1:C:714:TRP:CD2	1:C:762:LEU:HD22	2.55	0.41
1:C:2466:ASP:OD1	1:C:2466:ASP:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1977:ASP:OD1	1:D:1977:ASP:N	2.50	0.41
1:E:828:ASN:OD1	1:E:828:ASN:N	2.51	0.41
2:F:1442:THR:OG1	2:F:1443:ALA:N	2.54	0.41
2:F:1549:ASN:OD1	2:F:1549:ASN:N	2.50	0.41
1:C:542:SER:OG	1:C:543:THR:N	2.50	0.41
1:C:935:HIS:O	1:C:936:ALA:C	2.63	0.41
1:D:1840:VAL:C	1:D:1841:ALA:O	2.61	0.41
1:E:1242:GLU:O	1:E:1243:ASP:C	2.62	0.41
1:E:2081:GLU:O	1:E:2082:LYS:C	2.63	0.41
1:E:2255:ARG:O	1:E:2256:GLY:C	2.61	0.41
1:B:308:TYR:CZ	1:B:311:ASN:HA	2.56	0.41
1:B:832:ALA:O	1:B:833:GLU:HB2	2.21	0.41
1:B:1977:ASP:N	1:B:1977:ASP:OD1	2.42	0.41
1:C:315:THR:HA	1:C:316:PRO:HD2	1.93	0.41
1:C:1333:TYR:CD1	1:C:1360:ILE:HB	2.56	0.41
1:D:696:ILE:O	1:D:700:LEU:HG	2.21	0.41
1:D:1503:LYS:NZ	1:D:1508:GLU:OE2	2.48	0.41
1:E:766:TYR:CD2	1:E:771:ILE:HD11	2.56	0.41
1:E:912:TYR:CG	1:E:913:ALA:N	2.89	0.41
2:F:904:SER:O	2:F:905:ARG:C	2.62	0.41
2:F:1909:ASN:OD1	2:F:1909:ASN:N	2.53	0.41
1:A:858:HIS:O	1:A:859:LEU:C	2.61	0.40
1:B:597:ILE:HG13	1:B:598:HIS:CD2	2.55	0.40
1:B:1124:ARG:HD3	1:B:1144:TRP:CD2	2.56	0.40
1:D:2430:GLN:O	1:D:2487:PRO:HD2	2.20	0.40
1:A:971:LEU:O	1:A:972:LEU:HB2	2.21	0.40
1:A:1507:LYS:NZ	1:A:1538:ASP:OD2	2.37	0.40
1:A:2374:ASN:OD1	1:A:2374:ASN:C	2.64	0.40
1:B:990:ILE:O	1:B:992:SER:N	2.54	0.40
1:C:2013:PHE:O	1:C:2015:SER:N	2.54	0.40
1:D:581:ASN:OD1	1:D:581:ASN:C	2.64	0.40
1:E:1104:ASP:N	1:E:1104:ASP:OD1	2.43	0.40
2:F:618:SER:OG	2:F:619:GLY:N	2.51	0.40
2:F:1872:TYR:CD1	2:F:1872:TYR:N	2.90	0.40
1:B:1836:ASP:C	1:B:1836:ASP:OD1	2.61	0.40
1:C:1860:LEU:O	1:C:1862:ALA:N	2.55	0.40
1:D:1872:GLU:O	1:D:1873:ARG:C	2.63	0.40
1:E:1878:GLU:O	1:E:1879:ALA:C	2.63	0.40
1:A:1027:ARG:O	1:A:1028:TYR:C	2.62	0.40
1:C:368:LEU:HB3	1:C:381:THR:HB	2.04	0.40
1:C:872:THR:O	1:C:873:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:ILE:O	1:C:990:ILE:HG22	2.20	0.40
1:C:1513:ALA:O	1:C:1514:ASP:C	2.64	0.40
1:A:693:ALA:HB3	1:A:694:PRO:HD3	2.04	0.40
1:A:1836:ASP:OD1	1:A:1836:ASP:C	2.65	0.40
1:C:1333:TYR:O	1:C:1334:ASN:C	2.65	0.40
1:C:2382:ASP:OD1	1:C:2382:ASP:N	2.46	0.40
2:F:1347:ASP:C	2:F:1347:ASP:OD1	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2286/2516 (91%)	2220 (97%)	58 (2%)	8 (0%)	36	65
1	B	2286/2516 (91%)	2222 (97%)	61 (3%)	3 (0%)	48	78
1	C	2286/2516 (91%)	2228 (98%)	51 (2%)	7 (0%)	36	65
1	D	2286/2516 (91%)	2223 (97%)	57 (2%)	6 (0%)	36	65
1	E	2286/2516 (91%)	2230 (98%)	49 (2%)	7 (0%)	36	65
2	F	2143/2439 (88%)	2089 (98%)	50 (2%)	4 (0%)	43	71
All	All	13573/15019 (90%)	13212 (97%)	326 (2%)	35 (0%)	37	65

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	891	PRO
1	B	891	PRO
1	D	101	SER
1	D	891	PRO
1	D	1138	ALA

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Mol	Chain	Res	Type
2	F	956	GLN
2	F	2144	VAL
1	A	991	ALA
1	A	1711	PHE
1	B	2493	GLU
1	C	991	ALA
1	C	1292	GLN
1	C	1334	ASN
1	D	991	ALA
1	E	991	ALA
1	E	2154	TRP
1	C	1138	ALA
1	A	1273	MET
1	C	1758	MET
1	C	1953	ASN
1	D	1953	ASN
1	E	1953	ASN
1	A	2154	TRP
1	B	1334	ASN
1	D	1758	MET
1	E	101	SER
1	E	659	TYR
1	E	1758	MET
2	F	530	ASP
1	A	739	THR
1	A	890	ALA
1	A	215	ASP
1	C	215	ASP
1	E	215	ASP
2	F	801	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1960/2157 (91%)	1960 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1960/2157 (91%)	1960 (100%)	0	100	100
1	C	1960/2157 (91%)	1960 (100%)	0	100	100
1	D	1960/2157 (91%)	1960 (100%)	0	100	100
1	E	1960/2157 (91%)	1960 (100%)	0	100	100
2	F	1854/2109 (88%)	1854 (100%)	0	100	100
All	All	11654/12894 (90%)	11654 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	635	ASN
1	A	709	HIS
1	A	751	HIS
1	A	767	HIS
1	A	852	GLN
1	A	854	GLN
1	A	1240	GLN
1	A	1252	GLN
1	A	1671	ASN
1	A	1781	GLN
1	A	1808	HIS
1	A	1888	HIS
1	A	1951	GLN
1	A	2093	GLN
1	A	2248	GLN
1	A	2497	GLN
1	B	201	HIS
1	B	571	HIS
1	B	679	GLN
1	B	690	HIS
1	B	1189	GLN
1	B	1252	GLN
1	B	1265	GLN
1	B	1289	ASN
1	B	1520	GLN
1	B	1631	ASN
1	B	1671	ASN

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Mol	Chain	Res	Type
1	B	1685	ASN
1	B	1743	HIS
1	B	1787	GLN
1	B	1842	GLN
1	B	1888	HIS
1	B	1951	GLN
1	B	1965	GLN
1	B	1969	ASN
1	B	2057	GLN
1	B	2093	GLN
1	B	2348	ASN
1	C	295	GLN
1	C	312	GLN
1	C	361	ASN
1	C	394	ASN
1	C	749	GLN
1	C	757	GLN
1	C	1252	GLN
1	C	1361	HIS
1	C	1520	GLN
1	C	1599	GLN
1	C	1655	HIS
1	C	1842	GLN
1	C	1951	GLN
1	C	2032	GLN
1	C	2093	GLN
1	C	2223	GLN
1	C	2348	ASN
1	D	361	ASN
1	D	441	ASN
1	D	635	ASN
1	D	644	GLN
1	D	854	GLN
1	D	886	GLN
1	D	1132	ASN
1	D	1252	GLN
1	D	1293	GLN
1	D	1781	GLN
1	D	1842	GLN
1	D	1888	HIS
1	D	2093	GLN
1	D	2235	GLN

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Mol	Chain	Res	Type
1	D	2348	ASN
1	E	352	ASN
1	E	404	GLN
1	E	441	ASN
1	E	527	GLN
1	E	735	ASN
1	E	886	GLN
1	E	892	GLN
1	E	1132	ASN
1	E	1240	GLN
1	E	1252	GLN
1	E	1951	GLN
1	E	2181	GLN
1	E	2205	GLN
1	E	2348	ASN
1	E	2372	ASN
2	F	137	HIS
2	F	183	GLN
2	F	222	GLN
2	F	502	GLN
2	F	796	ASN
2	F	943	GLN
2	F	947	GLN
2	F	951	GLN
2	F	1050	GLN
2	F	1378	GLN
2	F	1459	ASN
2	F	1534	ASN
2	F	1535	GLN
2	F	1825	ASN
2	F	1935	HIS
2	F	1943	GLN
2	F	1992	ASN
2	F	2010	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

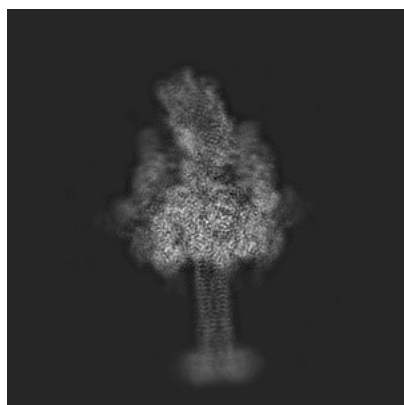
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10313. These allow visual inspection of the internal detail of the map and identification of artifacts.

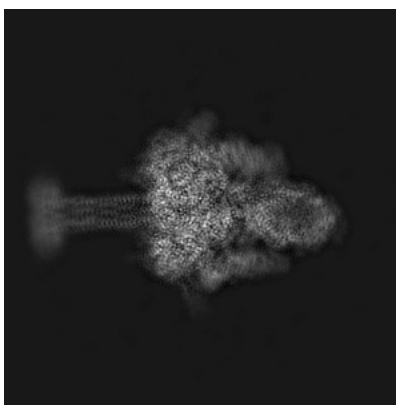
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

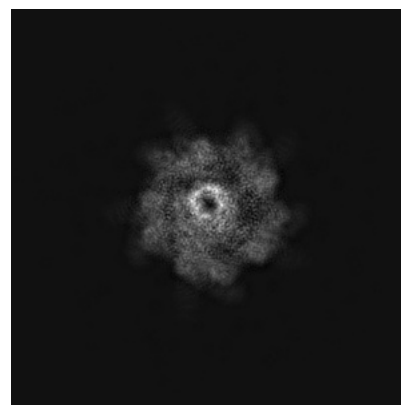
6.1.1 Primary map



X



Y

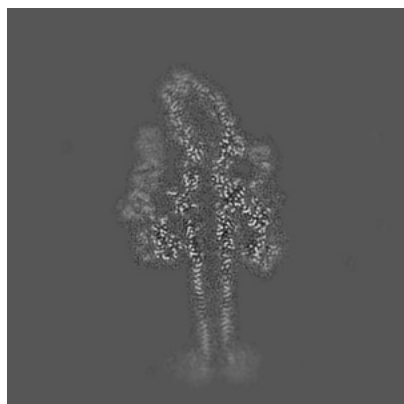


Z

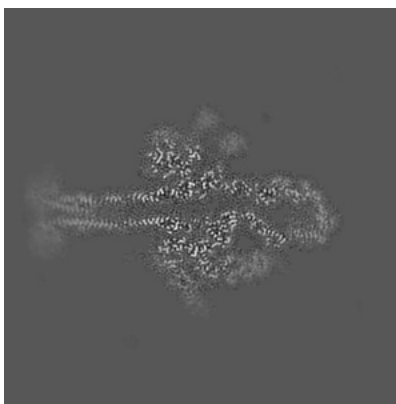
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

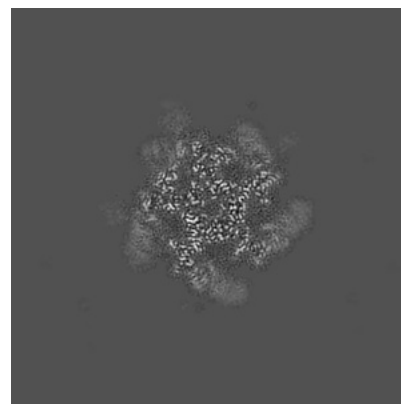
6.2.1 Primary map



X Index: 210



Y Index: 210

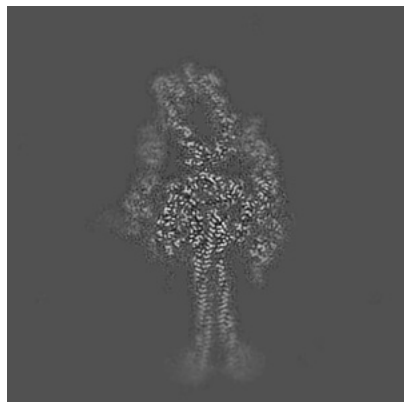


Z Index: 210

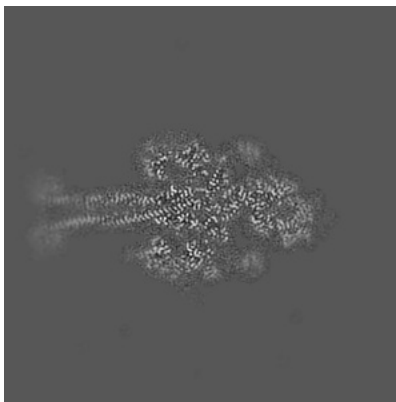
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

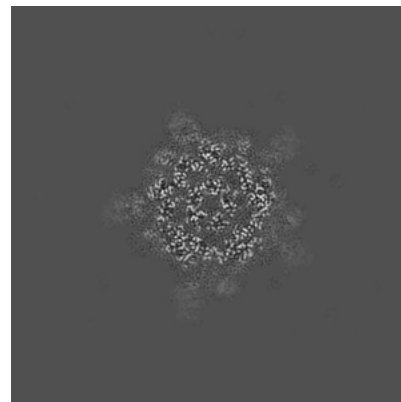
6.3.1 Primary map



X Index: 197



Y Index: 225

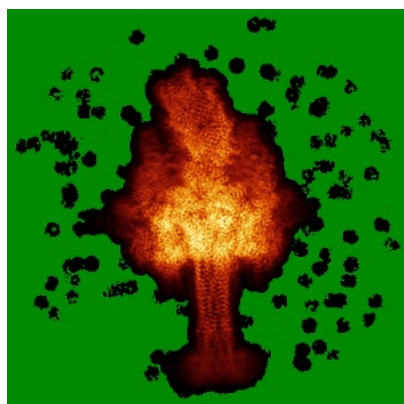


Z Index: 196

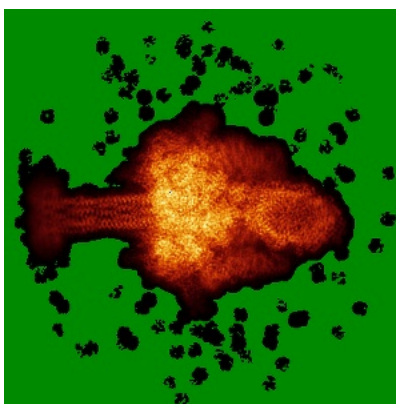
The images above show the largest variance slices of the map in three orthogonal directions.

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

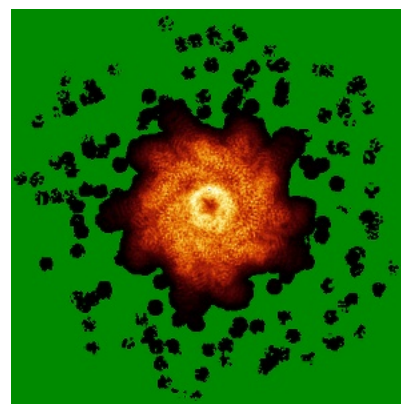
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

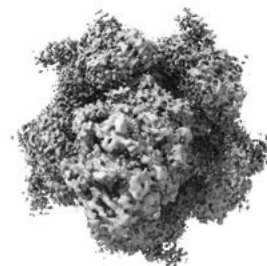
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

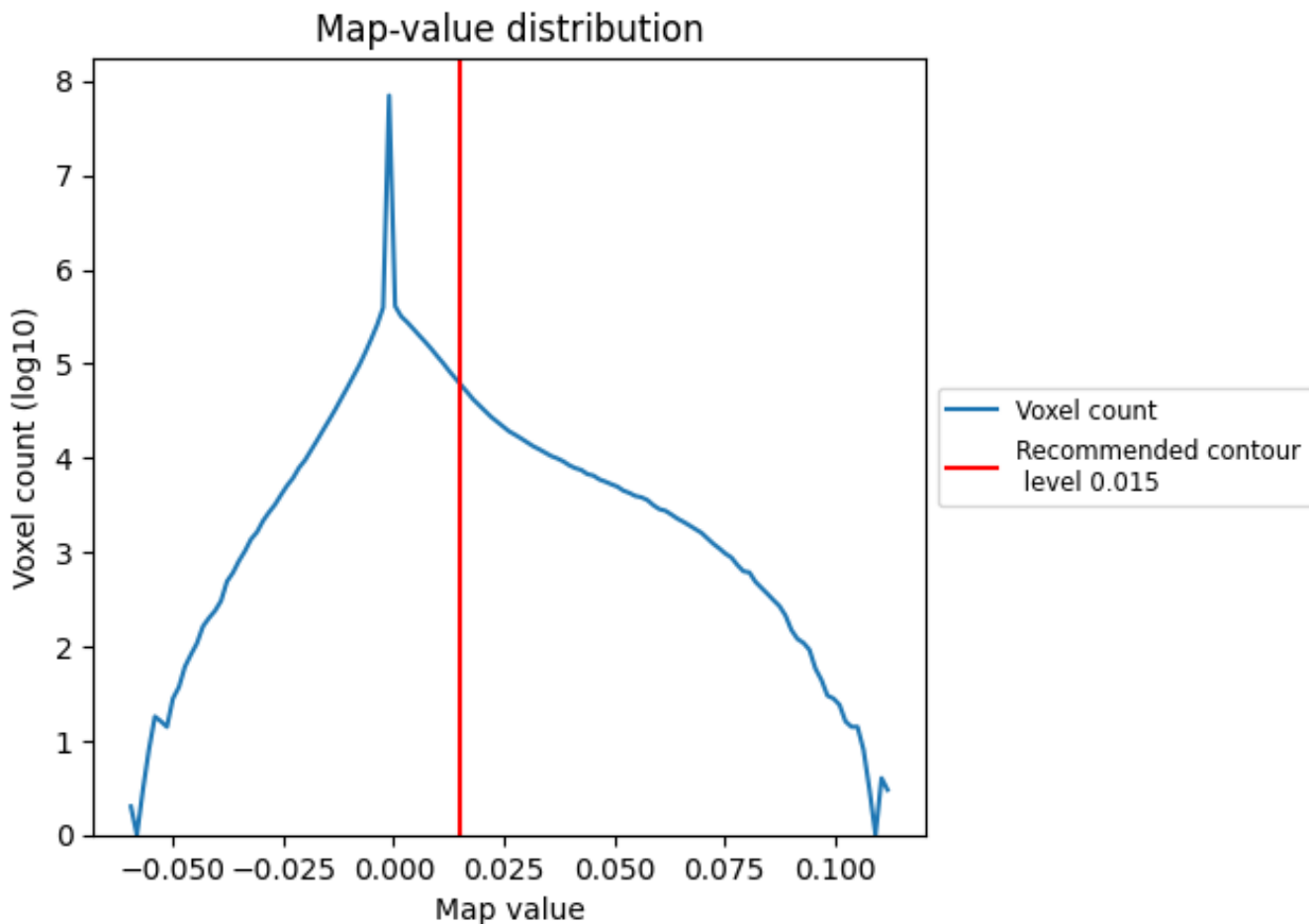
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

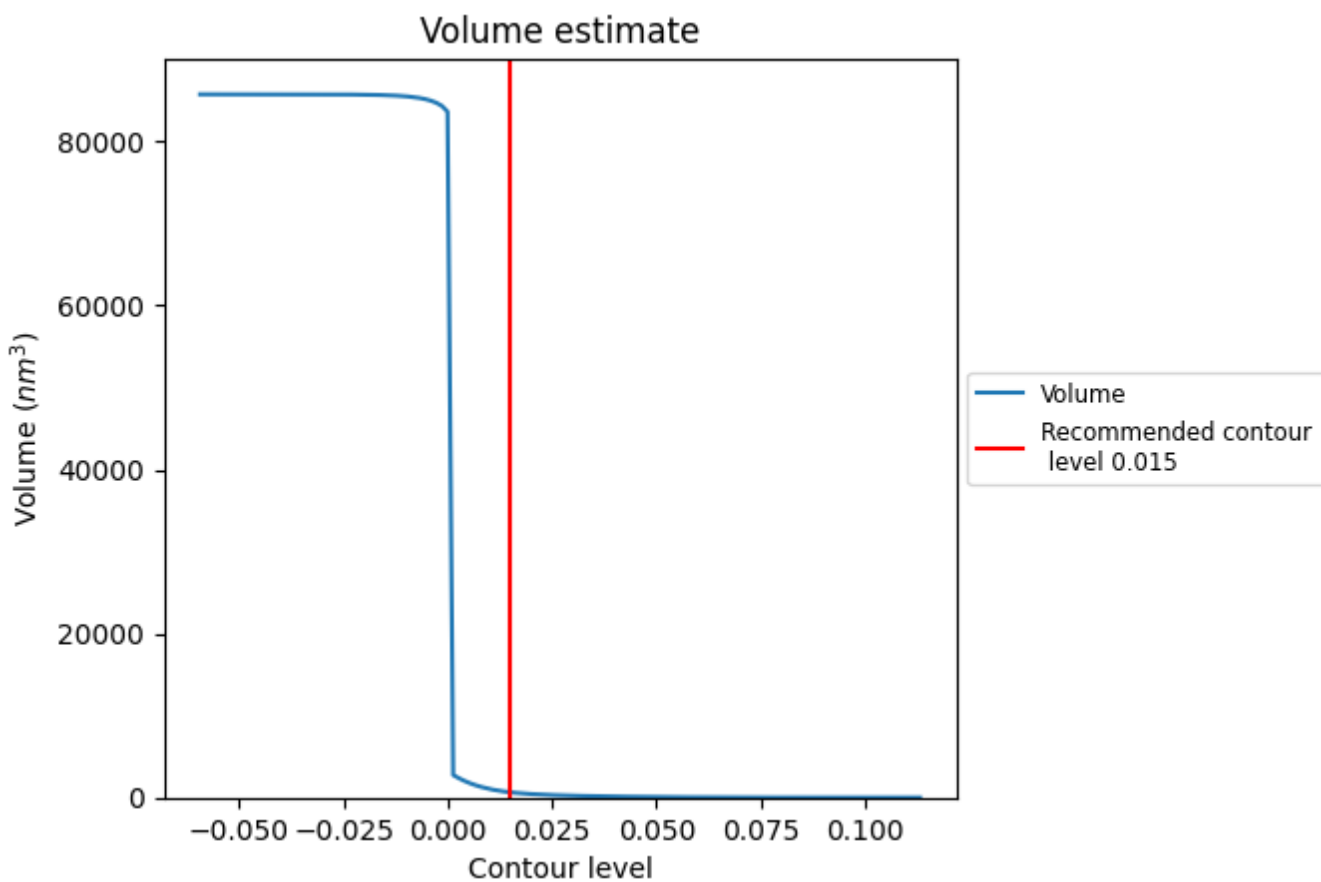
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

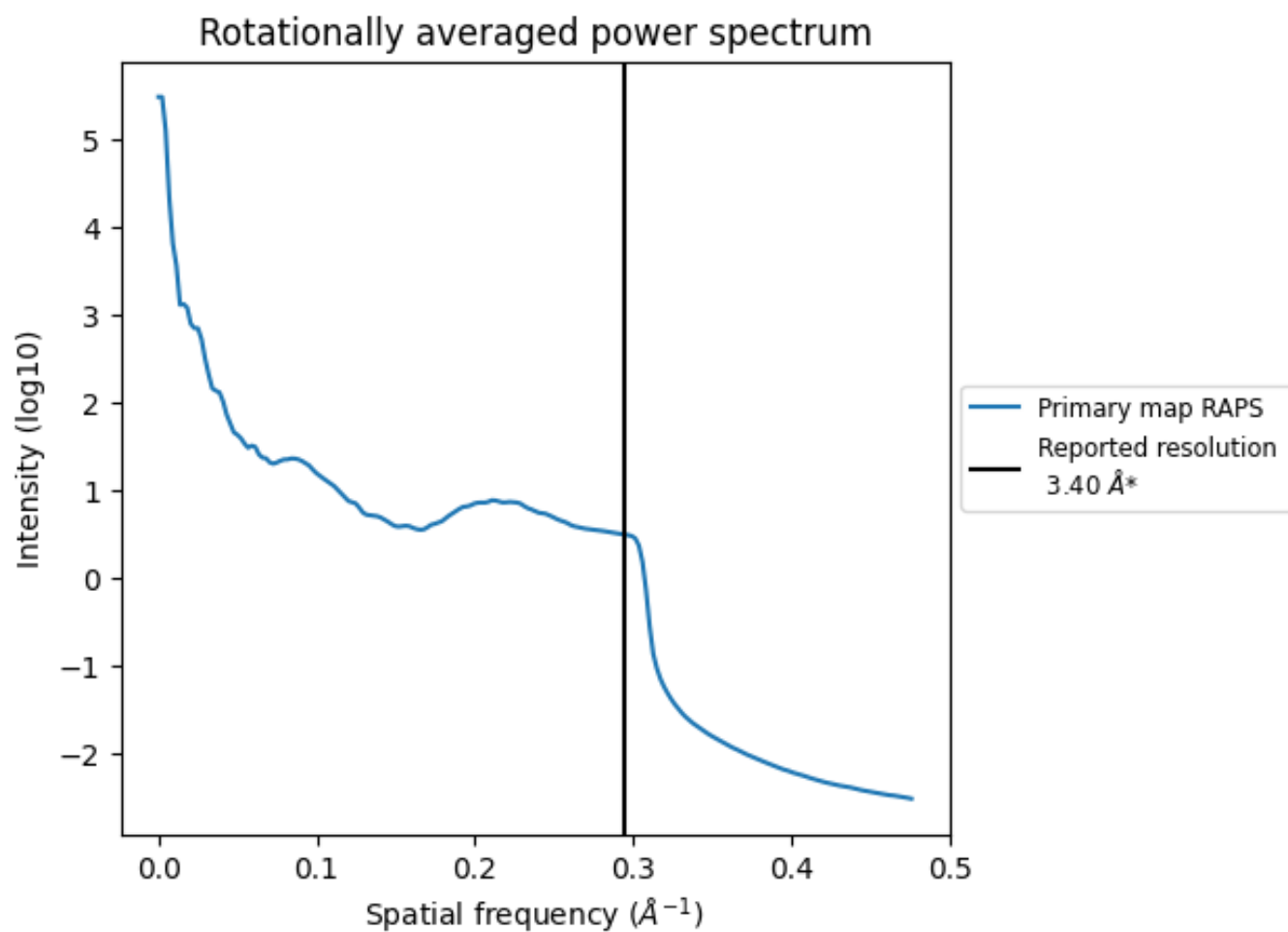
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 639 nm³; this corresponds to an approximate mass of 577 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

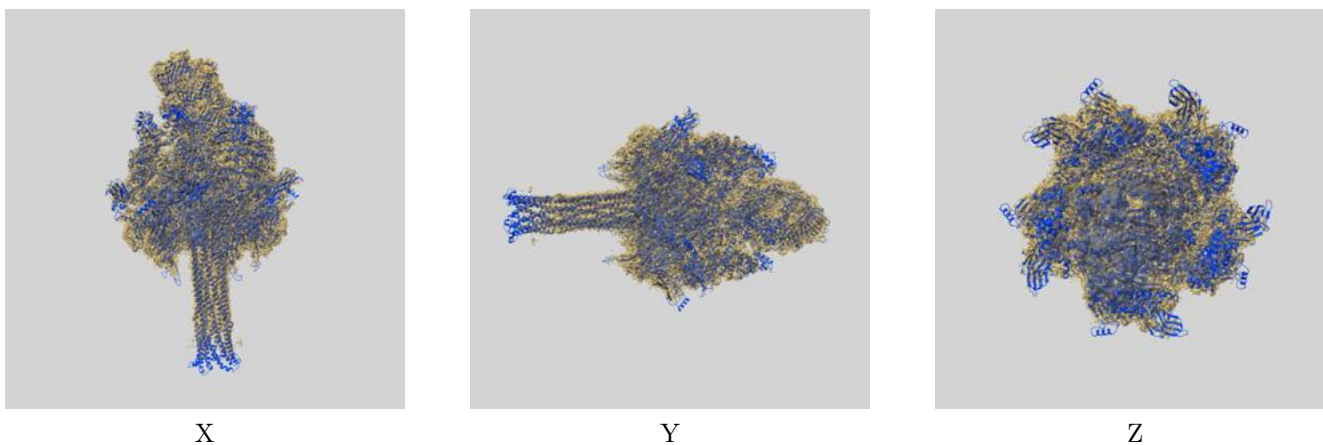
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

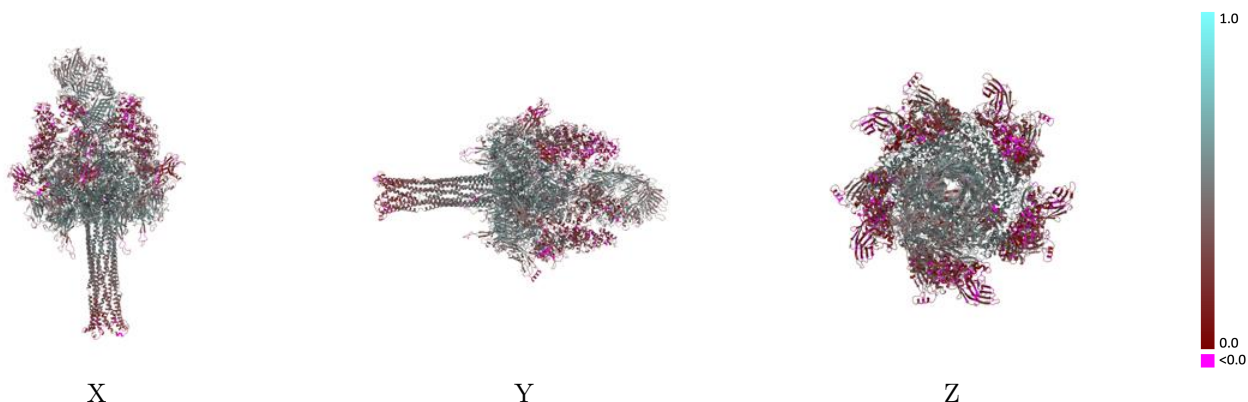
This section contains information regarding the fit between EMDB map EMD-10313 and PDB model 6SUF. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



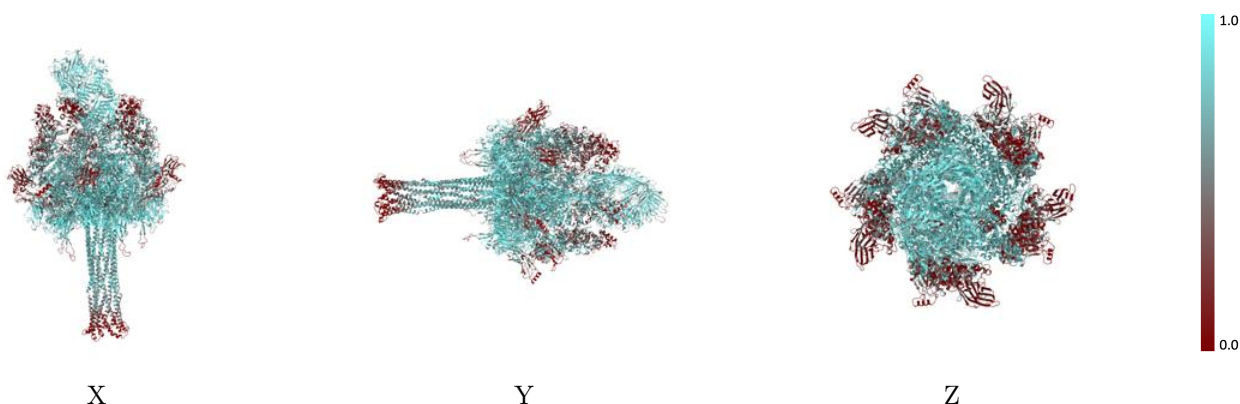
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



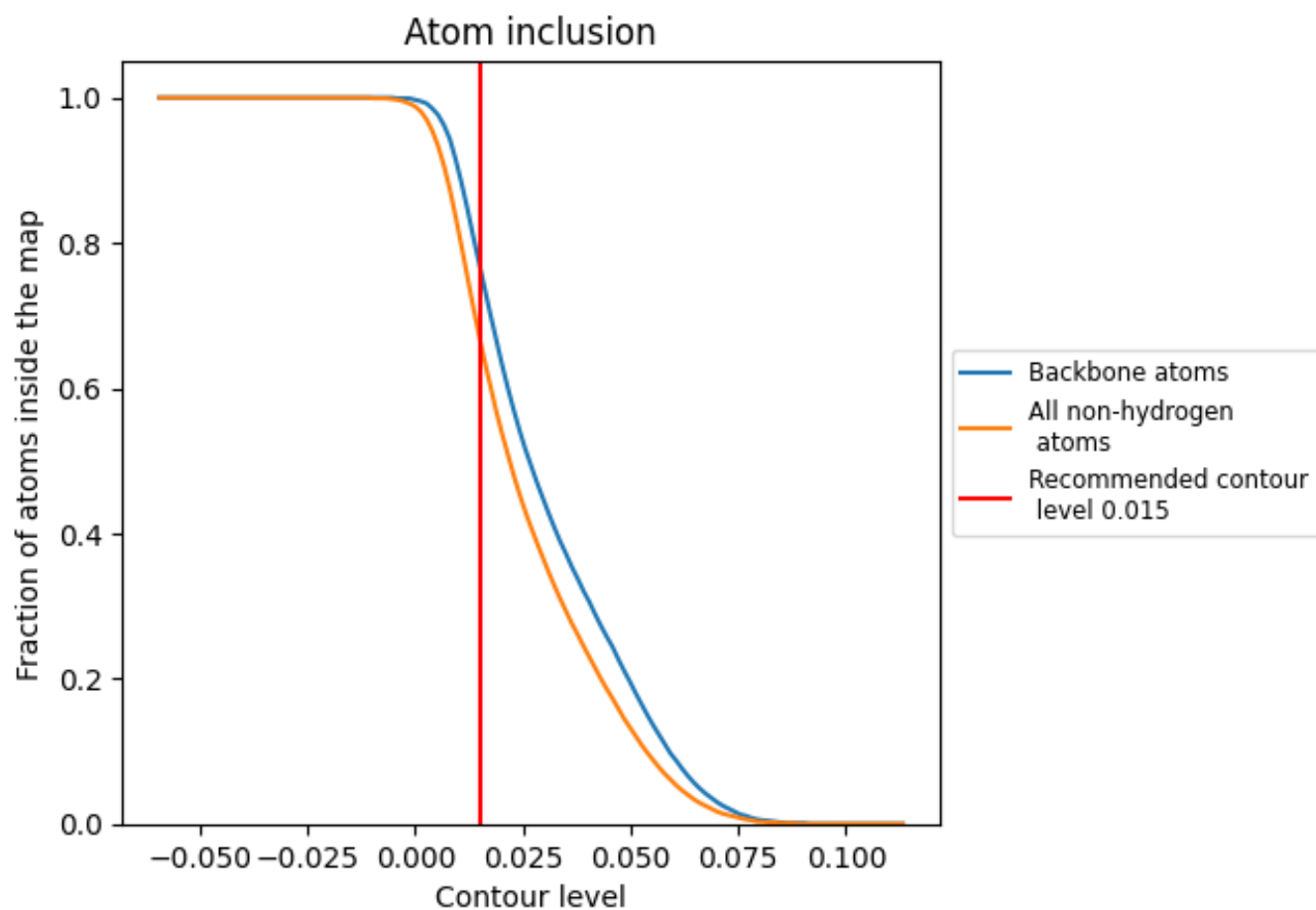
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).















9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.3960
A	 0.6460	 0.3870
B	 0.6360	 0.3810
C	 0.6390	 0.3850
D	 0.6310	 0.3760
E	 0.6650	 0.3940
F	 0.7970	 0.4590

