



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:52 AM EDT

PDB ID : 5LP7 / pdb_00005lp7
Title : Crystal structure of 3-Ketoacyl-CoA Thiolase (MmgA) from Bacillus subtilis.
Authors : Baker, G.E.; Race, P.R.
Deposited on : 2016-08-11
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

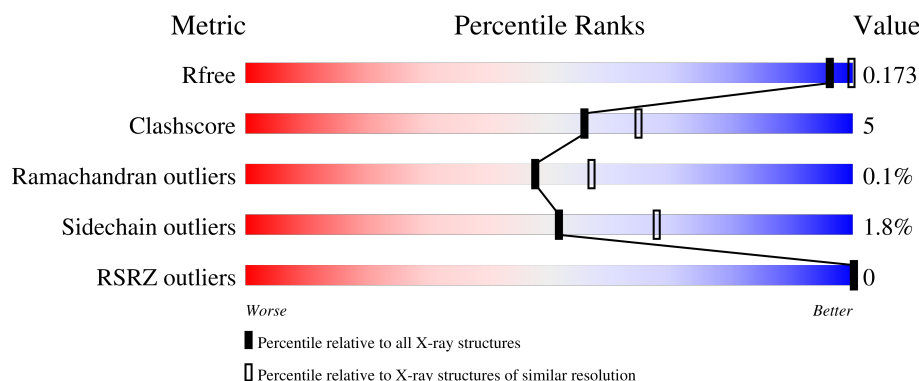
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



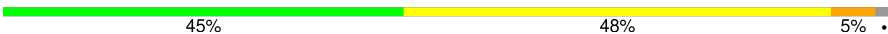
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	
1	B	393	
1	C	393	
1	D	393	
1	E	393	

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Mol	Chain	Length	Quality of chain
1	F	393	
1	G	393	
1	H	393	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	401	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22740 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	386	Total	C	N	O	S	0	0	0
			2733	1707	484	524	18			
1	E	386	Total	C	N	O	S	0	0	0
			2740	1702	490	531	17			
1	A	386	Total	C	N	O	S	0	0	0
			2730	1703	486	523	18			
1	B	388	Total	C	N	O	S	0	0	0
			2753	1716	491	528	18			
1	C	387	Total	C	N	O	S	0	0	0
			2749	1713	497	522	17			
1	F	380	Total	C	N	O	S	0	0	0
			2641	1648	468	507	18			
1	G	385	Total	C	N	O	S	0	0	0
			2728	1702	482	528	16			
1	D	386	Total	C	N	O	S	0	0	0
			2740	1710	491	521	18			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	82	Total	O	0	0
			82	82		
3	E	80	Total	O	0	0
			80	80		
3	A	110	Total	O	0	0
			110	110		
3	B	146	Total	O	0	0
			146	146		

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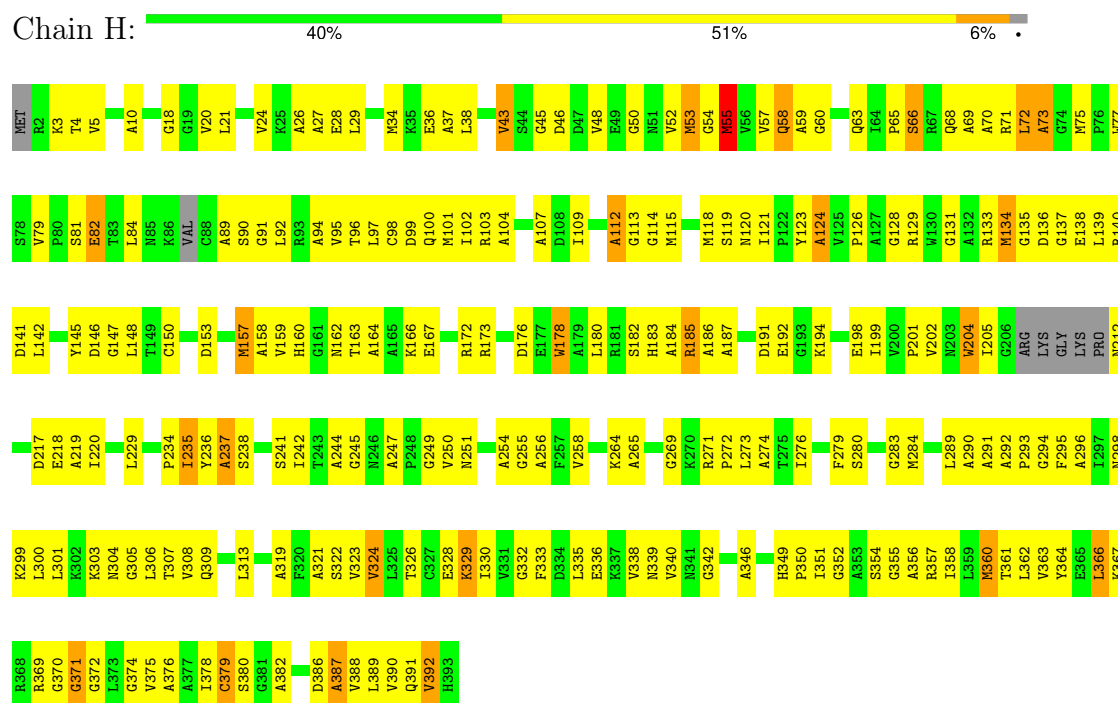
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	136	Total 136	O 136	0	0
3	F	80	Total 80	O 80	0	0
3	G	119	Total 119	O 119	0	0
3	D	125	Total 125	O 125	0	0

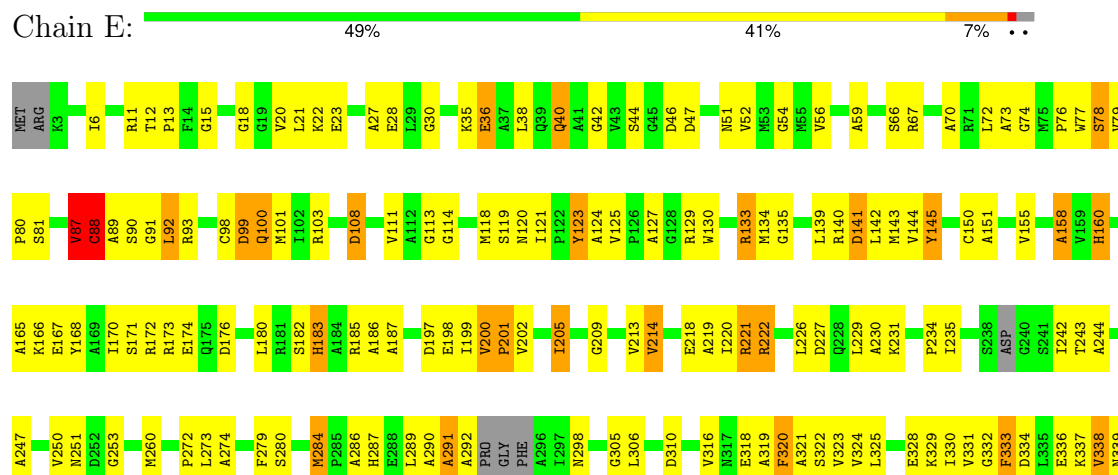
3 Residue-property plots

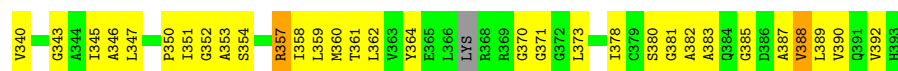
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Acetyl-CoA acetyltransferase



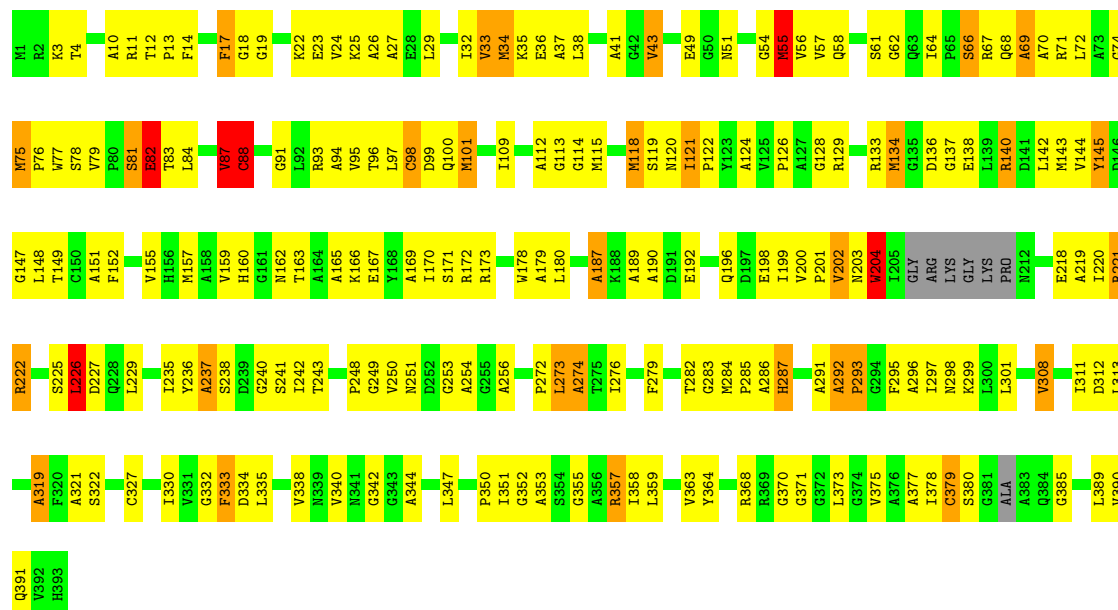
• Molecule 1: Acetyl-CoA acetyltransferase





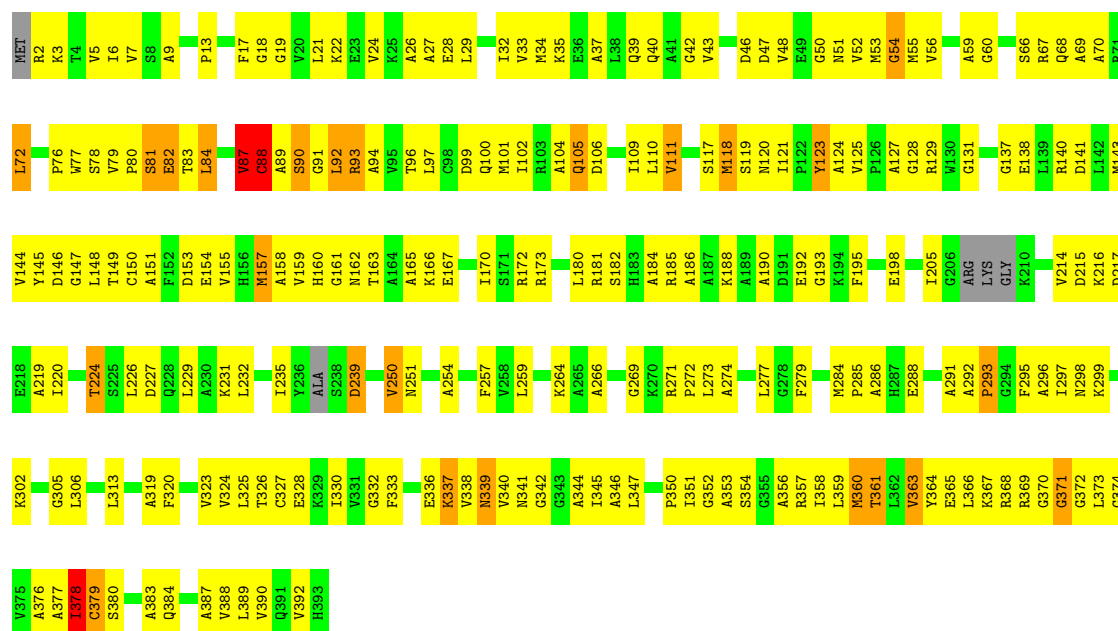
• Molecule 1: Acetyl-CoA acetyltransferase

Chain A: 45% 44% 8% ..



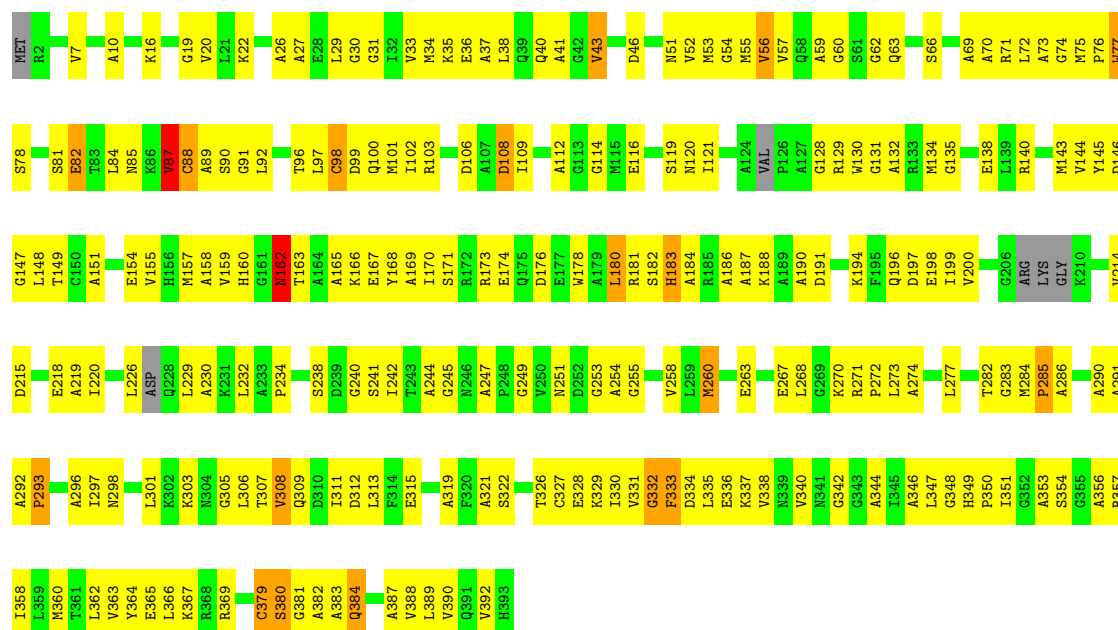
• Molecule 1: Acetyl-CoA acetyltransferase

Chain B: 41% 51% 6% ..



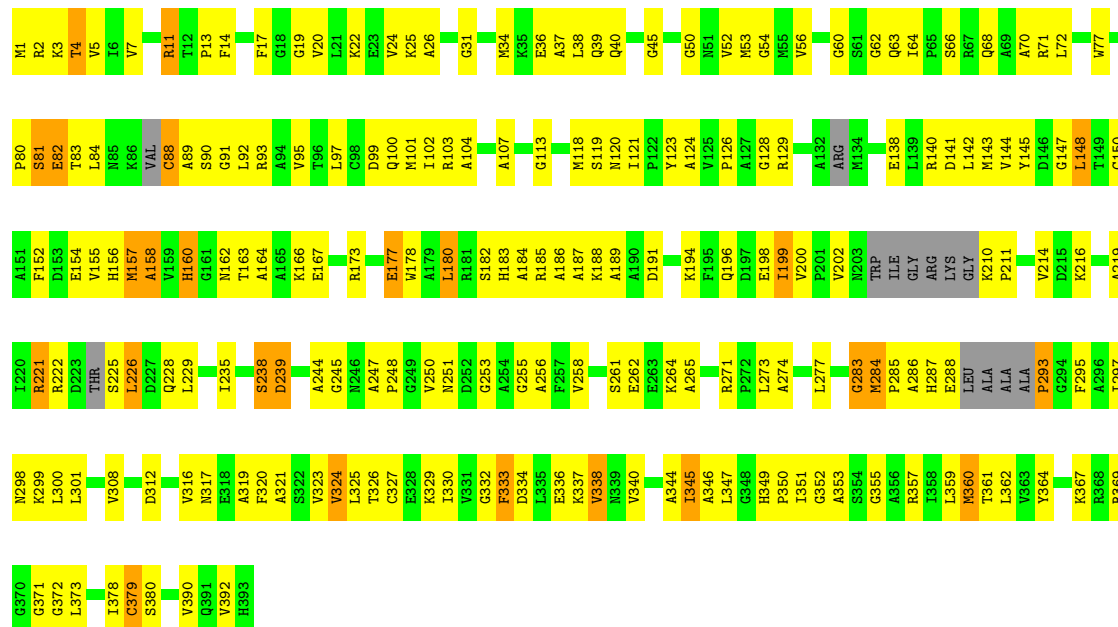
• Molecule 1: Acetyl-CoA acetyltransferase

Chain C: 41% 53% 5% ..



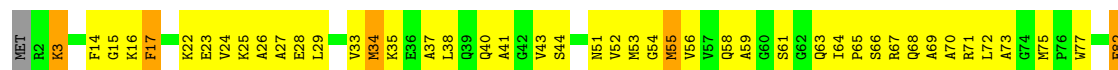
• Molecule 1: Acetyl-CoA acetyltransferase

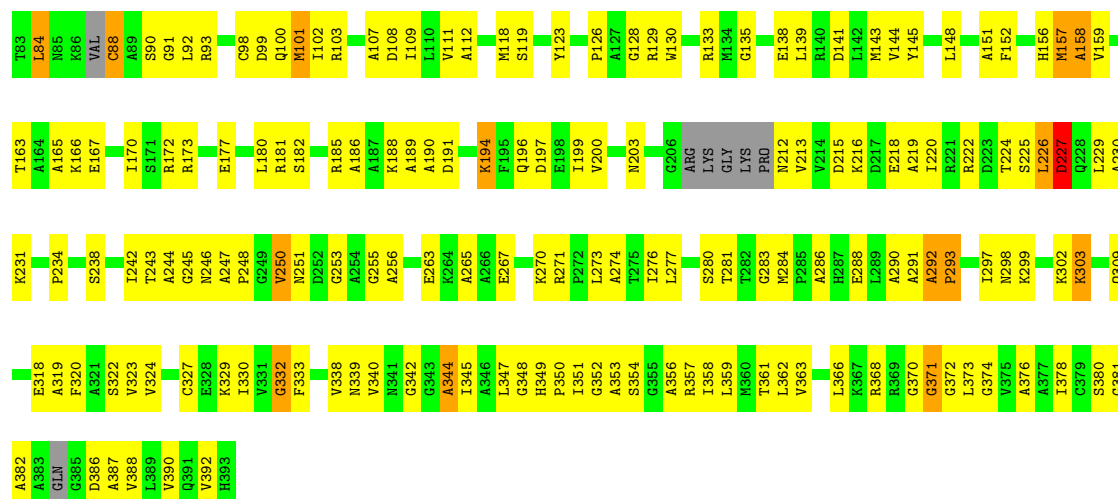
Chain F: 45% 45% 6% .



• Molecule 1: Acetyl-CoA acetyltransferase

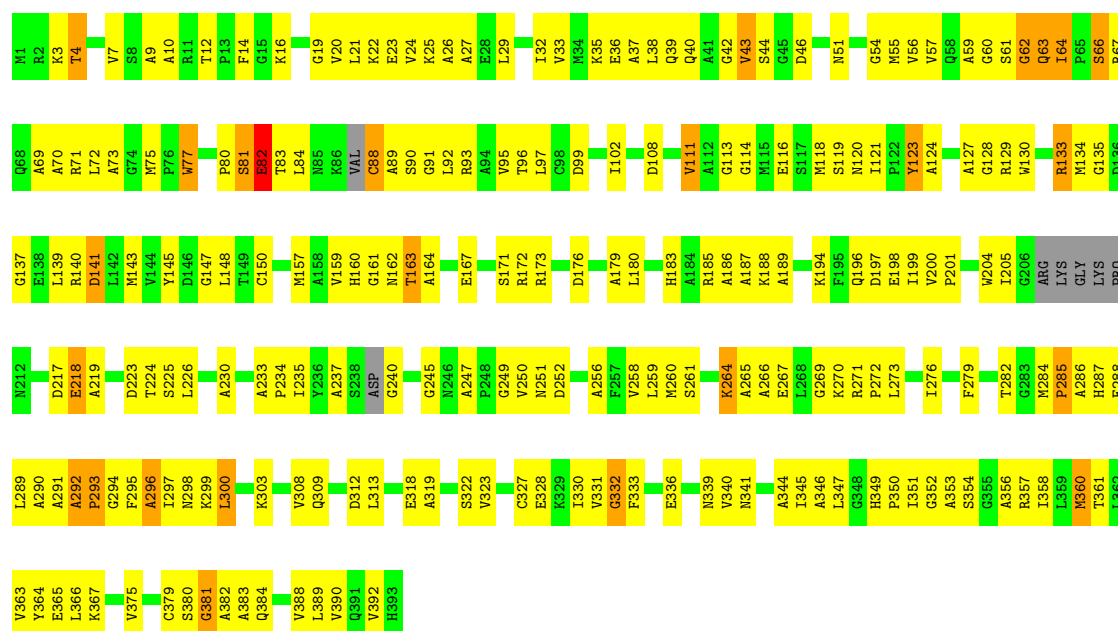
Chain G: 45% 48% 5% .





• Molecule 1: Acetyl-CoA acetyltransferase

Chain D: 41% 51% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.18Å 141.12Å 211.46Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	31.92 – 2.20 31.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (31.92-2.20) 98.3 (31.92-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.150 , 0.205 0.169 , 0.173	Depositor DCC
R_{free} test set	7962 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 8.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.426 for h,-k,-l	Xtriage
Reported twinning fraction	0.425 for H, K, L 0.575 for -h,-k,l	Depositor
Outliers	5 of 161152 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22740	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2.85	179/2769 (6.5%)	2.22	110/3742 (2.9%)
1	B	2.78	201/2792 (7.2%)	1.99	97/3773 (2.6%)
1	C	2.70	205/2787 (7.4%)	1.85	84/3762 (2.2%)
1	D	2.75	187/2778 (6.7%)	1.92	79/3753 (2.1%)
1	E	2.72	169/2777 (6.1%)	1.95	73/3756 (1.9%)
1	F	2.68	163/2675 (6.1%)	1.98	92/3614 (2.5%)
1	G	2.70	178/2766 (6.4%)	1.89	75/3733 (2.0%)
1	H	2.58	193/2772 (7.0%)	1.96	80/3741 (2.1%)
All	All	2.72	1475/22116 (6.7%)	1.97	690/29874 (2.3%)

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	6
1	C	0	4
1	D	0	6
1	E	0	4
1	F	0	4
1	G	0	3
1	H	0	2
All	All	0	38

All (1475) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	307	THR	C-N	-40.01	0.90	1.34
1	B	87	VAL	C-N	-33.82	0.91	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	101	MET	C-N	-32.61	0.92	1.33
1	A	87	VAL	C-N	-31.64	0.93	1.33
1	E	99	ASP	C-N	-31.29	0.93	1.33
1	F	225	SER	C-N	-31.07	0.94	1.33
1	B	91	GLY	C-N	-30.88	0.91	1.33
1	B	2	ARG	C-N	-30.13	0.94	1.33
1	D	22	LYS	C-N	-29.82	0.88	1.33
1	E	87	VAL	C-N	-28.86	0.97	1.33
1	B	336	GLU	C-N	-28.54	0.90	1.33
1	D	162	ASN	C-N	-27.76	1.00	1.33
1	A	240	GLY	C-N	-27.36	0.92	1.33
1	H	360	MET	C-N	-26.59	0.97	1.34
1	D	62	GLY	C-N	26.53	1.70	1.33
1	F	155	VAL	C-N	-26.23	0.99	1.33
1	A	225	SER	C-N	-25.83	1.02	1.33
1	F	91	GLY	C-N	-25.49	0.96	1.33
1	D	23	GLU	C-N	-25.47	0.95	1.33
1	A	120	ASN	C-N	-24.62	1.05	1.33
1	G	165	ALA	C-N	-24.57	0.99	1.33
1	E	273	LEU	C-N	-24.13	1.03	1.33
1	E	91	GLY	C-N	-24.00	1.01	1.33
1	G	23	GLU	C-N	-23.96	1.01	1.33
1	F	360	MET	C-N	-23.54	0.99	1.33
1	D	63	GLN	C-N	-22.74	1.07	1.33
1	C	270	LYS	C-N	-22.63	0.94	1.33
1	C	360	MET	C-N	-21.58	1.00	1.33
1	A	241	SER	C-N	-21.17	1.07	1.33
1	D	270	LYS	C-N	-20.80	1.06	1.33
1	A	272	PRO	C-N	-20.64	1.07	1.33
1	A	82	GLU	C-N	-20.41	1.07	1.33
1	A	222	ARG	C-N	-20.23	1.07	1.33
1	E	230	ALA	C-N	-20.19	1.06	1.33
1	G	166	LYS	C-N	-19.77	1.07	1.34
1	F	154	GLU	C-N	19.61	1.60	1.33
1	G	34	MET	C-N	-19.31	1.09	1.33
1	D	42	GLY	C-N	-19.22	1.09	1.33
1	F	226	LEU	C-N	-18.85	1.10	1.33
1	C	273	LEU	C-N	-18.76	1.09	1.33
1	E	221	ARG	C-N	-18.43	1.07	1.33
1	H	205	ILE	C-N	-18.33	1.07	1.33
1	F	211	PRO	C-N	-17.80	1.06	1.33
1	G	63	GLN	C-N	-17.60	1.13	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	224	THR	C-N	-17.58	1.12	1.33
1	A	389	LEU	C-N	-17.31	1.08	1.33
1	E	337	LYS	C-N	-17.27	1.10	1.33
1	H	124	ALA	C-N	-16.84	1.14	1.33
1	C	334	ASP	C-N	-16.59	1.11	1.33
1	A	273	LEU	C-N	-16.59	1.13	1.33
1	E	222	ARG	C-N	-15.94	1.11	1.33
1	H	305	GLY	C-N	-15.85	1.10	1.33
1	E	360	MET	C-N	-15.82	1.13	1.33
1	E	98	CYS	C-N	-15.64	1.14	1.33
1	F	145	TYR	C-N	15.42	1.55	1.33
1	G	283	GLY	C-N	-15.33	1.15	1.33
1	H	284	MET	C-N	15.28	1.54	1.33
1	A	226	LEU	C-N	-15.19	1.14	1.33
1	D	226	LEU	C-N	-14.99	1.13	1.33
1	A	75	MET	C-N	14.86	1.52	1.33
1	A	83	THR	C-N	-14.85	1.13	1.33
1	A	33	VAL	C-N	14.85	1.54	1.34
1	F	337	LYS	C-N	-14.80	1.15	1.33
1	C	389	LEU	C-N	-14.75	1.10	1.33
1	A	333	PHE	C-N	14.68	1.54	1.33
1	G	54	GLY	C-N	-14.60	1.15	1.33
1	A	84	LEU	C-N	-14.57	1.14	1.33
1	A	221	ARG	C-N	-14.50	1.07	1.33
1	B	42	GLY	C-N	-14.38	1.15	1.33
1	G	270	LYS	C-N	-14.24	1.12	1.33
1	E	174	GLU	C-N	-13.88	1.15	1.33
1	D	92	LEU	C-N	-13.71	1.15	1.34
1	D	82	GLU	C-N	-13.67	1.16	1.33
1	G	33	VAL	C-N	-13.58	1.15	1.33
1	A	121	ILE	C-N	-13.54	1.17	1.33
1	F	222	ARG	C-N	13.52	1.52	1.33
1	F	338	VAL	C-N	-13.31	1.14	1.33
1	B	389	LEU	C-N	-13.15	1.13	1.33
1	B	216	LYS	C-N	-13.11	1.14	1.33
1	H	367	LYS	C-N	-12.99	1.16	1.34
1	E	231	LYS	C-N	-12.97	1.16	1.33
1	E	142	LEU	C-N	-12.92	1.16	1.33
1	C	306	LEU	C-N	-12.91	1.15	1.33
1	E	92	LEU	C-N	-12.64	1.17	1.34
1	H	272	PRO	C-N	-12.63	1.17	1.33
1	G	167	GLU	C-N	-12.60	1.15	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	163	THR	C-N	-12.59	1.17	1.33
1	H	283	GLY	C-N	-12.28	1.17	1.32
1	E	141	ASP	C-N	-12.14	1.17	1.34
1	F	361	THR	C-N	-12.10	1.17	1.33
1	G	22	LYS	C-N	-11.86	1.17	1.33
1	C	332	GLY	C-N	11.81	1.49	1.33
1	E	272	PRO	C-N	-11.70	1.18	1.33
1	A	237	ALA	C-N	-11.54	1.17	1.33
1	F	144	VAL	C-N	-11.42	1.17	1.33
1	A	334	ASP	C-N	-11.28	1.18	1.33
1	H	55	MET	C-O	-11.08	1.10	1.23
1	H	362	LEU	C-N	-11.03	1.20	1.33
1	H	363	VAL	C-N	-11.01	1.19	1.33
1	C	271	ARG	C-N	-10.97	1.19	1.33
1	B	378	ILE	C-N	-10.92	1.18	1.33
1	H	306	LEU	C-N	-10.89	1.18	1.33
1	B	227	ASP	C-N	10.88	1.48	1.33
1	C	46	ASP	C-N	-10.85	1.19	1.33
1	B	250	VAL	C-N	-10.83	1.19	1.33
1	F	202	VAL	C-N	-10.65	1.18	1.33
1	C	72	LEU	C-O	-10.28	1.11	1.24
1	D	4	THR	C-N	-10.25	1.17	1.33
1	E	173	ARG	C-N	-10.24	1.20	1.33
1	F	129	ARG	C-O	-10.20	1.12	1.24
1	D	201	PRO	N-CD	10.16	1.61	1.47
1	C	333	PHE	C-N	10.14	1.48	1.33
1	A	129	ARG	C-O	-10.03	1.12	1.24
1	H	133	ARG	C-N	-9.99	1.21	1.33
1	B	306	LEU	C-N	-9.94	1.19	1.33
1	F	221	ARG	C-N	-9.91	1.19	1.33
1	B	332	GLY	C-N	9.85	1.46	1.33
1	H	4	THR	C-N	-9.81	1.18	1.33
1	B	350	PRO	C-O	-9.76	1.16	1.24
1	H	352	GLY	C-O	-9.70	1.13	1.24
1	C	74	GLY	C-N	-9.66	1.17	1.33
1	F	82	GLU	C-N	-9.59	1.20	1.33
1	B	163	THR	C-O	-9.57	1.12	1.24
1	B	217	ASP	C-N	-9.52	1.19	1.33
1	G	227	ASP	C-N	-9.49	1.21	1.33
1	G	88	CYS	C-N	-9.45	1.19	1.33
1	C	242	ILE	C-O	-9.43	1.13	1.24
1	C	383	ALA	C-N	-9.38	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	LEU	C-O	-9.26	1.11	1.24
1	E	129	ARG	C-O	-9.25	1.13	1.24
1	B	198	GLU	C-O	-9.24	1.12	1.24
1	B	377	ALA	C-N	-9.24	1.21	1.33
1	G	362	LEU	C-N	-9.21	1.22	1.33
1	G	327	CYS	C-N	9.10	1.45	1.33
1	A	43	VAL	C-N	-9.03	1.21	1.33
1	B	388	VAL	C-N	-8.95	1.21	1.33
1	B	333	PHE	C-N	-8.85	1.20	1.33
1	B	145	TYR	C-O	-8.84	1.14	1.24
1	B	88	CYS	C-N	8.83	1.46	1.33
1	F	92	LEU	C-N	-8.80	1.22	1.34
1	D	91	GLY	C-N	-8.71	1.21	1.33
1	D	293	PRO	C-O	-8.70	1.12	1.24
1	B	337	LYS	C-N	-8.64	1.22	1.33
1	A	55	MET	C-N	-8.60	1.23	1.33
1	G	332	GLY	C-N	8.58	1.45	1.33
1	B	88	CYS	C-O	-8.58	1.13	1.24
1	D	69	ALA	C-O	-8.57	1.14	1.24
1	A	55	MET	C-O	-8.56	1.13	1.24
1	G	284	MET	C-O	-8.55	1.16	1.24
1	G	93	ARG	C-O	-8.47	1.14	1.24
1	F	145	TYR	C-O	-8.45	1.14	1.24
1	A	282	THR	C-O	-8.41	1.13	1.23
1	B	97	LEU	C-N	-8.40	1.23	1.33
1	H	3	LYS	C-N	-8.37	1.22	1.33
1	E	388	VAL	C-O	-8.37	1.15	1.24
1	A	292	ALA	C-O	-8.36	1.16	1.24
1	A	99	ASP	C-O	-8.35	1.14	1.24
1	H	292	ALA	C-O	-8.34	1.16	1.24
1	A	159	VAL	C-O	-8.31	1.14	1.24
1	G	273	LEU	C-N	-8.28	1.23	1.33
1	D	290	ALA	C-O	-8.28	1.13	1.24
1	B	220	ILE	C-O	-8.23	1.15	1.24
1	F	34	MET	C-O	-8.23	1.14	1.24
1	E	81	SER	C-N	-8.22	1.23	1.33
1	C	71	ARG	C-O	-8.21	1.14	1.24
1	A	254	ALA	C-O	-8.20	1.14	1.23
1	F	333	PHE	C-N	-8.14	1.22	1.33
1	E	35	LYS	C-O	-8.13	1.14	1.24
1	D	3	LYS	C-N	-8.11	1.22	1.33
1	A	119	SER	C-O	-8.09	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	ALA	C-O	-8.07	1.16	1.24
1	A	38	LEU	C-O	-8.05	1.14	1.24
1	A	198	GLU	C-O	-8.05	1.14	1.24
1	H	301	LEU	C-O	-8.02	1.14	1.24
1	G	247	ALA	C-O	-8.01	1.15	1.24
1	F	200	VAL	N-CA	-8.00	1.39	1.46
1	A	340	VAL	C-O	-7.97	1.13	1.24
1	H	66	SER	C-O	-7.97	1.14	1.24
1	C	116	GLU	C-O	-7.96	1.14	1.23
1	C	290	ALA	C-O	-7.91	1.14	1.24
1	B	363	VAL	C-O	-7.91	1.15	1.24
1	A	56	VAL	C-O	-7.91	1.16	1.24
1	G	271	ARG	C-N	-7.90	1.23	1.33
1	B	119	SER	C-O	-7.89	1.14	1.24
1	C	305	GLY	C-N	-7.88	1.22	1.33
1	B	77	TRP	C-O	-7.87	1.14	1.24
1	B	361	THR	C-N	-7.87	1.44	1.33
1	C	159	VAL	C-O	-7.86	1.15	1.24
1	C	145	TYR	C-O	-7.85	1.15	1.24
1	B	291	ALA	C-O	-7.84	1.15	1.24
1	A	284	MET	C-O	-7.83	1.17	1.24
1	H	82	GLU	C-N	-7.79	1.44	1.33
1	H	284	MET	C-O	-7.77	1.17	1.24
1	H	346	ALA	C-O	-7.76	1.15	1.24
1	C	99	ASP	C-O	-7.74	1.15	1.24
1	B	344	ALA	C-O	-7.72	1.14	1.24
1	B	131	GLY	C-O	-7.70	1.15	1.24
1	H	296	ALA	C-O	-7.69	1.15	1.24
1	E	56	VAL	C-O	-7.69	1.15	1.24
1	B	352	GLY	C-O	-7.68	1.14	1.23
1	B	26	ALA	C-O	-7.67	1.15	1.24
1	A	378	ILE	C-O	-7.67	1.16	1.24
1	B	378	ILE	C-O	-7.67	1.15	1.24
1	G	225	SER	C-N	-7.66	1.24	1.33
1	B	392	VAL	C-O	-7.66	1.15	1.24
1	H	81	SER	C-N	-7.65	1.24	1.33
1	B	22	LYS	C-O	-7.65	1.15	1.24
1	H	367	LYS	C-O	-7.63	1.15	1.24
1	E	143	MET	C-O	-7.63	1.15	1.24
1	F	371	GLY	C-O	-7.63	1.16	1.23
1	D	352	GLY	C-O	-7.62	1.14	1.23
1	C	91	GLY	C-O	-7.61	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	345	ILE	C-O	-7.61	1.15	1.24
1	E	27	ALA	C-O	-7.60	1.15	1.24
1	C	358	ILE	C-O	-7.59	1.15	1.24
1	G	381	GLY	C-O	-7.59	1.16	1.23
1	B	97	LEU	C-O	-7.58	1.15	1.24
1	G	363	VAL	C-O	-7.56	1.15	1.24
1	E	99	ASP	C-O	-7.53	1.15	1.24
1	B	274	ALA	C-O	-7.53	1.15	1.23
1	A	238	SER	C-N	-7.53	1.23	1.33
1	H	129	ARG	C-O	-7.52	1.15	1.24
1	H	357	ARG	C-O	-7.52	1.15	1.24
1	E	119	SER	C-O	-7.52	1.14	1.24
1	A	134	MET	C-O	-7.52	1.13	1.23
1	F	350	PRO	C-O	-7.51	1.18	1.24
1	G	159	VAL	C-O	-7.50	1.15	1.24
1	C	147	GLY	C-O	-7.49	1.13	1.23
1	G	99	ASP	C-O	-7.49	1.15	1.24
1	C	360	MET	C-O	-7.48	1.15	1.24
1	F	99	ASP	C-O	-7.48	1.15	1.24
1	D	33	VAL	C-O	-7.48	1.15	1.24
1	D	72	LEU	C-O	-7.48	1.14	1.24
1	F	392	VAL	C-O	-7.48	1.15	1.24
1	E	305	GLY	C-N	-7.48	1.22	1.33
1	E	352	GLY	C-O	-7.48	1.14	1.23
1	A	298	ASN	C-O	-7.47	1.15	1.24
1	C	296	ALA	C-O	-7.46	1.15	1.24
1	G	250	VAL	C-O	-7.45	1.16	1.24
1	A	203	ASN	C-N	-7.45	1.24	1.33
1	A	138	GLU	C-O	-7.45	1.15	1.23
1	G	37	ALA	C-O	-7.45	1.15	1.24
1	G	151	ALA	C-O	-7.44	1.14	1.24
1	B	217	ASP	C-O	-7.43	1.15	1.24
1	B	93	ARG	C-O	-7.42	1.15	1.24
1	E	87	VAL	N-CA	-7.42	1.37	1.46
1	G	54	GLY	C-O	-7.41	1.16	1.23
1	E	145	TYR	C-O	-7.40	1.15	1.24
1	F	162	ASN	C-O	-7.40	1.15	1.24
1	A	133	ARG	C-N	7.39	1.42	1.33
1	B	70	ALA	C-O	-7.39	1.15	1.24
1	F	346	ALA	C-O	-7.39	1.14	1.24
1	G	66	SER	C-O	-7.38	1.15	1.24
1	D	135	GLY	C-O	-7.35	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	ALA	C-O	-7.35	1.15	1.24
1	D	185	ARG	C-O	-7.34	1.15	1.24
1	D	21	LEU	C-O	-7.34	1.14	1.24
1	C	293	PRO	C-O	-7.33	1.15	1.24
1	C	340	VAL	C-O	-7.33	1.15	1.24
1	B	172	ARG	C-O	-7.32	1.15	1.24
1	B	125	VAL	C-O	-7.31	1.16	1.23
1	G	38	LEU	C-O	-7.30	1.15	1.24
1	G	281	THR	C-N	-7.30	1.22	1.33
1	B	150	CYS	C-O	-7.30	1.15	1.23
1	H	94	ALA	C-O	-7.29	1.15	1.24
1	G	64	ILE	C-N	-7.29	1.24	1.34
1	D	66	SER	C-O	-7.29	1.15	1.24
1	E	378	ILE	C-O	-7.28	1.16	1.24
1	D	102	ILE	C-O	-7.27	1.16	1.24
1	B	72	LEU	C-O	-7.25	1.15	1.24
1	C	143	MET	C-O	-7.25	1.15	1.24
1	F	166	LYS	C-O	-7.25	1.15	1.24
1	B	48	VAL	C-O	-7.24	1.15	1.24
1	H	290	ALA	C-O	-7.24	1.15	1.24
1	H	150	CYS	C-O	-7.24	1.15	1.23
1	D	145	TYR	C-O	-7.23	1.15	1.24
1	A	287	HIS	C-O	-7.22	1.14	1.24
1	A	93	ARG	C-O	-7.22	1.15	1.24
1	D	40	GLN	C-O	-7.21	1.15	1.24
1	C	59	ALA	C-O	-7.21	1.15	1.23
1	C	76	PRO	C-O	-7.21	1.15	1.23
1	F	352	GLY	C-O	-7.21	1.14	1.24
1	G	352	GLY	C-O	-7.19	1.15	1.23
1	C	354	SER	C-O	-7.19	1.15	1.24
1	E	381	GLY	C-O	-7.18	1.14	1.23
1	A	144	VAL	C-O	-7.17	1.16	1.24
1	C	146	ASP	C-O	-7.17	1.15	1.24
1	B	167	GLU	C-O	-7.17	1.15	1.24
1	B	33	VAL	C-O	-7.17	1.15	1.24
1	B	81	SER	C-O	-7.17	1.15	1.23
1	D	256	ALA	C-O	-7.16	1.15	1.23
1	C	100	GLN	C-O	-7.16	1.15	1.24
1	G	349	HIS	C-O	-7.14	1.16	1.24
1	H	387	ALA	C-O	-7.13	1.15	1.23
1	A	87	VAL	C-O	-7.12	1.15	1.24
1	F	90	SER	C-O	-7.12	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	157	MET	C-O	-7.12	1.15	1.24
1	C	230	ALA	C-O	-7.11	1.15	1.24
1	G	290	ALA	C-O	-7.11	1.15	1.24
1	E	186	ALA	C-O	-7.11	1.15	1.24
1	D	292	ALA	C-O	-7.11	1.17	1.24
1	C	284	MET	C-O	-7.11	1.15	1.24
1	C	356	ALA	C-O	-7.11	1.16	1.24
1	B	284	MET	C-O	-7.10	1.18	1.24
1	B	144	VAL	C-O	-7.10	1.16	1.24
1	F	26	ALA	C-O	-7.09	1.15	1.24
1	H	27	ALA	C-O	-7.09	1.15	1.24
1	H	180	LEU	C-O	-7.08	1.15	1.24
1	B	190	ALA	C-O	-7.08	1.15	1.24
1	G	92	LEU	C-O	-7.08	1.15	1.24
1	D	7	VAL	C-O	-7.08	1.16	1.24
1	D	194	LYS	C-O	-7.08	1.15	1.24
1	D	354	SER	C-O	-7.07	1.15	1.24
1	F	126	PRO	C-O	-7.07	1.15	1.24
1	F	298	ASN	C-O	-7.07	1.15	1.24
1	C	34	MET	C-O	-7.07	1.16	1.24
1	C	69	ALA	C-O	-7.07	1.15	1.24
1	B	299	LYS	C-O	-7.06	1.15	1.24
1	E	290	ALA	C-O	-7.05	1.15	1.24
1	E	250	VAL	C-O	-7.05	1.16	1.24
1	D	198	GLU	C-O	-7.05	1.15	1.24
1	F	39	GLN	C-O	-7.04	1.16	1.24
1	F	103	ARG	C-O	-7.03	1.15	1.24
1	H	54	GLY	C-O	-7.02	1.16	1.23
1	E	364	TYR	C-O	-7.02	1.15	1.24
1	F	118	MET	C-O	-7.02	1.15	1.24
1	G	40	GLN	C-O	-7.02	1.16	1.24
1	B	298	ASN	C-O	-7.01	1.15	1.24
1	D	273	LEU	C-O	-7.01	1.16	1.24
1	G	185	ARG	C-O	-7.00	1.15	1.24
1	B	157	MET	C-O	-7.00	1.16	1.24
1	E	151	ALA	C-O	-6.99	1.15	1.24
1	G	172	ARG	C-O	-6.99	1.16	1.24
1	G	230	ALA	C-O	-6.99	1.15	1.24
1	G	182	SER	C-O	-6.99	1.16	1.24
1	D	179	ALA	C-O	-6.97	1.16	1.24
1	C	247	ALA	C-O	-6.97	1.17	1.24
1	G	181	ARG	C-O	-6.96	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	358	ILE	C-O	-6.96	1.16	1.24
1	B	224	THR	C-O	-6.96	1.15	1.24
1	A	173	ARG	C-O	-6.96	1.16	1.24
1	G	102	ILE	C-O	-6.95	1.16	1.24
1	B	91	GLY	C-O	-6.95	1.14	1.23
1	E	38	LEU	C-O	-6.94	1.15	1.24
1	D	363	VAL	C-O	-6.94	1.16	1.24
1	E	214	VAL	C-O	-6.94	1.16	1.24
1	D	95	VAL	C-O	-6.94	1.16	1.24
1	F	196	GLN	C-O	-6.93	1.16	1.24
1	C	77	TRP	C-O	-6.92	1.15	1.24
1	E	332	GLY	C-N	6.92	1.43	1.33
1	C	30	GLY	C-O	-6.92	1.15	1.23
1	H	69	ALA	C-O	-6.92	1.16	1.24
1	A	126	PRO	C-O	-6.92	1.15	1.24
1	B	147	GLY	C-O	-6.91	1.14	1.23
1	E	382	ALA	C-O	-6.91	1.15	1.24
1	B	19	GLY	C-O	-6.90	1.17	1.24
1	H	131	GLY	C-O	-6.89	1.14	1.23
1	H	163	THR	C-O	-6.89	1.16	1.24
1	H	329	LYS	C-O	-6.88	1.16	1.24
1	E	200	VAL	C-O	-6.88	1.17	1.23
1	C	292	ALA	C-O	-6.88	1.18	1.24
1	H	198	GLU	C-O	-6.88	1.15	1.24
1	H	380	SER	C-O	-6.88	1.15	1.23
1	E	370	GLY	C-O	-6.87	1.16	1.24
1	G	234	PRO	C-O	-6.87	1.15	1.23
1	E	183	HIS	C-O	-6.87	1.16	1.24
1	F	253	GLY	C-O	-6.87	1.16	1.23
1	F	38	LEU	C-O	-6.86	1.16	1.24
1	G	298	ASN	C-O	-6.86	1.16	1.24
1	C	66	SER	C-O	-6.85	1.16	1.24
1	H	336	GLU	C-O	-6.85	1.15	1.24
1	D	77	TRP	C-O	-6.85	1.15	1.24
1	A	68	GLN	C-O	-6.85	1.16	1.24
1	B	232	LEU	C-O	-6.85	1.15	1.23
1	G	371	GLY	C-O	-6.84	1.17	1.23
1	B	365	GLU	C-O	-6.84	1.16	1.24
1	H	90	SER	C-O	-6.84	1.16	1.24
1	E	40	GLN	C-O	-6.84	1.16	1.24
1	B	180	LEU	C-O	-6.84	1.16	1.24
1	C	87	VAL	C-O	-6.83	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	ALA	C-O	-6.83	1.16	1.24
1	H	276	ILE	C-O	-6.81	1.16	1.23
1	F	188	LYS	C-O	-6.81	1.16	1.24
1	D	141	ASP	C-O	-6.81	1.15	1.24
1	B	360	MET	C-N	-6.80	1.23	1.33
1	E	121	ILE	C-O	-6.80	1.16	1.25
1	E	220	ILE	C-O	-6.80	1.17	1.24
1	H	121	ILE	C-O	-6.80	1.15	1.24
1	G	27	ALA	C-O	-6.80	1.16	1.24
1	B	76	PRO	C-O	-6.79	1.15	1.23
1	F	157	MET	C-O	-6.79	1.16	1.24
1	D	313	LEU	C-O	-6.79	1.15	1.23
1	F	228	GLN	C-O	-6.78	1.16	1.24
1	A	368	ARG	C-O	-6.77	1.15	1.24
1	F	325	LEU	C-O	-6.76	1.16	1.24
1	D	120	ASN	C-O	-6.76	1.14	1.24
1	D	264	LYS	C-O	-6.76	1.16	1.24
1	B	32	ILE	C-O	-6.76	1.16	1.24
1	C	331	VAL	C-O	-6.76	1.16	1.24
1	F	4	THR	C-O	-6.75	1.15	1.24
1	H	204	TRP	C-N	-6.75	1.20	1.33
1	E	174	GLU	C-O	-6.75	1.16	1.24
1	B	165	ALA	C-O	-6.74	1.16	1.24
1	H	134	MET	C-O	-6.74	1.15	1.23
1	D	27	ALA	C-O	-6.74	1.16	1.24
1	C	75	MET	C-N	6.73	1.41	1.33
1	D	133	ARG	C-O	-6.73	1.15	1.24
1	D	164	ALA	C-O	-6.72	1.16	1.24
1	E	118	MET	C-O	-6.72	1.15	1.24
1	B	34	MET	C-O	-6.72	1.16	1.24
1	D	360	MET	C-O	-6.71	1.16	1.24
1	H	324	VAL	C-O	-6.71	1.16	1.24
1	H	57	VAL	C-O	-6.71	1.16	1.24
1	G	91	GLY	C-O	-6.71	1.15	1.23
1	E	72	LEU	C-O	-6.70	1.16	1.24
1	H	389	LEU	C-N	-6.70	1.24	1.33
1	A	43	VAL	C-O	-6.70	1.16	1.24
1	C	379	CYS	C-O	-6.70	1.16	1.23
1	G	166	LYS	C-O	-6.70	1.16	1.24
1	E	133	ARG	C-O	-6.69	1.15	1.24
1	C	190	ALA	C-O	-6.69	1.16	1.24
1	E	361	THR	C-O	-6.69	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	183	HIS	C-O	-6.69	1.16	1.24
1	G	53	MET	C-O	-6.68	1.16	1.24
1	C	274	ALA	C-O	-6.68	1.16	1.23
1	C	214	VAL	C-O	-6.67	1.17	1.24
1	F	60	GLY	C-O	-6.67	1.14	1.23
1	G	324	VAL	C-O	-6.67	1.16	1.24
1	D	56	VAL	C-O	-6.67	1.16	1.24
1	D	276	ILE	C-O	-6.67	1.16	1.23
1	H	218	GLU	C-O	-6.67	1.16	1.24
1	B	143	MET	C-O	-6.67	1.16	1.24
1	B	235	ILE	C-O	-6.67	1.16	1.24
1	D	298	ASN	C-O	-6.67	1.16	1.24
1	B	390	VAL	C-O	-6.67	1.17	1.24
1	G	118	MET	C-O	-6.66	1.15	1.24
1	A	313	LEU	C-O	-6.66	1.15	1.23
1	G	145	TYR	C-O	-6.66	1.16	1.24
1	D	75	MET	C-O	-6.66	1.15	1.23
1	H	38	LEU	C-O	-6.65	1.16	1.24
1	C	184	ALA	C-O	-6.65	1.16	1.24
1	E	73	ALA	C-O	-6.64	1.15	1.24
1	C	160	HIS	C-O	-6.64	1.16	1.24
1	F	64	ILE	C-O	-6.64	1.16	1.24
1	H	147	GLY	C-O	-6.64	1.15	1.23
1	E	70	ALA	C-O	-6.63	1.16	1.24
1	C	381	GLY	C-O	-6.63	1.17	1.23
1	A	322	SER	C-O	-6.63	1.15	1.24
1	B	53	MET	C-O	-6.63	1.16	1.24
1	F	53	MET	C-O	-6.62	1.16	1.24
1	H	119	SER	C-O	-6.62	1.15	1.24
1	A	293	PRO	C-O	-6.62	1.15	1.24
1	A	311	ILE	C-O	-6.61	1.16	1.24
1	B	59	ALA	C-O	-6.61	1.15	1.23
1	C	291	ALA	C-O	-6.61	1.15	1.24
1	C	390	VAL	C-O	-6.61	1.17	1.24
1	H	392	VAL	C-O	-6.61	1.16	1.24
1	B	99	ASP	C-O	-6.61	1.16	1.24
1	B	117	SER	C-O	-6.61	1.16	1.23
1	B	376	ALA	C-O	-6.61	1.16	1.24
1	C	33	VAL	C-O	-6.61	1.16	1.24
1	C	54	GLY	C-O	-6.61	1.17	1.24
1	H	95	VAL	C-O	-6.61	1.16	1.24
1	C	82	GLU	C-N	6.60	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	187	ALA	C-O	-6.60	1.16	1.24
1	D	282	THR	C-O	-6.60	1.15	1.23
1	E	359	LEU	C-O	-6.59	1.16	1.24
1	G	191	ASP	C-O	-6.59	1.16	1.24
1	E	345	ILE	C-O	-6.59	1.16	1.24
1	E	387	ALA	C-O	-6.59	1.16	1.24
1	C	285	PRO	C-O	-6.59	1.16	1.23
1	E	328	GLU	C-O	-6.59	1.16	1.24
1	E	357	ARG	C-O	-6.59	1.16	1.24
1	B	151	ALA	C-O	-6.59	1.15	1.24
1	E	21	LEU	C-O	-6.59	1.15	1.24
1	G	340	VAL	C-O	-6.59	1.15	1.24
1	E	98	CYS	C-O	-6.58	1.16	1.24
1	B	162	ASN	C-O	-6.58	1.16	1.24
1	H	91	GLY	C-O	-6.57	1.16	1.23
1	G	390	VAL	C-O	-6.57	1.17	1.24
1	C	362	LEU	C-O	-6.57	1.16	1.24
1	C	96	THR	C-O	-6.57	1.16	1.24
1	B	140	ARG	C-O	-6.56	1.16	1.24
1	H	162	ASN	C-O	-6.56	1.16	1.24
1	A	72	LEU	C-O	-6.55	1.16	1.24
1	E	227	ASP	C-O	-6.55	1.16	1.24
1	B	37	ALA	C-O	-6.55	1.16	1.24
1	C	196	GLN	C-O	-6.54	1.16	1.24
1	H	102	ILE	C-O	-6.54	1.16	1.24
1	B	339	ASN	C-O	-6.54	1.16	1.23
1	F	77	TRP	C-O	-6.54	1.16	1.24
1	F	121	ILE	C-O	-6.54	1.16	1.24
1	B	166	LYS	C-O	-6.54	1.16	1.24
1	C	22	LYS	C-O	-6.53	1.16	1.24
1	D	118	MET	C-O	-6.53	1.15	1.24
1	D	364	TYR	C-O	-6.53	1.16	1.24
1	A	101	MET	C-N	6.53	1.42	1.33
1	G	59	ALA	C-O	-6.53	1.16	1.23
1	A	276	ILE	C-O	-6.53	1.16	1.23
1	B	149	THR	C-O	-6.53	1.16	1.24
1	G	354	SER	C-O	-6.53	1.16	1.24
1	A	11	ARG	C-O	-6.52	1.15	1.23
1	G	216	LYS	C-N	-6.52	1.24	1.33
1	D	26	ALA	C-O	-6.52	1.16	1.24
1	D	54	GLY	C-O	-6.51	1.16	1.23
1	H	96	THR	C-O	-6.51	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	336	GLU	C-O	-6.51	1.15	1.24
1	C	157	MET	C-O	-6.51	1.16	1.24
1	D	119	SER	C-O	-6.51	1.16	1.24
1	A	218	GLU	C-O	-6.50	1.15	1.24
1	G	376	ALA	C-O	-6.50	1.16	1.24
1	F	102	ILE	C-O	-6.50	1.16	1.24
1	D	127	ALA	C-O	-6.50	1.15	1.24
1	G	288	GLU	C-O	-6.50	1.14	1.24
1	E	124	ALA	C-O	-6.49	1.15	1.23
1	H	160	HIS	C-O	-6.49	1.16	1.24
1	G	163	THR	C-O	-6.48	1.16	1.24
1	E	202	VAL	C-O	-6.48	1.17	1.24
1	F	63	GLN	C-O	-6.48	1.16	1.23
1	F	143	MET	C-O	-6.48	1.16	1.24
1	G	323	VAL	C-O	-6.48	1.16	1.24
1	C	255	GLY	C-O	-6.48	1.16	1.24
1	H	115	MET	C-O	-6.47	1.16	1.23
1	G	165	ALA	C-O	-6.47	1.16	1.24
1	A	243	THR	C-O	-6.46	1.15	1.23
1	C	382	ALA	C-O	-6.46	1.15	1.24
1	C	135	GLY	C-O	-6.46	1.15	1.23
1	A	364	TYR	C-O	-6.46	1.16	1.24
1	A	284	MET	N-CA	6.45	1.50	1.46
1	A	199	ILE	C-O	-6.45	1.16	1.24
1	C	162	ASN	C-O	-6.45	1.16	1.24
1	F	150	CYS	C-O	-6.45	1.16	1.24
1	E	322	SER	C-O	-6.45	1.15	1.24
1	H	24	VAL	C-O	-6.44	1.16	1.24
1	H	52	VAL	C-O	-6.44	1.17	1.24
1	C	46	ASP	C-O	-6.44	1.15	1.24
1	B	336	GLU	C-O	-6.44	1.16	1.24
1	G	286	ALA	C-O	-6.43	1.16	1.24
1	E	88	CYS	C-O	-6.42	1.16	1.24
1	B	186	ALA	C-O	-6.42	1.16	1.24
1	H	184	ALA	C-O	-6.42	1.16	1.24
1	H	238	SER	CA-C	-6.42	1.44	1.52
1	F	210	LYS	C-N	6.42	1.41	1.33
1	G	17	PHE	C-O	-6.42	1.16	1.23
1	D	296	ALA	C-O	-6.42	1.16	1.24
1	B	55	MET	C-O	-6.41	1.16	1.24
1	A	115	MET	C-O	-6.41	1.16	1.23
1	H	303	LYS	C-O	-6.40	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	ILE	C-O	-6.40	1.17	1.24
1	B	29	LEU	C-O	-6.40	1.16	1.24
1	C	114	GLY	C-O	-6.39	1.17	1.24
1	H	300	LEU	C-O	-6.39	1.16	1.24
1	B	155	VAL	C-O	-6.39	1.16	1.23
1	H	279	PHE	C-O	-6.38	1.16	1.23
1	F	301	LEU	C-O	-6.38	1.16	1.24
1	F	101	MET	C-O	-6.38	1.16	1.24
1	E	125	VAL	C-O	-6.38	1.16	1.24
1	D	322	SER	C-O	-6.37	1.16	1.24
1	A	26	ALA	C-O	-6.37	1.16	1.24
1	B	323	VAL	C-O	-6.37	1.17	1.24
1	D	330	ILE	C-O	-6.37	1.17	1.24
1	B	21	LEU	C-O	-6.36	1.15	1.24
1	B	160	HIS	C-O	-6.36	1.16	1.24
1	B	324	VAL	C-O	-6.36	1.16	1.24
1	H	18	GLY	C-O	-6.36	1.15	1.24
1	G	107	ALA	C-O	-6.36	1.16	1.23
1	A	137	GLY	C-O	-6.36	1.16	1.23
1	G	73	ALA	C-O	-6.36	1.15	1.24
1	D	89	ALA	C-O	-6.35	1.15	1.24
1	D	300	LEU	C-O	-6.35	1.16	1.24
1	F	361	THR	C-O	-6.35	1.15	1.24
1	D	186	ALA	C-O	-6.35	1.16	1.24
1	H	126	PRO	C-O	-6.34	1.15	1.24
1	C	149	THR	C-O	-6.34	1.16	1.24
1	C	60	GLY	C-O	-6.34	1.15	1.24
1	H	271	ARG	C-O	-6.34	1.16	1.24
1	B	345	ILE	C-O	-6.34	1.16	1.24
1	H	60	GLY	C-O	-6.33	1.15	1.24
1	E	354	SER	C-O	-6.33	1.16	1.24
1	H	299	LYS	C-O	-6.33	1.16	1.24
1	E	15	GLY	C-O	-6.33	1.14	1.23
1	E	242	ILE	C-O	-6.33	1.16	1.24
1	H	46	ASP	C-O	-6.32	1.16	1.24
1	G	129	ARG	C-O	-6.32	1.16	1.24
1	A	166	LYS	C-O	-6.32	1.16	1.24
1	C	140	ARG	C-O	-6.32	1.16	1.24
1	C	245	GLY	C-O	-6.32	1.16	1.23
1	G	291	ALA	C-O	-6.31	1.16	1.24
1	D	163	THR	C-O	-6.31	1.16	1.24
1	C	26	ALA	C-O	-6.30	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	71	ARG	C-O	-6.30	1.16	1.24
1	G	353	ALA	C-O	-6.30	1.15	1.24
1	D	328	GLU	C-O	-6.30	1.16	1.24
1	D	93	ARG	C-O	-6.30	1.16	1.24
1	B	90	SER	C-O	-6.29	1.16	1.24
1	B	185	ARG	C-O	-6.29	1.16	1.24
1	G	75	MET	C-O	-6.29	1.15	1.23
1	A	91	GLY	C-O	-6.29	1.16	1.23
1	B	266	ALA	C-O	-6.28	1.16	1.24
1	D	180	LEU	C-O	-6.28	1.16	1.24
1	A	35	LYS	C-O	-6.28	1.16	1.24
1	D	366	LEU	C-O	-6.28	1.16	1.24
1	D	67	ARG	C-O	-6.28	1.16	1.24
1	C	220	ILE	C-O	-6.28	1.17	1.24
1	D	150	CYS	C-O	-6.28	1.16	1.23
1	H	103	ARG	C-O	-6.28	1.16	1.24
1	H	360	MET	C-O	-6.27	1.16	1.24
1	D	333	PHE	C-O	-6.27	1.16	1.23
1	G	366	LEU	C-O	-6.27	1.16	1.24
1	D	139	LEU	C-O	-6.27	1.16	1.23
1	G	119	SER	C-O	-6.27	1.16	1.24
1	H	53	MET	C-O	-6.27	1.16	1.24
1	B	170	ILE	C-O	-6.27	1.17	1.24
1	C	40	GLN	C-O	-6.26	1.16	1.24
1	G	133	ARG	C-N	-6.26	1.25	1.33
1	D	39	GLN	C-O	-6.25	1.17	1.24
1	D	59	ALA	C-O	-6.25	1.16	1.23
1	A	128	GLY	C-O	-6.25	1.16	1.23
1	D	299	LYS	C-O	-6.25	1.17	1.24
1	D	140	ARG	C-O	-6.25	1.16	1.24
1	B	84	LEU	C-O	-6.24	1.16	1.24
1	G	72	LEU	C-O	-6.24	1.16	1.24
1	B	326	THR	C-O	-6.23	1.16	1.24
1	C	70	ALA	C-O	-6.23	1.16	1.24
1	D	381	GLY	C-O	-6.23	1.17	1.23
1	A	363	VAL	C-O	-6.22	1.16	1.24
1	F	123	TYR	C-O	-6.22	1.16	1.23
1	G	368	ARG	C-O	-6.22	1.16	1.24
1	B	5	VAL	C-O	-6.22	1.18	1.24
1	F	299	LYS	C-O	-6.21	1.16	1.24
1	F	124	ALA	C-O	-6.21	1.16	1.23
1	G	203	ASN	CA-C	-6.21	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	349	HIS	C-O	-6.21	1.17	1.24
1	B	28	GLU	C-O	-6.21	1.17	1.24
1	A	51	ASN	C-O	-6.21	1.16	1.23
1	B	120	ASN	C-O	-6.21	1.15	1.24
1	B	351	ILE	C-O	-6.21	1.16	1.24
1	C	187	ALA	C-O	-6.21	1.16	1.24
1	E	325	LEU	C-O	-6.19	1.16	1.24
1	A	69	ALA	C-O	-6.19	1.16	1.24
1	C	35	LYS	C-O	-6.19	1.17	1.24
1	C	173	ARG	C-O	-6.19	1.17	1.24
1	D	250	VAL	C-O	-6.19	1.17	1.24
1	H	291	ALA	C-O	-6.19	1.16	1.24
1	C	106	ASP	C-O	-6.19	1.15	1.24
1	C	191	ASP	C-O	-6.19	1.16	1.24
1	C	97	LEU	C-O	-6.19	1.16	1.24
1	D	388	VAL	C-O	-6.19	1.17	1.24
1	G	56	VAL	C-O	-6.18	1.17	1.24
1	G	292	ALA	C-O	-6.18	1.18	1.24
1	G	388	VAL	C-O	-6.18	1.17	1.24
1	B	67	ARG	C-O	-6.18	1.16	1.24
1	B	387	ALA	C-O	-6.17	1.16	1.23
1	C	62	GLY	C-O	-6.17	1.14	1.23
1	A	17	PHE	C-O	-6.17	1.16	1.23
1	C	244	ALA	C-O	-6.17	1.16	1.24
1	E	180	LEU	C-O	-6.16	1.17	1.24
1	A	143	MET	C-O	-6.16	1.17	1.24
1	B	269	GLY	C-O	-6.16	1.15	1.23
1	C	130	TRP	C-O	-6.16	1.16	1.24
1	G	126	PRO	C-O	-6.16	1.16	1.24
1	G	329	LYS	C-O	-6.16	1.17	1.24
1	D	129	ARG	C-O	-6.16	1.17	1.24
1	H	319	ALA	C-O	-6.16	1.17	1.24
1	G	65	PRO	C-O	-6.16	1.16	1.24
1	A	321	ALA	C-O	-6.15	1.17	1.24
1	F	329	LYS	C-O	-6.15	1.17	1.24
1	D	297	ILE	C-O	-6.15	1.17	1.24
1	H	220	ILE	C-O	-6.15	1.17	1.24
1	G	173	ARG	C-O	-6.15	1.17	1.24
1	F	184	ALA	C-O	-6.15	1.17	1.24
1	D	340	VAL	C-O	-6.15	1.16	1.24
1	H	71	ARG	C-O	-6.14	1.16	1.24
1	A	338	VAL	C-O	-6.14	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	322	SER	C-O	-6.14	1.16	1.24
1	H	354	SER	C-O	-6.14	1.17	1.24
1	H	167	GLU	C-O	-6.13	1.17	1.24
1	H	114	GLY	C-O	-6.13	1.17	1.24
1	C	163	THR	C-O	-6.13	1.17	1.24
1	B	66	SER	C-O	-6.13	1.17	1.24
1	D	258	VAL	N-CA	-6.13	1.38	1.46
1	C	89	ALA	C-O	-6.13	1.16	1.24
1	G	238	SER	C-O	-6.13	1.16	1.24
1	D	303	LYS	C-O	-6.12	1.16	1.24
1	D	356	ALA	C-O	-6.12	1.16	1.24
1	A	344	ALA	C-O	-6.12	1.16	1.24
1	H	295	PHE	C-O	-6.12	1.16	1.24
1	H	363	VAL	C-O	-6.12	1.17	1.24
1	G	255	GLY	C-O	-6.12	1.17	1.24
1	A	357	ARG	C-O	-6.12	1.17	1.24
1	C	166	LYS	C-O	-6.12	1.17	1.24
1	E	336	GLU	C-O	-6.11	1.16	1.24
1	C	199	ILE	C-O	-6.11	1.16	1.24
1	F	379	CYS	C-O	-6.11	1.16	1.23
1	E	142	LEU	C-O	-6.10	1.16	1.24
1	B	273	LEU	C-O	-6.10	1.17	1.24
1	C	129	ARG	C-O	-6.10	1.17	1.24
1	H	356	ALA	C-O	-6.10	1.17	1.24
1	C	272	PRO	C-N	-6.09	1.25	1.34
1	B	229	LEU	C-O	-6.09	1.17	1.24
1	A	330	ILE	C-O	-6.09	1.17	1.24
1	F	326	THR	C-O	-6.09	1.17	1.24
1	A	121	ILE	C-O	-6.09	1.16	1.24
1	B	357	ARG	C-O	-6.09	1.17	1.24
1	H	173	ARG	C-O	-6.09	1.17	1.24
1	C	144	VAL	C-O	-6.09	1.17	1.24
1	D	383	ALA	C-O	-6.09	1.15	1.23
1	A	10	ALA	C-O	-6.09	1.16	1.23
1	A	71	ARG	C-O	-6.08	1.16	1.24
1	E	213	VAL	C-O	-6.08	1.17	1.24
1	C	188	LYS	C-O	-6.08	1.17	1.24
1	G	29	LEU	C-O	-6.08	1.17	1.24
1	H	159	VAL	C-O	-6.08	1.17	1.24
1	F	271	ARG	C-O	-6.08	1.17	1.24
1	E	321	ALA	C-O	-6.07	1.17	1.24
1	E	139	LEU	C-O	-6.07	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	100	GLN	C-O	-6.07	1.17	1.24
1	G	109	ILE	C-O	-6.07	1.17	1.24
1	D	35	LYS	C-O	-6.07	1.17	1.24
1	B	92	LEU	C-O	-6.07	1.16	1.23
1	B	153	ASP	C-O	-6.07	1.16	1.24
1	G	263	GLU	C-O	-6.07	1.17	1.24
1	H	321	ALA	C-O	-6.07	1.16	1.24
1	G	190	ALA	C-O	-6.07	1.17	1.24
1	E	130	TRP	C-O	-6.06	1.15	1.24
1	C	234	PRO	C-O	-6.06	1.16	1.23
1	D	351	ILE	C-O	-6.06	1.17	1.24
1	G	25	LYS	C-O	-6.06	1.15	1.23
1	E	52	VAL	C-O	-6.06	1.17	1.24
1	C	366	LEU	C-O	-6.06	1.17	1.24
1	F	138	GLU	C-O	-6.06	1.16	1.23
1	D	61	SER	C-O	-6.06	1.15	1.24
1	C	10	ALA	C-O	-6.05	1.16	1.23
1	D	312	ASP	C-O	-6.05	1.17	1.24
1	A	41	ALA	C-O	-6.05	1.15	1.24
1	F	91	GLY	C-O	-6.05	1.16	1.23
1	F	247	ALA	C-O	-6.05	1.16	1.24
1	D	96	THR	C-O	-6.05	1.17	1.24
1	G	152	PHE	C-O	-6.04	1.16	1.23
1	E	358	ILE	C-O	-6.04	1.17	1.24
1	B	330	ILE	C-O	-6.04	1.17	1.24
1	C	92	LEU	C-O	-6.04	1.17	1.24
1	F	19	GLY	C-O	-6.04	1.17	1.24
1	G	111	VAL	C-O	-6.04	1.17	1.24
1	E	229	LEU	C-O	-6.04	1.17	1.24
1	D	265	ALA	C-O	-6.03	1.17	1.24
1	H	118	MET	C-O	-6.03	1.16	1.24
1	H	138	GLU	C-O	-6.03	1.16	1.23
1	E	93	ARG	C-O	-6.03	1.16	1.24
1	B	173	ARG	C-O	-6.03	1.17	1.24
1	A	37	ALA	C-O	-6.03	1.17	1.24
1	A	67	ARG	C-O	-6.03	1.17	1.24
1	A	291	ALA	C-O	-6.03	1.16	1.24
1	E	144	VAL	C-O	-6.03	1.17	1.24
1	F	229	LEU	C-O	-6.02	1.16	1.24
1	E	114	GLY	C-O	-6.02	1.17	1.24
1	C	38	LEU	C-O	-6.02	1.17	1.24
1	F	119	SER	C-O	-6.01	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	135	GLY	C-O	-6.01	1.15	1.23
1	D	130	TRP	C-O	-6.01	1.16	1.24
1	F	351	ILE	C-O	-6.00	1.17	1.24
1	G	16	LYS	C-O	-6.00	1.16	1.23
1	G	90	SER	C-O	-6.00	1.17	1.24
1	G	70	ALA	C-O	-6.00	1.17	1.24
1	G	245	GLY	C-O	-6.00	1.16	1.23
1	H	21	LEU	C-O	-5.99	1.16	1.24
1	G	293	PRO	C-O	-5.99	1.16	1.24
1	G	197	ASP	C-O	-5.99	1.17	1.24
1	C	134	MET	C-O	-5.99	1.16	1.23
1	G	265	ALA	C-O	-5.99	1.17	1.24
1	F	5	VAL	C-O	-5.99	1.18	1.24
1	D	91	GLY	C-O	-5.99	1.16	1.23
1	H	388	VAL	C-O	-5.98	1.18	1.24
1	B	358	ILE	C-O	-5.98	1.17	1.24
1	A	373	LEU	C-O	-5.97	1.16	1.24
1	B	102	ILE	C-O	-5.97	1.17	1.24
1	H	101	MET	C-O	-5.97	1.17	1.24
1	H	323	VAL	C-O	-5.96	1.17	1.24
1	H	5	VAL	C-O	-5.96	1.17	1.24
1	B	302	LYS	C-O	-5.96	1.17	1.24
1	F	71	ARG	C-O	-5.96	1.17	1.24
1	D	384	GLN	C-O	-5.95	1.16	1.23
1	A	163	THR	C-O	-5.95	1.17	1.24
1	F	164	ALA	C-O	-5.95	1.17	1.24
1	C	168	TYR	C-O	-5.95	1.15	1.23
1	F	56	VAL	C-O	-5.95	1.17	1.24
1	E	88	CYS	N-CA	-5.94	1.39	1.46
1	H	255	GLY	C-O	-5.94	1.16	1.23
1	H	313	LEU	C-O	-5.94	1.16	1.23
1	D	159	VAL	C-O	-5.94	1.17	1.24
1	C	283	GLY	C-N	-5.93	1.21	1.33
1	D	357	ARG	C-O	-5.93	1.17	1.24
1	F	107	ALA	C-O	-5.92	1.16	1.23
1	G	103	ARG	C-O	-5.92	1.16	1.24
1	G	342	GLY	C-O	-5.92	1.14	1.23
1	A	274	ALA	C-O	-5.92	1.16	1.23
1	B	288	GLU	C-N	-5.92	1.26	1.33
1	C	181	ARG	CZ-NH2	-5.92	1.25	1.33
1	C	351	ILE	C-O	-5.92	1.17	1.24
1	B	295	PHE	C-O	-5.91	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	GLY	C-O	-5.91	1.16	1.23
1	B	296	ALA	C-O	-5.91	1.17	1.24
1	C	56	VAL	C-O	-5.91	1.17	1.24
1	E	135	GLY	C-O	-5.91	1.16	1.23
1	A	308	VAL	C-O	-5.91	1.17	1.24
1	B	128	GLY	C-O	-5.91	1.16	1.23
1	B	368	ARG	C-O	-5.91	1.16	1.24
1	C	180	LEU	C-O	-5.90	1.17	1.24
1	E	66	SER	C-O	-5.90	1.17	1.24
1	C	329	LYS	C-O	-5.90	1.17	1.24
1	E	247	ALA	C-O	-5.90	1.16	1.24
1	H	379	CYS	C-O	-5.90	1.16	1.23
1	A	301	LEU	C-O	-5.90	1.17	1.24
1	C	109	ILE	C-O	-5.90	1.18	1.24
1	D	19	GLY	C-O	-5.90	1.17	1.24
1	F	141	ASP	C-O	-5.89	1.16	1.23
1	H	36	GLU	C-O	-5.89	1.17	1.24
1	E	329	LYS	C-O	-5.89	1.17	1.24
1	F	7	VAL	C-O	-5.89	1.17	1.24
1	D	197	ASP	C-O	-5.89	1.17	1.24
1	B	297	ILE	C-O	-5.89	1.17	1.24
1	A	14	PHE	C-O	-5.89	1.16	1.24
1	A	220	ILE	C-O	-5.89	1.18	1.24
1	H	339	ASN	C-O	-5.88	1.16	1.23
1	F	68	GLN	C-O	-5.88	1.17	1.24
1	D	90	SER	C-O	-5.88	1.17	1.24
1	E	187	ALA	C-O	-5.88	1.17	1.24
1	B	24	VAL	C-O	-5.88	1.17	1.24
1	B	80	PRO	C-O	-5.88	1.17	1.23
1	D	97	LEU	C-O	-5.88	1.17	1.24
1	C	389	LEU	C-O	-5.87	1.16	1.24
1	A	24	VAL	C-O	-5.87	1.17	1.24
1	F	66	SER	C-O	-5.87	1.17	1.24
1	F	330	ILE	C-O	-5.87	1.17	1.24
1	G	246	ASN	C-O	-5.87	1.16	1.24
1	H	280	SER	C-O	-5.87	1.17	1.23
1	E	316	VAL	C-O	-5.87	1.17	1.24
1	G	77	TRP	C-O	-5.87	1.16	1.24
1	D	279	PHE	C-O	-5.86	1.16	1.23
1	C	170	ILE	C-O	-5.86	1.17	1.24
1	F	97	LEU	C-O	-5.86	1.17	1.24
1	A	19	GLY	C-O	-5.86	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	199	ILE	C-N	-5.86	1.29	1.33
1	E	6	ILE	C-O	-5.86	1.17	1.24
1	B	158	ALA	C-O	-5.86	1.16	1.24
1	E	362	LEU	C-O	-5.85	1.17	1.24
1	F	344	ALA	C-O	-5.85	1.16	1.24
1	F	95	VAL	C-O	-5.85	1.17	1.24
1	B	264	LYS	C-O	-5.85	1.17	1.24
1	G	158	ALA	C-O	-5.85	1.16	1.24
1	F	22	LYS	C-O	-5.85	1.17	1.24
1	F	327	CYS	C-O	-5.85	1.17	1.24
1	H	274	ALA	C-O	-5.84	1.17	1.23
1	E	323	VAL	C-O	-5.84	1.17	1.24
1	C	321	ALA	C-O	-5.84	1.17	1.24
1	H	178	TRP	C-O	-5.84	1.17	1.24
1	C	218	GLU	C-O	-5.84	1.16	1.24
1	D	173	ARG	C-O	-5.83	1.17	1.24
1	B	379	CYS	C-O	-5.83	1.16	1.23
1	F	173	ARG	C-O	-5.83	1.17	1.24
1	E	197	ASP	C-O	-5.83	1.17	1.24
1	A	165	ALA	C-O	-5.83	1.17	1.24
1	D	287	HIS	C-O	-5.83	1.16	1.24
1	H	351	ILE	C-O	-5.83	1.17	1.24
1	G	61	SER	C-O	-5.83	1.16	1.24
1	B	137	GLY	C-O	-5.82	1.16	1.23
1	F	286	ALA	C-O	-5.82	1.17	1.24
1	F	158	ALA	C-O	-5.82	1.16	1.24
1	D	44	SER	C-O	-5.82	1.16	1.23
1	G	361	THR	C-O	-5.82	1.17	1.24
1	G	382	ALA	C-O	-5.82	1.15	1.23
1	D	176	ASP	C-O	-5.82	1.17	1.24
1	C	388	VAL	C-O	-5.81	1.17	1.24
1	A	180	LEU	C-O	-5.81	1.17	1.24
1	C	182	SER	C-O	-5.81	1.17	1.24
1	A	196	GLN	C-O	-5.81	1.17	1.24
1	E	44	SER	C-O	-5.80	1.16	1.23
1	H	81	SER	C-O	-5.80	1.16	1.23
1	H	185	ARG	C-O	-5.80	1.17	1.24
1	E	150	CYS	C-O	-5.80	1.17	1.23
1	A	18	GLY	C-O	-5.80	1.15	1.23
1	A	124	ALA	C-O	-5.80	1.16	1.23
1	F	359	LEU	C-O	-5.80	1.17	1.24
1	G	330	ILE	C-O	-5.80	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	351	ILE	C-O	-5.79	1.17	1.24
1	A	202	VAL	C-O	-5.79	1.17	1.24
1	C	336	GLU	C-O	-5.79	1.16	1.24
1	F	128	GLY	C-O	-5.79	1.16	1.23
1	B	325	LEU	C-O	-5.78	1.17	1.24
1	B	251	ASN	C-O	-5.78	1.17	1.23
1	D	99	ASP	C-O	-5.78	1.17	1.24
1	A	335	LEU	C-N	-5.77	1.25	1.34
1	E	172	ARG	C-O	-5.77	1.17	1.24
1	F	378	ILE	C-O	-5.77	1.18	1.24
1	G	356	ALA	C-O	-5.77	1.17	1.24
1	A	98	CYS	C-O	-5.77	1.17	1.24
1	H	309	GLN	C-O	-5.76	1.16	1.24
1	E	101	MET	C-O	-5.76	1.17	1.24
1	F	82	GLU	C-O	-5.76	1.16	1.24
1	G	359	LEU	C-O	-5.76	1.17	1.24
1	F	31	GLY	C-O	-5.75	1.16	1.23
1	D	358	ILE	C-O	-5.75	1.17	1.24
1	A	151	ALA	C-O	-5.75	1.16	1.24
1	B	188	LYS	C-O	-5.75	1.17	1.24
1	C	138	GLU	C-O	-5.75	1.17	1.23
1	C	31	GLY	C-O	-5.75	1.17	1.23
1	B	111	VAL	C-O	-5.75	1.18	1.24
1	G	196	GLN	C-O	-5.75	1.17	1.24
1	E	243	THR	C-O	-5.75	1.16	1.23
1	G	270	LYS	C-O	-5.75	1.16	1.23
1	C	263	GLU	C-O	-5.74	1.17	1.24
1	G	112	ALA	C-O	-5.74	1.16	1.23
1	E	324	VAL	C-O	-5.74	1.17	1.24
1	C	108	ASP	C-O	-5.74	1.16	1.24
1	C	181	ARG	C-O	-5.74	1.17	1.24
1	G	82	GLU	C-O	-5.74	1.16	1.23
1	H	107	ALA	C-O	-5.74	1.16	1.23
1	H	192	GLU	C-O	-5.74	1.16	1.24
1	F	362	LEU	C-O	-5.73	1.17	1.24
1	H	43	VAL	C-O	-5.72	1.18	1.24
1	C	277	LEU	C-O	-5.72	1.17	1.24
1	F	11	ARG	C-O	-5.72	1.16	1.23
1	B	138	GLU	C-O	-5.72	1.17	1.23
1	E	289	LEU	C-O	-5.72	1.17	1.24
1	A	379	CYS	C-O	-5.72	1.16	1.23
1	C	258	VAL	C-O	-5.72	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	294	GLY	C-O	-5.72	1.17	1.23
1	H	366	LEU	C-O	-5.72	1.17	1.24
1	A	200	VAL	C-O	-5.72	1.17	1.24
1	B	46	ASP	C-O	-5.71	1.16	1.24
1	C	37	ALA	C-O	-5.71	1.17	1.24
1	G	322	SER	C-O	-5.71	1.17	1.24
1	A	187	ALA	C-O	-5.71	1.17	1.24
1	E	353	ALA	C-O	-5.71	1.16	1.24
1	D	218	GLU	C-O	-5.71	1.17	1.24
1	H	157	MET	C-O	-5.71	1.17	1.24
1	E	284	MET	C-O	-5.71	1.18	1.24
1	C	200	VAL	C-O	-5.71	1.18	1.23
1	B	35	LYS	C-O	-5.70	1.17	1.24
1	G	52	VAL	C-O	-5.70	1.18	1.24
1	E	389	LEU	C-O	-5.70	1.17	1.24
1	G	387	ALA	C-O	-5.70	1.17	1.23
1	C	286	ALA	C-O	-5.70	1.17	1.24
1	H	273	LEU	C-N	-5.69	1.26	1.33
1	F	155	VAL	C-O	-5.69	1.17	1.23
1	E	334	ASP	C-O	-5.69	1.17	1.24
1	F	216	LYS	C-O	-5.69	1.16	1.23
1	A	13	PRO	C-O	-5.68	1.17	1.23
1	E	337	LYS	C-O	-5.68	1.16	1.23
1	F	92	LEU	C-O	-5.68	1.16	1.24
1	F	245	GLY	C-O	-5.68	1.17	1.23
1	H	364	TYR	C-O	-5.68	1.17	1.24
1	B	154	GLU	C-O	-5.68	1.16	1.23
1	H	99	ASP	C-O	-5.67	1.17	1.24
1	G	218	GLU	C-O	-5.67	1.16	1.24
1	A	114	GLY	C-O	-5.67	1.17	1.24
1	E	87	VAL	C-O	-5.67	1.17	1.24
1	E	390	VAL	C-O	-5.67	1.18	1.24
1	B	364	TYR	C-O	-5.67	1.17	1.24
1	C	273	LEU	C-O	-5.67	1.17	1.24
1	D	36	GLU	C-O	-5.66	1.17	1.24
1	D	249	GLY	C-O	-5.66	1.17	1.24
1	B	121	ILE	C-O	-5.66	1.17	1.24
1	E	351	ILE	C-O	-5.66	1.17	1.24
1	G	67	ARG	C-O	-5.66	1.17	1.24
1	G	350	PRO	C-O	-5.66	1.19	1.24
1	D	349	HIS	C-O	-5.66	1.17	1.24
1	H	109	ILE	C-O	-5.65	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	353	ALA	C-O	-5.65	1.16	1.24
1	A	297	ILE	C-O	-5.65	1.17	1.24
1	B	6	ILE	C-O	-5.65	1.17	1.23
1	H	172	ARG	C-O	-5.65	1.17	1.24
1	H	158	ALA	C-O	-5.64	1.17	1.24
1	E	59	ALA	C-O	-5.64	1.17	1.23
1	E	176	ASP	C-O	-5.64	1.17	1.24
1	E	18	GLY	C-O	-5.64	1.16	1.23
1	E	318	GLU	C-O	-5.63	1.17	1.23
1	A	149	THR	C-O	-5.63	1.17	1.24
1	C	337	LYS	C-O	-5.63	1.16	1.24
1	E	230	ALA	C-O	-5.63	1.17	1.24
1	B	271	ARG	C-O	-5.63	1.17	1.24
1	C	16	LYS	C-O	-5.63	1.16	1.23
1	C	120	ASN	C-O	-5.63	1.16	1.24
1	F	194	LYS	C-O	-5.62	1.17	1.24
1	D	284	MET	C-O	-5.62	1.18	1.24
1	E	103	ARG	C-O	-5.62	1.17	1.24
1	A	299	LYS	C-O	-5.62	1.17	1.24
1	H	249	GLY	C-O	-5.62	1.18	1.23
1	C	154	GLU	C-O	-5.61	1.16	1.23
1	G	299	LYS	C-O	-5.61	1.17	1.24
1	H	72	LEU	C-O	-5.61	1.17	1.24
1	G	177	GLU	C-O	-5.61	1.17	1.24
1	E	340	VAL	C-O	-5.61	1.16	1.24
1	A	100	GLN	C-O	-5.61	1.17	1.24
1	G	194	LYS	C-O	-5.61	1.16	1.24
1	D	327	CYS	C-O	-5.60	1.17	1.24
1	C	119	SER	C-O	-5.60	1.17	1.24
1	H	361	THR	C-O	-5.60	1.17	1.24
1	H	45	GLY	C-O	-5.60	1.16	1.23
1	A	327	CYS	C-O	-5.60	1.17	1.24
1	D	70	ALA	C-O	-5.60	1.17	1.24
1	H	113	GLY	C-O	-5.59	1.17	1.23
1	D	331	VAL	C-O	-5.59	1.17	1.24
1	B	159	VAL	C-O	-5.59	1.17	1.24
1	C	307	THR	C-O	-5.59	1.16	1.23
1	B	367	LYS	C-O	-5.58	1.17	1.24
1	E	226	LEU	C-O	-5.58	1.17	1.24
1	B	342	GLY	C-O	-5.58	1.16	1.24
1	D	247	ALA	C-O	-5.58	1.16	1.24
1	F	185	ARG	C-O	-5.58	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	THR	C-N	-5.58	1.26	1.33
1	G	229	LEU	C-O	-5.58	1.17	1.24
1	A	242	ILE	C-O	-5.58	1.17	1.24
1	H	92	LEU	C-O	-5.57	1.17	1.24
1	D	134	MET	C-O	-5.57	1.16	1.23
1	A	140	ARG	C-O	-5.56	1.17	1.24
1	H	58	GLN	C-O	-5.56	1.16	1.24
1	D	71	ARG	C-O	-5.56	1.17	1.24
1	H	265	ALA	C-O	-5.56	1.17	1.24
1	E	67	ARG	C-O	-5.56	1.17	1.24
1	A	78	SER	C-O	-5.56	1.17	1.24
1	C	57	VAL	C-O	-5.56	1.17	1.24
1	G	28	GLU	C-O	-5.56	1.17	1.24
1	D	14	PHE	C-O	-5.56	1.17	1.24
1	G	344	ALA	C-O	-5.55	1.17	1.24
1	C	348	GLY	C-O	-5.55	1.17	1.23
1	B	366	LEU	C-O	-5.55	1.17	1.24
1	C	178	TRP	C-O	-5.55	1.17	1.24
1	D	347	LEU	C-O	-5.55	1.16	1.24
1	A	169	ALA	C-O	-5.55	1.16	1.23
1	G	339	ASN	C-O	-5.54	1.16	1.23
1	F	93	ARG	C-O	-5.54	1.17	1.24
1	B	94	ALA	C-O	-5.54	1.17	1.24
1	B	341	ASN	C-O	-5.54	1.16	1.24
1	D	32	ILE	C-O	-5.54	1.17	1.24
1	H	153	ASP	C-O	-5.54	1.16	1.24
1	E	90	SER	C-O	-5.54	1.17	1.24
1	D	379	CYS	C-O	-5.54	1.16	1.23
1	A	190	ALA	C-O	-5.53	1.17	1.24
1	C	215	ASP	C-O	-5.53	1.16	1.24
1	D	160	HIS	C-O	-5.53	1.17	1.24
1	G	156	HIS	C-O	-5.53	1.17	1.23
1	E	120	ASN	C-O	-5.53	1.16	1.23
1	H	104	ALA	C-O	-5.53	1.16	1.24
1	H	234	PRO	C-O	-5.53	1.17	1.23
1	F	198	GLU	C-O	-5.53	1.17	1.23
1	D	172	ARG	C-O	-5.53	1.17	1.24
1	D	365	GLU	C-O	-5.53	1.17	1.24
1	E	134	MET	C-O	-5.53	1.17	1.23
1	F	160	HIS	C-O	-5.53	1.17	1.24
1	D	143	MET	C-O	-5.53	1.17	1.24
1	C	251	ASN	C-O	-5.52	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	140	ARG	C-O	-5.52	1.17	1.24
1	G	358	ILE	C-O	-5.52	1.17	1.24
1	D	147	GLY	C-O	-5.52	1.16	1.23
1	C	103	ARG	C-O	-5.52	1.16	1.24
1	G	41	ALA	C-O	-5.52	1.16	1.24
1	C	36	GLU	C-O	-5.52	1.17	1.24
1	D	62	GLY	C-O	-5.52	1.16	1.23
1	F	54	GLY	C-O	-5.51	1.17	1.23
1	C	229	LEU	C-O	-5.51	1.17	1.24
1	G	26	ALA	C-O	-5.51	1.17	1.24
1	C	364	TYR	C-O	-5.51	1.17	1.24
1	C	90	SER	C-O	-5.51	1.17	1.24
1	C	268	LEU	C-O	-5.50	1.16	1.24
1	D	38	LEU	C-O	-5.50	1.17	1.24
1	A	178	TRP	C-O	-5.50	1.17	1.24
1	F	189	ALA	C-O	-5.50	1.17	1.24
1	E	298	ASN	C-O	-5.50	1.17	1.24
1	B	254	ALA	C-O	-5.50	1.17	1.23
1	F	187	ALA	C-O	-5.50	1.17	1.24
1	C	335	LEU	C-O	-5.49	1.17	1.24
1	G	144	VAL	C-O	-5.49	1.18	1.24
1	F	214	VAL	C-O	-5.49	1.18	1.24
1	H	137	GLY	C-O	-5.49	1.16	1.23
1	B	60	GLY	C-O	-5.49	1.17	1.24
1	C	158	ALA	C-O	-5.48	1.17	1.24
1	F	62	GLY	C-O	-5.48	1.17	1.23
1	C	19	GLY	C-O	-5.48	1.16	1.23
1	F	324	VAL	C-O	-5.48	1.17	1.24
1	A	66	SER	C-O	-5.47	1.17	1.24
1	A	235	ILE	C-O	-5.47	1.18	1.24
1	C	121	ILE	C-O	-5.47	1.17	1.24
1	C	301	LEU	C-O	-5.47	1.17	1.24
1	F	340	VAL	C-O	-5.46	1.17	1.24
1	D	137	GLY	C-O	-5.46	1.16	1.23
1	A	391	GLN	C-O	-5.46	1.17	1.24
1	C	165	ALA	C-O	-5.46	1.17	1.24
1	C	78	SER	C-O	-5.46	1.17	1.24
1	A	79	VAL	C-O	-5.46	1.17	1.24
1	C	197	ASP	C-O	-5.46	1.17	1.24
1	D	288	GLU	C-O	-5.46	1.15	1.23
1	A	389	LEU	C-O	-5.45	1.17	1.24
1	D	43	VAL	C-O	-5.45	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	251	ASN	C-O	-5.45	1.16	1.23
1	B	106	ASP	C-O	-5.45	1.17	1.24
1	F	264	LYS	C-O	-5.45	1.17	1.24
1	A	352	GLY	C-O	-5.45	1.16	1.23
1	D	259	LEU	C-O	-5.45	1.17	1.23
1	D	309	GLN	C-O	-5.45	1.17	1.24
1	B	18	GLY	C-O	-5.45	1.16	1.24
1	A	155	VAL	C-O	-5.45	1.18	1.23
1	D	113	GLY	C-O	-5.45	1.17	1.23
1	F	182	SER	C-O	-5.44	1.17	1.24
1	G	170	ILE	C-O	-5.44	1.18	1.24
1	A	113	GLY	C-O	-5.44	1.18	1.23
1	B	47	ASP	C-O	-5.44	1.16	1.24
1	G	213	VAL	C-O	-5.44	1.18	1.24
1	H	77	TRP	C-O	-5.44	1.17	1.24
1	E	182	SER	C-O	-5.44	1.17	1.24
1	E	286	ALA	C-O	-5.44	1.17	1.24
1	A	201	PRO	C-O	-5.44	1.17	1.23
1	C	383	ALA	C-O	-5.44	1.16	1.23
1	F	104	ALA	C-O	-5.44	1.16	1.24
1	G	347	LEU	C-O	-5.44	1.16	1.24
1	H	59	ALA	C-O	-5.44	1.17	1.23
1	A	162	ASN	C-O	-5.44	1.17	1.24
1	A	284	MET	C-N	5.43	1.41	1.33
1	D	60	GLY	C-O	-5.43	1.16	1.24
1	G	100	GLN	C-N	5.43	1.41	1.33
1	C	247	ALA	N-CA	-5.43	1.41	1.45
1	A	229	LEU	C-O	-5.43	1.17	1.24
1	F	152	PHE	C-O	-5.43	1.16	1.23
1	D	375	VAL	C-O	-5.42	1.18	1.24
1	E	330	ILE	C-O	-5.42	1.17	1.24
1	E	274	ALA	N-CA	-5.42	1.39	1.46
1	F	251	ASN	C-O	-5.42	1.17	1.23
1	A	96	THR	C-O	-5.41	1.17	1.24
1	F	238	SER	CA-C	-5.41	1.46	1.52
1	H	97	LEU	C-O	-5.41	1.17	1.24
1	H	194	LYS	C-O	-5.41	1.17	1.24
1	B	354	SER	C-O	-5.41	1.17	1.24
1	D	92	LEU	C-O	-5.41	1.17	1.24
1	H	89	ALA	C-O	-5.40	1.16	1.24
1	E	185	ARG	C-O	-5.40	1.17	1.24
1	H	378	ILE	C-O	-5.40	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	338	VAL	C-O	-5.40	1.18	1.24
1	H	382	ALA	C-O	-5.40	1.16	1.23
1	F	255	GLY	C-O	-5.40	1.18	1.24
1	E	279	PHE	C-O	-5.40	1.17	1.23
1	H	390	VAL	C-O	-5.39	1.18	1.24
1	C	328	GLU	C-O	-5.39	1.17	1.24
1	G	138	GLU	C-O	-5.39	1.17	1.24
1	A	167	GLU	C-O	-5.39	1.17	1.24
1	B	340	VAL	C-O	-5.39	1.16	1.24
1	G	280	SER	C-O	-5.39	1.17	1.23
1	A	109	ILE	C-O	-5.38	1.18	1.24
1	B	56	VAL	C-O	-5.38	1.18	1.24
1	F	52	VAL	C-O	-5.38	1.18	1.24
1	H	176	ASP	C-O	-5.38	1.17	1.24
1	E	166	LYS	C-O	-5.38	1.18	1.24
1	D	187	ALA	C-O	-5.38	1.18	1.24
1	E	218	GLU	C-O	-5.38	1.17	1.24
1	B	184	ALA	C-O	-5.38	1.18	1.24
1	F	140	ARG	C-O	-5.38	1.17	1.24
1	F	226	LEU	C-O	-5.37	1.18	1.24
1	E	78	SER	C-O	-5.37	1.17	1.24
1	A	36	GLU	C-O	-5.37	1.17	1.24
1	C	194	LYS	C-O	-5.37	1.17	1.24
1	F	70	ALA	C-O	-5.37	1.17	1.24
1	B	346	ALA	C-O	-5.37	1.17	1.24
1	A	118	MET	C-O	-5.37	1.17	1.24
1	A	170	ILE	C-O	-5.37	1.18	1.24
1	C	238	SER	C-O	-5.37	1.17	1.24
1	B	219	ALA	C-O	-5.37	1.17	1.24
1	F	186	ALA	C-O	-5.37	1.17	1.24
1	A	192	GLU	C-O	-5.37	1.16	1.24
1	A	342	GLY	C-O	-5.37	1.17	1.23
1	G	130	TRP	C-O	-5.37	1.16	1.24
1	G	309	GLN	C-O	-5.37	1.17	1.24
1	D	20	VAL	C-O	-5.36	1.17	1.24
1	D	332	GLY	C-O	-5.36	1.17	1.24
1	D	339	ASN	C-O	-5.36	1.16	1.23
1	G	226	LEU	C-N	5.36	1.41	1.34
1	E	201	PRO	C-O	-5.36	1.17	1.23
1	G	220	ILE	C-O	-5.36	1.18	1.24
1	C	267	GLU	C-O	-5.36	1.17	1.24
1	B	109	ILE	C-O	-5.36	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	364	TYR	C-O	-5.35	1.17	1.24
1	F	191	ASP	C-O	-5.35	1.17	1.24
1	F	369	ARG	C-O	-5.35	1.16	1.24
1	B	27	ALA	C-O	-5.35	1.17	1.24
1	F	180	LEU	C-O	-5.35	1.17	1.24
1	G	372	GLY	C-O	-5.34	1.16	1.23
1	G	108	ASP	C-O	-5.34	1.17	1.24
1	E	76	PRO	C-O	-5.34	1.17	1.23
1	B	100	GLN	C-O	-5.34	1.18	1.24
1	A	32	ILE	C-O	-5.34	1.18	1.24
1	H	386	ASP	CA-C	5.34	1.58	1.52
1	D	64	ILE	C-O	-5.34	1.17	1.24
1	C	183	HIS	C-O	-5.33	1.18	1.24
1	A	296	ALA	C-O	-5.33	1.18	1.24
1	A	34	MET	C-O	-5.33	1.17	1.24
1	F	283	GLY	C-O	-5.33	1.16	1.23
1	E	20	VAL	C-O	-5.33	1.17	1.24
1	E	79	VAL	C-O	-5.33	1.17	1.24
1	E	168	TYR	C-O	-5.33	1.16	1.24
1	H	166	LYS	C-O	-5.32	1.18	1.24
1	B	359	LEU	C-O	-5.32	1.18	1.24
1	D	269	GLY	C-O	-5.32	1.16	1.23
1	H	217	ASP	C-O	-5.32	1.17	1.24
1	H	375	VAL	C-O	-5.32	1.18	1.24
1	E	36	GLU	C-O	-5.32	1.17	1.24
1	D	46	ASP	C-O	-5.32	1.17	1.24
1	D	200	VAL	C-O	-5.32	1.18	1.24
1	H	349	HIS	C-O	-5.32	1.18	1.24
1	E	108	ASP	C-O	-5.32	1.17	1.24
1	A	57	VAL	C-O	-5.32	1.17	1.24
1	B	320	PHE	C-O	-5.32	1.17	1.23
1	D	341	ASN	C-O	-5.32	1.17	1.24
1	C	169	ALA	C-O	-5.31	1.17	1.23
1	H	322	SER	C-O	-5.31	1.17	1.24
1	G	188	LYS	C-O	-5.31	1.18	1.24
1	D	319	ALA	C-O	-5.31	1.18	1.24
1	E	170	ILE	C-O	-5.31	1.18	1.24
1	B	87	VAL	C-O	-5.31	1.17	1.24
1	F	367	LYS	C-O	-5.31	1.18	1.24
1	H	10	ALA	C-O	-5.30	1.17	1.23
1	H	100	GLN	C-O	-5.30	1.18	1.24
1	A	23	GLU	C-O	-5.30	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	323	VAL	C-O	-5.30	1.17	1.24
1	E	280	SER	C-O	-5.30	1.17	1.23
1	C	186	ALA	C-O	-5.30	1.18	1.24
1	D	252	ASP	C-O	-5.30	1.17	1.24
1	C	29	LEU	C-O	-5.30	1.18	1.24
1	H	183	HIS	C-O	-5.30	1.18	1.24
1	D	57	VAL	C-O	-5.30	1.17	1.24
1	D	121	ILE	C-O	-5.30	1.17	1.24
1	A	253	GLY	C-O	-5.29	1.18	1.24
1	C	384	GLN	C-O	-5.29	1.17	1.23
1	D	344	ALA	C-O	-5.29	1.17	1.24
1	C	176	ASP	C-O	-5.29	1.17	1.24
1	F	274	ALA	C-O	-5.29	1.17	1.23
1	G	297	ILE	C-O	-5.29	1.18	1.24
1	D	346	ALA	C-O	-5.29	1.17	1.24
1	H	182	SER	C-O	-5.29	1.18	1.24
1	C	151	ALA	C-O	-5.29	1.17	1.24
1	H	250	VAL	C-O	-5.28	1.18	1.24
1	E	113	GLY	C-O	-5.28	1.17	1.23
1	A	286	ALA	C-O	-5.28	1.17	1.24
1	E	46	ASP	C-O	-5.28	1.17	1.24
1	B	68	GLN	C-O	-5.28	1.18	1.24
1	F	351	ILE	N-CA	-5.28	1.40	1.46
1	G	167	GLU	C-O	-5.28	1.17	1.24
1	D	308	VAL	C-O	-5.28	1.18	1.24
1	F	300	LEU	C-O	-5.28	1.18	1.24
1	B	124	ALA	C-O	-5.28	1.17	1.23
1	F	273	LEU	C-O	-5.28	1.18	1.24
1	B	285	PRO	C-O	-5.27	1.17	1.23
1	G	51	ASN	CG-OD1	-5.27	1.13	1.23
1	C	53	MET	C-O	-5.27	1.18	1.24
1	G	143	MET	C-O	-5.27	1.18	1.24
1	B	371	GLY	C-O	-5.27	1.15	1.23
1	C	282	THR	C-O	-5.27	1.17	1.23
1	A	62	GLY	C-O	-5.27	1.16	1.23
1	B	82	GLU	C-O	-5.27	1.17	1.24
1	F	40	GLN	C-O	-5.27	1.18	1.24
1	H	374	GLY	C-O	-5.27	1.17	1.23
1	A	94	ALA	C-O	-5.26	1.18	1.24
1	H	298	ASN	C-O	-5.26	1.18	1.24
1	H	326	THR	C-O	-5.26	1.18	1.24
1	H	202	VAL	C-O	-5.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	297	ILE	C-O	-5.26	1.18	1.24
1	E	209	GLY	C-O	-5.25	1.17	1.24
1	G	215	ASP	C-N	-5.25	1.25	1.33
1	A	279	PHE	C-O	-5.25	1.17	1.23
1	D	80	PRO	C-O	-5.25	1.18	1.23
1	B	118	MET	C-O	-5.25	1.17	1.24
1	D	29	LEU	C-O	-5.25	1.18	1.24
1	H	361	THR	C-N	5.25	1.40	1.33
1	E	165	ALA	C-O	-5.25	1.18	1.24
1	A	359	LEU	C-O	-5.25	1.18	1.24
1	C	311	ILE	C-O	-5.25	1.18	1.24
1	E	234	PRO	C-O	-5.24	1.17	1.23
1	B	181	ARG	C-O	-5.24	1.18	1.24
1	F	163	THR	C-O	-5.24	1.18	1.24
1	H	68	GLN	C-O	-5.24	1.18	1.24
1	A	385	GLY	C-O	-5.24	1.16	1.23
1	B	6	ILE	N-CA	-5.24	1.40	1.46
1	B	79	VAL	C-O	-5.24	1.17	1.24
1	C	298	ASN	C-O	-5.24	1.18	1.24
1	C	303	LYS	C-O	-5.24	1.17	1.24
1	C	167	GLU	C-O	-5.23	1.18	1.24
1	H	264	LYS	C-O	-5.23	1.18	1.24
1	F	355	GLY	C-O	-5.23	1.17	1.23
1	D	266	ALA	C-O	-5.23	1.18	1.24
1	H	145	TYR	C-O	-5.23	1.18	1.24
1	G	33	VAL	C-O	-5.22	1.18	1.24
1	D	272	PRO	C-N	-5.22	1.27	1.33
1	E	158	ALA	C-O	-5.22	1.17	1.24
1	C	342	GLY	C-O	-5.22	1.15	1.23
1	F	72	LEU	C-O	-5.22	1.17	1.24
1	H	65	PRO	C-O	-5.22	1.17	1.24
1	H	186	ALA	C-O	-5.22	1.18	1.24
1	B	146	ASP	C-O	-5.22	1.17	1.24
1	B	192	GLU	C-O	-5.22	1.17	1.24
1	C	297	ILE	C-O	-5.22	1.18	1.24
1	A	256	ALA	C-O	-5.21	1.17	1.23
1	C	241	SER	C-O	-5.21	1.17	1.24
1	E	47	ASP	C-O	-5.21	1.17	1.24
1	D	285	PRO	C-O	-5.21	1.17	1.23
1	F	25	LYS	C-O	-5.21	1.16	1.23
1	E	30	GLY	C-O	-5.21	1.17	1.23
1	C	380	SER	C-N	-5.21	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	MET	C-O	-5.21	1.17	1.24
1	C	381	GLY	N-CA	-5.20	1.40	1.45
1	H	50	GLY	C-O	-5.20	1.18	1.24
1	B	279	PHE	C-O	-5.20	1.17	1.23
1	G	251	ASN	C-O	-5.20	1.17	1.23
1	F	178	TRP	C-O	-5.20	1.18	1.24
1	H	355	GLY	C-O	-5.20	1.17	1.23
1	D	189	ALA	C-O	-5.19	1.18	1.24
1	B	96	THR	C-O	-5.19	1.17	1.24
1	B	52	VAL	C-O	-5.19	1.18	1.24
1	C	174	GLU	C-O	-5.19	1.18	1.24
1	D	225	SER	C-N	-5.19	1.26	1.34
1	D	124	ALA	C-O	-5.18	1.17	1.23
1	E	74	GLY	C-O	-5.18	1.17	1.24
1	E	28	GLU	C-O	-5.18	1.18	1.24
1	H	362	LEU	C-O	-5.18	1.18	1.24
1	A	179	ALA	C-O	-5.18	1.18	1.24
1	F	80	PRO	C-O	-5.18	1.17	1.23
1	F	277	LEU	C-O	-5.18	1.18	1.24
1	G	253	GLY	C-O	-5.18	1.16	1.23
1	E	123	TYR	C-O	-5.18	1.17	1.23
1	B	50	GLY	C-O	-5.18	1.17	1.23
1	B	81	SER	C-N	-5.17	1.26	1.33
1	B	54	GLY	C-O	-5.17	1.17	1.23
1	G	35	LYS	C-O	-5.17	1.18	1.24
1	H	244	ALA	C-O	-5.17	1.17	1.24
1	E	89	ALA	C-O	-5.17	1.17	1.24
1	C	363	VAL	C-O	-5.17	1.18	1.24
1	F	317	ASN	C-O	-5.17	1.17	1.23
1	D	10	ALA	C-O	-5.17	1.17	1.23
1	E	88	CYS	CA-CB	5.17	1.61	1.53
1	C	27	ALA	C-O	-5.17	1.18	1.24
1	G	371	GLY	CA-C	-5.17	1.44	1.52
1	C	387	ALA	C-O	-5.17	1.18	1.23
1	G	15	GLY	C-O	-5.17	1.16	1.23
1	B	83	THR	C-O	-5.17	1.17	1.24
1	B	161	GLY	C-O	-5.16	1.17	1.23
1	B	259	LEU	C-O	-5.16	1.17	1.24
1	C	87	VAL	C-N	-5.16	1.27	1.33
1	D	295	PHE	C-O	-5.16	1.18	1.24
1	A	95	VAL	C-O	-5.16	1.18	1.24
1	A	375	VAL	C-O	-5.16	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	PHE	C-O	-5.16	1.18	1.24
1	C	319	ALA	C-O	-5.16	1.18	1.24
1	D	367	LYS	C-O	-5.16	1.18	1.24
1	H	120	ASN	C-O	-5.15	1.17	1.24
1	F	81	SER	C-O	-5.15	1.17	1.23
1	E	339	ASN	C-O	-5.15	1.17	1.23
1	A	285	PRO	C-O	-5.15	1.17	1.23
1	C	260	MET	C-O	-5.15	1.17	1.23
1	F	20	VAL	C-O	-5.15	1.17	1.24
1	F	349	HIS	C-O	-5.15	1.18	1.24
1	D	55	MET	C-O	-5.14	1.17	1.23
1	H	79	VAL	C-O	-5.14	1.18	1.24
1	D	230	ALA	C-O	-5.14	1.17	1.24
1	E	291	ALA	C-O	-5.14	1.17	1.24
1	G	348	GLY	C-O	-5.14	1.17	1.23
1	H	112	ALA	C-O	-5.14	1.17	1.23
1	E	320	PHE	C-O	-5.14	1.17	1.23
1	H	26	ALA	C-O	-5.14	1.18	1.24
1	E	310	ASP	C-O	-5.13	1.17	1.24
1	F	24	VAL	C-O	-5.13	1.18	1.24
1	F	37	ALA	C-O	-5.13	1.18	1.24
1	D	273	LEU	C-N	-5.13	1.27	1.33
1	H	128	GLY	C-O	-5.13	1.17	1.23
1	E	54	GLY	C-O	-5.12	1.16	1.23
1	H	391	GLN	C-O	-5.12	1.17	1.24
1	A	25	LYS	C-O	-5.12	1.17	1.23
1	D	217	ASP	C-O	-5.12	1.18	1.24
1	E	91	GLY	C-O	-5.12	1.17	1.23
1	A	97	LEU	C-O	-5.12	1.18	1.24
1	D	392	VAL	C-O	-5.12	1.18	1.24
1	D	188	LYS	C-O	-5.11	1.18	1.24
1	G	68	GLN	C-O	-5.11	1.18	1.24
1	H	201	PRO	C-O	-5.11	1.17	1.23
1	F	36	GLU	C-O	-5.11	1.18	1.24
1	H	164	ALA	C-O	-5.11	1.18	1.24
1	A	88	CYS	C-N	5.11	1.41	1.33
1	F	248	PRO	C-O	-5.11	1.17	1.23
1	B	356	ALA	C-O	-5.10	1.18	1.24
1	D	73	ALA	C-O	-5.10	1.17	1.24
1	E	361	THR	CA-C	-5.10	1.46	1.52
1	A	358	ILE	C-O	-5.10	1.18	1.24
1	B	127	ALA	C-O	-5.10	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	GLY	C-O	-5.10	1.18	1.23
1	G	370	GLY	C-O	-5.10	1.17	1.23
1	E	23	GLU	C-O	-5.10	1.17	1.24
1	H	247	ALA	CA-C	-5.10	1.47	1.52
1	A	77	TRP	C-O	-5.10	1.17	1.24
1	A	152	PHE	C-O	-5.09	1.17	1.23
1	A	27	ALA	C-O	-5.09	1.18	1.24
1	F	89	ALA	C-O	-5.09	1.17	1.24
1	G	200	VAL	C-O	-5.09	1.18	1.24
1	G	267	GLU	C-O	-5.09	1.17	1.24
1	D	114	GLY	C-O	-5.09	1.18	1.24
1	C	132	ALA	C-O	-5.09	1.17	1.24
1	C	344	ALA	C-O	-5.09	1.17	1.24
1	F	265	ALA	C-O	-5.08	1.18	1.24
1	B	361	THR	C-O	-5.08	1.17	1.24
1	G	256	ALA	C-O	-5.08	1.17	1.23
1	H	37	ALA	C-O	-5.08	1.18	1.24
1	A	249	GLY	C-O	-5.08	1.17	1.24
1	B	338	VAL	C-O	-5.08	1.18	1.24
1	B	39	GLN	C-O	-5.08	1.18	1.24
1	E	155	VAL	C-O	-5.08	1.18	1.23
1	B	89	ALA	C-O	-5.07	1.17	1.24
1	A	172	ARG	C-O	-5.07	1.18	1.24
1	C	98	CYS	C-O	-5.07	1.18	1.24
1	A	189	ALA	C-O	-5.07	1.18	1.24
1	C	102	ILE	C-O	-5.07	1.18	1.24
1	E	42	GLY	C-O	-5.07	1.17	1.23
1	B	182	SER	C-O	-5.07	1.18	1.24
1	G	180	LEU	C-O	-5.07	1.18	1.24
1	E	160	HIS	C-O	-5.06	1.18	1.24
1	H	342	GLY	C-O	-5.06	1.16	1.23
1	E	22	LYS	C-O	-5.06	1.18	1.24
1	A	142	LEU	C-O	-5.06	1.17	1.24
1	A	355	GLY	C-O	-5.06	1.17	1.23
1	H	48	VAL	C-O	-5.06	1.18	1.24
1	B	327	CYS	C-O	-5.06	1.17	1.24
1	G	44	SER	C-O	-5.06	1.17	1.23
1	C	101	MET	C-O	-5.06	1.18	1.24
1	A	238	SER	C-O	-5.05	1.16	1.23
1	C	55	MET	C-O	-5.05	1.17	1.23
1	G	276	ILE	C-O	-5.05	1.18	1.23
1	H	135	GLY	C-O	-5.05	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	307	THR	C-O	-5.05	1.17	1.23
1	A	136	ASP	C-O	-5.05	1.17	1.23
1	B	195	PHE	C-O	-5.05	1.17	1.23
1	C	367	LYS	C-O	-5.05	1.18	1.24
1	B	40	GLN	C-O	-5.05	1.18	1.24
1	B	214	VAL	C-O	-5.05	1.18	1.24
1	G	243	THR	C-O	-5.05	1.16	1.23
1	D	22	LYS	C-O	-5.05	1.17	1.24
1	B	193	GLY	C-O	-5.04	1.16	1.24
1	G	319	ALA	C-O	-5.04	1.18	1.24
1	D	16	LYS	C-O	-5.04	1.17	1.23
1	H	124	ALA	C-O	-5.04	1.17	1.23
1	A	347	LEU	C-O	-5.04	1.17	1.24
1	B	293	PRO	C-O	-5.04	1.18	1.24
1	C	309	GLN	C-O	-5.04	1.17	1.24
1	F	147	GLY	C-O	-5.04	1.17	1.23
1	H	191	ASP	C-O	-5.04	1.17	1.24
1	H	241	SER	C-O	-5.04	1.17	1.24
1	G	186	ALA	C-O	-5.04	1.18	1.24
1	C	327	CYS	C-O	-5.04	1.17	1.24
1	F	372	GLY	C-O	-5.04	1.17	1.23
1	H	305	GLY	C-O	-5.03	1.17	1.24
1	C	392	VAL	C-O	-5.03	1.17	1.24
1	A	4	THR	C-O	-5.03	1.18	1.23
1	F	45	GLY	C-O	-5.03	1.17	1.23
1	G	386	ASP	C-O	-5.03	1.18	1.24
1	E	392	VAL	C-O	-5.03	1.18	1.24
1	B	205	ILE	C-O	-5.02	1.18	1.24
1	D	233	ALA	C-O	-5.02	1.17	1.24
1	D	111	VAL	C-O	-5.02	1.18	1.24
1	E	100	GLN	C-O	-5.02	1.18	1.24
1	D	267	GLU	C-O	-5.02	1.18	1.24
1	B	353	ALA	C-O	-5.02	1.17	1.24
1	H	136	ASP	C-O	-5.01	1.17	1.23
1	C	155	VAL	C-O	-5.01	1.18	1.23
1	D	116	GLU	C-O	-5.01	1.17	1.23
1	A	172	ARG	N-CA	-5.01	1.40	1.46
1	H	269	GLY	C-O	-5.01	1.17	1.24
1	C	326	THR	C-O	-5.01	1.18	1.24
1	H	73	ALA	C-O	-5.01	1.17	1.24
1	H	146	ASP	C-O	-5.01	1.18	1.24
1	C	52	VAL	C-O	-5.01	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	142	LEU	C-O	-5.01	1.17	1.24
1	C	73	ALA	C-O	-5.00	1.17	1.24
1	F	177	GLU	C-O	-5.00	1.18	1.24

All (690) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	222	ARG	O-C-N	-34.59	76.58	122.59
1	D	82	GLU	O-C-N	-25.01	98.70	123.46
1	A	371	GLY	N-CA-C	22.28	136.83	112.33
1	D	332	GLY	O-C-N	-22.02	100.83	122.41
1	G	101	MET	CA-C-O	-20.69	98.49	120.42
1	E	337	LYS	CA-C-N	20.42	150.49	123.13
1	E	337	LYS	C-N-CA	20.42	150.49	123.13
1	F	235	ILE	N-CA-C	20.18	129.50	110.53
1	B	215	ASP	CA-C-N	19.71	155.45	122.33
1	B	215	ASP	C-N-CA	19.71	155.45	122.33
1	H	305	GLY	O-C-N	-19.49	103.31	122.41
1	F	238	SER	N-CA-C	-19.28	78.02	109.07
1	H	238	SER	N-CA-C	-19.04	79.72	109.23
1	A	333	PHE	O-C-N	18.98	147.12	122.82
1	D	332	GLY	CA-C-N	18.77	147.36	120.90
1	D	332	GLY	C-N-CA	18.77	147.36	120.90
1	A	87	VAL	CA-C-N	18.63	148.76	120.82
1	A	87	VAL	C-N-CA	18.63	148.76	120.82
1	B	305	GLY	O-C-N	-18.40	107.61	122.51
1	G	34	MET	CA-C-O	-18.38	100.94	120.42
1	F	210	LYS	CA-C-N	18.13	138.94	119.90
1	F	210	LYS	C-N-CA	18.13	138.94	119.90
1	A	82	GLU	O-C-N	-18.10	105.19	123.29
1	G	227	ASP	O-C-N	-17.95	101.74	122.20
1	H	305	GLY	CA-C-N	17.93	150.96	122.81
1	H	305	GLY	C-N-CA	17.93	150.96	122.81
1	A	389	LEU	CA-C-N	17.80	147.69	122.94
1	A	389	LEU	C-N-CA	17.80	147.69	122.94
1	A	55	MET	O-C-N	-17.27	101.85	123.26
1	F	81	SER	O-C-N	-17.21	102.78	122.92
1	E	235	ILE	N-CA-C	16.97	126.71	110.42
1	E	230	ALA	O-C-N	-16.48	104.65	122.12
1	D	3	LYS	CA-C-N	16.37	145.97	123.05
1	D	3	LYS	C-N-CA	16.37	145.97	123.05
1	A	241	SER	O-C-N	-16.31	104.40	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3	LYS	CA-C-N	16.30	145.49	123.00
1	H	3	LYS	C-N-CA	16.30	145.49	123.00
1	B	215	ASP	O-C-N	-16.30	101.67	122.20
1	G	332	GLY	O-C-N	-16.29	100.68	122.35
1	A	55	MET	CA-C-O	16.12	139.65	119.98
1	D	82	GLU	CA-C-N	15.91	147.00	121.86
1	D	82	GLU	C-N-CA	15.91	147.00	121.86
1	G	226	LEU	O-C-N	-15.89	105.70	122.07
1	B	378	ILE	O-C-N	-15.66	103.00	122.57
1	A	84	LEU	O-C-N	-15.06	105.38	123.30
1	H	371	GLY	N-CA-C	14.95	132.28	112.25
1	F	82	GLU	CB-CA-C	14.70	139.68	110.42
1	H	204	TRP	O-C-N	-14.67	107.05	123.48
1	B	305	GLY	CA-C-N	14.57	145.68	122.81
1	B	305	GLY	C-N-CA	14.57	145.68	122.81
1	H	134	MET	O-C-N	-14.09	107.42	123.48
1	B	332	GLY	O-C-N	-14.04	104.55	122.39
1	E	87	VAL	CA-C-N	13.75	139.10	120.54
1	E	87	VAL	C-N-CA	13.75	139.10	120.54
1	A	272	PRO	CA-C-N	13.74	139.21	120.38
1	A	272	PRO	C-N-CA	13.74	139.21	120.38
1	E	305	GLY	CA-C-N	13.52	143.71	122.62
1	E	305	GLY	C-N-CA	13.52	143.71	122.62
1	F	333	PHE	O-C-N	13.46	139.37	122.81
1	F	338	VAL	O-C-N	-13.46	109.97	123.03
1	F	332	GLY	O-C-N	-13.38	106.02	122.34
1	A	120	ASN	CA-C-N	13.31	146.75	122.13
1	A	120	ASN	C-N-CA	13.31	146.75	122.13
1	G	333	PHE	O-C-N	13.30	140.27	122.59
1	H	55	MET	O-C-N	-13.29	108.27	123.42
1	H	55	MET	CA-C-O	13.22	136.27	120.14
1	B	87	VAL	CA-C-N	13.05	140.40	120.82
1	B	87	VAL	C-N-CA	13.05	140.40	120.82
1	E	333	PHE	O-C-N	13.04	139.94	122.59
1	C	271	ARG	O-C-N	-12.95	107.77	120.85
1	C	333	PHE	O-C-N	12.77	138.55	122.97
1	A	120	ASN	O-C-N	-12.76	106.39	122.34
1	E	222	ARG	N-CA-C	12.69	137.84	110.80
1	F	332	GLY	CA-C-N	12.62	139.81	120.75
1	F	332	GLY	C-N-CA	12.62	139.81	120.75
1	A	101	MET	O-C-N	-12.51	108.86	122.12
1	A	34	MET	O-C-N	-12.48	106.92	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	LEU	O-C-N	-12.46	108.56	123.27
1	E	371	GLY	N-CA-C	12.34	133.02	112.30
1	A	81	SER	O-C-N	-12.31	107.44	122.96
1	A	134	MET	O-C-N	-12.29	110.01	123.52
1	H	237	ALA	CB-CA-C	12.08	136.79	111.91
1	H	204	TRP	CA-C-N	11.97	139.66	121.71
1	H	204	TRP	C-N-CA	11.97	139.66	121.71
1	A	75	MET	CA-C-O	11.95	130.98	119.75
1	A	370	GLY	CA-C-N	11.91	133.43	120.44
1	A	370	GLY	C-N-CA	11.91	133.43	120.44
1	C	75	MET	CA-C-O	11.84	133.03	120.25
1	A	43	VAL	O-C-N	-11.83	110.33	122.99
1	F	222	ARG	O-C-N	11.81	136.68	123.22
1	B	360	MET	O-C-N	11.67	135.88	122.22
1	F	3	LYS	CA-C-N	11.59	139.00	123.00
1	F	3	LYS	C-N-CA	11.59	139.00	123.00
1	A	273	LEU	O-C-N	-11.59	109.84	122.12
1	G	22	LYS	CA-C-N	-11.27	104.63	122.65
1	G	22	LYS	C-N-CA	-11.27	104.63	122.65
1	B	42	GLY	CA-C-N	11.26	138.97	122.98
1	B	42	GLY	C-N-CA	11.26	138.97	122.98
1	E	337	LYS	O-C-N	-11.18	108.37	122.34
1	C	308	VAL	O-C-N	-11.16	107.43	122.05
1	C	270	LYS	CA-C-N	11.12	146.52	122.17
1	C	270	LYS	C-N-CA	11.12	146.52	122.17
1	C	384	GLN	O-C-N	11.02	135.78	123.10
1	D	235	ILE	N-CA-C	11.01	121.69	111.45
1	H	82	GLU	O-C-N	10.97	135.73	123.33
1	D	294	GLY	N-CA-C	-10.95	81.56	113.30
1	C	383	ALA	CA-C-N	10.79	140.98	122.64
1	C	383	ALA	C-N-CA	10.79	140.98	122.64
1	B	361	THR	CA-C-N	10.78	135.10	120.44
1	B	361	THR	C-N-CA	10.78	135.10	120.44
1	B	337	LYS	O-C-N	-10.76	107.14	122.41
1	H	218	GLU	N-CA-C	10.76	123.08	111.36
1	E	230	ALA	CA-C-N	10.67	142.31	121.18
1	E	230	ALA	C-N-CA	10.67	142.31	121.18
1	A	134	MET	CA-C-O	10.66	132.35	120.31
1	F	154	GLU	O-C-N	-10.65	109.35	122.55
1	C	333	PHE	N-CA-C	10.64	125.25	110.24
1	A	82	GLU	CB-CA-C	10.64	130.10	110.95
1	E	174	GLU	O-C-N	-10.59	110.90	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	PRO	O-C-N	-10.57	110.41	123.10
1	A	237	ALA	CB-CA-C	10.46	128.01	110.43
1	F	145	TYR	O-C-N	10.39	134.74	122.17
1	F	211	PRO	O-C-N	10.34	134.68	123.10
1	G	281	THR	O-C-N	-10.32	110.69	123.27
1	A	83	THR	CA-C-N	10.31	137.53	122.99
1	A	83	THR	C-N-CA	10.31	137.53	122.99
1	E	99	ASP	O-C-N	-10.24	111.44	122.09
1	C	383	ALA	O-C-N	-10.23	109.86	122.55
1	G	251	ASN	N-CA-C	10.21	124.35	109.14
1	C	251	ASN	N-CA-C	10.17	124.12	108.96
1	B	333	PHE	O-C-N	10.15	134.48	123.11
1	E	332	GLY	O-C-N	-10.13	109.15	122.42
1	G	55	MET	O-C-N	-9.96	110.91	123.26
1	A	284	MET	N-CA-C	9.95	126.77	109.06
1	D	83	THR	N-CA-CB	9.94	126.99	110.59
1	H	134	MET	CA-C-O	9.93	132.14	120.43
1	C	87	VAL	CA-C-N	9.92	133.93	120.54
1	C	87	VAL	C-N-CA	9.92	133.93	120.54
1	H	333	PHE	O-C-N	9.90	134.33	122.75
1	D	42	GLY	CA-C-N	9.90	136.26	123.10
1	D	42	GLY	C-N-CA	9.90	136.26	123.10
1	B	217	ASP	O-C-N	-9.86	109.89	123.01
1	E	98	CYS	CA-C-N	9.84	133.82	120.54
1	E	98	CYS	C-N-CA	9.84	133.82	120.54
1	A	55	MET	CA-C-N	9.80	132.84	120.88
1	A	55	MET	C-N-CA	9.80	132.84	120.88
1	D	218	GLU	N-CA-C	9.79	122.03	111.36
1	H	205	ILE	O-C-N	-9.77	111.19	122.72
1	G	222	ARG	N-CA-C	-9.73	96.11	110.52
1	G	372	GLY	N-CA-C	9.72	136.22	113.18
1	C	56	VAL	N-CA-C	9.68	119.63	110.53
1	H	351	ILE	N-CA-C	9.65	120.49	110.36
1	A	75	MET	O-C-N	9.65	129.88	121.30
1	C	270	LYS	O-C-N	-9.64	111.13	122.89
1	B	332	GLY	CA-C-N	9.59	136.51	121.56
1	B	332	GLY	C-N-CA	9.59	136.51	121.56
1	H	134	MET	CA-C-N	9.55	133.69	121.85
1	H	134	MET	C-N-CA	9.55	133.69	121.85
1	E	272	PRO	O-C-N	9.54	135.15	123.13
1	H	251	ASN	N-CA-C	9.48	123.09	108.96
1	A	84	LEU	CA-C-N	9.46	136.30	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LEU	C-N-CA	9.46	136.30	122.86
1	F	56	VAL	N-CA-C	9.46	119.43	110.53
1	F	200	VAL	CB-CA-C	9.44	119.29	110.13
1	G	242	ILE	N-CA-CB	9.42	120.99	110.72
1	E	305	GLY	O-C-N	-9.42	110.46	122.70
1	G	350	PRO	N-CA-C	-9.40	95.13	110.74
1	A	204	TRP	O-C-N	-9.34	113.66	123.56
1	H	3	LYS	O-C-N	-9.31	110.19	122.94
1	H	332	GLY	O-C-N	-9.30	110.62	122.43
1	A	101	MET	CA-C-O	9.29	130.40	120.55
1	G	3	LYS	CA-C-N	9.27	136.06	122.99
1	G	3	LYS	C-N-CA	9.27	136.06	122.99
1	D	293	PRO	CA-C-N	9.25	138.36	121.70
1	D	293	PRO	C-N-CA	9.25	138.36	121.70
1	D	286	ALA	N-CA-C	9.22	122.49	111.33
1	F	371	GLY	N-CA-C	9.21	126.95	112.31
1	D	226	LEU	O-C-N	-9.19	110.97	122.27
1	A	34	MET	CA-C-O	9.15	130.49	119.97
1	G	63	GLN	CA-C-N	9.05	138.88	122.13
1	G	63	GLN	C-N-CA	9.05	138.88	122.13
1	E	284	MET	N-CA-C	9.04	118.73	108.25
1	A	332	GLY	O-C-N	-9.01	111.15	122.41
1	A	225	SER	O-C-N	-8.92	111.16	123.11
1	A	350	PRO	N-CA-C	-8.89	95.98	110.74
1	C	74	GLY	O-C-N	-8.89	111.14	122.43
1	G	216	LYS	CA-C-N	8.88	133.38	120.95
1	G	216	LYS	C-N-CA	8.88	133.38	120.95
1	A	87	VAL	O-C-N	-8.84	111.52	122.57
1	E	218	GLU	N-CA-C	8.83	120.99	111.36
1	C	333	PHE	CB-CA-C	-8.83	95.48	109.70
1	B	371	GLY	N-CA-C	8.79	127.01	112.85
1	F	284	MET	N-CA-C	8.76	116.11	108.22
1	F	390	VAL	N-CA-C	8.73	120.70	108.12
1	C	350	PRO	N-CA-C	-8.71	96.28	110.74
1	H	237	ALA	N-CA-C	-8.69	96.65	108.38
1	A	147	GLY	N-CA-C	8.68	123.00	112.49
1	B	336	GLU	CA-C-N	8.64	138.13	122.06
1	B	336	GLU	C-N-CA	8.64	138.13	122.06
1	D	293	PRO	N-CA-C	8.64	125.83	113.47
1	E	273	LEU	O-C-N	-8.64	112.30	122.15
1	A	312	ASP	N-CA-C	8.63	120.46	111.14
1	D	3	LYS	O-C-N	-8.57	111.20	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	VAL	O-C-N	-8.51	114.18	123.20
1	H	124	ALA	CA-C-N	8.45	137.77	122.13
1	H	124	ALA	C-N-CA	8.45	137.77	122.13
1	A	148	LEU	N-CA-C	8.44	123.77	112.88
1	A	56	VAL	N-CA-C	8.43	118.41	110.74
1	B	337	LYS	CA-C-N	8.41	134.06	123.12
1	B	337	LYS	C-N-CA	8.41	134.06	123.12
1	C	305	GLY	CA-C-N	8.41	138.05	122.74
1	C	305	GLY	C-N-CA	8.41	138.05	122.74
1	E	145	TYR	N-CA-C	8.41	120.22	111.14
1	B	378	ILE	CA-C-N	8.38	135.30	121.39
1	B	378	ILE	C-N-CA	8.38	135.30	121.39
1	C	74	GLY	CA-C-N	8.32	132.31	120.49
1	C	74	GLY	C-N-CA	8.32	132.31	120.49
1	F	210	LYS	O-C-N	-8.31	109.70	123.00
1	B	388	VAL	O-C-N	-8.31	114.23	123.20
1	D	333	PHE	O-C-N	8.31	133.10	122.97
1	G	148	LEU	N-CA-C	8.29	123.12	112.92
1	A	226	LEU	CA-C-N	-8.29	109.02	120.38
1	A	226	LEU	C-N-CA	-8.29	109.02	120.38
1	C	284	MET	CA-C-N	8.26	128.29	119.78
1	C	284	MET	C-N-CA	8.26	128.29	119.78
1	D	56	VAL	N-CA-C	8.24	118.28	110.53
1	B	360	MET	CA-C-N	-8.24	105.52	121.58
1	B	360	MET	C-N-CA	-8.24	105.52	121.58
1	H	128	GLY	N-CA-C	8.20	122.01	112.50
1	D	284	MET	N-CA-C	8.13	123.24	109.09
1	F	225	SER	CA-C-N	8.11	130.99	120.44
1	F	225	SER	C-N-CA	8.11	130.99	120.44
1	C	7	VAL	N-CA-C	8.11	118.15	110.53
1	E	221	ARG	O-C-N	-8.11	112.74	122.63
1	C	332	GLY	O-C-N	-8.09	111.84	122.28
1	F	319	ALA	N-CA-C	-8.08	102.48	111.28
1	E	199	ILE	N-CA-C	8.06	120.18	108.58
1	A	251	ASN	N-CA-C	8.04	121.12	109.14
1	B	373	LEU	N-CA-C	8.02	122.77	109.46
1	D	291	ALA	N-CA-C	7.99	122.29	112.23
1	E	173	ARG	CA-C-N	7.92	131.23	120.38
1	E	173	ARG	C-N-CA	7.92	131.23	120.38
1	G	56	VAL	N-CA-C	7.91	118.49	110.82
1	G	332	GLY	CA-C-N	7.90	136.63	121.54
1	G	332	GLY	C-N-CA	7.90	136.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	ILE	N-CA-C	7.87	119.28	108.89
1	A	225	SER	CA-C-N	7.85	131.70	120.79
1	A	225	SER	C-N-CA	7.85	131.70	120.79
1	E	219	ALA	N-CA-C	7.83	122.41	113.01
1	G	101	MET	O-C-N	7.82	131.06	122.15
1	B	227	ASP	O-C-N	7.81	131.05	122.15
1	E	56	VAL	N-CA-C	7.80	118.39	110.82
1	F	350	PRO	N-CA-C	-7.80	97.79	110.74
1	A	330	ILE	N-CA-C	7.77	117.83	110.53
1	G	371	GLY	N-CA-C	7.76	124.66	112.31
1	D	225	SER	CA-C-N	7.76	132.10	120.31
1	D	225	SER	C-N-CA	7.76	132.10	120.31
1	D	23	GLU	O-C-N	-7.71	111.46	122.41
1	D	350	PRO	N-CA-C	-7.71	97.95	110.74
1	G	22	LYS	O-C-N	7.68	132.32	122.33
1	C	284	MET	O-C-N	-7.66	112.51	121.32
1	E	88	CYS	O-C-N	7.65	130.05	122.09
1	D	351	ILE	N-CA-C	7.65	117.77	110.42
1	B	216	LYS	O-C-N	7.63	132.67	123.36
1	C	82	GLU	O-C-N	-7.63	112.44	122.59
1	H	199	ILE	N-CA-C	7.56	118.87	108.89
1	E	251	ASN	N-CA-C	7.56	120.40	109.14
1	B	350	PRO	N-CA-C	-7.54	98.22	110.74
1	C	219	ALA	N-CA-C	7.51	122.44	113.28
1	G	219	ALA	N-CA-C	7.49	122.25	113.18
1	B	148	LEU	N-CA-C	7.46	123.30	113.30
1	B	384	GLN	CA-C-N	7.45	126.72	121.65
1	B	384	GLN	C-N-CA	7.45	126.72	121.65
1	F	154	GLU	CA-C-N	7.42	134.40	122.68
1	F	154	GLU	C-N-CA	7.42	134.40	122.68
1	A	198	GLU	N-CA-C	7.36	119.38	111.36
1	B	336	GLU	O-C-N	-7.36	113.22	122.27
1	E	98	CYS	O-C-N	-7.30	114.39	122.12
1	H	283	GLY	O-C-N	7.28	132.17	122.70
1	B	2	ARG	CA-C-N	7.28	134.75	121.94
1	B	2	ARG	C-N-CA	7.28	134.75	121.94
1	C	82	GLU	CA-C-N	7.28	132.45	122.19
1	C	82	GLU	C-N-CA	7.28	132.45	122.19
1	D	219	ALA	N-CA-C	7.28	121.74	113.01
1	B	372	GLY	N-CA-C	7.27	130.41	113.18
1	E	12	THR	N-CA-C	-7.25	101.79	110.13
1	E	361	THR	N-CA-CB	7.25	120.78	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	ARG	CB-CA-C	7.24	116.96	110.44
1	F	148	LEU	N-CA-C	7.23	122.98	113.30
1	H	350	PRO	N-CA-C	-7.18	98.81	110.74
1	G	216	LYS	O-C-N	-7.18	113.86	123.19
1	B	374	GLY	N-CA-C	7.16	121.85	110.90
1	E	350	PRO	N-CA-C	-7.15	97.74	112.47
1	H	346	ALA	N-CA-C	7.14	118.85	111.14
1	A	145	TYR	N-CA-C	7.14	118.75	110.97
1	D	128	GLY	N-CA-C	7.14	121.30	112.73
1	A	84	LEU	N-CA-C	7.13	120.52	108.90
1	F	286	ALA	N-CA-C	7.12	119.04	111.28
1	A	3	LYS	N-CA-C	7.11	120.55	109.52
1	E	361	THR	CB-CA-C	-7.10	99.00	110.79
1	C	357	ARG	N-CA-C	7.10	118.67	111.07
1	C	291	ALA	N-CA-C	7.10	120.05	111.82
1	H	372	GLY	N-CA-C	7.08	129.97	113.18
1	B	145	TYR	N-CA-C	7.08	118.65	111.07
1	E	253	GLY	N-CA-C	7.06	121.19	110.18
1	E	319	ALA	N-CA-C	-7.05	103.59	111.28
1	A	238	SER	N-CA-C	-7.02	105.25	113.88
1	E	351	ILE	N-CA-C	7.01	117.78	110.62
1	A	219	ALA	N-CA-C	7.00	121.65	113.18
1	C	271	ARG	CA-C-N	7.00	127.56	120.14
1	C	271	ARG	C-N-CA	7.00	127.56	120.14
1	G	55	MET	CA-C-N	6.97	130.71	120.74
1	G	55	MET	C-N-CA	6.97	130.71	120.74
1	H	284	MET	O-C-N	-6.96	115.40	121.32
1	F	83	THR	N-CA-CB	6.95	122.23	110.49
1	A	83	THR	N-CA-CB	6.94	122.04	110.59
1	B	347	LEU	N-CA-C	6.93	121.00	112.54
1	G	227	ASP	CA-C-N	6.92	130.11	120.29
1	G	227	ASP	C-N-CA	6.92	130.11	120.29
1	A	74	GLY	CA-C-N	6.91	130.04	120.65
1	A	74	GLY	C-N-CA	6.91	130.04	120.65
1	G	145	TYR	N-CA-C	6.88	118.43	111.07
1	E	20	VAL	N-CA-C	6.87	119.64	111.05
1	E	198	GLU	N-CA-C	6.87	118.84	111.36
1	F	351	ILE	N-CA-C	6.86	117.56	110.36
1	H	330	ILE	N-CA-C	6.84	118.46	111.00
1	B	216	LYS	CA-C-N	6.84	131.14	121.02
1	B	216	LYS	C-N-CA	6.84	131.14	121.02
1	C	199	ILE	N-CA-C	6.84	118.40	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	390	VAL	N-CA-C	6.82	119.34	108.85
1	C	306	LEU	O-C-N	-6.81	115.33	123.03
1	D	92	LEU	O-C-N	-6.81	113.20	122.33
1	B	129	ARG	N-CA-C	6.80	118.49	111.14
1	B	313	LEU	N-CA-C	6.79	119.66	108.99
1	C	75	MET	O-C-N	6.77	129.01	121.43
1	F	82	GLU	N-CA-C	-6.77	96.39	110.80
1	F	251	ASN	N-CA-C	6.76	119.03	108.96
1	E	205	ILE	N-CA-C	-6.76	98.13	107.99
1	D	145	TYR	N-CA-C	6.75	118.29	111.07
1	A	332	GLY	CA-C-N	6.73	130.72	120.82
1	A	332	GLY	C-N-CA	6.73	130.72	120.82
1	B	378	ILE	N-CA-C	6.72	123.31	109.34
1	D	81	SER	CA-C-N	-6.72	108.27	121.91
1	D	81	SER	C-N-CA	-6.72	108.27	121.91
1	D	245	GLY	N-CA-C	6.71	121.35	112.77
1	F	211	PRO	CA-C-N	-6.70	112.17	122.62
1	F	211	PRO	C-N-CA	-6.70	112.17	122.62
1	F	50	GLY	N-CA-C	6.68	120.86	110.91
1	F	353	ALA	N-CA-C	6.66	121.70	113.50
1	A	74	GLY	O-C-N	-6.64	114.70	122.60
1	B	56	VAL	N-CA-C	6.62	117.24	110.82
1	F	219	ALA	N-CA-C	6.61	121.35	113.28
1	G	374	GLY	N-CA-C	6.61	123.03	111.46
1	F	338	VAL	CA-C-N	6.59	131.50	122.34
1	F	338	VAL	C-N-CA	6.59	131.50	122.34
1	H	124	ALA	O-C-N	-6.57	114.30	123.11
1	F	323	VAL	N-CA-C	6.55	116.69	110.53
1	D	251	ASN	N-CA-C	6.53	118.69	108.96
1	F	244	ALA	CA-C-N	6.52	127.18	120.00
1	F	244	ALA	C-N-CA	6.52	127.18	120.00
1	G	253	GLY	N-CA-C	6.50	120.06	110.63
1	A	171	SER	N-CA-C	6.49	119.10	110.53
1	H	81	SER	CA-C-N	6.48	133.33	121.85
1	H	81	SER	C-N-CA	6.48	133.33	121.85
1	G	29	LEU	N-CA-C	-6.48	104.22	111.28
1	B	291	ALA	N-CA-C	6.47	118.33	111.28
1	F	361	THR	CA-C-N	6.45	129.21	120.44
1	F	361	THR	C-N-CA	6.45	129.21	120.44
1	C	308	VAL	CA-C-N	6.45	131.49	120.72
1	C	308	VAL	C-N-CA	6.45	131.49	120.72
1	C	20	VAL	N-CA-C	6.43	117.18	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	129	ARG	N-CA-C	6.43	118.08	111.14
1	C	120	ASN	N-CA-C	6.40	120.80	112.92
1	G	302	LYS	N-CA-C	6.40	118.26	111.28
1	A	319	ALA	N-CA-C	-6.39	104.31	111.28
1	B	333	PHE	N-CA-C	6.39	119.75	110.42
1	E	221	ARG	CA-C-N	6.37	133.70	121.54
1	E	221	ARG	C-N-CA	6.37	133.70	121.54
1	H	361	THR	CA-C-N	6.36	129.05	120.65
1	H	361	THR	C-N-CA	6.36	129.05	120.65
1	F	140	ARG	N-CA-C	6.35	119.86	109.76
1	A	308	VAL	CB-CA-C	-6.33	103.60	112.14
1	E	338	VAL	N-CA-C	6.32	117.33	107.28
1	G	274	ALA	N-CA-C	6.32	118.46	108.79
1	C	263	GLU	N-CA-C	6.32	118.24	111.36
1	H	254	ALA	CA-C-N	6.31	127.46	121.46
1	H	254	ALA	C-N-CA	6.31	127.46	121.46
1	C	344	ALA	N-CA-C	6.31	118.97	111.71
1	B	319	ALA	N-CA-C	-6.31	104.40	111.28
1	H	332	GLY	CA-C-N	6.31	131.53	120.87
1	H	332	GLY	C-N-CA	6.31	131.53	120.87
1	C	51	ASN	N-CA-C	6.31	119.01	109.23
1	B	91	GLY	CA-C-N	6.30	135.42	121.80
1	B	91	GLY	C-N-CA	6.30	135.42	121.80
1	G	24	VAL	N-CA-C	6.30	117.19	107.99
1	D	223	ASP	N-CA-C	-6.30	103.23	111.74
1	H	219	ALA	N-CA-C	6.29	120.80	113.18
1	H	205	ILE	CA-C-N	6.28	133.00	121.70
1	H	205	ILE	C-N-CA	6.28	133.00	121.70
1	C	388	VAL	O-C-N	-6.28	116.48	123.26
1	F	378	ILE	N-CA-C	6.26	117.72	108.45
1	D	353	ALA	N-CA-C	6.25	121.07	113.38
1	D	271	ARG	CA-C-N	6.25	126.19	119.76
1	D	271	ARG	C-N-CA	6.25	126.19	119.76
1	G	277	LEU	N-CA-C	6.24	119.06	111.82
1	C	330	ILE	N-CA-C	6.22	116.38	110.53
1	G	245	GLY	N-CA-C	6.22	120.73	112.77
1	G	330	ILE	N-CA-C	6.22	116.38	110.53
1	H	258	VAL	N-CA-CB	6.21	118.44	110.99
1	B	370	GLY	CA-C-N	6.21	130.62	121.05
1	B	370	GLY	C-N-CA	6.21	130.62	121.05
1	F	373	LEU	N-CA-C	6.21	119.76	109.46
1	A	351	ILE	N-CA-C	6.20	116.86	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	ARG	N-CA-C	6.19	118.72	109.25
1	F	155	VAL	O-C-N	6.19	129.91	123.04
1	C	244	ALA	CA-C-N	6.16	128.05	120.22
1	C	244	ALA	C-N-CA	6.16	128.05	120.22
1	F	92	LEU	CA-C-N	6.16	129.14	120.28
1	F	92	LEU	C-N-CA	6.16	129.14	120.28
1	A	390	VAL	CB-CA-C	-6.15	101.03	110.50
1	B	384	GLN	N-CA-C	-6.15	100.17	109.95
1	A	82	GLU	CA-C-N	6.15	131.58	121.86
1	A	82	GLU	C-N-CA	6.15	131.58	121.86
1	D	361	THR	N-CA-CB	6.14	119.15	110.12
1	F	261	SER	N-CA-C	-6.14	101.85	110.50
1	D	205	ILE	N-CA-C	6.13	117.29	107.73
1	E	370	GLY	N-CA-C	-6.12	102.73	113.76
1	A	237	ALA	N-CA-C	-6.12	98.99	108.42
1	E	357	ARG	N-CA-C	6.12	117.62	111.07
1	D	323	VAL	N-CA-C	6.11	116.89	110.72
1	H	136	ASP	N-CA-C	6.10	118.64	110.35
1	F	288	GLU	CB-CA-C	6.10	121.69	110.10
1	C	128	GLY	N-CA-C	6.09	120.04	112.73
1	B	226	LEU	CA-C-N	6.07	128.90	120.29
1	B	226	LEU	C-N-CA	6.07	128.90	120.29
1	F	92	LEU	O-C-N	-6.07	113.36	122.28
1	B	388	VAL	CA-C-N	6.04	131.34	123.00
1	B	388	VAL	C-N-CA	6.04	131.34	123.00
1	B	338	VAL	N-CA-C	6.04	116.55	107.80
1	F	167	GLU	N-CA-C	6.03	117.86	111.28
1	B	219	ALA	N-CA-C	6.03	120.48	113.18
1	A	333	PHE	CA-C-N	-6.02	112.89	121.50
1	A	333	PHE	C-N-CA	-6.02	112.89	121.50
1	G	281	THR	CA-C-N	6.02	132.01	122.62
1	G	281	THR	C-N-CA	6.02	132.01	122.62
1	G	388	VAL	N-CA-C	6.02	116.78	108.12
1	C	148	LEU	N-CA-C	6.01	121.35	113.30
1	A	240	GLY	CA-C-N	5.98	131.62	122.24
1	A	240	GLY	C-N-CA	5.98	131.62	122.24
1	A	242	ILE	N-CA-C	5.98	117.29	109.58
1	F	338	VAL	N-CA-C	5.98	117.28	107.24
1	G	34	MET	CA-C-N	5.98	128.21	120.44
1	G	34	MET	C-N-CA	5.98	128.21	120.44
1	D	196	GLN	N-CA-C	5.96	117.78	111.28
1	F	277	LEU	N-CA-C	5.96	117.86	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	81	SER	O-C-N	-5.96	116.36	123.27
1	E	81	SER	O-C-N	-5.95	116.61	123.33
1	B	353	ALA	N-CA-C	5.95	120.81	113.50
1	B	81	SER	N-CA-C	5.94	118.22	109.24
1	A	54	GLY	O-C-N	-5.94	116.72	122.84
1	C	109	ILE	CB-CA-C	5.93	118.18	110.12
1	H	304	ASN	N-CA-C	5.92	120.21	112.92
1	C	334	ASP	CA-C-N	5.91	130.05	120.60
1	C	334	ASP	C-N-CA	5.91	130.05	120.60
1	C	307	THR	CA-C-N	5.90	130.44	120.64
1	C	307	THR	C-N-CA	5.90	130.44	120.64
1	C	90	SER	N-CA-C	5.89	118.46	111.33
1	B	167	GLU	N-CA-C	5.89	117.70	111.28
1	D	12	THR	N-CA-CB	5.89	117.21	109.55
1	F	20	VAL	N-CA-C	5.89	118.41	111.05
1	H	370	GLY	CA-C-N	5.86	128.68	121.06
1	H	370	GLY	C-N-CA	5.86	128.68	121.06
1	H	338	VAL	N-CA-C	5.86	116.56	108.12
1	G	373	LEU	N-CA-C	5.86	118.28	108.96
1	A	138	GLU	N-CA-C	5.84	119.34	109.76
1	G	338	VAL	N-CA-C	5.83	116.26	107.80
1	B	13	PRO	N-CA-C	-5.83	102.67	111.41
1	H	140	ARG	N-CA-C	5.82	119.12	109.46
1	E	330	ILE	N-CA-C	5.82	116.60	110.72
1	D	383	ALA	N-CA-C	5.81	119.26	111.24
1	D	148	LEU	N-CA-C	5.80	120.47	113.17
1	H	245	GLY	N-CA-C	5.79	120.19	112.77
1	C	349	HIS	N-CA-CB	-5.79	103.91	111.09
1	D	198	GLU	N-CA-C	5.78	118.80	111.69
1	E	118	MET	CA-C-N	5.78	128.60	120.28
1	E	118	MET	C-N-CA	5.78	128.60	120.28
1	H	306	LEU	CA-C-N	5.78	131.66	122.59
1	H	306	LEU	C-N-CA	5.78	131.66	122.59
1	F	333	PHE	CA-C-N	-5.78	113.24	121.50
1	F	333	PHE	C-N-CA	-5.78	113.24	121.50
1	B	131	GLY	N-CA-C	5.77	119.91	112.18
1	H	29	LEU	CA-C-N	5.76	126.34	120.00
1	H	29	LEU	C-N-CA	5.76	126.34	120.00
1	G	128	GLY	N-CA-C	5.75	119.63	112.73
1	D	4	THR	O-C-N	-5.75	116.48	123.27
1	H	148	LEU	N-CA-C	5.75	120.45	113.38
1	G	271	ARG	CA-C-N	5.75	125.66	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	271	ARG	C-N-CA	5.75	125.66	119.85
1	B	29	LEU	CA-C-N	5.75	126.36	119.98
1	B	29	LEU	C-N-CA	5.75	126.36	119.98
1	F	245	GLY	N-CA-C	5.74	120.11	112.77
1	B	140	ARG	N-CA-C	5.73	118.87	109.76
1	G	138	GLU	N-CA-C	5.73	118.81	109.59
1	D	23	GLU	CA-C-N	5.71	130.12	122.93
1	D	23	GLU	C-N-CA	5.71	130.12	122.93
1	B	92	LEU	CA-C-N	5.70	128.19	120.38
1	B	92	LEU	C-N-CA	5.70	128.19	120.38
1	D	354	SER	CA-C-N	5.69	126.30	119.98
1	D	354	SER	C-N-CA	5.69	126.30	119.98
1	H	20	VAL	N-CA-C	5.69	120.08	111.89
1	D	29	LEU	CA-C-N	5.69	126.29	119.98
1	D	29	LEU	C-N-CA	5.69	126.29	119.98
1	B	286	ALA	N-CA-C	5.68	118.20	111.33
1	A	204	TRP	CA-C-N	5.67	131.91	121.70
1	A	204	TRP	C-N-CA	5.67	131.91	121.70
1	F	372	GLY	N-CA-C	5.67	126.62	113.18
1	E	88	CYS	N-CA-C	5.67	117.91	111.11
1	E	373	LEU	N-CA-C	5.66	117.91	109.25
1	F	81	SER	N-CA-C	5.66	116.55	108.74
1	D	162	ASN	CA-C-N	5.66	128.65	120.79
1	D	162	ASN	C-N-CA	5.66	128.65	120.79
1	G	363	VAL	N-CA-CB	5.65	117.16	110.55
1	H	357	ARG	N-CA-C	5.65	117.11	111.07
1	H	363	VAL	N-CA-CB	5.63	116.53	110.62
1	F	4	THR	O-C-N	-5.62	116.66	123.29
1	E	250	VAL	CB-CA-C	5.60	118.97	110.62
1	D	318	GLU	N-CA-C	5.60	118.46	110.68
1	A	129	ARG	N-CA-C	5.59	117.18	111.14
1	A	4	THR	O-C-N	-5.59	116.65	123.19
1	G	33	VAL	CA-C-N	5.59	128.23	120.29
1	G	33	VAL	C-N-CA	5.59	128.23	120.29
1	H	43	VAL	N-CA-C	5.59	116.78	108.46
1	B	351	ILE	N-CA-C	5.59	116.99	110.62
1	C	347	LEU	N-CA-C	5.59	120.16	113.23
1	C	145	TYR	N-CA-C	5.56	117.15	111.14
1	D	84	LEU	N-CA-C	5.55	118.44	109.40
1	H	258	VAL	N-CA-C	-5.54	100.44	108.36
1	B	43	VAL	O-C-N	-5.53	117.42	123.18
1	C	272	PRO	CA-C-N	5.53	128.72	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	PRO	C-N-CA	5.53	128.72	120.31
1	C	232	LEU	N-CA-C	5.53	117.87	110.35
1	F	330	ILE	N-CA-C	5.53	116.31	110.72
1	H	390	VAL	N-CA-C	5.53	116.44	108.48
1	F	361	THR	O-C-N	-5.53	114.92	122.33
1	H	84	LEU	N-CA-C	5.53	117.97	109.07
1	H	131	GLY	N-CA-C	5.52	119.16	112.48
1	B	138	GLU	N-CA-C	5.51	119.04	110.17
1	C	84	LEU	N-CA-C	5.51	118.38	109.40
1	C	135	GLY	CA-C-O	-5.50	117.84	122.29
1	F	256	ALA	N-CA-C	5.49	117.42	109.07
1	A	43	VAL	N-CA-C	5.48	116.00	107.28
1	C	63	GLN	CA-CB-CG	5.48	125.06	114.10
1	A	274	ALA	N-CA-C	5.48	117.17	108.79
1	F	293	PRO	CA-N-CD	-5.48	104.33	112.00
1	F	262	GLU	N-CA-C	-5.47	105.32	111.28
1	A	235	ILE	N-CA-C	5.46	115.75	108.11
1	G	215	ASP	CA-C-N	5.45	131.37	122.81
1	G	215	ASP	C-N-CA	5.45	131.37	122.81
1	E	244	ALA	CA-C-N	5.44	125.99	120.00
1	E	244	ALA	C-N-CA	5.44	125.99	120.00
1	G	284	MET	N-CA-C	5.44	117.03	108.55
1	D	171	SER	N-CA-C	5.43	117.70	110.53
1	F	347	LEU	N-CA-C	5.43	119.75	113.18
1	A	76	PRO	CA-C-O	-5.42	115.18	121.95
1	A	378	ILE	N-CA-C	5.41	116.46	108.45
1	C	81	SER	CA-C-N	-5.41	111.21	121.54
1	C	81	SER	C-N-CA	-5.41	111.21	121.54
1	C	254	ALA	CA-C-N	5.41	127.98	121.38
1	C	254	ALA	C-N-CA	5.41	127.98	121.38
1	D	225	SER	O-C-N	-5.41	117.09	123.25
1	B	121	ILE	N-CA-CB	5.40	115.10	110.08
1	B	239	ASP	CB-CA-C	5.40	115.18	109.83
1	H	244	ALA	CA-C-N	5.40	125.94	120.00
1	H	244	ALA	C-N-CA	5.40	125.94	120.00
1	C	171	SER	N-CA-C	5.40	118.11	110.50
1	C	253	GLY	N-CA-C	5.40	118.61	110.18
1	D	330	ILE	N-CA-C	5.40	115.60	110.53
1	E	113	GLY	N-CA-C	5.39	119.82	111.08
1	B	76	PRO	CA-C-N	5.39	128.04	120.28
1	B	76	PRO	C-N-CA	5.39	128.04	120.28
1	C	286	ALA	N-CA-C	5.39	117.85	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	91	GLY	O-C-N	5.39	127.36	122.19
1	A	49	GLU	N-CA-C	5.38	119.56	112.89
1	B	7	VAL	N-CA-C	5.38	116.03	110.82
1	D	24	VAL	N-CA-C	5.38	116.05	108.36
1	B	254	ALA	CA-C-N	5.38	126.57	121.46
1	B	254	ALA	C-N-CA	5.38	126.57	121.46
1	A	240	GLY	N-CA-C	5.37	121.50	112.85
1	A	353	ALA	N-CA-C	5.37	119.89	113.23
1	E	331	VAL	CB-CA-C	-5.36	105.06	112.24
1	A	199	ILE	N-CA-C	5.36	115.96	108.89
1	F	312	ASP	N-CA-C	5.36	117.20	111.36
1	G	244	ALA	CA-C-N	5.35	125.88	120.00
1	G	244	ALA	C-N-CA	5.35	125.88	120.00
1	D	81	SER	N-CA-C	5.34	117.09	109.14
1	A	373	LEU	N-CA-C	5.33	117.44	108.96
1	D	258	VAL	N-CA-CB	5.33	117.45	111.21
1	G	347	LEU	N-CA-C	5.33	119.49	112.89
1	A	256	ALA	N-CA-C	5.32	117.28	109.24
1	A	22	LYS	N-CA-C	5.32	117.08	111.28
1	D	250	VAL	N-CA-C	-5.31	100.83	108.53
1	B	2	ARG	O-C-N	-5.30	114.51	123.00
1	B	84	LEU	N-CA-C	5.29	118.11	109.59
1	C	383	ALA	N-CA-C	5.29	118.69	111.39
1	A	284	MET	CB-CA-C	-5.29	101.58	109.56
1	C	198	GLU	N-CA-C	5.29	117.85	111.40
1	G	212	ASN	N-CA-CB	5.28	119.48	110.50
1	G	213	VAL	N-CA-C	5.28	115.73	108.12
1	H	229	LEU	N-CA-C	5.28	117.04	111.28
1	A	282	THR	O-C-N	-5.28	117.15	123.27
1	C	315	GLU	N-CA-C	-5.28	100.30	108.90
1	D	167	GLU	N-CA-C	5.28	117.03	111.28
1	E	343	GLY	CA-C-N	5.27	127.86	120.28
1	E	343	GLY	C-N-CA	5.27	127.86	120.28
1	B	251	ASN	N-CA-C	5.26	116.01	108.74
1	F	361	THR	N-CA-CB	5.25	118.39	110.30
1	G	139	LEU	N-CA-C	-5.25	97.28	107.62
1	D	390	VAL	N-CA-C	5.25	116.28	108.46
1	G	349	HIS	N-CA-CB	-5.25	104.58	111.09
1	D	344	ALA	N-CA-C	5.25	117.74	111.71
1	D	163	THR	N-CA-CB	5.24	117.78	109.82
1	E	387	ALA	N-CA-C	5.23	117.61	108.76
1	A	377	ALA	N-CA-C	5.22	117.94	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	351	ILE	N-CA-C	5.22	116.57	110.62
1	G	199	ILE	N-CA-C	5.21	116.30	109.21
1	D	120	ASN	N-CA-C	5.21	119.33	112.92
1	F	113	GLY	CA-C-N	5.21	126.41	121.46
1	F	113	GLY	C-N-CA	5.21	126.41	121.46
1	D	261	SER	N-CA-C	-5.21	103.15	110.50
1	F	235	ILE	CB-CA-C	-5.21	105.20	112.02
1	F	321	ALA	N-CA-C	-5.20	105.10	111.75
1	B	123	TYR	N-CA-C	-5.19	103.54	110.55
1	C	226	LEU	N-CA-C	-5.19	96.46	111.00
1	G	319	ALA	N-CA-C	-5.19	105.62	111.28
1	E	127	ALA	CA-C-N	5.19	125.71	120.00
1	E	127	ALA	C-N-CA	5.19	125.71	120.00
1	H	374	GLY	N-CA-C	5.19	119.84	111.38
1	E	331	VAL	N-CA-C	5.19	116.65	111.00
1	G	51	ASN	N-CA-C	5.19	117.27	109.23
1	E	347	LEU	N-CA-C	5.18	119.45	113.18
1	F	239	ASP	N-CA-CB	-5.18	108.92	114.10
1	A	56	VAL	N-CA-CB	5.17	116.85	110.64
1	F	129	ARG	N-CA-C	5.17	116.60	111.07
1	C	305	GLY	O-C-N	-5.17	115.95	122.41
1	B	383	ALA	N-CA-C	5.17	118.37	111.24
1	B	90	SER	CA-C-N	5.16	126.59	120.14
1	B	90	SER	C-N-CA	5.16	126.59	120.14
1	H	4	THR	O-C-N	-5.16	117.20	123.29
1	B	161	GLY	CA-C-N	5.16	127.14	120.44
1	B	161	GLY	C-N-CA	5.16	127.14	120.44
1	B	333	PHE	CB-CA-C	-5.15	102.55	109.71
1	H	306	LEU	O-C-N	-5.15	116.50	123.19
1	D	282	THR	O-C-N	-5.15	117.30	123.27
1	A	390	VAL	N-CA-C	5.14	116.11	108.46
1	B	277	LEU	N-CA-C	5.12	119.24	112.89
1	F	258	VAL	N-CA-C	-5.12	100.52	107.99
1	E	139	LEU	N-CA-C	-5.12	97.40	107.69
1	A	291	ALA	N-CA-C	5.11	117.75	111.82
1	E	321	ALA	N-CA-C	-5.11	105.72	111.28
1	C	36	GLU	N-CA-C	5.10	116.92	111.36
1	E	171	SER	N-CA-C	5.10	117.69	110.50
1	A	203	ASN	CA-C-N	-5.10	110.45	121.87
1	A	203	ASN	C-N-CA	-5.10	110.45	121.87
1	F	83	THR	N-CA-C	-5.09	99.95	110.80
1	C	85	ASN	N-CA-C	5.09	117.27	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LEU	CA-C-N	5.09	125.63	119.98
1	A	29	LEU	C-N-CA	5.09	125.63	119.98
1	B	272	PRO	N-CA-C	5.08	119.29	111.21
1	F	226	LEU	CA-C-N	-5.08	113.69	120.54
1	F	226	LEU	C-N-CA	-5.08	113.69	120.54
1	G	177	GLU	N-CA-C	-5.07	105.75	111.28
1	D	123	TYR	N-CA-C	-5.06	103.03	110.52
1	H	139	LEU	N-CA-C	-5.05	97.53	107.69
1	G	378	ILE	N-CA-C	5.05	115.02	108.35
1	C	131	GLY	N-CA-C	5.04	118.94	112.18
1	H	145	TYR	N-CA-C	5.04	116.62	111.03
1	E	81	SER	CA-C-N	5.04	130.80	121.94
1	E	81	SER	C-N-CA	5.04	130.80	121.94
1	A	238	SER	O-C-N	-5.03	115.62	122.36
1	F	81	SER	N-CA-CB	-5.03	102.81	111.21
1	F	156	HIS	CA-C-N	5.03	127.02	120.28
1	F	156	HIS	C-N-CA	5.03	127.02	120.28
1	D	293	PRO	CA-C-O	-5.03	112.74	120.03
1	F	360	MET	N-CA-CB	-5.03	102.73	110.12
1	F	84	LEU	N-CA-C	5.02	117.75	109.72
1	F	120	ASN	N-CA-C	5.02	119.49	113.17
1	A	83	THR	O-C-N	-5.01	116.47	123.34
1	F	337	LYS	O-C-N	-5.01	116.19	122.35
1	H	55	MET	N-CA-C	-5.01	100.11	108.32
1	H	256	ALA	N-CA-C	5.01	116.68	109.07

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	MET	Mainchain
1	A	204	TRP	Mainchain
1	A	221	ARG	Mainchain
1	A	226	LEU	Mainchain
1	A	43	VAL	Mainchain
1	A	55	MET	Mainchain
1	A	81	SER	Mainchain
1	A	82	GLU	Mainchain
1	A	88	CYS	Mainchain
1	B	337	LYS	Mainchain
1	B	361	THR	Mainchain
1	B	378	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	B	81	SER	Mainchain
1	B	82	GLU	Mainchain
1	B	88	CYS	Mainchain
1	C	308	VAL	Mainchain
1	C	332	GLY	Mainchain
1	C	82	GLU	Mainchain
1	C	88	CYS	Mainchain
1	D	163	THR	Mainchain
1	D	332	GLY	Mainchain,Peptide
1	D	4	THR	Mainchain
1	D	82	GLU	Mainchain,Peptide
1	E	221	ARG	Mainchain
1	E	222	ARG	Mainchain
1	E	306	LEU	Mainchain
1	E	88	CYS	Mainchain
1	F	4	THR	Mainchain
1	F	81	SER	Mainchain
1	F	82	GLU	Mainchain
1	F	88	CYS	Mainchain
1	G	226	LEU	Mainchain
1	G	227	ASP	Mainchain
1	G	332	GLY	Mainchain
1	H	134	MET	Mainchain
1	H	55	MET	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	2730	0	2591	35	0
1	B	2753	0	2631	22	0
1	C	2749	0	2636	20	0
1	D	2740	0	2642	22	0
1	E	2740	0	2625	30	0
1	F	2641	0	2480	32	0
1	G	2728	0	2603	24	0
1	H	2733	0	2622	24	0
2	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	G	6	0	8	0	0
3	A	110	0	0	0	0
3	B	146	0	0	0	0
3	C	136	0	0	0	0
3	D	125	0	0	0	0
3	E	80	0	0	0	0
3	F	80	0	0	0	0
3	G	119	0	0	0	0
3	H	82	0	0	0	0
All	All	22740	0	20894	201	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 5.

All (201) 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:62:GLY:C	1:D:63:GLN:N	1.70	1.50
1:A:66:SER:OG	1:A:82:GLU:O	1.62	1.15
1:F:333:PHE:CD1	1:F:338:VAL:HG21	1.90	1.05
1:F:333:PHE:CE1	1:F:338:VAL:HG21	1.93	1.03
1:E:333:PHE:CD1	1:E:338:VAL:HG21	1.95	1.01
1:E:333:PHE:CE1	1:E:338:VAL:HG21	2.02	0.95
1:F:283:GLY:O	1:F:284:MET:HG2	1.72	0.88
1:E:88:CYS:HB2	1:E:380:SER:HA	1.59	0.84
1:A:88:CYS:HB2	1:A:380:SER:HA	1.62	0.82
1:F:333:PHE:CD1	1:F:338:VAL:CG2	2.64	0.80
1:A:66:SER:CB	1:A:82:GLU:O	2.33	0.77
1:E:333:PHE:CD1	1:E:338:VAL:CG2	2.68	0.76
1:G:88:CYS:HB2	1:G:380:SER:HA	1.69	0.74
1:G:189:ALA:HB1	1:G:194:LYS:HB2	1.70	0.73
1:C:293:PRO:HG3	1:C:379:CYS:HB3	1.71	0.73
1:B:360:MET:HA	1:B:363:VAL:HG22	1.70	0.71
1:F:88:CYS:HB2	1:F:380:SER:HA	1.74	0.69
1:C:333:PHE:CE1	1:C:338:VAL:HG21	2.27	0.69
1:F:88:CYS:HB2	1:F:380:SER:CB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:CYS:HA	1:A:101:MET:HE3	1.76	0.68
1:A:293:PRO:HG3	1:A:379:CYS:HB3	1.74	0.68
1:G:34:MET:CE	1:G:69:ALA:HB1	2.24	0.67
1:A:118:MET:HA	1:A:121:ILE:HD12	1.75	0.67
1:H:55:MET:HE2	1:H:58:GLN:HA	1.78	0.65
1:G:55:MET:HE2	1:G:58:GLN:HA	1.77	0.65
1:A:70:ALA:HB1	1:A:75:MET:HE3	1.78	0.64
1:B:157:MET:HE2	1:B:157:MET:HA	1.78	0.64
1:C:333:PHE:CD1	1:C:338:VAL:HG21	2.32	0.64
1:E:88:CYS:HB2	1:E:380:SER:CB	2.28	0.64
1:G:34:MET:HE1	1:G:69:ALA:CB	2.29	0.63
1:A:55:MET:HE2	1:A:58:GLN:HA	1.82	0.62
1:F:160:HIS:CE1	1:F:287:HIS:HA	2.35	0.62
1:F:283:GLY:C	1:F:284:MET:HG2	2.23	0.62
1:E:88:CYS:HB2	1:E:380:SER:CA	2.29	0.62
1:B:101:MET:HE3	1:B:110:LEU:HD13	1.81	0.61
1:H:371:GLY:O	1:H:392:VAL:O	2.17	0.61
1:B:88:CYS:HB2	1:B:380:SER:CB	2.29	0.61
1:F:284:MET:HE1	1:F:295:PHE:CD2	2.36	0.61
1:F:316:VAL:HG12	1:F:324:VAL:HG12	1.84	0.60
1:C:162:ASN:HD21	1:C:240:GLY:HA2	1.65	0.60
1:F:11:ARG:HB3	1:F:360:MET:SD	2.42	0.59
1:A:55:MET:HE1	1:A:61:SER:OG	2.02	0.59
1:F:333:PHE:HD1	1:F:338:VAL:HG21	1.65	0.59
1:E:140:ARG:HD3	1:E:145:TYR:CG	2.38	0.57
1:E:284:MET:O	1:E:383:ALA:HB3	2.04	0.57
1:F:88:CYS:HB2	1:F:380:SER:CA	2.33	0.57
1:C:312:ASP:O	1:C:313:LEU:HD23	2.05	0.56
1:F:238:SER:O	1:F:239:ASP:CB	2.53	0.56
1:C:333:PHE:CD1	1:C:333:PHE:O	2.59	0.55
1:D:63:GLN:O	1:D:64:ILE:C	2.46	0.55
1:A:88:CYS:HB2	1:A:380:SER:CA	2.35	0.55
1:C:88:CYS:HB2	1:C:380:SER:CB	2.36	0.55
1:E:291:ALA:O	1:E:292:ALA:HB2	2.07	0.54
1:A:292:ALA:N	1:A:293:PRO:HD2	2.21	0.54
1:C:56:VAL:HG13	1:C:87:VAL:HA	1.90	0.53
1:G:14:PHE:CE2	1:G:357:ARG:HD3	2.43	0.53
1:E:291:ALA:O	1:E:292:ALA:CB	2.57	0.53
1:D:9:ALA:HB1	1:D:360:MET:HG3	1.91	0.53
1:D:62:GLY:C	1:D:63:GLN:CA	2.73	0.52
1:E:13:PRO:HG2	1:E:214:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:GLN:NE2	1:D:81:SER:H	2.07	0.52
1:B:104:ALA:C	1:B:105:GLN:HG2	2.34	0.52
1:C:98:CYS:SG	1:C:112:ALA:HB2	2.50	0.52
1:D:123:TYR:CE2	1:D:141:ASP:HB2	2.45	0.52
1:B:17:PHE:CD1	1:B:250:VAL:HG23	2.44	0.52
1:A:88:CYS:CB	1:A:380:SER:HA	2.38	0.51
1:H:366:LEU:O	1:H:371:GLY:HA3	2.10	0.51
1:C:88:CYS:HB2	1:C:380:SER:HB2	1.93	0.51
1:G:34:MET:CE	1:G:69:ALA:CB	2.89	0.51
1:F:283:GLY:C	1:F:284:MET:CG	2.84	0.50
1:D:88:CYS:SG	1:D:380:SER:HA	2.52	0.50
1:A:34:MET:CE	1:A:69:ALA:HB1	2.41	0.50
1:D:204:TRP:N	1:D:204:TRP:CD1	2.79	0.50
1:H:236:TYR:O	1:H:237:ALA:HB2	2.11	0.50
1:A:98:CYS:HA	1:A:101:MET:CE	2.41	0.50
1:C:333:PHE:CD1	1:C:338:VAL:CG2	2.94	0.50
1:B:293:PRO:HG3	1:B:379:CYS:HB3	1.93	0.50
1:B:369:ARG:C	1:B:371:GLY:N	2.70	0.49
1:G:248:PRO:HB3	1:G:344:ALA:O	2.13	0.49
1:H:98:CYS:SG	1:H:112:ALA:HB2	2.52	0.49
1:A:283:GLY:HA2	1:B:78:SER:HA	1.94	0.49
1:B:369:ARG:C	1:B:371:GLY:H	2.19	0.49
1:D:234:PRO:HB3	1:D:240:GLY:O	2.12	0.49
1:A:118:MET:HA	1:A:121:ILE:CD1	2.42	0.49
1:B:101:MET:HE3	1:B:110:LEU:CD1	2.43	0.49
1:C:88:CYS:HB2	1:C:380:SER:HA	1.95	0.49
1:F:333:PHE:CE1	1:F:338:VAL:CG2	2.81	0.49
1:F:160:HIS:ND1	1:F:287:HIS:HA	2.27	0.48
1:H:82:GLU:HG3	1:G:84:LEU:HD21	1.93	0.48
1:A:202:VAL:HG12	1:A:204:TRP:HD1	1.79	0.48
1:A:88:CYS:HB2	1:A:380:SER:CB	2.42	0.48
1:H:34:MET:HB2	1:H:73:ALA:HB2	1.95	0.48
1:C:56:VAL:HG22	1:C:87:VAL:O	2.13	0.48
1:E:333:PHE:CE1	1:E:338:VAL:CG2	2.89	0.48
1:G:17:PHE:HB2	1:G:250:VAL:HG23	1.95	0.48
1:G:371:GLY:O	1:G:392:VAL:O	2.31	0.48
1:A:17:PHE:HB2	1:A:250:VAL:O	2.15	0.47
1:E:36:GLU:O	1:E:40:GLN:HG3	2.15	0.47
1:F:13:PRO:HD3	1:F:199:ILE:HG23	1.95	0.47
1:B:88:CYS:HB2	1:B:380:SER:HB2	1.97	0.47
1:H:328:GLU:HG3	1:H:335:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:CYS:CB	1:E:380:SER:HA	2.39	0.46
1:A:187:ALA:HB1	1:A:222:ARG:NH1	2.31	0.46
1:G:303:LYS:HB3	1:G:303:LYS:HE3	1.70	0.46
1:D:293:PRO:O	1:D:296:ALA:HB3	2.15	0.46
1:G:34:MET:HE1	1:G:69:ALA:HB3	1.97	0.46
1:G:123:TYR:CE2	1:G:141:ASP:HB2	2.49	0.46
1:C:77:TRP:CD2	1:D:285:PRO:HA	2.50	0.46
1:H:53:MET:HB2	1:H:66:SER:HB3	1.98	0.46
1:E:78:SER:O	1:E:80:PRO:HD3	2.16	0.46
1:E:123:TYR:CE2	1:E:141:ASP:HB2	2.50	0.46
1:A:98:CYS:SG	1:A:112:ALA:HB2	2.56	0.46
1:F:316:VAL:CG1	1:F:324:VAL:HG12	2.46	0.46
1:H:123:TYR:CE2	1:H:141:ASP:HB2	2.51	0.46
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.69	0.46
1:A:248:PRO:HD2	1:A:319:ALA:O	2.15	0.46
1:B:118:MET:HE2	1:B:250:VAL:HB	1.98	0.46
1:A:121:ILE:HA	1:A:122:PRO:HD3	1.68	0.45
1:D:157:MET:HE3	1:D:289:LEU:CD2	2.46	0.45
1:B:84:LEU:HD21	1:B:93:ARG:HG3	1.98	0.45
1:F:14:PHE:CE2	1:F:357:ARG:HD3	2.51	0.45
1:F:183:HIS:CE1	1:F:221:ARG:HG2	2.51	0.45
1:E:200:VAL:CG2	1:E:201:PRO:HD2	2.47	0.45
1:A:70:ALA:CB	1:A:75:MET:HE3	2.45	0.45
1:F:333:PHE:HE1	1:F:338:VAL:HG21	1.71	0.45
1:H:63:GLN:HE22	1:G:157:MET:HE3	1.81	0.45
1:H:178:TRP:CZ2	1:H:324:VAL:HG11	2.52	0.45
1:G:318:GLU:HB3	1:G:345:ILE:HG13	1.98	0.45
1:G:227:ASP:O	1:G:231:LYS:HD2	2.16	0.45
1:E:284:MET:HE1	1:E:291:ALA:O	2.16	0.45
1:E:160:HIS:ND1	1:E:287:HIS:HA	2.32	0.45
1:A:34:MET:HE2	1:A:69:ALA:HB1	1.99	0.44
1:D:292:ALA:N	1:D:293:PRO:CD	2.80	0.44
1:H:235:ILE:HD11	1:H:242:ILE:HG22	1.98	0.44
1:B:51:ASN:HA	1:B:111:VAL:O	2.17	0.44
1:H:204:TRP:O	1:H:212:ASN:N	2.50	0.44
1:F:1:MET:HA	1:F:2:ARG:C	2.38	0.44
1:A:273:LEU:O	1:A:274:ALA:HB2	2.18	0.44
1:H:28:GLU:HA	1:H:72:LEU:HD13	2.00	0.44
1:E:292:ALA:HB1	1:E:385:GLY:HA3	1.99	0.44
1:B:88:CYS:HB2	1:B:380:SER:HA	2.00	0.44
1:E:11:ARG:HD3	1:E:357:ARG:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:MET:CE	1:A:69:ALA:CB	2.95	0.44
1:E:140:ARG:HD3	1:E:145:TYR:CD1	2.53	0.44
1:B:9:ALA:HB2	1:B:257:PHE:CD1	2.53	0.43
1:D:51:ASN:HA	1:D:111:VAL:O	2.18	0.43
1:G:88:CYS:HB2	1:G:380:SER:CB	2.48	0.43
1:G:88:CYS:HB2	1:G:380:SER:CA	2.44	0.43
1:G:158:ALA:HA	1:G:320:PHE:CZ	2.53	0.43
1:D:157:MET:HE3	1:D:289:LEU:HD21	2.00	0.43
1:H:124:ALA:HB2	1:H:142:LEU:HD11	1.99	0.43
1:A:236:TYR:O	1:A:237:ALA:HB2	2.18	0.43
1:E:158:ALA:HA	1:E:320:PHE:CZ	2.53	0.43
1:E:183:HIS:CE1	1:E:346:ALA:HA	2.54	0.43
1:B:92:LEU:HD23	1:B:378:ILE:HG22	1.98	0.43
1:C:183:HIS:CE1	1:C:346:ALA:HA	2.53	0.43
1:F:334:ASP:OD2	1:F:336:GLU:HB2	2.18	0.43
1:A:160:HIS:ND1	1:A:287:HIS:HA	2.33	0.43
1:F:158:ALA:HA	1:F:320:PHE:CZ	2.54	0.43
1:D:108:ASP:HB3	1:D:264:LYS:HB2	1.99	0.43
1:H:70:ALA:O	1:H:75:MET:HB2	2.19	0.43
1:H:376:ALA:O	1:H:387:ALA:HA	2.18	0.43
1:A:140:ARG:HD3	1:A:145:TYR:CG	2.54	0.43
1:D:234:PRO:HB2	1:D:237:ALA:O	2.19	0.43
1:D:300:LEU:HD21	1:D:389:LEU:N	2.34	0.43
1:A:226:LEU:O	1:A:227:ASP:C	2.55	0.43
1:F:180:LEU:HD22	1:F:226:LEU:HG	2.01	0.42
1:F:88:CYS:HB2	1:F:380:SER:HB2	2.01	0.42
1:G:292:ALA:N	1:G:293:PRO:HD2	2.35	0.42
1:A:202:VAL:HG12	1:A:204:TRP:CD1	2.54	0.42
1:C:365:GLU:O	1:C:369:ARG:HG3	2.19	0.42
1:F:17:PHE:CD1	1:F:250:VAL:HG23	2.54	0.42
1:D:66:SER:CB	1:D:82:GLU:O	2.68	0.42
1:A:308:VAL:HG11	1:A:333:PHE:HA	2.00	0.42
1:A:12:THR:HG23	1:A:33:VAL:HG13	2.01	0.42
1:H:185:ARG:HD3	1:H:340:VAL:O	2.20	0.42
1:E:92:LEU:HD11	1:E:388:VAL:HG21	2.02	0.42
1:E:108:ASP:O	1:E:260:MET:HA	2.20	0.42
1:G:34:MET:HE2	1:G:69:ALA:HB1	2.01	0.41
1:E:77:TRP:CD2	1:F:285:PRO:HA	2.54	0.41
1:H:293:PRO:HD3	1:H:379:CYS:HB3	2.03	0.41
1:F:11:ARG:HD3	1:F:357:ARG:HG3	2.02	0.41
1:F:148:LEU:O	1:F:157:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:GLY:O	1:D:382:ALA:HB3	2.21	0.41
1:H:157:MET:HE3	1:H:289:LEU:CD2	2.50	0.41
1:F:293:PRO:HD3	1:F:379:CYS:HB3	2.01	0.41
1:D:43:VAL:HG21	1:D:260:MET:CE	2.51	0.41
1:E:99:ASP:O	1:E:100:GLN:C	2.49	0.41
1:B:92:LEU:HD23	1:B:378:ILE:CG2	2.51	0.41
1:H:34:MET:HE2	1:H:75:MET:HE1	2.03	0.41
1:G:98:CYS:HA	1:G:101:MET:HE3	2.02	0.41
1:B:54:GLY:HA3	1:B:90:SER:HB3	2.02	0.41
1:B:123:TYR:CE2	1:B:141:ASP:HB2	2.55	0.41
1:C:285:PRO:HA	1:D:77:TRP:CD2	2.56	0.40
1:H:63:GLN:NE2	1:G:157:MET:HE3	2.37	0.40
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.86	0.40
1:C:41:ALA:HB1	1:C:43:VAL:HG13	2.04	0.40
1:H:360:MET:HE3	1:H:360:MET:HB2	1.97	0.40
1:E:11:ARG:CD	1:E:357:ARG:HG3	2.51	0.40
1:E:51:ASN:HA	1:E:111:VAL:O	2.22	0.40
1:C:108:ASP:O	1:C:260:MET:HA	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	380/393 (97%)	375 (99%)	4 (1%)	1 (0%)	36	42
1	B	382/393 (97%)	374 (98%)	7 (2%)	1 (0%)	36	42
1	C	379/393 (96%)	373 (98%)	5 (1%)	1 (0%)	36	42
1	D	378/393 (96%)	370 (98%)	8 (2%)	0	100	100
1	E	378/393 (96%)	370 (98%)	7 (2%)	1 (0%)	36	42
1	F	368/393 (94%)	361 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	377/393 (96%)	370 (98%)	7 (2%)	0	100	100
1	H	380/393 (97%)	374 (98%)	6 (2%)	0	100	100
All	All	3022/3144 (96%)	2967 (98%)	51 (2%)	4 (0%)	48	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	87	VAL
1	B	87	VAL
1	C	87	VAL
1	A	87	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	256/291 (88%)	254 (99%)	2 (1%)	73	85
1	B	259/291 (89%)	251 (97%)	8 (3%)	35	48
1	C	255/291 (88%)	252 (99%)	3 (1%)	63	78
1	D	255/291 (88%)	250 (98%)	5 (2%)	48	64
1	E	259/291 (89%)	255 (98%)	4 (2%)	57	73
1	F	239/291 (82%)	236 (99%)	3 (1%)	61	76
1	G	256/291 (88%)	250 (98%)	6 (2%)	44	59
1	H	257/291 (88%)	252 (98%)	5 (2%)	50	66
All	All	2036/2328 (88%)	2000 (98%)	36 (2%)	51	68

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	43	VAL
1	H	235	ILE
1	H	308	VAL

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Mol	Chain	Res	Type
1	H	329	LYS
1	H	369	ARG
1	E	87	VAL
1	E	133	ARG
1	E	167	GLU
1	E	205	ILE
1	A	64	ILE
1	A	87	VAL
1	B	3	LYS
1	B	87	VAL
1	B	105	GLN
1	B	224	THR
1	B	231	LYS
1	B	239	ASP
1	B	328	GLU
1	B	339	ASN
1	C	43	VAL
1	C	162	ASN
1	C	180	LEU
1	F	177	GLU
1	F	308	VAL
1	F	345	ILE
1	G	3	LYS
1	G	43	VAL
1	G	82	GLU
1	G	84	LEU
1	G	224	THR
1	G	303	LYS
1	D	25	LYS
1	D	88	CYS
1	D	133	ARG
1	D	218	GLU
1	D	345	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	63	GLN
1	H	317	ASN
1	E	175	GLN
1	E	212	ASN
1	A	251	ASN

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Mol	Chain	Res	Type
1	A	317	ASN
1	B	39	GLN
1	B	175	GLN
1	C	120	ASN
1	C	212	ASN
1	C	317	ASN
1	F	120	ASN
1	F	183	HIS
1	F	341	ASN
1	G	203	ASN
1	D	175	GLN
1	D	317	ASN

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	C	401	-	5,5,5	0.36	0	5,5,5	0.92	0
2	GOL	G	401	-	5,5,5	0.48	0	5,5,5	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	401	-	5,5,5	0.47	0	5,5,5	0.86	0
2	GOL	B	401	-	5,5,5	0.46	0	5,5,5	1.81	2 (40%)
2	GOL	F	401	-	5,5,5	0.24	0	5,5,5	0.55	0
2	GOL	E	401	-	5,5,5	0.84	0	5,5,5	0.68	0
2	GOL	A	401	-	5,5,5	0.62	0	5,5,5	1.04	0
2	GOL	B	402	-	5,5,5	0.43	0	5,5,5	0.39	0

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	GOL	C	401	-	-	0/4/4/4	-
2	GOL	G	401	-	-	0/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	4/4/4/4	-
2	GOL	F	401	-	-	4/4/4/4	-
2	GOL	E	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	B	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GOL	O3-C3-C2	3.14	124.53	110.38
2	B	401	GOL	O2-C2-C3	2.26	118.54	109.18

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	GOL	C1-C2-C3-O3
2	B	401	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	B	402	GOL	O2-C2-C3-O3
2	F	401	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3
2	F	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	F	401	GOL	O2-C2-C3-O3
2	E	401	GOL	O2-C2-C3-O3
2	F	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-O2
2	B	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	17
1	E	16
1	D	13
1	F	13
1	G	13
1	H	11
1	B	11
1	C	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	62:GLY	C	63:GLN	N	1.70
1	H	204:TRP	C	205:ILE	N	1.20
1	F	82:GLU	C	83:THR	N	1.20
1	H	363:VAL	C	364:TYR	N	1.19
1	B	217:ASP	C	218:GLU	N	1.19
1	B	250:VAL	C	251:ASN	N	1.19
1	B	306:LEU	C	307:THR	N	1.19
1	C	46:ASP	C	47:ASP	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	271:ARG	C	272:PRO	N	1.19
1	C	383:ALA	C	384:GLN	N	1.19
1	F	221:ARG	C	222:ARG	N	1.19
1	G	88:CYS	C	89:ALA	N	1.19
1	H	4:THR	C	5:VAL	N	1.18
1	H	306:LEU	C	307:THR	N	1.18
1	E	272:PRO	C	273:LEU	N	1.18
1	A	334:ASP	C	335:LEU	N	1.18
1	B	378:ILE	C	379:CYS	N	1.18
1	F	202:VAL	C	203:ASN	N	1.18
1	H	272:PRO	C	273:LEU	N	1.17
1	H	283:GLY	C	284:MET	N	1.17
1	E	92:LEU	C	93:ARG	N	1.17
1	E	141:ASP	C	142:LEU	N	1.17
1	A	121:ILE	C	122:PRO	N	1.17
1	A	237:ALA	C	238:SER	N	1.17
1	C	74:GLY	C	75:MET	N	1.17
1	F	144:VAL	C	145:TYR	N	1.17
1	F	361:THR	C	362:LEU	N	1.17
1	G	22:LYS	C	23:GLU	N	1.17
1	D	4:THR	C	5:VAL	N	1.17
1	D	163:THR	C	164:ALA	N	1.17
1	H	367:LYS	C	368:ARG	N	1.16
1	E	142:LEU	C	143:MET	N	1.16
1	E	231:LYS	C	232:LEU	N	1.16
1	D	82:GLU	C	83:THR	N	1.16
1	E	174:GLU	C	175:GLN	N	1.15
1	B	42:GLY	C	43:VAL	N	1.15
1	C	306:LEU	C	307:THR	N	1.15
1	F	337:LYS	C	338:VAL	N	1.15
1	G	33:VAL	C	34:MET	N	1.15
1	G	54:GLY	C	55:MET	N	1.15
1	G	167:GLU	C	168:TYR	N	1.15
1	G	283:GLY	C	284:MET	N	1.15
1	D	92:LEU	C	93:ARG	N	1.15
1	H	124:ALA	C	125:VAL	N	1.14
1	E	98:CYS	C	99:ASP	N	1.14
1	A	84:LEU	C	85:ASN	N	1.14
1	A	226:LEU	C	227:ASP	N	1.14
1	B	216:LYS	C	217:ASP	N	1.14
1	F	338:VAL	C	339:ASN	N	1.14
1	E	360:MET	C	361:THR	N	1.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	83:THR	C	84:LEU	N	1.13
1	A	273:LEU	C	274:ALA	N	1.13
1	B	389:LEU	C	390:VAL	N	1.13
1	G	63:GLN	C	64:ILE	N	1.13
1	D	226:LEU	C	227:ASP	N	1.13
1	G	270:LYS	C	271:ARG	N	1.12
1	D	224:THR	C	225:SER	N	1.12
1	E	222:ARG	C	223:ASP	N	1.11
1	C	334:ASP	C	335:LEU	N	1.11
1	H	305:GLY	C	306:LEU	N	1.10
1	E	337:LYS	C	338:VAL	N	1.10
1	C	389:LEU	C	390:VAL	N	1.10
1	F	226:LEU	C	227:ASP	N	1.10
1	C	273:LEU	C	274:ALA	N	1.09
1	G	34:MET	C	35:LYS	N	1.09
1	D	42:GLY	C	43:VAL	N	1.09
1	A	389:LEU	C	390:VAL	N	1.08
1	H	205:ILE	C	206:GLY	N	1.07
1	E	221:ARG	C	222:ARG	N	1.07
1	A	82:GLU	C	83:THR	N	1.07
1	A	221:ARG	C	222:ARG	N	1.07
1	A	222:ARG	C	223:ASP	N	1.07
1	A	241:SER	C	242:ILE	N	1.07
1	A	272:PRO	C	273:LEU	N	1.07
1	G	166:LYS	C	167:GLU	N	1.07
1	D	63:GLN	C	64:ILE	N	1.07
1	E	230:ALA	C	231:LYS	N	1.06
1	F	211:PRO	C	212:ASN	N	1.06
1	D	270:LYS	C	271:ARG	N	1.06
1	A	120:ASN	C	121:ILE	N	1.05
1	E	273:LEU	C	274:ALA	N	1.03
1	A	225:SER	C	226:LEU	N	1.02
1	E	91:GLY	C	92:LEU	N	1.01
1	G	23:GLU	C	24:VAL	N	1.01
1	C	360:MET	C	361:THR	N	1.00
1	D	162:ASN	C	163:THR	N	1.00
1	F	155:VAL	C	156:HIS	N	0.99
1	F	360:MET	C	361:THR	N	0.99
1	G	165:ALA	C	166:LYS	N	0.99
1	H	360:MET	C	361:THR	N	0.97
1	E	87:VAL	C	88:CYS	N	0.97
1	F	91:GLY	C	92:LEU	N	0.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	270:LYS	C	271:ARG	N	0.95
1	D	23:GLU	C	24:VAL	N	0.95
1	B	2:ARG	C	3:LYS	N	0.94
1	F	225:SER	C	226:LEU	N	0.94
1	E	99:ASP	C	100:GLN	N	0.93
1	A	87:VAL	C	88:CYS	N	0.93
1	A	240:GLY	C	241:SER	N	0.92
1	G	101:MET	C	102:ILE	N	0.92
1	B	91:GLY	C	92:LEU	N	0.91
1	B	87:VAL	C	88:CYS	N	0.90
1	B	336:GLU	C	337:LYS	N	0.90
1	C	307:THR	C	308:VAL	N	0.90
1	D	22:LYS	C	23:GLU	N	0.88

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/393 (98%)	-1.44	0 100 100	11, 21, 36, 58	0
1	B	388/393 (98%)	-1.50	0 100 100	10, 18, 32, 48	0
1	C	387/393 (98%)	-1.49	0 100 100	9, 17, 30, 62	0
1	D	386/393 (98%)	-1.49	0 100 100	10, 19, 37, 53	0
1	E	386/393 (98%)	-1.46	0 100 100	11, 21, 37, 51	0
1	F	380/393 (96%)	-1.44	0 100 100	12, 22, 40, 62	0
1	G	385/393 (97%)	-1.48	0 100 100	11, 19, 34, 58	0
1	H	386/393 (98%)	-1.50	0 100 100	10, 19, 33, 49	0
All	All	3084/3144 (98%)	-1.48	0 100 100	9, 19, 35, 62	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	402	6/6	0.98	0.05	36,37,40,42	0
2	GOL	C	401	6/6	0.98	0.06	35,43,45,50	0
2	GOL	F	401	6/6	0.98	0.06	49,52,56,63	0
2	GOL	E	401	6/6	0.99	0.05	25,29,35,38	0
2	GOL	A	401	6/6	0.99	0.05	28,32,34,36	0
2	GOL	B	401	6/6	0.99	0.05	25,25,28,32	0
2	GOL	G	401	6/6	0.99	0.04	14,16,17,18	0
2	GOL	D	401	6/6	0.99	0.03	31,35,36,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.