



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:14 AM EDT

PDB ID : 7REQ / pdb_00007req
Title : METHYLMALONYL-COA MUTASE, 2-CARBOXYPROPYL-COA INHIBITOR COMPLEX
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1998-09-10
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

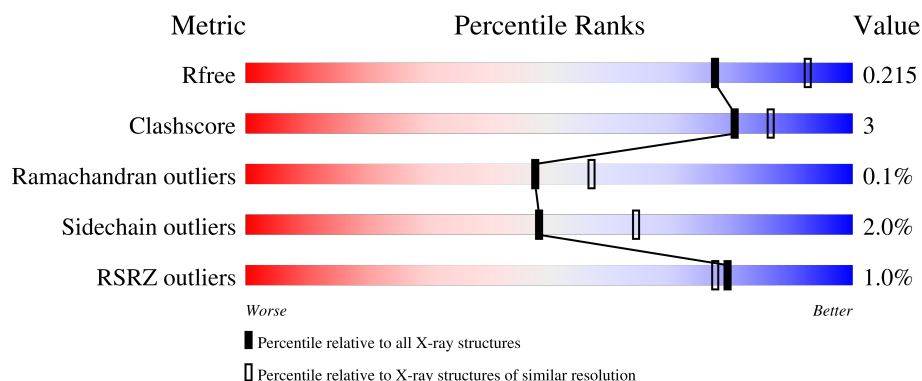
1 Overall quality at a glance

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	727	% 62% 35% .
1	C	727	% 61% 35% .
2	B	637	% 61% 33% .
2	D	637	% 61% 33% .

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
5	GOL	D	3004	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22203 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 PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5539	3507	952	1056	24			
1	C	725	Total	C	N	O	S	0	0	0
			5539	3507	952	1056	24			

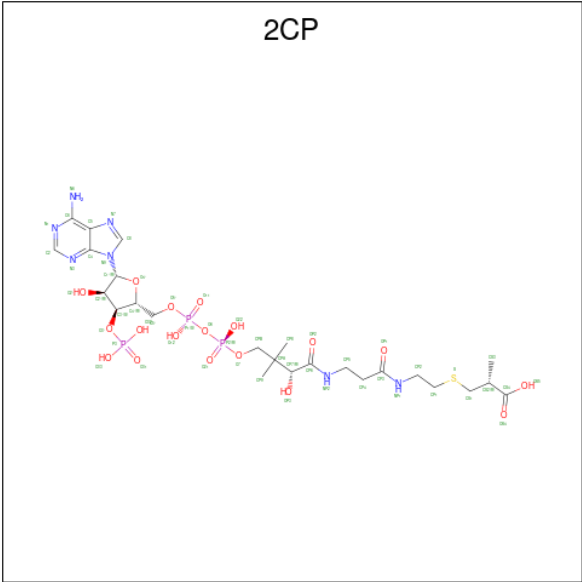
- Molecule 2 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	623	Total	C	N	O	S	0	0	0
			4744	2992	823	916	13			
2	D	623	Total	C	N	O	S	0	0	0
			4744	2992	823	916	13			

There are 6 discrepancies between the modelled and reference sequences:

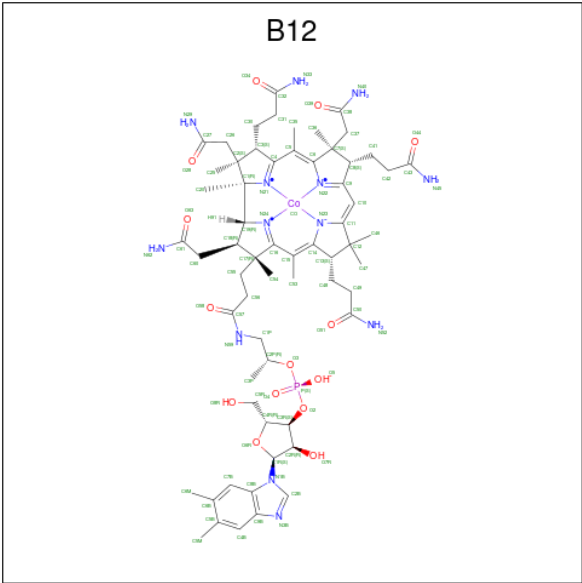
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is 2-CARBOXYPROPYL-COENZYME A (CCD ID: 2CP) (formula: C₂₅H₄₂N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 4 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
4	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			3	2	1		

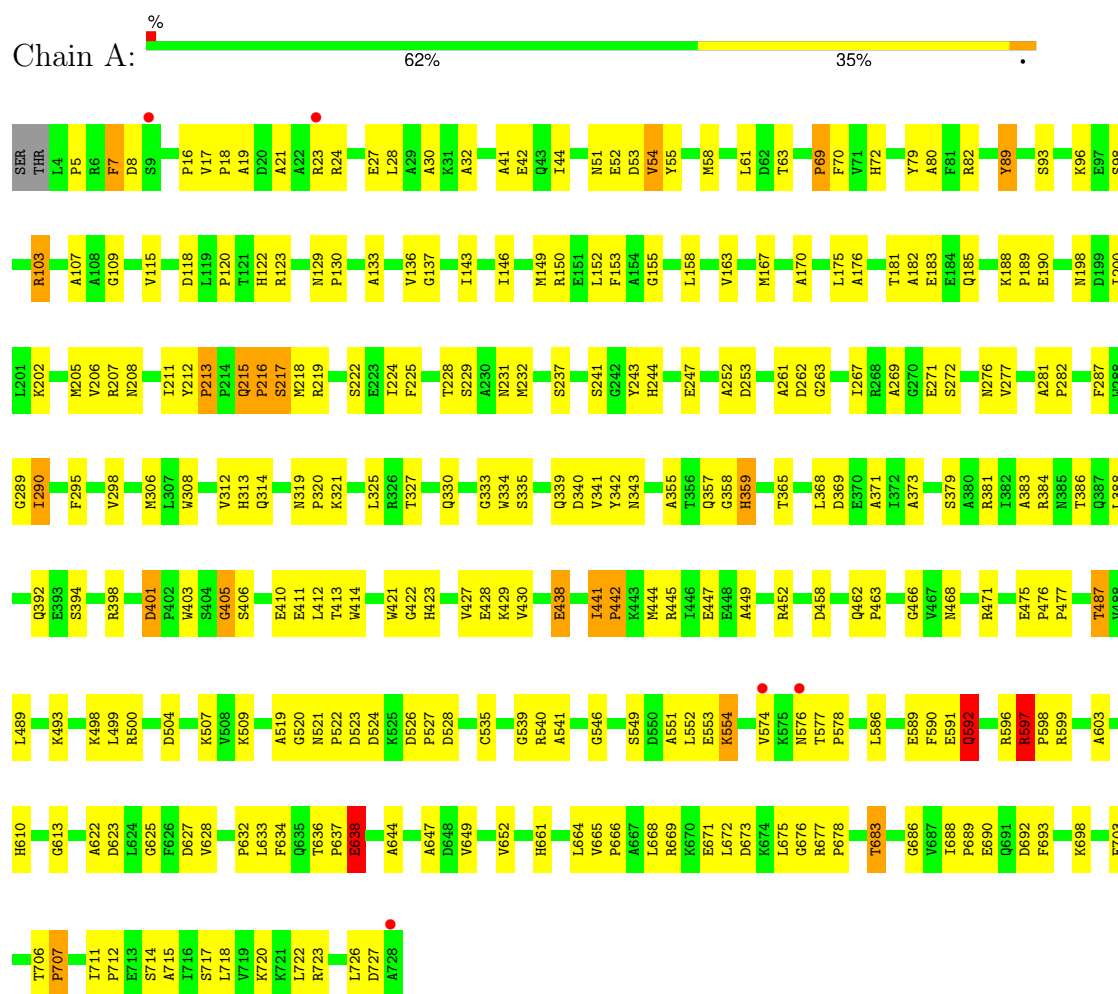
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	420	Total	O	0	0
			420	420		
6	B	243	Total	O	0	0
			243	243		
6	C	421	Total	O	0	0
			421	421		
6	D	242	Total	O	0	0
			242	242		

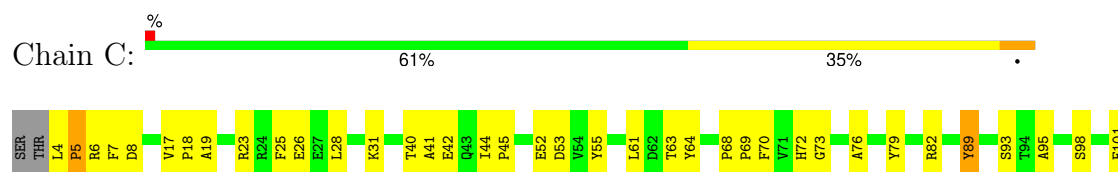
3 Residue-property plots

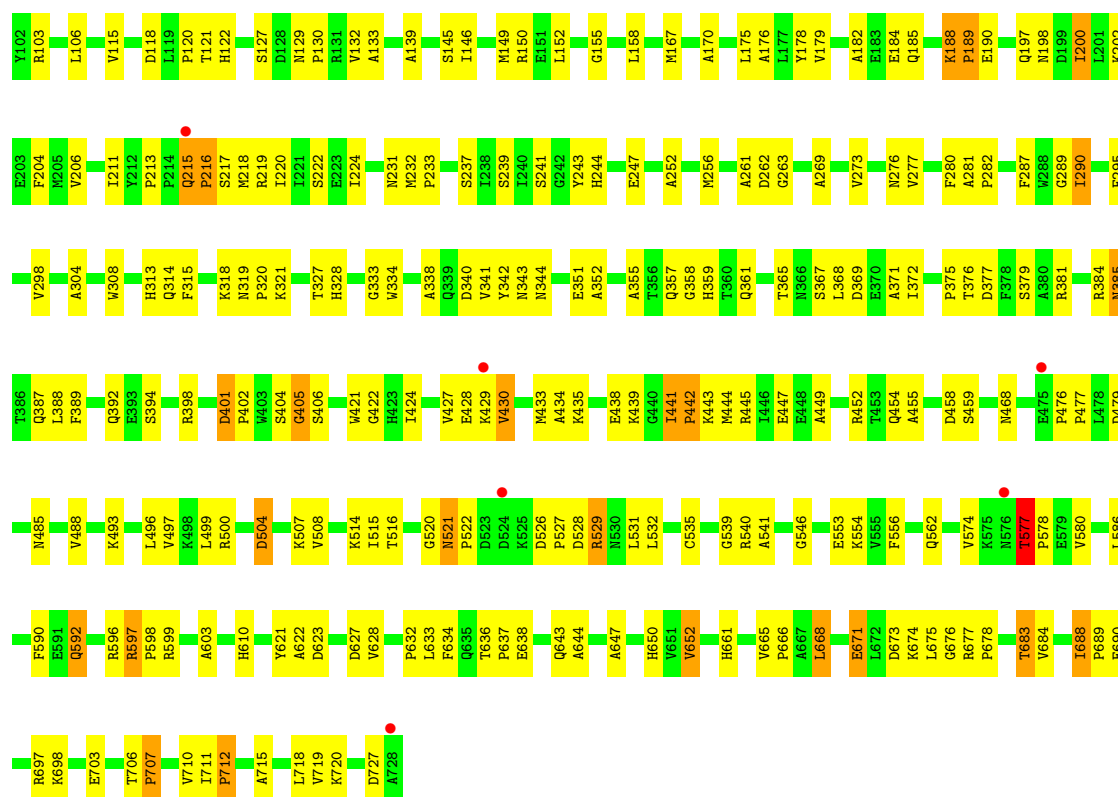
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (METHYLMALONYL-COA MUTASE)

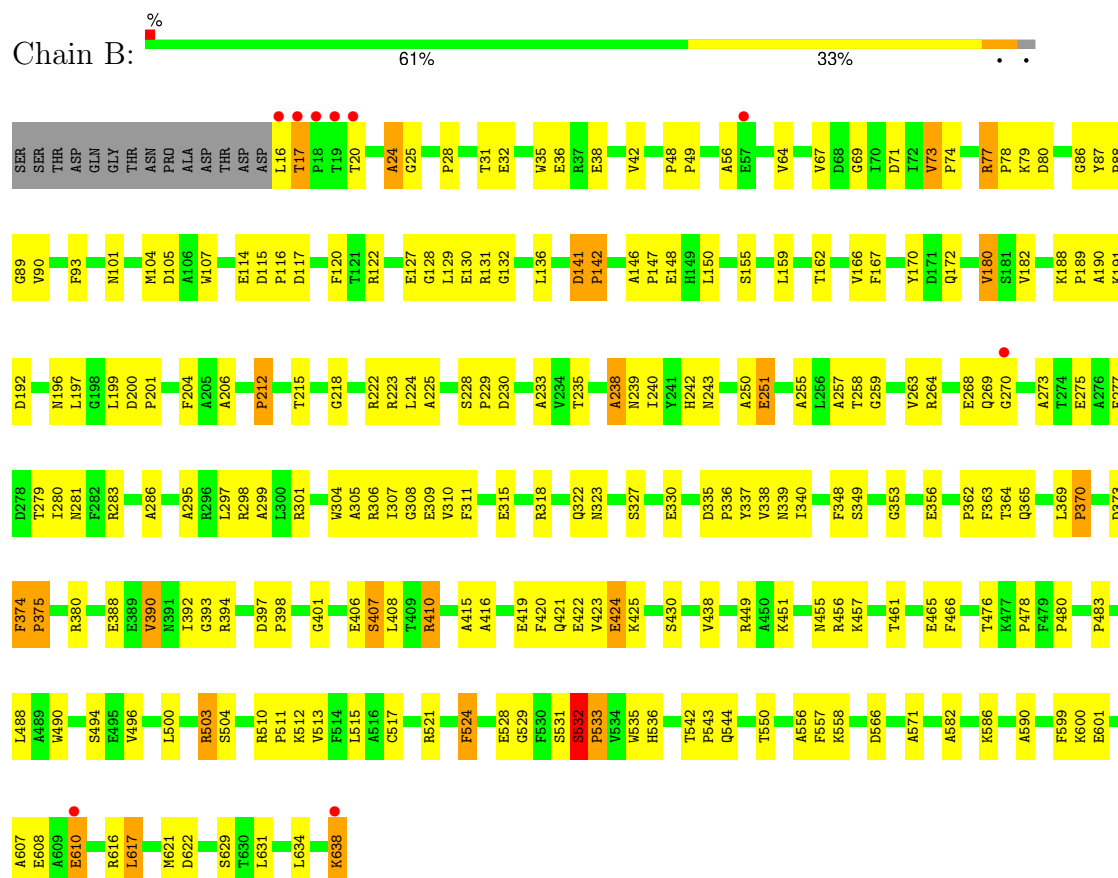


• Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE)

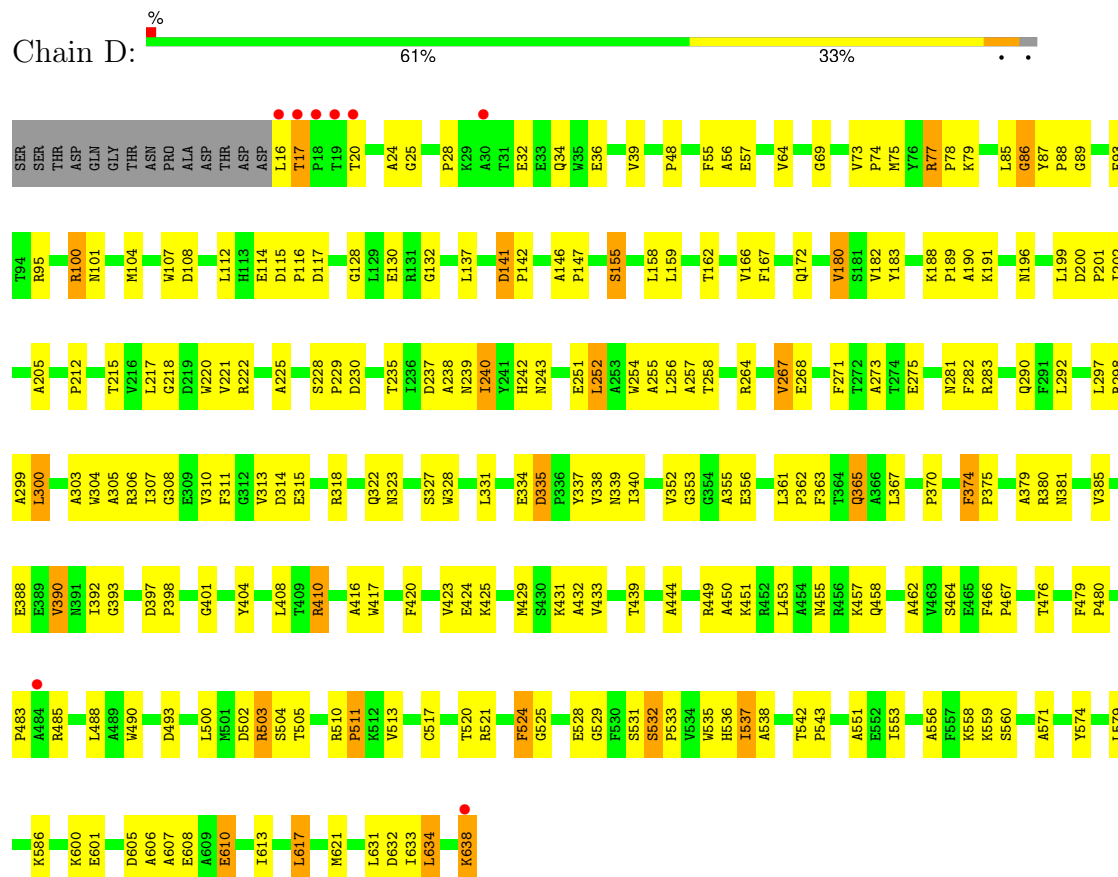




- Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)



● Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.53Å 161.40Å 86.97Å 90.00° 104.81° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-2.20) 95.3 (20.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.229 0.176 , 0.215	Depositor DCC
R_{free} test set	7983 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22203	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B12, 2CP, 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	0.84	1/5655 (0.0%)	2.57	481/7686 (6.3%)
1	C	0.83	0/5655	2.48	449/7686 (5.8%)
2	B	0.77	3/4835 (0.1%)	2.51	394/6569 (6.0%)
2	D	0.76	1/4835 (0.0%)	2.51	401/6569 (6.1%)
All	All	0.80	5/20980 (0.0%)	2.52	1725/28510 (6.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	466	PHE	CA-CB	6.73	1.58	1.52
2	B	466	PHE	CA-CB	6.41	1.57	1.52
2	B	87	TYR	CA-CB	5.41	1.61	1.54
2	B	410	ARG	CD-NE	-5.31	1.38	1.46
1	A	596	ARG	CD-NE	-5.04	1.39	1.46

All (1725) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	ARG	CD-NE-CZ	39.23	179.32	124.40
2	B	410	ARG	CD-NE-CZ	37.87	177.41	124.40
2	D	410	ARG	CD-NE-CZ	36.16	175.03	124.40
1	C	103	ARG	CD-NE-CZ	24.86	159.21	124.40
1	A	103	ARG	CD-NE-CZ	21.21	154.09	124.40
2	D	264	ARG	CD-NE-CZ	13.97	143.96	124.40
1	C	596	ARG	CD-NE-CZ	13.43	143.21	124.40
1	C	597	ARG	CD-NE-CZ	13.04	142.65	124.40
2	D	77	ARG	CD-NE-CZ	12.85	142.39	124.40
2	D	32	GLU	CA-C-N	12.08	136.14	120.44
2	D	32	GLU	C-N-CA	12.08	136.14	120.44
2	D	229	PRO	CA-C-N	11.90	141.96	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	229	PRO	C-N-CA	11.90	141.96	121.14
2	D	25	GLY	CA-C-N	11.89	138.38	120.31
2	D	25	GLY	C-N-CA	11.89	138.38	120.31
2	D	141	ASP	CA-CB-CG	11.80	124.40	112.60
2	B	17	THR	CA-C-O	11.77	136.29	120.16
2	B	77	ARG	CD-NE-CZ	11.54	140.56	124.40
2	D	17	THR	CA-C-O	11.46	135.86	120.16
1	C	63	THR	O-C-N	-11.46	109.55	122.84
2	D	17	THR	CA-C-N	11.28	131.38	119.76
2	D	17	THR	C-N-CA	11.28	131.38	119.76
2	B	600	LYS	CA-C-N	11.16	137.27	120.31
2	B	600	LYS	C-N-CA	11.16	137.27	120.31
1	A	241	SER	N-CA-C	11.08	127.42	109.59
2	B	229	PRO	CA-C-N	10.99	141.00	121.66
2	B	229	PRO	C-N-CA	10.99	141.00	121.66
1	C	727	ASP	CA-C-N	10.83	141.20	121.70
1	C	727	ASP	C-N-CA	10.83	141.20	121.70
2	B	238	ALA	CA-C-N	10.81	135.84	120.28
2	B	238	ALA	C-N-CA	10.81	135.84	120.28
2	B	17	THR	CA-C-N	10.76	130.87	119.78
2	B	17	THR	C-N-CA	10.76	130.87	119.78
1	A	678	PRO	CA-C-N	10.71	136.58	120.31
1	A	678	PRO	C-N-CA	10.71	136.58	120.31
1	A	597	ARG	CD-NE-CZ	10.63	139.29	124.40
2	B	141	ASP	CA-CB-CG	10.63	123.23	112.60
2	B	337	TYR	CA-C-N	10.52	137.09	120.47
2	B	337	TYR	C-N-CA	10.52	137.09	120.47
2	B	32	GLU	CA-C-N	10.44	134.27	120.28
2	B	32	GLU	C-N-CA	10.44	134.27	120.28
2	D	264	ARG	NE-CZ-NH2	-10.43	109.82	119.20
2	D	89	GLY	CA-C-N	10.39	137.38	122.94
2	D	89	GLY	C-N-CA	10.39	137.38	122.94
1	A	476	PRO	N-CA-CB	10.38	109.00	103.19
2	D	600	LYS	CA-C-N	10.31	137.94	120.72
2	D	600	LYS	C-N-CA	10.31	137.94	120.72
1	A	384	ARG	CD-NE-CZ	10.31	138.83	124.40
1	A	673	ASP	CA-C-N	10.27	135.07	120.28
1	A	673	ASP	C-N-CA	10.27	135.07	120.28
1	A	371	ALA	CA-C-N	10.25	134.03	123.16
1	A	371	ALA	C-N-CA	10.25	134.03	123.16
1	C	170	ALA	CA-C-N	10.22	134.46	120.46
1	C	170	ALA	C-N-CA	10.22	134.46	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	524	PHE	CA-CB-CG	10.21	124.01	113.80
1	A	637	PRO	CA-C-N	9.88	133.28	120.44
1	A	637	PRO	C-N-CA	9.88	133.28	120.44
1	C	241	SER	N-CA-C	9.84	125.43	109.59
1	C	637	PRO	O-C-N	-9.72	110.56	122.23
1	A	320	PRO	CA-C-N	9.71	134.26	120.28
1	A	320	PRO	C-N-CA	9.71	134.26	120.28
1	C	637	PRO	CA-C-N	9.69	134.05	120.29
1	C	637	PRO	C-N-CA	9.69	134.05	120.29
2	B	424	GLU	CA-C-N	9.61	134.12	120.28
2	B	424	GLU	C-N-CA	9.61	134.12	120.28
1	A	429	LYS	CA-C-N	9.58	136.89	121.09
1	A	429	LYS	C-N-CA	9.58	136.89	121.09
1	A	313	HIS	CA-C-N	9.54	134.02	120.28
1	A	313	HIS	C-N-CA	9.54	134.02	120.28
1	C	182	ALA	CA-C-N	9.50	133.40	120.38
1	C	182	ALA	C-N-CA	9.50	133.40	120.38
1	A	170	ALA	CA-C-N	9.46	133.42	120.46
1	A	170	ALA	C-N-CA	9.46	133.42	120.46
2	B	239	ASN	CA-C-N	9.40	132.40	120.56
2	B	239	ASN	C-N-CA	9.40	132.40	120.56
2	D	238	ALA	CA-C-N	9.37	134.55	120.31
2	D	238	ALA	C-N-CA	9.37	134.55	120.31
1	C	333	GLY	O-C-N	-9.34	113.13	122.19
1	C	277	VAL	O-C-N	-9.30	112.78	121.89
1	C	623	ASP	CA-CB-CG	9.21	121.81	112.60
1	C	452	ARG	CD-NE-CZ	9.16	137.23	124.40
2	D	93	PHE	CA-C-N	9.16	132.34	120.44
2	D	93	PHE	C-N-CA	9.16	132.34	120.44
1	A	82	ARG	CD-NE-CZ	9.15	137.21	124.40
1	C	41	ALA	O-C-N	-9.15	111.52	122.22
2	B	69	GLY	N-CA-C	9.12	128.44	115.30
2	B	117	ASP	CA-C-N	9.05	134.06	120.31
2	B	117	ASP	C-N-CA	9.05	134.06	120.31
2	B	264	ARG	CD-NE-CZ	8.95	136.93	124.40
1	C	215	GLN	CA-C-O	8.90	127.54	119.08
1	A	52	GLU	CA-C-N	8.86	133.03	120.28
1	A	52	GLU	C-N-CA	8.86	133.03	120.28
1	C	369	ASP	CA-C-N	8.85	132.50	120.38
1	C	369	ASP	C-N-CA	8.85	132.50	120.38
1	A	638	GLU	CB-CG-CD	8.84	127.63	112.60
1	C	70	PHE	CA-CB-CG	8.81	122.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	PHE	CA-C-N	8.80	132.43	120.54
2	B	93	PHE	C-N-CA	8.80	132.43	120.54
2	D	86	GLY	O-C-N	-8.80	113.36	122.60
2	D	600	LYS	O-C-N	-8.76	111.00	122.39
1	A	541	ALA	CA-C-N	8.74	135.33	122.74
1	A	541	ALA	C-N-CA	8.74	135.33	122.74
1	C	198	ASN	N-CA-CB	-8.73	99.13	111.62
1	A	41	ALA	CA-C-N	8.73	138.60	121.58
1	A	41	ALA	C-N-CA	8.73	138.60	121.58
2	D	307	ILE	CA-C-N	8.69	129.62	119.98
2	D	307	ILE	C-N-CA	8.69	129.62	119.98
1	C	678	PRO	CA-C-N	8.68	133.50	120.31
1	C	678	PRO	C-N-CA	8.68	133.50	120.31
2	D	601	GLU	CA-C-N	8.67	136.31	121.14
2	D	601	GLU	C-N-CA	8.67	136.31	121.14
1	A	452	ARG	NE-CZ-NH2	-8.65	111.41	119.20
1	A	198	ASN	N-CA-CB	-8.65	99.25	111.62
2	D	531	SER	N-CA-C	8.65	120.78	111.36
2	D	128	GLY	O-C-N	-8.63	113.89	122.18
2	D	182	VAL	CA-C-N	8.62	131.83	120.28
2	D	182	VAL	C-N-CA	8.62	131.83	120.28
1	A	312	VAL	CA-C-N	8.61	132.18	120.38
1	A	312	VAL	C-N-CA	8.61	132.18	120.38
1	A	182	ALA	CA-C-N	8.60	131.81	120.28
1	A	182	ALA	C-N-CA	8.60	131.81	120.28
2	B	536	HIS	O-C-N	-8.60	111.21	122.39
1	C	553	GLU	CA-C-N	8.59	132.15	120.38
1	C	553	GLU	C-N-CA	8.59	132.15	120.38
2	B	327	SER	N-CA-C	8.55	122.15	109.59
1	C	439	LYS	CA-C-N	8.53	137.69	120.80
1	C	439	LYS	C-N-CA	8.53	137.69	120.80
1	C	540	ARG	O-C-N	-8.53	112.43	122.15
2	D	455	ASN	O-C-N	-8.49	111.73	122.34
1	A	637	PRO	O-C-N	-8.47	113.03	122.18
2	D	352	VAL	O-C-N	-8.47	112.23	121.80
1	C	313	HIS	CA-C-N	8.47	134.15	120.60
1	C	313	HIS	C-N-CA	8.47	134.15	120.60
1	C	452	ARG	NE-CZ-NH2	-8.46	111.59	119.20
1	A	343	ASN	CA-C-N	8.43	132.43	120.28
1	A	343	ASN	C-N-CA	8.43	132.43	120.28
1	C	231	ASN	O-C-N	-8.42	113.08	122.34
2	D	525	GLY	CA-C-N	8.40	129.27	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	525	GLY	C-N-CA	8.40	129.27	119.94
2	B	24	ALA	CA-C-N	8.40	135.18	120.74
2	B	24	ALA	C-N-CA	8.40	135.18	120.74
2	B	204	PHE	CA-C-N	8.36	131.48	120.28
2	B	204	PHE	C-N-CA	8.36	131.48	120.28
1	A	146	ILE	O-C-N	-8.32	113.47	121.87
1	A	413	THR	CA-C-N	8.31	131.24	120.44
1	A	413	THR	C-N-CA	8.31	131.24	120.44
1	C	313	HIS	O-C-N	-8.28	112.76	122.20
1	A	342	TYR	CA-C-N	8.27	132.18	120.28
1	A	342	TYR	C-N-CA	8.27	132.18	120.28
1	C	541	ALA	CA-C-N	8.20	137.19	121.54
1	C	541	ALA	C-N-CA	8.20	137.19	121.54
1	C	8	ASP	CA-C-N	8.18	135.27	122.26
1	C	8	ASP	C-N-CA	8.18	135.27	122.26
1	A	622	ALA	O-C-N	-8.16	113.66	122.07
2	D	524	PHE	CA-CB-CG	8.16	121.96	113.80
2	D	338	VAL	O-C-N	-8.14	113.64	121.87
2	D	25	GLY	O-C-N	-8.12	113.83	122.19
2	D	397	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	369	ASP	CA-C-N	8.11	131.48	120.38
1	A	369	ASP	C-N-CA	8.11	131.48	120.38
1	A	237	SER	N-CA-C	8.08	122.95	113.18
1	C	334	TRP	O-C-N	-8.08	113.56	122.12
1	C	280	PHE	CA-C-N	8.06	130.17	120.09
1	C	280	PHE	C-N-CA	8.06	130.17	120.09
1	C	438	GLU	O-C-N	-8.05	111.92	122.39
1	A	287	PHE	CA-CB-CG	8.04	121.84	113.80
1	A	553	GLU	CA-C-N	8.04	131.39	120.38
1	A	553	GLU	C-N-CA	8.04	131.39	120.38
1	A	212	TYR	CA-C-O	8.03	129.71	120.96
1	A	398	ARG	N-CA-C	8.01	120.92	111.71
1	C	398	ARG	N-CA-C	8.01	122.31	112.54
2	B	419	GLU	CA-C-N	8.00	131.00	120.28
2	B	419	GLU	C-N-CA	8.00	131.00	120.28
1	A	313	HIS	O-C-N	-8.00	113.64	122.12
1	A	727	ASP	CA-C-N	7.99	136.08	121.70
1	A	727	ASP	C-N-CA	7.99	136.08	121.70
2	D	423	VAL	CA-C-N	7.98	130.97	120.28
2	D	423	VAL	C-N-CA	7.98	130.97	120.28
1	A	321	LYS	CA-C-N	7.98	130.97	120.28
1	A	321	LYS	C-N-CA	7.98	130.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	ALA	CA-C-N	7.97	137.13	121.58
1	C	41	ALA	C-N-CA	7.97	137.13	121.58
2	D	521	ARG	O-C-N	-7.97	113.80	122.09
1	A	333	GLY	CA-C-N	7.96	130.94	120.28
1	A	333	GLY	C-N-CA	7.96	130.94	120.28
1	A	540	ARG	O-C-N	-7.95	113.69	122.12
2	B	48	PRO	CA-C-N	7.95	128.69	119.47
2	B	48	PRO	C-N-CA	7.95	128.69	119.47
1	A	277	VAL	O-C-N	-7.93	114.12	121.89
1	C	319	ASN	CA-C-N	7.92	128.00	119.28
1	C	319	ASN	C-N-CA	7.92	128.00	119.28
1	C	320	PRO	CA-C-N	7.91	131.68	120.28
1	C	320	PRO	C-N-CA	7.91	131.68	120.28
2	B	339	ASN	O-C-N	-7.91	112.11	122.39
1	C	215	GLN	N-CA-CB	7.91	121.50	110.11
2	B	86	GLY	O-C-N	-7.90	114.31	122.60
1	C	468	ASN	OD1-CG-ND2	-7.90	114.70	122.60
2	B	147	PRO	O-C-N	-7.90	113.16	122.24
1	C	556	PHE	CA-CB-CG	7.88	121.68	113.80
2	B	89	GLY	CA-C-N	7.88	134.05	122.71
2	B	89	GLY	C-N-CA	7.88	134.05	122.71
2	B	25	GLY	O-C-N	-7.87	113.88	122.54
2	B	496	VAL	O-C-N	-7.85	114.25	121.87
2	D	458	GLN	OE1-CD-NE2	7.84	130.44	122.60
2	B	438	VAL	CA-C-N	7.83	131.11	120.38
2	B	438	VAL	C-N-CA	7.83	131.11	120.38
2	B	258	THR	CA-C-N	7.83	128.63	119.94
2	B	258	THR	C-N-CA	7.83	128.63	119.94
2	D	500	LEU	CA-C-N	7.81	130.75	120.28
2	D	500	LEU	C-N-CA	7.81	130.75	120.28
1	C	372	ILE	CB-CG1-CD1	7.80	130.18	113.80
1	A	520	GLY	O-C-N	-7.79	112.90	122.71
1	C	520	GLY	CA-C-N	7.78	131.41	122.85
1	C	520	GLY	C-N-CA	7.78	131.41	122.85
1	C	675	LEU	CA-C-N	7.78	133.51	120.91
1	C	675	LEU	C-N-CA	7.78	133.51	120.91
2	D	78	PRO	CA-C-N	7.76	133.02	120.60
2	D	78	PRO	C-N-CA	7.76	133.02	120.60
1	A	261	ALA	CA-C-N	7.76	130.53	120.44
1	A	261	ALA	C-N-CA	7.76	130.53	120.44
2	B	86	GLY	CA-C-O	7.76	130.66	122.59
1	C	526	ASP	CA-C-O	7.76	126.73	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	455	ASN	CA-C-O	7.75	128.42	119.35
1	A	690	GLU	CA-C-N	7.75	132.99	120.60
1	A	690	GLU	C-N-CA	7.75	132.99	120.60
1	A	528	ASP	CA-CB-CG	-7.74	104.86	112.60
1	A	320	PRO	O-C-N	-7.73	112.25	122.22
1	C	79	TYR	CA-C-N	7.73	130.63	120.28
1	C	79	TYR	C-N-CA	7.73	130.63	120.28
2	B	24	ALA	O-C-N	-7.72	112.77	122.27
1	A	449	ALA	O-C-N	-7.72	113.94	122.12
1	C	526	ASP	CA-C-N	7.72	127.35	119.56
1	C	526	ASP	C-N-CA	7.72	127.35	119.56
2	D	108	ASP	CA-CB-CG	7.71	120.31	112.60
2	B	457	LYS	CA-C-N	7.71	134.40	123.30
2	B	457	LYS	C-N-CA	7.71	134.40	123.30
2	D	24	ALA	CA-C-N	7.69	129.81	120.13
2	D	24	ALA	C-N-CA	7.69	129.81	120.13
1	A	28	LEU	CA-C-N	7.68	130.43	120.44
1	A	28	LEU	C-N-CA	7.68	130.43	120.44
1	C	115	VAL	N-CA-C	7.68	119.65	108.58
1	C	185	GLN	CA-C-N	7.68	133.36	120.91
1	C	185	GLN	C-N-CA	7.68	133.36	120.91
1	A	281	ALA	O-C-N	-7.67	113.26	120.55
2	B	306	ARG	CA-C-N	7.67	131.31	120.42
2	B	306	ARG	C-N-CA	7.67	131.31	120.42
1	A	690	GLU	O-C-N	-7.66	114.00	122.12
2	D	117	ASP	CA-C-N	7.64	131.93	120.31
2	D	117	ASP	C-N-CA	7.64	131.93	120.31
1	A	333	GLY	O-C-N	-7.63	114.79	122.19
2	B	536	HIS	CA-C-N	7.62	130.90	120.46
2	B	536	HIS	C-N-CA	7.62	130.90	120.46
1	A	327	THR	N-CA-C	7.62	121.32	109.52
2	D	543	PRO	N-CA-CB	7.60	109.96	103.35
1	A	666	PRO	O-C-N	-7.59	113.13	122.23
1	A	222	SER	CA-C-N	7.57	131.03	120.29
1	A	222	SER	C-N-CA	7.57	131.03	120.29
1	A	677	ARG	O-C-N	-7.57	114.53	121.42
2	D	536	HIS	O-C-N	-7.56	112.56	122.39
1	A	271	GLU	O-C-N	-7.56	114.11	122.12
1	A	118	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	405	GLY	O-C-N	-7.52	114.55	122.52
2	D	77	ARG	CA-C-N	7.51	127.89	119.32
2	D	77	ARG	C-N-CA	7.51	127.89	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	527	PRO	N-CA-CB	7.51	110.72	103.51
1	A	63	THR	CA-C-N	7.50	134.19	122.94
1	A	63	THR	C-N-CA	7.50	134.19	122.94
1	A	175	LEU	CA-C-N	7.50	130.19	120.44
1	A	175	LEU	C-N-CA	7.50	130.19	120.44
1	A	636	THR	N-CA-C	-7.50	100.31	110.36
1	A	63	THR	O-C-N	-7.49	112.55	122.97
1	C	405	GLY	O-C-N	-7.49	114.86	122.65
2	D	420	PHE	CA-CB-CG	7.49	121.29	113.80
1	A	41	ALA	O-C-N	-7.49	113.06	122.27
1	A	215	GLN	CB-CG-CD	7.48	125.32	112.60
1	A	677	ARG	N-CA-C	7.48	122.58	108.97
1	A	359	HIS	N-CA-C	7.48	121.99	111.52
2	B	531	SER	N-CA-C	7.46	119.49	111.36
2	D	228	SER	CA-C-N	7.45	127.62	119.87
2	D	228	SER	C-N-CA	7.45	127.62	119.87
1	C	603	ALA	N-CA-C	7.45	121.80	109.95
1	C	155	GLY	O-C-N	-7.45	114.37	122.41
2	B	259	GLY	CA-C-N	7.44	130.25	120.28
2	B	259	GLY	C-N-CA	7.44	130.25	120.28
2	B	20	THR	CA-C-O	7.44	127.91	120.32
1	C	281	ALA	O-C-N	-7.43	113.72	120.71
2	B	93	PHE	O-C-N	-7.43	114.07	121.87
1	A	277	VAL	CA-C-N	7.42	132.47	120.60
1	A	277	VAL	C-N-CA	7.42	132.47	120.60
1	A	271	GLU	CA-C-N	7.41	132.46	120.60
1	A	271	GLU	C-N-CA	7.41	132.46	120.60
1	C	215	GLN	CB-CG-CD	7.41	125.20	112.60
2	B	77	ARG	CA-C-N	7.40	127.76	119.32
2	B	77	ARG	C-N-CA	7.40	127.76	119.32
2	B	364	THR	CA-C-N	7.40	132.54	120.63
2	B	364	THR	C-N-CA	7.40	132.54	120.63
1	A	683	THR	N-CA-CB	7.39	123.72	111.08
1	A	7	PHE	N-CA-C	7.39	122.14	113.20
2	D	17	THR	N-CA-C	7.37	126.11	109.81
1	A	394	SER	N-CA-C	7.37	120.37	111.82
1	C	392	GLN	N-CA-C	7.37	122.70	112.45
2	D	528	GLU	CA-C-N	7.37	128.16	119.98
2	D	528	GLU	C-N-CA	7.37	128.16	119.98
1	C	63	THR	CA-C-N	7.37	133.99	122.94
1	C	63	THR	C-N-CA	7.37	133.99	122.94
1	A	592	GLN	CG-CD-NE2	7.35	127.43	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261	ALA	O-C-N	-7.35	113.23	122.27
2	D	340	ILE	CA-C-N	7.35	130.73	120.29
2	D	340	ILE	C-N-CA	7.35	130.73	120.29
1	A	636	THR	CA-C-N	7.35	126.88	119.24
1	A	636	THR	C-N-CA	7.35	126.88	119.24
1	A	225	PHE	CA-CB-CG	7.35	121.15	113.80
1	C	7	PHE	N-CA-C	7.34	122.27	113.16
1	C	237	SER	N-CA-C	7.33	122.05	113.18
1	C	277	VAL	CA-C-N	7.33	132.96	120.72
1	C	277	VAL	C-N-CA	7.33	132.96	120.72
1	A	185	GLN	CA-C-N	7.33	132.64	121.51
1	A	185	GLN	C-N-CA	7.33	132.64	121.51
1	A	17	VAL	N-CA-C	-7.31	99.59	107.77
1	A	215	GLN	CA-C-O	7.30	126.02	119.08
1	C	55	TYR	N-CA-C	7.30	120.10	111.71
2	B	408	LEU	CA-C-N	7.29	129.92	120.44
2	B	408	LEU	C-N-CA	7.29	129.92	120.44
1	C	327	THR	N-CA-C	7.29	121.03	109.50
1	C	556	PHE	N-CA-C	7.28	121.92	112.89
2	B	222	ARG	O-C-N	-7.27	114.41	122.12
1	A	120	PRO	CA-C-N	7.27	129.89	120.44
1	A	120	PRO	C-N-CA	7.27	129.89	120.44
2	B	397	ASP	CA-C-N	7.27	127.27	119.28
2	B	397	ASP	C-N-CA	7.27	127.27	119.28
1	C	384	ARG	CD-NE-CZ	7.26	134.56	124.40
1	C	321	LYS	CA-C-N	7.25	130.72	120.28
1	C	321	LYS	C-N-CA	7.25	130.72	120.28
1	C	338	ALA	CA-C-N	7.25	133.44	122.93
1	C	338	ALA	C-N-CA	7.25	133.44	122.93
1	C	232	MET	CA-C-N	7.25	126.95	119.56
1	C	232	MET	C-N-CA	7.25	126.95	119.56
1	C	321	LYS	O-C-N	-7.25	113.74	122.22
2	B	511	PRO	N-CA-CB	7.24	109.65	103.35
2	D	337	TYR	CA-C-N	7.22	131.88	120.47
2	D	337	TYR	C-N-CA	7.22	131.88	120.47
1	C	89	TYR	CA-CB-CG	7.21	126.88	113.90
2	D	141	ASP	CA-C-N	7.21	127.21	119.28
2	D	141	ASP	C-N-CA	7.21	127.21	119.28
1	A	526	ASP	CA-C-N	7.21	126.91	119.56
1	A	526	ASP	C-N-CA	7.21	126.91	119.56
1	C	698	LYS	O-C-N	-7.20	113.80	122.22
2	B	465	GLU	CA-C-N	7.20	130.60	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	465	GLU	C-N-CA	7.20	130.60	122.83
1	C	333	GLY	CA-C-N	7.20	130.24	120.38
1	C	333	GLY	C-N-CA	7.20	130.24	120.38
2	D	132	GLY	N-CA-C	7.18	124.54	115.21
2	B	601	GLU	CA-C-N	7.17	135.57	121.58
2	B	601	GLU	C-N-CA	7.17	135.57	121.58
2	B	269	GLN	CA-C-N	7.17	134.47	121.85
2	B	269	GLN	C-N-CA	7.17	134.47	121.85
1	A	319	ASN	CA-C-N	7.17	127.17	119.28
1	A	319	ASN	C-N-CA	7.17	127.17	119.28
2	D	424	GLU	CA-C-N	7.16	131.19	120.31
2	D	424	GLU	C-N-CA	7.16	131.19	120.31
2	B	550	THR	CA-C-N	7.15	129.74	120.44
2	B	550	THR	C-N-CA	7.15	129.74	120.44
1	C	179	VAL	CA-C-N	7.15	130.58	120.42
1	C	179	VAL	C-N-CA	7.15	130.58	120.42
1	A	152	LEU	O-C-N	-7.14	114.55	122.12
1	A	675	LEU	CA-C-N	7.14	133.84	121.07
1	A	675	LEU	C-N-CA	7.14	133.84	121.07
1	A	553	GLU	O-C-N	-7.13	113.88	122.22
2	D	78	PRO	O-C-N	-7.12	114.06	122.24
2	D	188	LYS	N-CA-C	-7.12	101.14	110.39
2	D	397	ASP	CA-C-N	7.11	126.82	119.56
2	D	397	ASP	C-N-CA	7.11	126.82	119.56
1	A	678	PRO	O-C-N	-7.11	112.49	122.38
2	B	566	ASP	CA-CB-CG	7.11	119.70	112.60
2	D	69	GLY	N-CA-C	7.10	125.83	114.90
2	B	616	ARG	CD-NE-CZ	7.09	134.33	124.40
1	A	158	LEU	N-CA-C	7.08	121.51	113.01
1	A	522	PRO	N-CA-CB	7.07	109.92	103.34
2	D	172	GLN	N-CA-C	7.07	118.99	111.28
2	D	229	PRO	O-C-N	-7.06	112.47	122.35
2	B	390	VAL	O-C-N	-7.06	113.85	122.18
2	D	222	ARG	O-C-N	-7.05	114.64	122.12
1	C	206	VAL	CB-CA-C	-7.04	99.74	111.29
2	B	318	ARG	CD-NE-CZ	7.04	134.25	124.40
1	A	54	VAL	CA-C-N	7.03	130.40	120.28
1	A	54	VAL	C-N-CA	7.03	130.40	120.28
1	A	55	TYR	N-CA-C	7.03	119.79	111.71
2	B	374	PHE	CA-C-N	7.02	126.84	119.05
2	B	374	PHE	C-N-CA	7.02	126.84	119.05
1	A	499	LEU	CA-C-N	7.01	130.25	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	LEU	C-N-CA	7.01	130.25	120.29
2	D	93	PHE	O-C-N	-7.01	114.51	121.87
1	C	371	ALA	CA-C-N	7.01	130.59	123.16
1	C	371	ALA	C-N-CA	7.01	130.59	123.16
1	C	521	ASN	O-C-N	-7.01	115.55	121.23
1	A	590	PHE	N-CA-C	-7.00	103.58	111.07
1	C	401	ASP	CA-C-N	6.99	126.97	119.28
1	C	401	ASP	C-N-CA	6.99	126.97	119.28
1	A	452	ARG	CD-NE-CZ	6.99	134.18	124.40
1	A	334	TRP	O-C-N	-6.98	114.72	122.12
1	A	261	ALA	O-C-N	-6.98	114.20	122.15
1	C	677	ARG	CA-C-N	6.96	126.67	119.64
1	C	677	ARG	C-N-CA	6.96	126.67	119.64
2	B	305	ALA	CA-C-N	6.96	130.17	120.29
2	B	305	ALA	C-N-CA	6.96	130.17	120.29
2	B	225	ALA	CA-C-N	6.96	132.34	120.72
2	B	225	ALA	C-N-CA	6.96	132.34	120.72
1	C	394	SER	N-CA-C	6.95	119.89	111.82
2	B	307	ILE	CA-C-N	6.95	127.66	119.94
2	B	307	ILE	C-N-CA	6.95	127.66	119.94
2	D	86	GLY	CA-C-O	6.95	129.82	122.59
2	D	159	LEU	CA-C-N	6.94	132.31	120.72
2	D	159	LEU	C-N-CA	6.94	132.31	120.72
2	D	335	ASP	CA-C-N	6.94	126.57	119.56
2	D	335	ASP	C-N-CA	6.94	126.57	119.56
1	A	340	ASP	CA-C-N	6.93	131.43	120.47
1	A	340	ASP	C-N-CA	6.93	131.43	120.47
2	B	180	VAL	N-CA-CB	6.93	119.97	110.54
2	D	337	TYR	O-C-N	-6.93	113.14	122.43
1	C	541	ALA	O-C-N	-6.93	112.13	122.39
2	D	420	PHE	CA-C-N	6.93	129.57	120.28
2	D	420	PHE	C-N-CA	6.93	129.57	120.28
1	A	133	ALA	O-C-N	-6.92	114.15	122.11
2	B	275	GLU	CA-C-N	6.92	129.44	120.44
2	B	275	GLU	C-N-CA	6.92	129.44	120.44
1	C	454	GLN	CA-C-N	6.92	129.44	120.44
1	C	454	GLN	C-N-CA	6.92	129.44	120.44
2	D	356	GLU	CB-CG-CD	6.92	124.37	112.60
2	D	374	PHE	CA-C-N	6.92	126.73	119.05
2	D	374	PHE	C-N-CA	6.92	126.73	119.05
1	C	522	PRO	N-CA-CB	6.92	109.47	103.31
1	C	574	VAL	N-CA-CB	6.92	120.52	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	443	LYS	O-C-N	-6.92	114.79	122.12
2	D	370	PRO	N-CA-CB	6.91	109.46	103.31
1	A	28	LEU	O-C-N	-6.90	114.80	122.12
1	C	352	ALA	O-C-N	-6.89	114.81	122.12
1	A	262	ASP	CA-C-N	6.88	127.62	119.98
1	A	262	ASP	C-N-CA	6.88	127.62	119.98
1	C	677	ARG	O-C-N	-6.88	115.18	121.37
1	A	5	PRO	N-CA-CB	6.88	109.30	103.25
1	A	79	TYR	CA-C-N	6.88	130.19	120.28
1	A	79	TYR	C-N-CA	6.88	130.19	120.28
1	A	592	GLN	CB-CG-CD	6.88	124.30	112.60
1	A	341	VAL	N-CA-C	6.88	119.65	111.05
1	A	592	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	C	129	ASN	CA-C-N	6.86	127.14	119.32
1	C	129	ASN	C-N-CA	6.86	127.14	119.32
2	D	255	ALA	N-CA-C	-6.86	103.74	111.14
2	B	115	ASP	CA-C-N	6.85	126.65	119.05
2	B	115	ASP	C-N-CA	6.85	126.65	119.05
1	A	342	TYR	O-C-N	-6.84	113.26	122.43
1	C	167	MET	O-C-N	-6.84	115.03	123.44
1	A	216	PRO	CA-C-N	6.84	129.44	120.28
1	A	216	PRO	C-N-CA	6.84	129.44	120.28
2	B	196	ASN	CA-CB-CG	6.83	119.43	112.60
2	B	532	SER	CA-C-N	6.83	127.10	119.32
2	B	532	SER	C-N-CA	6.83	127.10	119.32
1	A	603	ALA	N-CA-C	6.82	120.80	109.95
2	B	420	PHE	CA-CB-CG	6.82	120.62	113.80
1	A	541	ALA	O-C-N	-6.81	111.45	122.42
2	D	338	VAL	CA-C-N	6.81	131.50	120.60
2	D	338	VAL	C-N-CA	6.81	131.50	120.60
1	C	45	PRO	O-C-N	-6.81	115.47	123.10
1	A	368	LEU	CA-C-N	6.80	133.94	122.65
1	A	368	LEU	C-N-CA	6.80	133.94	122.65
2	D	532	SER	CA-C-N	6.80	126.60	119.05
2	D	532	SER	C-N-CA	6.80	126.60	119.05
1	C	520	GLY	O-C-N	-6.80	113.10	122.68
1	A	129	ASN	CA-C-N	6.79	126.75	119.28
1	A	129	ASN	C-N-CA	6.79	126.75	119.28
1	A	52	GLU	O-C-N	-6.79	113.56	122.39
2	D	258	THR	CA-C-N	6.79	127.47	119.94
2	D	258	THR	C-N-CA	6.79	127.47	119.94
1	A	577	THR	CA-C-N	6.78	126.58	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	THR	C-N-CA	6.78	126.58	119.05
2	B	337	TYR	O-C-N	-6.78	113.58	122.39
1	A	61	LEU	N-CA-C	6.78	120.65	112.38
1	A	625	GLY	CA-C-O	-6.77	111.49	119.01
2	B	353	GLY	CA-C-N	6.77	131.88	120.91
2	B	353	GLY	C-N-CA	6.77	131.88	120.91
2	D	304	TRP	CA-C-N	6.76	129.89	120.29
2	D	304	TRP	C-N-CA	6.76	129.89	120.29
2	D	162	THR	N-CA-C	6.75	119.91	108.90
1	C	361	GLN	OE1-CD-NE2	-6.75	115.85	122.60
1	C	385	ASN	CA-C-N	6.75	129.21	120.44
1	C	385	ASN	C-N-CA	6.75	129.21	120.44
1	C	98	SER	CA-C-N	6.75	129.21	120.44
1	C	98	SER	C-N-CA	6.75	129.21	120.44
2	D	633	ILE	O-C-N	-6.74	115.33	121.87
2	D	608	GLU	CA-C-N	6.74	129.20	120.44
2	D	608	GLU	C-N-CA	6.74	129.20	120.44
2	D	190	ALA	O-C-N	-6.74	114.98	122.12
2	D	513	VAL	N-CA-CB	6.73	121.96	111.99
1	A	379	SER	O-C-N	-6.73	114.00	122.27
1	A	686	GLY	N-CA-C	6.72	118.34	111.56
2	B	373	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	421	TRP	CA-C-N	6.71	127.43	119.98
1	A	421	TRP	C-N-CA	6.71	127.43	119.98
1	A	715	ALA	CA-C-N	6.71	129.02	120.56
1	A	715	ALA	C-N-CA	6.71	129.02	120.56
2	D	315	GLU	N-CA-C	6.71	119.43	111.71
1	C	634	PHE	N-CA-C	6.71	120.83	112.24
2	B	255	ALA	N-CA-C	-6.70	103.91	111.14
2	D	222	ARG	CA-C-N	6.69	129.92	120.28
2	D	222	ARG	C-N-CA	6.69	129.92	120.28
2	B	340	ILE	CA-C-N	6.69	129.13	120.44
2	B	340	ILE	C-N-CA	6.69	129.13	120.44
2	D	328	TRP	CA-C-N	6.68	129.91	120.28
2	D	328	TRP	C-N-CA	6.68	129.91	120.28
1	C	447	GLU	CA-C-N	6.68	129.12	120.44
1	C	447	GLU	C-N-CA	6.68	129.12	120.44
1	A	723	ARG	O-C-N	-6.67	115.20	122.07
1	A	188	LYS	CA-C-N	6.67	126.92	119.32
1	A	188	LYS	C-N-CA	6.67	126.92	119.32
2	B	339	ASN	CA-C-N	6.67	129.59	120.46
2	B	339	ASN	C-N-CA	6.67	129.59	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	PRO	N-CA-CB	6.66	109.24	103.31
1	C	496	LEU	CA-C-N	6.66	129.09	120.56
1	C	496	LEU	C-N-CA	6.66	129.09	120.56
1	A	181	THR	CA-C-N	6.66	129.21	120.28
1	A	181	THR	C-N-CA	6.66	129.21	120.28
1	A	252	ALA	N-CA-C	6.66	118.54	111.28
1	C	599	ARG	CD-NE-CZ	6.66	133.72	124.40
2	D	393	GLY	CA-C-N	6.65	130.42	120.31
2	D	393	GLY	C-N-CA	6.65	130.42	120.31
1	A	677	ARG	CA-C-N	6.65	126.35	119.64
1	A	677	ARG	C-N-CA	6.65	126.35	119.64
1	A	633	LEU	CA-C-O	6.64	129.58	121.94
2	B	309	GLU	CA-C-N	6.64	129.56	120.46
2	B	309	GLU	C-N-CA	6.64	129.56	120.46
1	C	444	MET	CA-C-N	6.64	129.18	120.28
1	C	444	MET	C-N-CA	6.64	129.18	120.28
1	A	183	GLU	O-C-N	-6.64	115.08	122.12
2	B	425	LYS	CA-C-N	6.63	135.20	121.94
2	B	425	LYS	C-N-CA	6.63	135.20	121.94
2	D	450	ALA	CA-C-N	6.63	129.16	120.28
2	D	450	ALA	C-N-CA	6.63	129.16	120.28
2	B	31	THR	CA-C-N	6.63	129.49	120.54
2	B	31	THR	C-N-CA	6.63	129.49	120.54
1	C	231	ASN	N-CA-C	6.62	122.85	114.31
1	A	335	SER	CA-C-N	6.61	130.87	121.42
1	A	335	SER	C-N-CA	6.61	130.87	121.42
2	B	218	GLY	CA-C-N	6.61	129.13	120.28
2	B	218	GLY	C-N-CA	6.61	129.13	120.28
2	B	420	PHE	CA-C-N	6.61	129.13	120.28
2	B	420	PHE	C-N-CA	6.61	129.13	120.28
1	A	30	ALA	O-C-N	-6.60	115.12	122.12
1	A	333	GLY	CA-C-O	6.60	127.66	120.66
1	A	449	ALA	CA-C-N	6.60	129.12	120.28
1	A	449	ALA	C-N-CA	6.60	129.12	120.28
2	B	88	PRO	N-CA-CB	6.60	109.48	103.34
2	B	141	ASP	CA-C-N	6.60	126.38	119.05
2	B	141	ASP	C-N-CA	6.60	126.38	119.05
2	B	348	PHE	CA-CB-CG	6.60	120.40	113.80
2	D	335	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	586	LEU	CA-C-N	6.59	129.79	120.42
1	C	586	LEU	C-N-CA	6.59	129.79	120.42
2	B	150	LEU	CA-C-N	6.59	129.43	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	150	LEU	C-N-CA	6.59	129.43	120.54
1	A	129	ASN	CA-C-O	6.58	124.53	119.46
1	C	367	SER	O-C-N	-6.58	115.59	123.03
1	A	211	ILE	CA-C-O	6.58	129.00	120.78
1	C	184	GLU	CA-C-N	6.58	133.39	122.54
1	C	184	GLU	C-N-CA	6.58	133.39	122.54
2	B	308	GLY	CA-C-N	6.57	128.99	120.44
2	B	308	GLY	C-N-CA	6.57	128.99	120.44
1	A	403	TRP	CA-C-N	6.57	130.45	121.05
1	A	403	TRP	C-N-CA	6.57	130.45	121.05
1	A	42	GLU	CA-C-N	6.57	131.94	122.35
1	A	42	GLU	C-N-CA	6.57	131.94	122.35
2	B	131	ARG	N-CA-C	6.56	120.68	111.30
1	C	146	ILE	O-C-N	-6.56	115.24	121.87
1	C	458	ASP	O-C-N	-6.56	115.31	122.07
1	A	576	ASN	N-CA-C	6.56	120.59	111.74
1	C	52	GLU	CA-C-N	6.55	131.66	120.72
1	C	52	GLU	C-N-CA	6.55	131.66	120.72
1	A	206	VAL	CA-CB-CG1	6.55	121.53	110.40
2	B	556	ALA	O-C-N	-6.55	115.32	122.07
2	B	190	ALA	CA-C-N	6.55	131.08	120.60
2	B	190	ALA	C-N-CA	6.55	131.08	120.60
1	C	449	ALA	CA-C-N	6.54	129.05	120.28
1	C	449	ALA	C-N-CA	6.54	129.05	120.28
2	D	48	PRO	CA-C-N	6.54	127.06	119.47
2	D	48	PRO	C-N-CA	6.54	127.06	119.47
2	B	610	GLU	CB-CG-CD	6.53	123.70	112.60
1	C	158	LEU	N-CA-C	6.52	120.84	113.01
2	D	339	ASN	CA-C-N	6.52	129.39	120.46
2	D	339	ASN	C-N-CA	6.52	129.39	120.46
2	B	200	ASP	CA-C-N	6.52	126.29	119.05
2	B	200	ASP	C-N-CA	6.52	126.29	119.05
1	C	488	VAL	N-CA-CB	6.52	118.18	110.55
2	D	479	PHE	CA-CB-CG	6.52	120.32	113.80
2	B	330	GLU	CB-CG-CD	6.52	123.68	112.60
1	C	158	LEU	CA-C-N	6.52	133.13	121.66
1	C	158	LEU	C-N-CA	6.52	133.13	121.66
2	D	408	LEU	CA-C-N	6.51	128.91	120.44
2	D	408	LEU	C-N-CA	6.51	128.91	120.44
1	C	158	LEU	O-C-N	-6.50	113.48	122.46
2	D	398	PRO	N-CA-CB	6.50	109.98	103.48
2	D	610	GLU	CA-C-N	6.50	129.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	610	GLU	C-N-CA	6.50	129.64	120.28
1	C	554	LYS	CA-C-N	6.50	130.01	122.35
1	C	554	LYS	C-N-CA	6.50	130.01	122.35
1	A	98	SER	CA-C-N	6.49	128.88	120.44
1	A	98	SER	C-N-CA	6.49	128.88	120.44
1	A	546	GLY	CA-C-N	6.49	128.98	120.28
1	A	546	GLY	C-N-CA	6.49	128.98	120.28
1	A	368	LEU	N-CA-C	6.49	119.17	111.71
2	B	273	ALA	CA-C-N	6.49	128.97	120.28
2	B	273	ALA	C-N-CA	6.49	128.97	120.28
2	B	147	PRO	CA-C-N	6.48	134.02	121.18
2	B	147	PRO	C-N-CA	6.48	134.02	121.18
1	C	152	LEU	O-C-N	-6.48	115.25	122.12
2	B	159	LEU	N-CA-C	6.48	119.16	111.71
1	A	388	LEU	O-C-N	-6.48	115.25	122.12
2	B	571	ALA	CA-C-N	6.48	129.25	120.38
2	B	571	ALA	C-N-CA	6.48	129.25	120.38
2	D	355	ALA	CA-C-N	6.48	129.49	120.29
2	D	355	ALA	C-N-CA	6.48	129.49	120.29
1	A	190	GLU	CA-C-N	6.47	134.10	122.06
1	A	190	GLU	C-N-CA	6.47	134.10	122.06
2	D	221	VAL	CA-C-N	6.47	128.96	120.28
2	D	221	VAL	C-N-CA	6.47	128.96	120.28
1	C	690	GLU	CA-C-N	6.47	130.95	120.60
1	C	690	GLU	C-N-CA	6.47	130.95	120.60
2	D	146	ALA	CA-C-N	6.47	126.39	119.28
2	D	146	ALA	C-N-CA	6.47	126.39	119.28
2	D	318	ARG	CD-NE-CZ	6.47	133.45	124.40
1	A	689	PRO	N-CA-CB	6.46	109.06	103.31
2	D	202	ILE	CA-C-N	6.46	127.16	119.98
2	D	202	ILE	C-N-CA	6.46	127.16	119.98
1	A	96	LYS	O-C-N	-6.46	115.41	122.07
2	B	191	LYS	CA-C-N	6.46	134.08	122.06
2	B	191	LYS	C-N-CA	6.46	134.08	122.06
1	A	507	LYS	CA-C-N	6.46	128.70	120.56
1	A	507	LYS	C-N-CA	6.46	128.70	120.56
2	B	362	PRO	N-CA-CB	6.46	108.97	103.35
2	B	225	ALA	O-C-N	-6.46	115.28	122.12
1	A	222	SER	O-C-N	-6.45	114.67	122.22
2	B	117	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	421	TRP	CA-C-N	6.45	127.10	119.94
1	C	421	TRP	C-N-CA	6.45	127.10	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	ALA	CA-C-N	6.44	128.82	120.44
1	C	95	ALA	C-N-CA	6.44	128.82	120.44
1	C	428	GLU	CA-C-N	6.44	130.10	120.31
1	C	428	GLU	C-N-CA	6.44	130.10	120.31
1	A	703	GLU	CA-CB-CG	6.44	126.97	114.10
2	D	455	ASN	CA-C-N	6.43	132.01	122.74
2	D	455	ASN	C-N-CA	6.43	132.01	122.74
1	A	314	GLN	CA-C-N	6.42	134.01	122.38
1	A	314	GLN	C-N-CA	6.42	134.01	122.38
1	A	638	GLU	O-C-N	-6.42	115.45	122.07
1	C	449	ALA	O-C-N	-6.42	115.31	122.12
2	B	600	LYS	O-C-N	-6.42	113.60	122.46
1	C	532	LEU	CA-C-N	6.42	129.21	120.54
1	C	532	LEU	C-N-CA	6.42	129.21	120.54
1	C	504	ASP	CA-C-N	6.42	125.64	118.97
1	C	504	ASP	C-N-CA	6.42	125.64	118.97
2	B	601	GLU	O-C-N	-6.41	114.38	122.27
1	A	712	PRO	CA-C-N	6.41	128.87	120.28
1	A	712	PRO	C-N-CA	6.41	128.87	120.28
1	C	262	ASP	CA-C-N	6.41	127.09	119.98
1	C	262	ASP	C-N-CA	6.41	127.09	119.98
1	C	298	VAL	CA-C-N	6.41	128.86	120.28
1	C	298	VAL	C-N-CA	6.41	128.86	120.28
2	B	146	ALA	CA-C-N	6.40	126.62	119.32
2	B	146	ALA	C-N-CA	6.40	126.62	119.32
1	A	282	PRO	O-C-N	-6.40	113.67	122.24
2	D	379	ALA	CA-C-O	-6.40	114.10	120.82
2	B	528	GLU	CA-C-N	6.39	128.13	120.14
2	B	528	GLU	C-N-CA	6.39	128.13	120.14
2	B	582	ALA	CA-C-N	6.39	128.75	120.44
2	B	582	ALA	C-N-CA	6.39	128.75	120.44
1	A	589	GLU	CA-C-N	6.39	128.75	120.44
1	A	589	GLU	C-N-CA	6.39	128.75	120.44
2	B	17	THR	N-CA-C	6.39	123.92	109.81
1	A	597	ARG	CA-C-O	6.38	127.21	120.64
1	C	636	THR	N-CA-C	-6.38	100.75	110.07
1	A	598	PRO	CA-C-O	-6.38	114.41	121.23
2	D	388	GLU	N-CA-C	6.38	121.14	113.23
2	B	257	ALA	CA-C-N	6.38	128.82	120.28
2	B	257	ALA	C-N-CA	6.38	128.82	120.28
1	A	438	GLU	O-C-N	-6.37	114.76	122.22
2	B	155	SER	CB-CA-C	-6.37	98.10	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ASN	O-C-N	-6.37	115.76	122.96
2	B	423	VAL	CA-C-N	6.37	128.72	120.44
2	B	423	VAL	C-N-CA	6.37	128.72	120.44
2	B	476	THR	CA-CB-CG2	6.36	121.31	110.50
1	A	386	THR	CA-C-O	-6.35	114.16	120.82
1	C	528	ASP	CA-C-N	6.34	133.00	122.54
1	C	528	ASP	C-N-CA	6.34	133.00	122.54
1	C	707	PRO	N-CA-CB	6.34	108.83	103.25
1	A	527	PRO	O-C-N	-6.33	113.75	122.24
2	B	42	VAL	O-C-N	-6.33	115.70	121.91
2	D	212	PRO	N-CA-CB	6.33	108.96	103.27
1	C	188	LYS	CA-C-N	6.32	126.53	119.32
1	C	188	LYS	C-N-CA	6.32	126.53	119.32
1	C	82	ARG	CD-NE-CZ	6.32	133.25	124.40
1	A	526	ASP	CA-C-O	6.32	126.28	120.09
2	B	461	THR	CA-C-O	6.32	128.13	120.92
1	C	146	ILE	CA-C-N	6.32	128.66	120.44
1	C	146	ILE	C-N-CA	6.32	128.66	120.44
2	B	235	THR	N-CA-CB	6.32	120.44	110.84
2	D	239	ASN	O-C-N	-6.31	114.50	122.27
2	B	78	PRO	O-C-N	-6.31	114.98	122.24
2	B	90	VAL	CA-CB-CG2	6.31	121.12	110.40
2	D	79	LYS	CA-C-N	6.30	133.87	121.58
2	D	79	LYS	C-N-CA	6.30	133.87	121.58
1	A	19	ALA	CA-C-N	6.30	132.88	122.73
1	A	19	ALA	C-N-CA	6.30	132.88	122.73
1	A	521	ASN	O-C-N	-6.30	115.73	121.34
1	C	61	LEU	N-CA-C	6.29	120.06	112.38
1	C	369	ASP	O-C-N	-6.29	114.32	122.37
1	A	232	MET	CA-CB-CG	6.29	126.68	114.10
2	D	297	LEU	CA-C-N	6.29	129.21	120.29
2	D	297	LEU	C-N-CA	6.29	129.21	120.29
2	D	340	ILE	O-C-N	-6.29	115.77	121.87
2	D	453	LEU	CA-C-N	6.29	129.21	120.29
2	D	453	LEU	C-N-CA	6.29	129.21	120.29
1	C	715	ALA	CA-C-N	6.28	128.48	120.56
1	C	715	ALA	C-N-CA	6.28	128.48	120.56
2	D	363	PHE	CA-CB-CG	6.28	120.08	113.80
2	D	381	ASN	CA-C-N	6.28	128.61	120.44
2	D	381	ASN	C-N-CA	6.28	128.61	120.44
2	D	79	LYS	O-C-N	-6.28	114.23	122.39
2	B	162	THR	N-CA-C	6.28	119.17	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ARG	CA-C-O	-6.27	114.23	120.82
2	B	425	LYS	O-C-N	-6.27	114.88	122.22
1	C	514	LYS	CA-C-N	6.27	128.58	120.56
1	C	514	LYS	C-N-CA	6.27	128.58	120.56
1	A	717	SER	CA-C-O	-6.26	113.78	120.42
2	B	529	GLY	CA-C-N	6.26	131.17	120.71
2	B	529	GLY	C-N-CA	6.26	131.17	120.71
1	C	674	LYS	O-C-N	-6.26	114.89	122.22
1	A	535	CYS	CA-C-N	6.26	128.45	120.56
1	A	535	CYS	C-N-CA	6.26	128.45	120.56
1	A	130	PRO	N-CA-CB	6.26	110.15	103.39
1	A	213	PRO	CA-C-N	6.25	125.99	119.05
1	A	213	PRO	C-N-CA	6.25	125.99	119.05
1	C	52	GLU	O-C-N	-6.25	114.12	122.43
2	D	601	GLU	O-C-N	-6.24	114.06	122.43
1	A	410	GLU	CA-C-N	6.24	128.55	120.44
1	A	410	GLU	C-N-CA	6.24	128.55	120.44
1	C	665	VAL	CA-C-N	6.23	125.97	119.05
1	C	665	VAL	C-N-CA	6.23	125.97	119.05
1	A	155	GLY	O-C-N	-6.23	115.68	122.41
1	A	23	ARG	NE-CZ-NH2	6.23	124.80	119.20
2	B	155	SER	N-CA-C	6.22	119.72	111.75
2	D	191	LYS	CA-C-N	6.22	132.61	121.66
2	D	191	LYS	C-N-CA	6.22	132.61	121.66
2	B	200	ASP	CA-CB-CG	6.22	118.82	112.60
2	D	239	ASN	CA-C-N	6.22	128.40	120.56
2	D	239	ASN	C-N-CA	6.22	128.40	120.56
2	D	256	LEU	CA-C-N	6.21	128.52	120.44
2	D	256	LEU	C-N-CA	6.21	128.52	120.44
1	C	190	GLU	O-C-N	-6.21	114.11	122.43
2	B	455	ASN	O-C-N	-6.21	114.58	122.34
2	B	494	SER	CA-C-N	6.21	128.60	120.28
2	B	494	SER	C-N-CA	6.21	128.60	120.28
1	C	351	GLU	CA-C-N	6.21	128.60	120.28
1	C	351	GLU	C-N-CA	6.21	128.60	120.28
2	D	536	HIS	CA-C-N	6.20	128.38	120.56
2	D	536	HIS	C-N-CA	6.20	128.38	120.56
1	C	44	ILE	N-CA-C	-6.20	100.97	107.60
2	B	268	GLU	O-C-N	-6.20	114.97	122.22
1	C	697	ARG	O-C-N	-6.20	115.55	122.12
2	B	311	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	281	ALA	CA-C-N	6.18	125.87	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ALA	C-N-CA	6.18	125.87	119.56
1	C	215	GLN	OE1-CD-NE2	-6.18	116.42	122.60
2	D	240	ILE	CA-C-N	6.18	129.06	120.29
2	D	240	ILE	C-N-CA	6.18	129.06	120.29
2	D	95	ARG	CG-CD-NE	6.18	125.59	112.00
2	D	86	GLY	CA-C-N	6.16	137.27	122.36
2	D	86	GLY	C-N-CA	6.16	137.27	122.36
1	C	586	LEU	O-C-N	-6.16	115.01	122.22
1	C	577	THR	CA-C-N	6.16	125.38	118.97
1	C	577	THR	C-N-CA	6.16	125.38	118.97
2	D	439	THR	CA-C-N	6.16	129.03	120.29
2	D	439	THR	C-N-CA	6.16	129.03	120.29
1	A	665	VAL	CA-C-N	6.15	125.88	119.05
1	A	665	VAL	C-N-CA	6.15	125.88	119.05
1	A	427	VAL	O-C-N	-6.15	115.88	121.91
2	D	483	PRO	N-CA-CB	6.15	108.79	103.31
1	C	204	PHE	CA-CB-CG	-6.15	107.65	113.80
2	B	608	GLU	CA-C-N	6.15	128.43	120.44
2	B	608	GLU	C-N-CA	6.15	128.43	120.44
2	B	78	PRO	CA-C-N	6.14	130.43	120.60
2	B	78	PRO	C-N-CA	6.14	130.43	120.60
1	C	281	ALA	N-CA-CB	6.14	119.95	110.43
2	D	158	LEU	CA-C-N	6.13	129.33	120.38
2	D	158	LEU	C-N-CA	6.13	129.33	120.38
1	A	365	THR	O-C-N	-6.13	116.06	123.29
1	C	262	ASP	N-CA-C	-6.12	104.52	111.07
1	C	497	VAL	N-CA-C	-6.12	104.77	110.53
1	C	690	GLU	O-C-N	-6.12	115.63	122.12
1	C	130	PRO	O-C-N	-6.12	115.20	122.24
2	B	375	PRO	CA-C-N	6.12	128.98	120.29
2	B	375	PRO	C-N-CA	6.12	128.98	120.29
1	A	343	ASN	O-C-N	-6.12	115.06	122.22
1	C	522	PRO	CB-CA-C	-6.11	103.58	111.46
1	A	726	LEU	CA-C-O	6.11	127.00	119.79
2	B	513	VAL	N-CA-CB	6.11	120.13	111.82
2	D	130	GLU	CA-C-N	6.11	133.21	121.54
2	D	130	GLU	C-N-CA	6.11	133.21	121.54
1	C	698	LYS	CA-C-N	6.11	130.92	120.72
1	C	698	LYS	C-N-CA	6.11	130.92	120.72
2	B	586	LYS	CA-C-N	6.10	129.58	120.31
2	B	586	LYS	C-N-CA	6.10	129.58	120.31
1	C	666	PRO	N-CA-CB	6.10	110.04	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	417	TRP	CA-C-N	6.09	128.36	120.44
2	D	417	TRP	C-N-CA	6.09	128.36	120.44
2	B	390	VAL	CA-C-O	6.09	126.25	119.42
2	D	503	ARG	CA-C-N	6.09	128.44	120.28
2	D	503	ARG	C-N-CA	6.09	128.44	120.28
2	B	422	GLU	CA-C-N	6.09	128.24	120.56
2	B	422	GLU	C-N-CA	6.09	128.24	120.56
2	D	117	ASP	CA-CB-CG	6.09	118.69	112.60
1	C	276	ASN	N-CA-C	-6.08	101.48	110.48
2	B	268	GLU	CA-C-N	6.08	134.47	122.31
2	B	268	GLU	C-N-CA	6.08	134.47	122.31
2	D	449	ARG	CA-C-N	6.08	128.34	120.44
2	D	449	ARG	C-N-CA	6.08	128.34	120.44
1	A	219	ARG	CA-C-N	6.08	128.22	120.56
1	A	219	ARG	C-N-CA	6.08	128.22	120.56
1	C	170	ALA	O-C-N	-6.08	111.81	121.53
1	A	673	ASP	O-C-N	-6.07	115.68	122.12
2	B	229	PRO	O-C-N	-6.07	112.03	122.17
2	D	420	PHE	O-C-N	-6.07	115.81	122.07
1	C	31	LYS	O-C-N	-6.07	115.12	122.22
1	C	636	THR	CA-C-N	6.07	125.78	119.05
1	C	636	THR	C-N-CA	6.07	125.78	119.05
1	C	381	ARG	O-C-N	-6.06	115.24	122.15
2	B	335	ASP	CA-C-N	6.06	125.68	119.56
2	B	335	ASP	C-N-CA	6.06	125.68	119.56
1	A	487	THR	N-CA-CB	6.06	119.63	110.30
1	C	129	ASN	CA-C-O	6.06	124.13	119.46
1	C	673	ASP	CA-C-N	6.06	129.00	120.28
1	C	673	ASP	C-N-CA	6.06	129.00	120.28
1	C	231	ASN	CA-C-O	6.05	125.49	118.77
1	A	466	GLY	CA-C-N	6.05	128.90	122.97
1	A	466	GLY	C-N-CA	6.05	128.90	122.97
1	C	121	THR	O-C-N	-6.05	115.84	122.07
2	B	35	TRP	CA-C-N	6.04	128.66	120.38
2	B	35	TRP	C-N-CA	6.04	128.66	120.38
2	B	283	ARG	N-CA-CB	6.03	120.48	110.47
2	D	34	GLN	O-C-N	-6.03	115.73	122.12
1	A	678	PRO	N-CA-CB	6.03	109.06	103.46
2	D	116	PRO	N-CA-CB	6.02	109.96	103.33
2	D	560	SER	O-C-N	-6.02	115.74	122.12
2	D	196	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	21	ALA	O-C-N	-6.01	115.88	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	298	ARG	CA-C-N	6.01	128.34	120.28
2	B	298	ARG	C-N-CA	6.01	128.34	120.28
1	C	320	PRO	N-CA-CB	6.01	109.88	103.39
1	C	64	TYR	N-CA-C	6.00	119.19	109.40
1	C	106	LEU	O-C-N	-6.00	115.31	122.15
1	C	514	LYS	O-C-N	-6.00	115.76	122.12
2	D	200	ASP	CA-C-N	6.00	125.71	119.05
2	D	200	ASP	C-N-CA	6.00	125.71	119.05
2	B	189	PRO	N-CA-CB	6.00	108.51	103.17
2	D	352	VAL	CA-C-N	5.99	134.56	121.19
2	D	352	VAL	C-N-CA	5.99	134.56	121.19
2	D	476	THR	CA-CB-CG2	5.99	120.68	110.50
1	A	158	LEU	CA-C-N	5.99	131.62	121.14
1	A	158	LEU	C-N-CA	5.99	131.62	121.14
1	C	233	PRO	N-CA-CB	5.99	109.47	103.48
1	A	381	ARG	O-C-N	-5.99	115.33	122.15
2	B	622	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	598	PRO	N-CA-CB	5.98	108.65	103.27
1	A	217	SER	CA-C-N	5.98	128.78	120.29
1	A	217	SER	C-N-CA	5.98	128.78	120.29
1	C	320	PRO	O-C-N	-5.98	114.50	122.22
2	D	242	HIS	O-C-N	-5.98	115.91	122.07
1	A	401	ASP	CA-C-N	5.98	125.86	119.28
1	A	401	ASP	C-N-CA	5.98	125.86	119.28
1	C	118	ASP	CA-CB-CG	5.97	118.58	112.60
1	C	222	SER	O-C-N	-5.97	115.23	122.22
1	C	387	GLN	CA-C-N	5.97	128.20	120.44
1	C	387	GLN	C-N-CA	5.97	128.20	120.44
1	A	475	GLU	CA-C-N	5.97	124.02	119.66
1	A	475	GLU	C-N-CA	5.97	124.02	119.66
2	B	488	LEU	N-CA-C	5.97	119.01	110.24
1	C	314	GLN	O-C-N	-5.97	114.63	122.39
2	B	218	GLY	O-C-N	-5.96	116.22	122.13
1	C	504	ASP	CA-C-O	5.96	123.73	119.32
2	D	28	PRO	N-CA-CB	5.96	108.33	103.32
1	C	590	PHE	O-C-N	-5.96	115.93	122.07
2	D	634	LEU	CA-C-N	5.96	131.74	121.07
2	D	634	LEU	C-N-CA	5.96	131.74	121.07
1	C	340	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	263	GLY	CA-C-N	5.95	128.62	120.46
1	A	263	GLY	C-N-CA	5.95	128.62	120.46
2	D	607	ALA	CA-C-N	5.95	128.18	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	607	ALA	C-N-CA	5.95	128.18	120.44
2	B	215	THR	N-CA-C	5.95	119.80	112.54
2	D	36	GLU	CA-C-O	-5.95	114.57	120.82
1	A	357	GLN	CA-C-N	5.95	135.51	121.82
1	A	357	GLN	C-N-CA	5.95	135.51	121.82
1	C	430	VAL	O-C-N	-5.95	115.13	122.57
2	D	267	VAL	O-C-N	-5.95	115.70	121.83
1	C	422	GLY	O-C-N	-5.95	116.47	122.18
2	D	363	PHE	CA-C-N	5.95	133.14	122.38
2	D	363	PHE	C-N-CA	5.95	133.14	122.38
2	B	251	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	633	LEU	O-C-N	-5.93	115.35	122.65
1	C	220	ILE	CA-C-N	5.93	128.04	120.56
1	C	220	ILE	C-N-CA	5.93	128.04	120.56
2	D	202	ILE	O-C-N	-5.93	115.73	121.90
2	B	457	LYS	O-C-N	-5.93	114.98	122.27
1	A	123	ARG	CA-C-N	5.93	131.86	120.66
1	A	123	ARG	C-N-CA	5.93	131.86	120.66
1	A	215	GLN	CA-C-N	5.93	125.63	119.05
1	A	215	GLN	C-N-CA	5.93	125.63	119.05
2	B	130	GLU	CA-C-N	5.93	133.27	123.25
2	B	130	GLU	C-N-CA	5.93	133.27	123.25
2	D	117	ASP	CA-C-O	5.93	128.99	120.51
1	A	468	ASN	OD1-CG-ND2	-5.92	116.68	122.60
2	B	483	PRO	N-CA-CB	5.92	108.58	103.31
1	A	693	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	676	GLY	O-C-N	-5.92	114.98	122.32
2	D	189	PRO	N-CA-CB	5.92	108.60	103.27
1	A	707	PRO	N-CA-CB	5.92	108.46	103.25
1	C	211	ILE	N-CA-CB	5.92	120.99	111.23
1	C	683	THR	N-CA-CB	5.91	121.18	111.08
1	A	282	PRO	CA-C-N	5.91	131.81	122.60
1	A	282	PRO	C-N-CA	5.91	131.81	122.60
2	D	159	LEU	O-C-N	-5.91	115.47	122.20
1	A	149	MET	CA-C-N	5.90	128.47	120.44
1	A	149	MET	C-N-CA	5.90	128.47	120.44
1	C	424	ILE	CA-C-N	5.90	128.11	120.44
1	C	424	ILE	C-N-CA	5.90	128.11	120.44
2	D	586	LYS	CA-C-N	5.90	130.57	120.72
2	D	586	LYS	C-N-CA	5.90	130.57	120.72
1	A	107	ALA	CA-C-N	5.90	132.70	122.56
1	A	107	ALA	C-N-CA	5.90	132.70	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	LEU	CA-C-N	5.89	128.18	120.28
1	A	672	LEU	C-N-CA	5.89	128.18	120.28
2	B	456	ARG	CA-C-N	5.89	129.27	120.31
2	B	456	ARG	C-N-CA	5.89	129.27	120.31
1	A	527	PRO	N-CA-CB	5.89	109.37	103.48
2	D	553	ILE	CA-C-N	5.89	127.98	120.56
2	D	553	ILE	C-N-CA	5.89	127.98	120.56
2	B	521	ARG	O-C-N	-5.88	115.89	122.12
1	C	76	ALA	N-CA-C	5.88	117.69	111.28
2	D	365	GLN	O-C-N	-5.88	114.69	122.33
1	A	675	LEU	O-C-N	-5.88	114.81	122.39
1	C	282	PRO	N-CA-CB	5.87	109.35	103.48
2	D	147	PRO	CA-C-N	5.87	133.03	121.58
2	D	147	PRO	C-N-CA	5.87	133.03	121.58
2	B	128	GLY	O-C-N	-5.87	116.55	122.18
2	D	172	GLN	CA-C-N	5.87	126.34	119.94
2	D	172	GLN	C-N-CA	5.87	126.34	119.94
2	B	304	TRP	CA-C-N	5.87	128.62	120.29
2	B	304	TRP	C-N-CA	5.87	128.62	120.29
1	A	597	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	C	23	ARG	O-C-N	-5.86	115.91	122.12
2	B	228	SER	CA-C-N	5.86	126.62	120.12
2	B	228	SER	C-N-CA	5.86	126.62	120.12
2	B	338	VAL	CA-C-N	5.86	129.97	120.60
2	B	338	VAL	C-N-CA	5.86	129.97	120.60
2	B	190	ALA	O-C-N	-5.85	115.39	122.11
1	C	219	ARG	CA-C-N	5.85	127.93	120.56
1	C	219	ARG	C-N-CA	5.85	127.93	120.56
2	D	292	LEU	CA-C-O	-5.84	114.23	120.42
2	B	310	VAL	O-C-N	-5.84	116.21	121.87
2	B	307	ILE	N-CA-C	-5.83	104.83	110.72
2	B	480	PRO	N-CA-CB	5.83	108.75	103.33
1	C	628	VAL	N-CA-C	5.83	116.33	108.17
2	B	299	ALA	CA-C-N	5.83	128.02	120.44
2	B	299	ALA	C-N-CA	5.83	128.02	120.44
2	B	610	GLU	O-C-N	-5.83	115.40	122.22
2	B	365	GLN	CA-C-N	5.83	131.92	121.66
2	B	365	GLN	C-N-CA	5.83	131.92	121.66
2	D	190	ALA	CA-C-N	5.83	132.72	121.18
2	D	190	ALA	C-N-CA	5.83	132.72	121.18
2	B	297	LEU	CA-C-N	5.83	128.56	120.29
2	B	297	LEU	C-N-CA	5.83	128.56	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	627	ASP	N-CA-C	-5.83	98.24	108.20
1	C	633	LEU	CA-C-N	5.83	130.85	122.40
1	C	633	LEU	C-N-CA	5.83	130.85	122.40
2	B	449	ARG	CA-C-N	5.82	128.09	120.28
2	B	449	ARG	C-N-CA	5.82	128.09	120.28
2	B	607	ALA	CA-C-N	5.82	128.08	120.28
2	B	607	ALA	C-N-CA	5.82	128.08	120.28
2	B	543	PRO	N-CA-CB	5.82	108.75	103.34
2	D	353	GLY	CA-C-N	5.82	130.34	120.91
2	D	353	GLY	C-N-CA	5.82	130.34	120.91
1	C	385	ASN	O-C-N	-5.82	115.42	122.22
1	A	591	GLU	O-C-N	-5.81	116.04	122.09
2	D	315	GLU	CA-C-N	5.81	131.31	121.14
2	D	315	GLU	C-N-CA	5.81	131.31	121.14
1	A	53	ASP	O-C-N	-5.81	115.42	122.22
1	A	208	ASN	N-CA-C	5.81	119.68	112.24
1	A	392	GLN	N-CA-C	5.81	120.53	112.45
1	A	215	GLN	N-CA-CB	5.80	118.47	110.11
1	A	269	ALA	CA-C-N	5.80	126.38	119.94
1	A	269	ALA	C-N-CA	5.80	126.38	119.94
2	D	432	ALA	CA-C-N	5.80	129.84	120.55
2	D	432	ALA	C-N-CA	5.80	129.84	120.55
2	B	263	VAL	N-CA-C	-5.80	105.08	110.53
2	D	390	VAL	O-C-N	-5.80	115.33	122.18
1	A	477	PRO	N-CA-CB	5.80	108.47	103.31
2	B	270	GLY	N-CA-C	5.80	123.61	115.43
1	A	253	ASP	CA-C-N	5.80	129.82	120.55
1	A	253	ASP	C-N-CA	5.80	129.82	120.55
1	A	447	GLU	CA-C-N	5.80	127.97	120.44
1	A	447	GLU	C-N-CA	5.80	127.97	120.44
2	D	505	THR	CA-C-N	5.80	130.40	120.72
2	D	505	THR	C-N-CA	5.80	130.40	120.72
1	A	727	ASP	O-C-N	-5.79	115.23	122.35
1	C	368	LEU	CA-C-N	5.79	132.26	122.65
1	C	368	LEU	C-N-CA	5.79	132.26	122.65
2	D	339	ASN	O-C-N	-5.79	114.86	122.39
1	A	153	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	167	MET	O-C-N	-5.78	116.33	123.44
1	A	647	ALA	O-C-N	-5.78	113.99	122.43
1	C	477	PRO	N-CA-CB	5.78	108.38	103.35
2	D	215	THR	N-CA-C	5.78	119.59	112.54
1	C	343	ASN	CA-C-N	5.77	128.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	343	ASN	C-N-CA	5.77	128.59	120.28
2	B	212	PRO	N-CA-CB	5.77	108.30	103.17
1	C	441	ILE	CA-C-N	5.77	125.24	119.24
1	C	441	ILE	C-N-CA	5.77	125.24	119.24
2	D	571	ALA	CA-C-N	5.77	128.32	120.54
2	D	571	ALA	C-N-CA	5.77	128.32	120.54
2	D	243	ASN	O-C-N	-5.76	115.48	122.22
1	A	554	LYS	CA-CB-CG	5.76	125.61	114.10
2	B	380	ARG	CA-C-N	5.76	129.06	120.31
2	B	380	ARG	C-N-CA	5.76	129.06	120.31
1	C	652	VAL	N-CA-CB	5.76	118.60	111.41
2	D	128	GLY	CA-C-N	5.76	128.57	120.28
2	D	128	GLY	C-N-CA	5.76	128.57	120.28
2	D	537	ILE	O-C-N	-5.76	116.27	121.91
1	A	93	SER	N-CA-CB	-5.75	100.77	110.49
1	C	435	LYS	O-C-N	-5.75	116.02	122.12
1	C	129	ASN	N-CA-C	-5.75	100.91	109.42
2	D	431	LYS	CA-C-N	5.74	127.97	120.28
2	D	431	LYS	C-N-CA	5.74	127.97	120.28
1	C	443	LYS	CA-C-N	5.74	127.97	120.28
1	C	443	LYS	C-N-CA	5.74	127.97	120.28
1	C	93	SER	N-CA-CB	-5.74	100.80	110.49
2	D	362	PRO	N-CA-CB	5.74	108.34	103.35
1	A	320	PRO	N-CA-CB	5.73	109.58	103.39
2	B	238	ALA	O-C-N	-5.73	114.55	122.46
1	C	546	GLY	CA-C-N	5.73	127.89	120.44
1	C	546	GLY	C-N-CA	5.73	127.89	120.44
2	B	558	LYS	CA-C-N	5.72	129.01	120.31
2	B	558	LYS	C-N-CA	5.72	129.01	120.31
1	C	499	LEU	CA-C-N	5.72	127.95	120.28
1	C	499	LEU	C-N-CA	5.72	127.95	120.28
1	A	677	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	C	404	SER	CA-C-O	5.72	126.97	120.80
2	B	148	GLU	CA-C-N	5.71	131.97	122.54
2	B	148	GLU	C-N-CA	5.71	131.97	122.54
2	D	220	TRP	CA-C-N	5.71	127.76	120.56
2	D	220	TRP	C-N-CA	5.71	127.76	120.56
1	A	441	ILE	CA-C-N	5.71	125.18	119.24
1	A	441	ILE	C-N-CA	5.71	125.18	119.24
2	D	457	LYS	CA-C-N	5.71	131.53	123.30
2	D	457	LYS	C-N-CA	5.71	131.53	123.30
1	A	504	ASP	CA-C-N	5.71	125.39	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ASP	C-N-CA	5.71	125.39	119.05
1	C	281	ALA	CA-C-N	5.71	125.38	119.56
1	C	281	ALA	C-N-CA	5.71	125.38	119.56
2	B	590	ALA	CA-C-O	5.71	126.96	120.80
1	C	438	GLU	CA-C-N	5.71	132.67	122.06
1	C	438	GLU	C-N-CA	5.71	132.67	122.06
2	B	28	PRO	N-CA-CB	5.70	108.31	103.35
2	B	335	ASP	CA-CB-CG	5.70	118.30	112.60
2	B	610	GLU	CA-C-N	5.70	128.49	120.28
2	B	610	GLU	C-N-CA	5.70	128.49	120.28
1	C	150	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	B	86	GLY	N-CA-C	-5.70	103.49	112.61
2	B	599	PHE	O-C-N	-5.70	115.55	122.22
1	A	412	LEU	CA-C-N	5.70	127.84	120.44
1	A	412	LEU	C-N-CA	5.70	127.84	120.44
2	B	136	LEU	N-CA-C	5.70	118.76	109.59
2	B	315	GLU	N-CA-C	5.70	119.04	111.75
2	D	444	ALA	CA-C-N	5.69	127.84	120.44
2	D	444	ALA	C-N-CA	5.69	127.84	120.44
2	B	629	SER	CA-C-N	5.69	127.84	120.44
2	B	629	SER	C-N-CA	5.69	127.84	120.44
1	A	549	SER	CA-C-N	5.69	127.91	120.28
1	A	549	SER	C-N-CA	5.69	127.91	120.28
2	B	116	PRO	N-CA-CB	5.69	109.59	103.33
1	A	330	GLN	CA-C-O	-5.69	114.12	120.66
2	D	78	PRO	N-CA-CB	5.68	109.74	103.26
1	C	488	VAL	CB-CA-C	-5.68	104.70	111.97
1	A	383	ALA	CA-C-N	5.68	128.35	120.29
1	A	383	ALA	C-N-CA	5.68	128.35	120.29
1	A	627	ASP	N-CA-C	-5.68	99.93	108.96
2	B	142	PRO	O-C-N	-5.67	115.42	122.23
1	C	26	GLU	CA-C-N	5.67	128.34	120.29
1	C	26	GLU	C-N-CA	5.67	128.34	120.29
1	A	120	PRO	O-C-N	-5.67	116.06	122.18
1	C	377	ASP	CA-C-N	5.67	128.15	120.44
1	C	377	ASP	C-N-CA	5.67	128.15	120.44
1	A	578	PRO	N-CA-CB	5.67	109.56	103.33
1	A	244	HIS	CA-C-N	5.67	127.80	120.44
1	A	244	HIS	C-N-CA	5.67	127.80	120.44
1	C	727	ASP	O-C-N	-5.66	115.12	122.37
1	A	462	GLN	CA-C-O	5.66	124.80	119.59
1	C	539	GLY	O-C-N	-5.66	116.76	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	88	PRO	N-CA-CB	5.66	108.59	103.33
2	D	56	ALA	O-C-N	-5.66	116.21	122.09
1	A	445	ARG	CA-C-N	5.65	128.44	120.42
1	A	445	ARG	C-N-CA	5.65	128.44	120.42
2	D	104	MET	N-CA-C	5.65	117.44	111.28
1	A	442	PRO	CA-C-N	5.65	127.85	120.28
1	A	442	PRO	C-N-CA	5.65	127.85	120.28
1	A	711	ILE	CA-C-N	5.65	125.32	119.05
1	A	711	ILE	C-N-CA	5.65	125.32	119.05
1	C	319	ASN	CA-C-O	5.65	125.65	119.32
2	D	104	MET	CA-C-O	-5.65	114.57	120.55
1	A	714	SER	N-CA-C	-5.64	105.21	111.36
2	D	305	ALA	CA-C-N	5.64	128.31	120.29
2	D	305	ALA	C-N-CA	5.64	128.31	120.29
1	A	379	SER	CA-C-N	5.64	128.89	120.31
1	A	379	SER	C-N-CA	5.64	128.89	120.31
1	C	688	ILE	CA-C-O	5.64	127.51	119.95
2	B	533	PRO	N-CA-CB	5.64	109.69	103.26
1	C	298	VAL	O-C-N	-5.64	116.38	121.91
1	A	623	ASP	O-C-N	-5.63	115.07	122.39
2	B	416	ALA	CA-C-N	5.63	128.29	120.29
2	B	416	ALA	C-N-CA	5.63	128.29	120.29
2	D	251	GLU	CB-CG-CD	5.63	122.18	112.60
2	B	617	LEU	N-CA-C	-5.63	99.72	108.90
2	B	104	MET	CA-C-O	-5.63	114.91	120.82
2	B	363	PHE	N-CA-C	5.63	119.41	112.54
1	A	358	GLY	CA-C-N	5.62	130.16	122.34
1	A	358	GLY	C-N-CA	5.62	130.16	122.34
1	A	698	LYS	O-C-N	-5.62	115.35	122.27
2	B	504	SER	CA-C-N	5.62	130.98	121.14
2	B	504	SER	C-N-CA	5.62	130.98	121.14
2	B	192	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	500	ARG	CA-C-N	5.62	128.27	120.29
1	C	500	ARG	C-N-CA	5.62	128.27	120.29
2	D	510	ARG	CA-C-N	5.62	125.57	119.78
2	D	510	ARG	C-N-CA	5.62	125.57	119.78
1	C	17	VAL	N-CA-C	-5.62	101.48	107.77
2	B	338	VAL	O-C-N	-5.61	116.20	121.87
2	D	254	TRP	CA-C-N	5.61	128.07	120.44
2	D	254	TRP	C-N-CA	5.61	128.07	120.44
1	A	428	GLU	O-C-N	-5.61	116.18	122.12
2	D	327	SER	N-CA-C	5.61	118.31	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	196	ASN	OD1-CG-ND2	-5.60	117.00	122.60
2	B	101	ASN	OD1-CG-ND2	-5.60	117.00	122.60
2	B	172	GLN	N-CA-C	5.59	117.46	111.36
2	B	182	VAL	CA-C-N	5.59	128.23	120.29
2	B	182	VAL	C-N-CA	5.59	128.23	120.29
2	B	322	GLN	CA-C-O	5.59	126.40	120.36
2	B	114	GLU	CA-CB-CG	5.59	125.29	114.10
1	C	711	ILE	CA-C-N	5.59	125.43	119.28
1	C	711	ILE	C-N-CA	5.59	125.43	119.28
2	D	504	SER	CA-C-N	5.59	130.06	120.72
2	D	504	SER	C-N-CA	5.59	130.06	120.72
2	D	283	ARG	N-CA-CB	5.59	119.75	110.47
1	A	539	GLY	CA-C-N	5.59	127.77	120.28
1	A	539	GLY	C-N-CA	5.59	127.77	120.28
1	C	553	GLU	O-C-N	-5.58	115.69	122.22
2	D	502	ASP	N-CA-CB	5.58	118.43	110.16
1	A	669	ARG	CA-C-N	5.58	127.76	120.28
1	A	669	ARG	C-N-CA	5.58	127.76	120.28
1	A	321	LYS	O-C-N	-5.58	115.69	122.22
1	C	72	HIS	CB-CG-ND1	5.58	131.07	122.70
1	C	28	LEU	CA-C-N	5.58	128.02	120.44
1	C	28	LEU	C-N-CA	5.58	128.02	120.44
2	D	367	LEU	CB-CA-C	-5.58	100.36	109.56
2	D	480	PRO	N-CA-CB	5.58	108.20	103.35
1	C	216	PRO	O-C-N	-5.57	115.54	122.23
1	C	358	GLY	N-CA-C	-5.57	106.97	115.66
1	A	677	ARG	CA-CB-CG	5.57	125.24	114.10
1	A	188	LYS	CA-C-O	5.57	127.11	120.88
1	A	463	PRO	N-CA-CB	5.56	108.26	103.31
2	D	183	TYR	CA-C-N	5.56	128.19	120.29
2	D	183	TYR	C-N-CA	5.56	128.19	120.29
1	A	632	PRO	N-CA-CB	5.56	109.22	103.38
2	B	36	GLU	CA-C-N	5.56	128.76	120.31
2	B	36	GLU	C-N-CA	5.56	128.76	120.31
1	C	344	ASN	CA-C-N	5.56	127.56	120.56
1	C	344	ASN	C-N-CA	5.56	127.56	120.56
2	B	250	ALA	O-C-N	-5.55	116.23	122.12
1	A	176	ALA	CB-CA-C	-5.55	102.17	110.88
1	A	89	TYR	CA-CB-CG	5.55	123.89	113.90
2	D	147	PRO	N-CA-CB	5.55	109.38	103.39
1	A	444	MET	CA-C-N	5.55	128.17	120.29
1	A	444	MET	C-N-CA	5.55	128.17	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	VAL	N-CA-CB	5.55	118.86	112.15
1	C	578	PRO	N-CA-CB	5.55	109.17	103.23
1	A	314	GLN	O-C-N	-5.54	115.73	122.22
2	B	201	PRO	N-CA-CB	5.54	109.43	103.33
1	C	73	GLY	CA-C-O	5.54	129.45	121.52
2	B	393	GLY	CA-C-N	5.54	128.73	120.31
2	B	393	GLY	C-N-CA	5.54	128.73	120.31
1	C	120	PRO	O-C-N	-5.54	115.91	122.17
1	C	342	TYR	CA-C-N	5.54	128.26	120.28
1	C	342	TYR	C-N-CA	5.54	128.26	120.28
2	D	268	GLU	O-C-N	-5.54	115.74	122.22
1	A	613	GLY	O-C-N	-5.54	116.86	122.18
2	D	137	LEU	N-CA-CB	5.54	119.26	110.84
2	B	132	GLY	N-CA-C	5.54	122.11	114.92
1	C	127	SER	O-C-N	-5.53	115.20	122.39
1	C	650	HIS	CA-CB-CG	-5.53	108.27	113.80
2	B	398	PRO	N-CA-CB	5.53	109.36	103.39
2	B	406	GLU	CB-CG-CD	5.53	122.00	112.60
1	A	394	SER	CA-C-N	5.53	130.96	121.07
1	A	394	SER	C-N-CA	5.53	130.96	121.07
1	A	500	ARG	CD-NE-CZ	5.53	132.13	124.40
1	A	524	ASP	CA-C-N	5.53	132.38	122.38
1	A	524	ASP	C-N-CA	5.53	132.38	122.38
2	D	467	PRO	CA-C-O	-5.53	115.27	122.12
1	C	376	THR	N-CA-C	-5.52	101.83	110.17
1	C	647	ALA	O-C-N	-5.52	114.57	122.41
1	A	70	PHE	N-CA-C	5.52	119.04	111.54
1	A	130	PRO	CA-C-N	5.52	129.93	120.72
1	A	130	PRO	C-N-CA	5.52	129.93	120.72
2	B	340	ILE	O-C-N	-5.51	116.52	121.87
2	B	503	ARG	O-C-N	-5.51	116.39	122.07
2	D	86	GLY	N-CA-C	-5.51	103.79	112.61
1	A	498	LYS	O-C-N	-5.51	116.28	122.12
1	A	554	LYS	CA-C-O	-5.50	114.68	120.63
2	D	55	PHE	CA-CB-CG	-5.50	108.30	113.80
2	D	416	ALA	O-C-N	-5.50	115.88	122.15
2	D	352	VAL	CA-C-O	5.50	126.41	120.47
2	B	305	ALA	N-CA-CB	5.50	118.30	110.16
1	C	155	GLY	CA-C-N	5.50	132.30	122.13
1	C	155	GLY	C-N-CA	5.50	132.30	122.13
1	A	136	VAL	O-C-N	-5.50	116.78	122.66
1	A	218	MET	O-C-N	-5.50	115.88	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	VAL	O-C-N	-5.50	116.52	121.91
2	D	230	ASP	CA-C-N	5.50	128.67	120.87
2	D	230	ASP	C-N-CA	5.50	128.67	120.87
1	A	634	PHE	N-CA-C	5.49	119.27	112.24
1	A	205	MET	O-C-N	-5.49	116.16	122.09
1	C	712	PRO	N-CA-CB	5.49	109.32	103.39
2	D	217	LEU	CA-C-N	5.49	126.07	119.98
2	D	217	LEU	C-N-CA	5.49	126.07	119.98
2	B	64	VAL	CA-C-O	5.49	127.20	120.84
2	B	264	ARG	NE-CZ-NH1	-5.49	116.01	121.50
2	B	455	ASN	CA-C-O	5.49	125.77	119.35
2	B	478	PRO	N-CA-CB	5.49	108.08	103.25
2	B	397	ASP	CA-C-O	5.48	127.67	120.16
1	A	290	ILE	CB-CA-C	-5.48	105.00	111.09
2	D	155	SER	N-CA-C	5.48	118.02	111.71
1	A	109	GLY	N-CA-C	5.48	122.89	115.00
2	D	257	ALA	CA-C-N	5.48	127.62	120.28
2	D	257	ALA	C-N-CA	5.48	127.62	120.28
1	A	628	VAL	N-CA-C	5.47	115.77	108.11
2	B	25	GLY	CA-C-N	5.47	132.25	121.58
2	B	25	GLY	C-N-CA	5.47	132.25	121.58
2	D	158	LEU	CA-C-O	5.47	126.61	120.92
1	A	80	ALA	CA-C-N	5.47	132.88	122.60
1	A	80	ALA	C-N-CA	5.47	132.88	122.60
2	B	240	ILE	N-CA-C	-5.47	105.17	110.42
1	C	621	TYR	CA-C-O	-5.47	114.62	120.42
1	A	319	ASN	CA-C-O	5.47	125.44	119.32
1	C	176	ALA	CB-CA-C	-5.47	101.72	110.79
2	D	306	ARG	CA-C-N	5.47	127.95	120.46
2	D	306	ARG	C-N-CA	5.47	127.95	120.46
2	B	512	LYS	CA-CB-CG	5.46	125.03	114.10
1	A	24	ARG	O-C-N	-5.46	115.92	122.15
1	A	115	VAL	N-CA-C	5.46	116.17	108.36
1	C	152	LEU	CA-C-N	5.46	131.38	122.65
1	C	152	LEU	C-N-CA	5.46	131.38	122.65
1	C	333	GLY	CA-C-O	5.46	126.44	120.66
1	C	622	ALA	O-C-N	-5.46	116.34	122.12
1	A	622	ALA	N-CA-C	-5.45	105.23	111.07
1	C	427	VAL	CA-C-N	5.45	127.58	120.28
1	C	427	VAL	C-N-CA	5.45	127.58	120.28
2	D	282	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	146	ILE	CA-C-N	5.45	127.89	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ILE	C-N-CA	5.45	127.89	120.54
1	A	688	ILE	CA-C-O	5.45	127.25	119.95
2	B	421	GLN	CA-C-N	5.45	128.03	120.29
2	B	421	GLN	C-N-CA	5.45	128.03	120.29
1	C	328	HIS	N-CA-C	-5.45	101.40	110.17
1	A	683	THR	N-CA-C	-5.45	101.01	109.72
2	B	277	PHE	O-C-N	-5.45	116.46	122.07
1	A	129	ASN	N-CA-C	-5.44	101.36	109.42
1	C	101	PHE	O-C-N	-5.44	115.94	122.15
1	C	357	GLN	O-C-N	-5.44	114.95	122.46
1	C	18	PRO	N-CA-CB	5.44	108.50	103.39
2	B	365	GLN	O-C-N	-5.44	115.26	122.33
1	C	42	GLU	CA-C-N	5.44	130.29	122.35
1	C	42	GLU	C-N-CA	5.44	130.29	122.35
1	A	551	ALA	CA-C-N	5.43	128.01	120.29
1	A	551	ALA	C-N-CA	5.43	128.01	120.29
1	A	18	PRO	CA-C-N	5.43	128.10	120.28
1	A	18	PRO	C-N-CA	5.43	128.10	120.28
2	D	20	THR	N-CA-CB	5.43	119.62	110.77
2	B	243	ASN	O-C-N	-5.43	115.87	122.22
2	D	524	PHE	CA-C-N	5.43	126.12	119.99
2	D	524	PHE	C-N-CA	5.43	126.12	119.99
1	C	643	GLN	O-C-N	-5.43	116.37	122.12
1	A	190	GLU	O-C-N	-5.42	115.16	122.43
1	A	429	LYS	O-C-N	-5.42	116.38	122.12
1	A	206	VAL	CB-CA-C	-5.42	102.41	111.29
2	B	206	ALA	CA-C-N	5.41	127.97	120.29
2	B	206	ALA	C-N-CA	5.41	127.97	120.29
1	C	200	ILE	CA-C-O	-5.41	114.41	120.25
1	A	143	ILE	N-CA-CB	5.40	118.67	111.64
1	C	103	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	122	HIS	CB-CA-C	-5.40	101.50	110.68
2	D	57	GLU	CA-C-N	5.40	127.46	120.44
2	D	57	GLU	C-N-CA	5.40	127.46	120.44
2	D	273	ALA	CA-C-N	5.40	127.46	120.44
2	D	273	ALA	C-N-CA	5.40	127.46	120.44
2	D	48	PRO	N-CA-CB	5.40	108.32	103.08
2	B	239	ASN	O-C-N	-5.40	115.90	122.22
1	C	689	PRO	O-C-N	-5.40	116.32	123.01
2	D	225	ALA	CA-C-N	5.40	129.24	120.60
2	D	225	ALA	C-N-CA	5.40	129.24	120.60
2	D	300	LEU	CA-C-N	5.40	127.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	LEU	C-N-CA	5.40	127.51	120.28
1	C	290	ILE	CB-CA-C	-5.39	105.10	111.09
2	B	230	ASP	CA-C-N	5.39	128.50	120.95
2	B	230	ASP	C-N-CA	5.39	128.50	120.95
1	C	308	TRP	O-C-N	-5.39	116.00	122.15
1	A	27	GLU	N-CA-C	-5.39	105.49	111.36
2	B	147	PRO	N-CA-CB	5.39	109.40	103.26
2	D	556	ALA	N-CA-C	-5.39	105.31	111.07
2	D	504	SER	N-CA-C	5.38	117.15	111.28
2	D	606	ALA	CA-C-N	5.38	127.81	120.54
2	D	606	ALA	C-N-CA	5.38	127.81	120.54
1	C	6	ARG	N-CA-C	-5.38	100.13	108.90
1	A	711	ILE	O-C-N	-5.38	114.96	121.10
2	B	631	LEU	CA-C-N	5.38	127.44	120.44
2	B	631	LEU	C-N-CA	5.38	127.44	120.44
1	C	507	LYS	CA-C-N	5.38	128.06	120.42
1	C	507	LYS	C-N-CA	5.38	128.06	120.42
2	B	490	TRP	O-C-N	-5.38	116.92	123.27
2	B	542	THR	CA-CB-CG2	5.38	119.64	110.50
1	C	79	TYR	O-C-N	-5.38	115.04	122.46
2	D	632	ASP	CA-C-N	5.38	127.83	120.46
2	D	632	ASP	C-N-CA	5.38	127.83	120.46
1	A	422	GLY	O-C-N	-5.37	117.03	122.19
1	C	224	ILE	N-CA-C	-5.37	105.30	110.72
1	C	218	MET	O-C-N	-5.37	116.43	122.12
1	C	676	GLY	O-C-N	-5.37	116.05	122.33
2	B	150	LEU	O-C-N	-5.36	116.55	122.07
1	C	206	VAL	N-CA-C	5.36	120.49	109.34
1	C	263	GLY	O-C-N	-5.36	117.04	122.19
2	B	159	LEU	CA-C-N	5.36	129.68	120.72
2	B	159	LEU	C-N-CA	5.36	129.68	120.72
2	D	201	PRO	N-CA-CB	5.36	109.22	103.33
2	B	322	GLN	N-CA-C	5.36	117.63	108.90
1	C	442	PRO	O-C-N	-5.36	116.39	122.18
2	D	189	PRO	CA-C-N	5.36	127.72	120.38
2	D	189	PRO	C-N-CA	5.36	127.72	120.38
2	B	336	PRO	O-C-N	-5.35	115.02	122.30
1	C	189	PRO	O-C-N	-5.35	116.08	122.24
1	A	189	PRO	CA-C-N	5.35	129.66	120.72
1	A	189	PRO	C-N-CA	5.35	129.66	120.72
2	B	369	LEU	CA-C-O	5.35	125.69	120.23
1	C	546	GLY	O-C-N	-5.35	117.05	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	ARG	CA-C-N	5.35	127.39	120.44
2	B	122	ARG	C-N-CA	5.35	127.39	120.44
1	C	53	ASP	CA-C-N	5.35	129.07	120.30
1	C	53	ASP	C-N-CA	5.35	129.07	120.30
1	A	32	ALA	CA-C-N	5.34	128.85	121.26
1	A	32	ALA	C-N-CA	5.34	128.85	121.26
1	C	175	LEU	CA-C-N	5.34	127.44	120.28
1	C	175	LEU	C-N-CA	5.34	127.44	120.28
2	B	67	VAL	CA-C-N	5.34	131.05	122.83
2	B	67	VAL	C-N-CA	5.34	131.05	122.83
2	D	101	ASN	OD1-CG-ND2	-5.34	117.26	122.60
2	D	533	PRO	N-CA-CB	5.34	109.20	103.33
1	A	652	VAL	N-CA-CB	5.34	118.08	111.41
2	B	128	GLY	CA-C-N	5.34	127.96	120.28
2	B	128	GLY	C-N-CA	5.34	127.96	120.28
2	D	239	ASN	OD1-CG-ND2	5.34	127.94	122.60
2	B	349	SER	O-C-N	-5.33	116.47	122.12
2	D	298	ARG	CA-C-N	5.33	127.42	120.28
2	D	298	ARG	C-N-CA	5.33	127.42	120.28
2	D	308	GLY	CA-C-N	5.33	127.37	120.44
2	D	308	GLY	C-N-CA	5.33	127.37	120.44
1	C	206	VAL	CA-CB-CG1	5.33	119.46	110.40
1	C	222	SER	CA-C-N	5.33	128.41	120.31
1	C	222	SER	C-N-CA	5.33	128.41	120.31
1	C	295	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	458	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	703	GLU	CA-CB-CG	5.32	124.75	114.10
1	C	256	MET	CB-CA-C	-5.32	102.52	110.88
1	C	632	PRO	N-CA-CB	5.32	108.97	103.38
2	D	34	GLN	CA-C-N	5.32	127.84	120.29
2	D	34	GLN	C-N-CA	5.32	127.84	120.29
1	A	216	PRO	O-C-N	-5.32	115.85	122.23
1	C	535	CYS	CA-C-N	5.32	127.26	120.56
1	C	535	CYS	C-N-CA	5.32	127.26	120.56
1	C	671	GLU	O-C-N	-5.32	116.09	122.15
1	A	224	ILE	CA-C-N	5.32	127.35	120.44
1	A	224	ILE	C-N-CA	5.32	127.35	120.44
1	A	216	PRO	N-CA-CB	5.31	109.17	103.33
1	C	493	LYS	CA-C-N	5.31	127.40	120.28
1	C	493	LYS	C-N-CA	5.31	127.40	120.28
1	C	535	CYS	O-C-N	-5.31	116.09	122.15
2	D	493	ASP	CA-CB-CG	5.31	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	LEU	O-C-N	-5.31	116.01	122.22
1	A	272	SER	O-C-N	-5.31	115.49	122.39
1	A	388	LEU	CA-C-N	5.31	127.34	120.44
1	A	388	LEU	C-N-CA	5.31	127.34	120.44
1	C	367	SER	CA-C-N	5.31	127.92	120.28
1	C	367	SER	C-N-CA	5.31	127.92	120.28
2	B	407	SER	O-C-N	-5.31	116.61	122.07
1	A	53	ASP	CA-C-N	5.30	128.85	120.47
1	A	53	ASP	C-N-CA	5.30	128.85	120.47
2	B	388	GLU	N-CA-C	5.30	119.84	112.90
1	A	666	PRO	CA-C-N	5.29	127.37	120.28
1	A	666	PRO	C-N-CA	5.29	127.37	120.28
2	B	188	LYS	N-CA-C	-5.29	103.52	110.39
1	C	40	THR	CA-C-N	5.29	127.90	120.28
1	C	40	THR	C-N-CA	5.29	127.90	120.28
1	C	261	ALA	CA-C-N	5.29	127.31	120.44
1	C	261	ALA	C-N-CA	5.29	127.31	120.44
1	A	498	LYS	CA-C-N	5.29	127.31	120.44
1	A	498	LYS	C-N-CA	5.29	127.31	120.44
2	B	370	PRO	N-CA-CB	5.29	108.01	103.31
1	A	369	ASP	O-C-N	-5.28	115.61	122.37
2	B	191	LYS	O-C-N	-5.28	115.52	122.39
1	A	590	PHE	CA-C-N	5.28	127.67	120.54
1	A	590	PHE	C-N-CA	5.28	127.67	120.54
2	B	146	ALA	CA-C-O	5.28	125.95	120.25
2	B	401	GLY	O-C-N	-5.28	117.16	122.65
2	D	158	LEU	O-C-N	-5.28	115.97	122.68
2	D	462	ALA	CA-C-N	5.28	131.47	121.97
2	D	462	ALA	C-N-CA	5.28	131.47	121.97
1	A	122	HIS	CB-CA-C	-5.28	102.37	110.81
1	A	219	ARG	O-C-N	-5.28	116.14	122.15
1	C	133	ALA	O-C-N	-5.28	115.82	122.20
1	C	644	ALA	CA-C-N	5.28	127.21	120.56
1	C	644	ALA	C-N-CA	5.28	127.21	120.56
2	D	218	GLY	CA-C-N	5.28	127.30	120.44
2	D	218	GLY	C-N-CA	5.28	127.30	120.44
2	B	120	PHE	CA-C-N	5.27	127.34	120.28
2	B	120	PHE	C-N-CA	5.27	127.34	120.28
1	C	429	LYS	CA-C-N	5.27	131.46	121.97
1	C	429	LYS	C-N-CA	5.27	131.46	121.97
1	C	445	ARG	CA-C-N	5.27	127.91	120.42
1	C	445	ARG	C-N-CA	5.27	127.91	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	ASP	N-CA-C	5.27	117.77	111.71
2	B	242	HIS	N-CA-CB	5.27	117.65	110.01
1	C	287	PHE	CA-CB-CG	5.27	119.07	113.80
1	C	529	ARG	N-CA-CB	-5.26	102.70	110.49
1	C	375	PRO	N-CA-CB	5.26	107.92	103.35
1	C	697	ARG	CA-C-N	5.26	127.85	120.28
1	C	697	ARG	C-N-CA	5.26	127.85	120.28
1	C	433	MET	N-CA-C	5.26	116.69	111.07
2	D	85	LEU	CA-C-N	-5.26	115.33	121.85
2	D	85	LEU	C-N-CA	-5.26	115.33	121.85
2	B	634	LEU	CA-C-N	5.25	131.20	120.80
2	B	634	LEU	C-N-CA	5.25	131.20	120.80
1	A	69	PRO	CA-C-N	5.25	129.57	122.07
1	A	69	PRO	C-N-CA	5.25	129.57	122.07
2	B	87	TYR	CA-C-N	5.25	125.01	119.76
2	B	87	TYR	C-N-CA	5.25	125.01	119.76
2	D	64	VAL	O-C-N	-5.25	117.37	122.93
2	B	170	TYR	N-CA-C	5.24	120.53	113.72
1	C	476	PRO	N-CA-CB	5.24	108.16	103.08
1	C	596	ARG	CG-CD-NE	5.24	123.53	112.00
1	A	72	HIS	CB-CG-ND1	5.24	130.56	122.70
1	A	633	LEU	CA-C-N	5.23	129.99	122.40
1	A	633	LEU	C-N-CA	5.23	129.99	122.40
1	A	689	PRO	O-C-N	-5.23	116.70	123.03
2	B	222	ARG	CA-C-N	5.23	127.81	120.28
2	B	222	ARG	C-N-CA	5.23	127.81	120.28
2	D	535	TRP	CA-C-N	5.23	128.97	120.60
2	D	535	TRP	C-N-CA	5.23	128.97	120.60
1	C	633	LEU	O-C-N	-5.23	116.27	122.65
1	A	150	ARG	CA-C-N	5.22	127.71	120.29
1	A	150	ARG	C-N-CA	5.22	127.71	120.29
2	B	365	GLN	N-CA-C	5.22	119.13	112.34
1	C	213	PRO	CA-C-N	5.22	124.85	119.05
1	C	213	PRO	C-N-CA	5.22	124.85	119.05
1	C	273	VAL	CA-C-N	5.22	131.04	121.85
1	C	273	VAL	C-N-CA	5.22	131.04	121.85
1	C	341	VAL	N-CA-C	5.22	119.41	111.89
2	D	488	LEU	N-CA-C	5.22	117.88	110.10
1	C	198	ASN	N-CA-C	5.22	118.40	111.30
2	B	557	PHE	O-C-N	-5.22	116.59	122.12
1	A	411	GLU	CA-C-O	-5.21	115.34	120.82
1	A	412	LEU	O-C-N	-5.21	116.60	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	ARG	O-C-N	-5.21	116.21	122.15
2	D	147	PRO	O-C-N	-5.21	115.50	122.22
1	C	627	ASP	N-CA-CB	5.21	118.96	110.37
2	B	500	LEU	CA-C-N	5.20	127.25	120.28
2	B	500	LEU	C-N-CA	5.20	127.25	120.28
1	C	276	ASN	OD1-CG-ND2	-5.20	117.40	122.60
2	D	542	THR	CA-CB-CG2	5.20	119.34	110.50
1	C	315	PHE	O-C-N	-5.20	115.19	122.37
2	D	586	LYS	O-C-N	-5.20	116.61	122.12
1	A	519	ALA	O-C-N	-5.20	116.61	122.12
2	D	310	VAL	CA-C-N	5.20	131.71	121.58
2	D	310	VAL	C-N-CA	5.20	131.71	121.58
2	B	336	PRO	CA-C-N	5.19	128.91	120.60
2	B	336	PRO	C-N-CA	5.19	128.91	120.60
2	B	438	VAL	O-C-N	-5.19	116.75	121.94
1	C	244	HIS	CA-C-O	-5.19	115.05	120.55
1	A	137	GLY	CA-C-N	5.19	129.45	120.58
1	A	137	GLY	C-N-CA	5.19	129.45	120.58
1	A	231	ASN	CB-CA-C	-5.19	100.67	109.38
2	D	235	THR	N-CA-CB	5.19	119.33	110.87
2	D	380	ARG	CA-C-N	5.19	128.19	120.31
2	D	380	ARG	C-N-CA	5.19	128.19	120.31
2	B	20	THR	N-CA-C	5.19	118.66	111.71
1	C	439	LYS	O-C-N	-5.19	115.05	122.41
2	D	167	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	644	ALA	CA-C-N	5.18	127.19	120.56
1	A	644	ALA	C-N-CA	5.18	127.19	120.56
2	D	538	ALA	O-C-N	-5.18	115.70	122.39
2	B	286	ALA	N-CA-C	-5.18	100.08	108.52
2	D	390	VAL	CA-C-O	5.18	125.22	119.42
2	D	559	LYS	O-C-N	-5.18	116.25	122.15
1	A	552	LEU	O-C-N	-5.17	116.25	122.15
2	B	89	GLY	O-C-N	-5.17	115.94	122.41
2	B	32	GLU	CA-C-O	5.17	126.44	120.90
1	C	515	ILE	O-C-N	-5.17	116.52	121.90
1	C	263	GLY	CA-C-N	5.17	127.54	120.46
1	C	263	GLY	C-N-CA	5.17	127.54	120.46
1	A	232	MET	CA-C-N	5.17	124.78	119.56
1	A	232	MET	C-N-CA	5.17	124.78	119.56
1	A	610	HIS	CA-C-O	-5.17	115.37	121.16
2	D	258	THR	O-C-N	-5.17	116.64	122.12
2	D	307	ILE	O-C-N	-5.17	116.86	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	384	ARG	CA-C-N	5.17	127.72	120.28
1	C	384	ARG	C-N-CA	5.17	127.72	120.28
2	D	290	GLN	N-CA-C	5.17	116.60	111.07
2	B	363	PHE	CA-C-N	5.17	131.73	122.38
2	B	363	PHE	C-N-CA	5.17	131.73	122.38
2	D	425	LYS	CA-C-N	5.17	132.27	121.94
2	D	425	LYS	C-N-CA	5.17	132.27	121.94
1	A	183	GLU	CA-C-N	5.16	129.34	120.72
1	A	183	GLU	C-N-CA	5.16	129.34	120.72
2	D	252	LEU	CA-C-N	5.16	127.20	120.28
2	D	252	LEU	C-N-CA	5.16	127.20	120.28
1	A	720	LYS	CA-C-N	5.16	127.15	120.44
1	A	720	LYS	C-N-CA	5.16	127.15	120.44
1	A	79	TYR	O-C-N	-5.16	115.52	122.43
1	A	623	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	23	ARG	CA-C-N	5.15	127.61	120.29
1	C	23	ARG	C-N-CA	5.15	127.61	120.29
2	D	39	VAL	O-C-N	-5.15	116.86	121.91
2	B	510	ARG	CA-C-N	5.15	125.09	119.78
2	B	510	ARG	C-N-CA	5.15	125.09	119.78
2	D	524	PHE	N-CA-C	5.15	119.56	113.28
1	C	459	SER	O-C-N	-5.15	115.35	122.46
2	D	529	GLY	CA-C-N	5.15	129.31	120.71
2	D	529	GLY	C-N-CA	5.15	129.31	120.71
2	D	490	TRP	O-C-N	-5.15	117.19	123.27
1	C	215	GLN	O-C-N	-5.15	116.31	120.38
2	D	521	ARG	CA-C-N	5.15	127.43	120.38
2	D	521	ARG	C-N-CA	5.15	127.43	120.38
2	B	280	ILE	N-CA-C	5.14	115.50	107.99
2	D	112	LEU	O-C-N	-5.14	117.36	123.22
2	B	264	ARG	CA-C-N	5.14	127.17	120.28
2	B	264	ARG	C-N-CA	5.14	127.17	120.28
1	C	190	GLU	CA-C-N	5.14	131.69	122.38
1	C	190	GLU	C-N-CA	5.14	131.69	122.38
1	C	677	ARG	CA-CB-CG	5.14	124.39	114.10
1	A	692	ASP	CA-C-N	5.14	127.48	120.54
1	A	692	ASP	C-N-CA	5.14	127.48	120.54
1	A	51	ASN	CA-C-N	5.14	128.82	120.60
1	A	51	ASN	C-N-CA	5.14	128.82	120.60
2	B	556	ALA	CA-C-N	5.14	127.42	120.38
2	B	556	ALA	C-N-CA	5.14	127.42	120.38
2	D	115	ASP	CA-C-N	5.14	124.75	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	115	ASP	C-N-CA	5.14	124.75	119.05
1	A	16	PRO	N-CA-CB	5.14	108.11	103.33
1	A	133	ALA	CA-C-N	5.13	129.57	120.74
1	A	133	ALA	C-N-CA	5.13	129.57	120.74
1	C	132	VAL	N-CA-C	-5.13	108.12	113.10
2	D	381	ASN	O-C-N	-5.13	115.96	122.27
1	A	263	GLY	O-C-N	-5.13	117.26	122.19
2	D	108	ASP	N-CA-CB	-5.13	101.69	110.16
2	B	607	ALA	O-C-N	-5.13	116.75	122.09
2	B	189	PRO	CA-C-N	5.13	128.51	120.82
2	B	189	PRO	C-N-CA	5.13	128.51	120.82
2	B	204	PHE	O-C-N	-5.13	116.79	122.07
1	C	661	HIS	N-CA-C	5.13	117.53	111.33
2	D	114	GLU	CB-CA-C	-5.13	101.55	109.80
1	A	622	ALA	CA-C-N	5.12	128.80	120.60
1	A	622	ALA	C-N-CA	5.12	128.80	120.60
1	C	63	THR	CA-C-O	5.12	128.40	121.89
1	A	163	VAL	CA-C-O	5.12	125.77	120.39
2	B	415	ALA	CA-C-N	5.12	128.09	120.31
2	B	415	ALA	C-N-CA	5.12	128.09	120.31
1	A	586	LEU	CA-C-N	5.12	127.69	120.42
1	A	586	LEU	C-N-CA	5.12	127.69	120.42
1	A	698	LYS	CA-C-N	5.12	130.10	121.14
1	A	698	LYS	C-N-CA	5.12	130.10	121.14
1	C	352	ALA	CA-C-O	5.12	125.98	120.55
1	A	198	ASN	N-CA-C	5.12	118.26	111.30
1	A	267	ILE	CA-C-O	-5.12	115.63	120.95
2	B	166	VAL	N-CA-CB	5.12	121.40	111.93
2	B	535	TRP	CA-C-N	5.11	128.78	120.60
2	B	535	TRP	C-N-CA	5.11	128.78	120.60
2	D	610	GLU	O-C-N	-5.11	116.70	122.12
2	B	129	LEU	N-CA-C	5.11	117.59	111.71
1	A	509	LYS	O-C-N	-5.11	116.81	122.07
1	C	304	ALA	CA-C-O	-5.11	115.13	120.55
1	C	554	LYS	O-C-N	-5.11	116.70	122.12
1	A	70	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	712	PRO	N-CA-CB	5.11	108.95	103.33
2	D	311	PHE	CA-C-N	5.11	129.18	120.91
2	D	311	PHE	C-N-CA	5.11	129.18	120.91
1	A	423	HIS	CA-C-N	5.10	127.45	120.46
1	A	423	HIS	C-N-CA	5.10	127.45	120.46
2	B	79	LYS	O-C-N	-5.10	115.76	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	PRO	N-CA-CB	5.10	109.08	103.26
2	B	56	ALA	O-C-N	-5.10	116.71	122.12
1	A	661	HIS	O-C-N	-5.10	116.71	122.12
1	A	664	LEU	CA-C-N	5.10	124.41	120.33
1	A	664	LEU	C-N-CA	5.10	124.41	120.33
2	D	520	THR	CB-CA-C	-5.10	101.28	110.36
2	B	295	ALA	CA-C-N	5.10	127.53	120.29
2	B	295	ALA	C-N-CA	5.10	127.53	120.29
1	C	531	LEU	N-CA-C	5.10	117.57	111.71
1	C	720	LYS	O-C-N	-5.10	116.82	122.07
1	A	24	ARG	CA-C-N	5.10	127.06	120.44
1	A	24	ARG	C-N-CA	5.10	127.06	120.44
1	C	327	THR	CA-C-O	5.09	127.07	121.11
2	D	205	ALA	O-C-N	-5.09	116.72	122.12
2	D	275	GLU	CA-C-N	5.09	127.11	120.28
2	D	275	GLU	C-N-CA	5.09	127.11	120.28
2	D	361	LEU	CA-C-O	5.09	125.75	120.25
2	B	223	ARG	O-C-N	-5.09	116.26	122.22
1	C	622	ALA	CA-C-N	5.09	129.23	120.72
1	C	622	ALA	C-N-CA	5.09	129.23	120.72
2	B	105	ASP	CA-C-N	5.09	129.34	120.68
2	B	105	ASP	C-N-CA	5.09	129.34	120.68
1	C	19	ALA	N-CA-C	5.09	116.83	111.28
2	B	167	PHE	CA-CB-CG	5.09	118.89	113.80
1	C	189	PRO	N-CA-CB	5.09	109.06	103.26
2	D	100	ARG	CD-NE-CZ	5.09	131.53	124.40
2	D	558	LYS	CA-C-N	5.09	127.52	120.29
2	D	558	LYS	C-N-CA	5.09	127.52	120.29
2	D	574	TYR	CA-C-N	5.09	128.05	120.31
2	D	574	TYR	C-N-CA	5.09	128.05	120.31
1	C	178	TYR	N-CA-C	-5.08	105.65	111.14
2	D	328	TRP	O-C-N	-5.08	115.62	122.23
1	C	678	PRO	CA-C-O	5.08	125.61	118.86
1	A	523	ASP	CA-C-N	5.07	127.59	120.28
1	A	523	ASP	C-N-CA	5.07	127.59	120.28
1	C	269	ALA	CA-C-N	5.07	125.57	119.94
1	C	269	ALA	C-N-CA	5.07	125.57	119.94
1	A	295	PHE	CA-C-N	5.07	127.48	120.29
1	A	295	PHE	C-N-CA	5.07	127.48	120.29
2	B	394	ARG	CA-C-N	5.07	130.05	123.06
2	B	394	ARG	C-N-CA	5.07	130.05	123.06
1	A	54	VAL	O-C-N	-5.07	116.75	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	THR	O-C-N	-5.06	116.38	122.15
2	D	631	LEU	CA-C-N	5.06	127.02	120.44
2	D	631	LEU	C-N-CA	5.06	127.02	120.44
2	D	303	ALA	CA-C-N	5.06	127.56	120.28
2	D	303	ALA	C-N-CA	5.06	127.56	120.28
2	B	142	PRO	N-CA-CB	5.06	108.89	103.33
1	A	373	ALA	N-CA-C	5.05	115.01	107.88
1	C	610	HIS	CA-C-O	-5.05	115.00	120.81
1	C	719	VAL	CA-C-O	-5.05	115.69	120.95
2	D	401	GLY	O-C-N	-5.05	116.94	122.65
2	D	556	ALA	CA-C-O	-5.05	115.51	120.82
2	B	504	SER	N-CA-C	5.05	117.52	111.71
2	D	242	HIS	CA-C-N	5.05	127.55	120.28
2	D	242	HIS	C-N-CA	5.05	127.55	120.28
1	C	516	THR	CA-C-N	5.05	127.00	120.44
1	C	516	THR	C-N-CA	5.05	127.00	120.44
1	A	306	MET	CA-C-N	5.05	127.04	120.28
1	A	306	MET	C-N-CA	5.05	127.04	120.28
1	A	136	VAL	CA-C-O	5.04	127.19	120.98
1	C	402	PRO	N-CA-CB	5.04	108.84	103.39
1	C	562	GLN	CA-C-O	-5.04	114.93	120.43
1	C	70	PHE	N-CA-C	5.04	118.39	111.54
1	C	252	ALA	CA-C-N	5.04	127.03	120.28
1	C	252	ALA	C-N-CA	5.04	127.03	120.28
1	C	439	LYS	CA-C-O	5.04	125.17	119.18
2	D	511	PRO	N-CA-CB	5.04	107.73	103.35
1	C	8	ASP	N-CA-C	5.04	118.53	112.38
2	D	551	ALA	CA-C-N	5.04	127.03	120.28
2	D	551	ALA	C-N-CA	5.04	127.03	120.28
1	A	722	LEU	CA-C-N	5.04	126.99	120.44
1	A	722	LEU	C-N-CA	5.04	126.99	120.44
2	B	38	GLU	CA-C-N	5.04	126.90	120.56
2	B	38	GLU	C-N-CA	5.04	126.90	120.56
2	D	180	VAL	CA-C-N	5.04	126.99	120.44
2	D	180	VAL	C-N-CA	5.04	126.99	120.44
2	D	617	LEU	N-CA-CB	5.04	118.50	110.65
1	A	207	ARG	N-CA-C	5.03	117.66	111.82
1	C	389	PHE	O-C-N	-5.03	116.89	122.07
1	C	455	ALA	O-C-N	-5.03	116.89	122.07
1	C	678	PRO	O-C-N	-5.03	115.38	122.38
2	D	166	VAL	N-CA-CB	5.03	120.90	112.44
2	D	299	ALA	O-C-N	-5.03	116.78	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	322	GLN	N-CA-C	5.03	117.11	108.90
2	D	36	GLU	CA-C-N	5.03	127.95	120.31
2	D	36	GLU	C-N-CA	5.03	127.95	120.31
2	D	503	ARG	O-C-N	-5.03	116.89	122.07
1	C	53	ASP	O-C-N	-5.03	115.69	122.43
1	A	414	TRP	CA-CB-CG	5.03	123.15	113.60
2	B	71	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	145	SER	N-CA-CB	-5.03	103.13	110.97
2	B	49	PRO	O-C-N	-5.03	116.09	122.17
1	A	8	ASP	CA-C-N	5.02	130.25	122.26
1	A	8	ASP	C-N-CA	5.02	130.25	122.26
1	C	434	ALA	CA-C-N	5.02	127.01	120.28
1	C	434	ALA	C-N-CA	5.02	127.01	120.28
1	C	675	LEU	O-C-N	-5.02	115.91	122.39
1	C	68	PRO	N-CA-CB	5.02	107.95	103.08
1	C	379	SER	CA-C-N	5.02	127.00	120.28
1	C	379	SER	C-N-CA	5.02	127.00	120.28
1	A	504	ASP	CA-CB-CG	5.02	117.62	112.60
2	D	303	ALA	O-C-N	-5.02	116.90	122.07
2	D	404	TYR	CA-CB-CG	5.02	122.93	113.90
1	A	44	ILE	N-CA-C	-5.01	102.23	107.60
2	B	73	VAL	CA-C-N	5.01	124.62	119.56
2	B	73	VAL	C-N-CA	5.01	124.62	119.56
1	C	427	VAL	O-C-N	-5.01	117.00	121.91
1	C	485	ASN	N-CA-C	5.01	117.12	111.11
2	D	229	PRO	N-CA-CB	5.01	108.12	103.41
2	D	613	ILE	N-CA-C	5.01	115.30	107.99
2	B	557	PHE	CA-C-N	5.01	127.92	120.31
2	B	557	PHE	C-N-CA	5.01	127.92	120.31
2	D	485	ARG	CG-CD-NE	-5.01	100.98	112.00
2	D	385	VAL	O-C-N	-5.01	116.67	121.83
2	B	364	THR	O-C-N	-5.00	115.47	122.37
2	B	375	PRO	N-CA-CB	5.00	108.83	103.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5539	0	5413	23	0
1	C	5539	0	5413	28	0
2	B	4744	0	4648	21	0
2	D	4744	0	4648	24	0
3	A	54	0	37	2	0
3	C	54	0	37	2	0
4	A	91	0	88	9	0
4	C	91	0	88	7	0
5	B	12	0	16	2	0
5	D	9	0	11	2	0
6	A	420	0	0	0	0
6	B	243	0	0	0	0
6	C	421	0	0	0	0
6	D	242	0	0	1	0
All	All	22203	0	20399	108	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 3.

All (108) 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)
4:C:2800:B12:H552	4:C:2800:B12:H531	1.48	0.92
1:A:638:GLU:HA	1:A:671:GLU:HG2	1.52	0.90
4:A:1800:B12:H531	4:A:1800:B12:H552	1.61	0.82
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.29	0.81
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.71	0.72
2:D:503:ARG:HD2	2:D:638:LYS:HD3	1.71	0.72
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.75	0.69
2:B:356:GLU:HA	5:B:3002:GOL:H2	1.75	0.68
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.77	0.67
1:C:638:GLU:HA	1:C:671:GLU:HG2	1.76	0.67
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.77	0.67
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.44	0.65
1:A:247:GLU:HB3	4:A:1800:B12:H532	1.77	0.64
2:B:617:LEU:HD22	2:B:621:MET:HE1	1.81	0.62
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.80	0.62
4:C:2800:B12:H531	4:C:2800:B12:C55	2.24	0.62
2:B:503:ARG:HD2	2:B:638:LYS:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1800:B12:H531	4:A:1800:B12:C55	2.30	0.61
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.84	0.59
2:B:515:LEU:HB2	2:B:544:GLN:HB3	1.84	0.59
1:C:706:THR:HB	1:C:707:PRO:HD2	1.84	0.58
1:A:706:THR:HB	1:A:707:PRO:HD2	1.85	0.58
1:C:706:THR:HB	1:C:707:PRO:CD	2.34	0.57
1:A:706:THR:HB	1:A:707:PRO:CD	2.35	0.57
4:A:1800:B12:H362	4:A:1800:B12:H351	1.87	0.56
3:C:2801:2CP:OP2	3:C:2801:2CP:HB1	2.04	0.56
2:D:141:ASP:HB3	2:D:142:PRO:HD2	1.86	0.56
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.87	0.56
1:C:359:HIS:CE1	1:C:401:ASP:H	2.24	0.56
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.88	0.56
2:D:617:LEU:HD22	2:D:621:MET:HE1	1.87	0.55
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.88	0.55
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.89	0.55
4:A:1800:B12:H351	4:A:1800:B12:H372	1.88	0.54
1:C:247:GLU:HB3	4:C:2800:B12:H532	1.90	0.54
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.90	0.54
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.90	0.54
2:B:107:TRP:HB3	5:B:3002:GOL:H11	1.92	0.51
1:A:359:HIS:CE1	1:A:401:ASP:H	2.29	0.51
2:D:107:TRP:HB3	5:D:3004:GOL:H11	1.93	0.51
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.76	0.50
2:D:237:ASP:HB3	2:D:240:ILE:HD12	1.93	0.50
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.95	0.49
4:A:1800:B12:H351	4:A:1800:B12:C36	2.41	0.48
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.95	0.48
3:A:1801:2CP:OP2	3:A:1801:2CP:HB1	2.13	0.48
2:D:100:ARG:HH21	5:D:3004:GOL:H12	1.78	0.48
2:D:511:PRO:HB3	2:D:634:LEU:HD13	1.96	0.48
2:B:238:ALA:HB1	2:B:251:GLU:HG3	1.95	0.48
1:A:308:TRP:HB2	1:A:325:LEU:HD12	1.96	0.47
2:B:212:PRO:HG2	2:B:430:SER:HB3	1.95	0.47
4:C:2800:B12:H353	4:C:2800:B12:H302	1.97	0.47
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.45	0.47
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.96	0.46
1:C:4:LEU:HA	1:C:5:PRO:HD3	1.85	0.46
1:A:89:TYR:CE2	3:A:1801:2CP:HS2	2.51	0.46
1:C:139:ALA:HB1	4:C:2800:B12:H362	1.97	0.45
1:A:69:PRO:HG3	2:B:24:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:VAL:HG12	2:D:392:ILE:HG23	1.99	0.45
1:C:197:GLN:HG3	1:C:239:SER:HB3	1.99	0.44
1:C:592:GLN:HE21	1:C:592:GLN:HA	1.83	0.44
1:A:200:ILE:HG12	1:A:217:SER:HB3	1.99	0.44
1:A:489:LEU:HG	1:A:493:LYS:HE3	1.99	0.44
2:D:579:LEU:HD22	2:D:605:ASP:HB3	1.98	0.44
4:A:1800:B12:H372	4:A:1800:B12:C35	2.48	0.44
2:B:224:LEU:HD12	2:B:233:ALA:HB2	2.00	0.44
1:C:577:THR:HG22	1:C:580:VAL:H	1.81	0.44
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.81	0.44
2:D:331:LEU:HD13	2:D:365:GLN:HB3	1.99	0.44
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.52	0.43
1:A:405:GLY:O	1:A:406:SER:C	2.61	0.43
4:A:1800:B12:H351	4:A:1800:B12:C37	2.47	0.43
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.99	0.43
1:A:592:GLN:HE21	1:A:592:GLN:HA	1.84	0.43
1:C:385:ASN:HD22	1:C:388:LEU:HD12	1.84	0.43
1:A:599:ARG:HD2	1:A:649:VAL:HA	1.99	0.43
1:C:710:VAL:HG12	1:C:712:PRO:HD2	2.00	0.43
1:A:597:ARG:HH11	1:A:597:ARG:HG2	1.83	0.43
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.48	0.43
2:B:180:VAL:HG13	2:B:197:LEU:HD21	2.00	0.43
2:D:429:MET:HE3	2:D:433:VAL:HG23	2.01	0.42
1:C:504:ASP:O	1:C:508:VAL:HG23	2.19	0.42
4:A:1800:B12:H412	4:A:1800:B12:H361	1.74	0.42
2:D:86:GLY:HA3	6:D:752:HOH:O	2.18	0.42
1:A:683:THR:HG21	1:A:718:LEU:HD13	2.02	0.42
1:A:213:PRO:HD2	1:A:216:PRO:HG2	2.02	0.42
1:C:385:ASN:HD22	1:C:385:ASN:HA	1.73	0.42
2:D:464:SER:HA	2:D:537:ILE:HG12	2.02	0.42
1:C:200:ILE:HG12	1:C:217:SER:HB3	2.03	0.41
1:A:54:VAL:O	1:A:58:MET:HE3	2.19	0.41
1:A:339:GLN:HG2	1:A:471:ARG:NH2	2.36	0.41
2:D:313:VAL:O	2:D:314:ASP:C	2.63	0.41
2:D:334:GLU:O	2:D:335:ASP:C	2.62	0.41
1:C:89:TYR:CE2	3:C:2801:2CP:HS2	2.55	0.41
1:C:683:THR:HG21	1:C:718:LEU:HD13	2.02	0.41
1:C:318:LYS:HA	1:C:318:LYS:HD3	1.95	0.41
4:C:2800:B12:H361	4:C:2800:B12:H412	1.62	0.41
2:B:80:ASP:HB3	2:B:407:SER:HB2	2.02	0.41
4:C:2800:B12:H372	4:C:2800:B12:H351	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:HB2	2:B:424:GLU:HG3	2.02	0.41
2:D:252:LEU:HD11	2:D:300:LEU:HA	2.03	0.41
1:C:188:LYS:HB3	1:C:189:PRO:HD2	2.03	0.40
1:C:521:ASN:O	1:C:529:ARG:HD3	2.20	0.40
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.56	0.40
1:C:652:VAL:HG11	1:C:668:LEU:HD11	2.03	0.40
1:C:405:GLY:O	1:C:406:SER:C	2.64	0.40
2:D:141:ASP:HB3	2:D:142:PRO:CD	2.50	0.40
2:D:267:VAL:HA	2:D:271:PHE:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	723/727 (99%)	701 (97%)	22 (3%)	0	100	100
1	C	723/727 (99%)	702 (97%)	21 (3%)	0	100	100
2	B	621/637 (98%)	606 (98%)	14 (2%)	1 (0%)	43	51
2	D	621/637 (98%)	605 (97%)	15 (2%)	1 (0%)	43	51
All	All	2688/2728 (98%)	2614 (97%)	72 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	THR
2	D	17	THR

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	563/590 (95%)	552 (98%)	11 (2%)	48	64
1	C	563/590 (95%)	553 (98%)	10 (2%)	51	68
2	B	480/509 (94%)	470 (98%)	10 (2%)	47	63
2	D	480/509 (94%)	469 (98%)	11 (2%)	44	59
All	All	2086/2198 (95%)	2044 (98%)	42 (2%)	48	64

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	202	LYS
1	A	229	SER
1	A	430	VAL
1	A	438	GLU
1	A	487	THR
1	A	554	LYS
1	A	592	GLN
1	A	597	ARG
1	A	638	GLU
1	A	668	LEU
2	B	16	LEU
2	B	77	ARG
2	B	127	GLU
2	B	199	LEU
2	B	279	THR
2	B	410	ARG
2	B	451	LYS
2	B	532	SER
2	B	610	GLU
2	B	638	LYS
1	C	69	PRO
1	C	149	MET
1	C	202	LYS

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Mol	Chain	Res	Type
1	C	365	THR
1	C	430	VAL
1	C	479	ASP
1	C	577	THR
1	C	592	GLN
1	C	597	ARG
1	C	668	LEU
2	D	16	LEU
2	D	75	MET
2	D	77	ARG
2	D	155	SER
2	D	180	VAL
2	D	199	LEU
2	D	410	ARG
2	D	451	LYS
2	D	532	SER
2	D	610	GLU
2	D	638	LYS

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

Mol	Chain	Res	Type
1	A	160	GLN
1	A	359	HIS
1	A	385	ASN
1	A	492	GLN
1	A	592	GLN
1	A	643	GLN
2	B	323	ASN
2	B	365	GLN
2	B	544	GLN
1	C	359	HIS
1	C	385	ASN
1	C	592	GLN
1	C	635	GLN
1	C	643	GLN
2	D	196	ASN
2	D	322	GLN
2	D	323	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$
5	GOL	D	3003	-	5,5,5	0.21	0	5,5,5	0.58	0
5	GOL	B	3002	-	5,5,5	0.26	0	5,5,5	0.55	0
4	B12	A	1800	6,1	94,101,101	0.98	5 (5%)	149,166,166	1.67	30 (20%)
5	GOL	B	3001	-	5,5,5	0.24	0	5,5,5	0.50	0
3	2CP	A	1801	-	53,56,56	1.14	8 (15%)	76,83,83	1.57	14 (18%)
5	GOL	D	3004	-	2,2,5	0.50	0	1,1,5	0.63	0
4	B12	C	2800	6,1	94,101,101	1.02	4 (4%)	149,166,166	1.63	24 (16%)
3	2CP	C	2801	-	53,56,56	1.25	7 (13%)	76,83,83	1.49	10 (13%)

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
5	GOL	D	3003	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	3002	-	-	2/4/4/4	-
4	B12	A	1800	6,1	-	8/56/223/223	0/3/11/11
5	GOL	B	3001	-	-	3/4/4/4	-
3	2CP	A	1801	-	-	4/56/72/72	0/3/3/3
4	B12	C	2800	6,1	-	10/56/223/223	0/3/11/11
3	2CP	C	2801	-	-	4/56/72/72	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2801	2CP	CP2-NP1	3.51	1.54	1.46
3	C	2801	2CP	CP5-NP2	2.97	1.52	1.46
3	A	1801	2CP	CP5-NP2	2.96	1.52	1.46
3	C	2801	2CP	P1-O6	2.90	1.62	1.59
3	C	2801	2CP	C2-N1	2.83	1.39	1.33
4	C	2800	B12	C14-N23	2.71	1.38	1.35
4	A	1800	B12	C54-C17	2.68	1.59	1.54
4	C	2800	B12	C54-C17	2.62	1.58	1.54
3	A	1801	2CP	CP2-NP1	2.60	1.52	1.46
3	C	2801	2CP	P2-O7	-2.59	1.49	1.59
4	C	2800	B12	C35-C5	2.53	1.56	1.50
4	A	1800	B12	C48-C13	2.53	1.60	1.54
3	A	1801	2CP	P2-O7	-2.51	1.49	1.59
3	A	1801	2CP	C2-N1	2.42	1.38	1.33
3	C	2801	2CP	OS4-CS4	2.41	1.29	1.22
3	A	1801	2CP	OS4-CS4	2.35	1.29	1.22
3	A	1801	2CP	C5-N7	-2.29	1.34	1.39
4	A	1800	B12	C2B-N1B	-2.28	1.33	1.37
4	C	2800	B12	C2B-N1B	-2.27	1.33	1.37
4	A	1800	B12	C6B-C5B	2.20	1.46	1.40
4	A	1800	B12	C46-C12	2.18	1.58	1.54
3	C	2801	2CP	P1-O12	-2.15	1.45	1.55
3	A	1801	2CP	P3-O32	-2.12	1.46	1.54
3	A	1801	2CP	P2-O22	-2.01	1.46	1.55

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2801	2CP	CP2-NP1-CP3	-6.08	111.50	122.82
3	A	1801	2CP	CP8-CPA-CPB	5.87	117.92	108.22
4	C	2800	B12	C19-N24-C16	5.87	113.70	107.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2801	2CP	CP8-CPA-CPB	5.52	117.33	108.22
4	A	1800	B12	C55-C17-C16	5.38	127.12	116.59
4	A	1800	B12	C54-C17-C55	-5.07	100.83	109.27
3	A	1801	2CP	CP2-NP1-CP3	-4.44	114.55	122.82
4	A	1800	B12	C19-N24-C16	4.42	112.12	107.29
4	A	1800	B12	C9B-C8B-N1B	4.29	107.21	105.30
4	C	2800	B12	C15-C16-N24	4.24	128.46	122.42
4	C	2800	B12	C16-C15-C14	-4.18	114.88	121.26
4	C	2800	B12	C9-N22-C6	4.14	110.27	105.28
4	C	2800	B12	C54-C17-C16	-4.08	91.29	112.41
3	A	1801	2CP	CP1-CP2-NP1	-4.05	103.96	112.41
3	C	2801	2CP	CP1-CP2-NP1	-3.92	104.23	112.41
3	A	1801	2CP	CP5-NP2-CP6	-3.80	115.71	122.55
4	A	1800	B12	C54-C17-C16	-3.78	92.81	112.41
4	C	2800	B12	C18-C17-C16	3.68	105.12	100.69
4	C	2800	B12	C1P-N59-C57	-3.67	114.80	122.69
4	C	2800	B12	C55-C17-C16	3.51	123.46	116.59
3	A	1801	2CP	CP9-CPA-CPB	3.46	113.94	108.22
3	C	2801	2CP	O7-CPB-CPA	-3.33	105.19	110.55
4	A	1800	B12	C55-C17-C18	3.33	117.48	111.12
4	C	2800	B12	C55-C17-C18	3.29	117.40	111.12
4	A	1800	B12	C41-C8-C9	-3.25	105.52	111.19
4	A	1800	B12	C9-N22-C6	3.24	109.17	105.28
4	A	1800	B12	C18-C19-N24	3.13	107.03	102.33
3	A	1801	2CP	O7-CPB-CPA	-3.04	105.65	110.55
4	C	2800	B12	C54-C17-C18	-3.02	108.66	112.99
4	A	1800	B12	C18-C17-C16	3.00	104.31	100.69
4	C	2800	B12	C5M-C5B-C6B	-2.93	114.78	120.76
4	C	2800	B12	C7B-C8B-C9B	2.92	125.97	122.47
4	A	1800	B12	C35-C5-C6	-2.89	117.76	122.41
4	A	1800	B12	C55-C56-C57	-2.87	104.84	111.25
4	A	1800	B12	C12-C11-C10	2.87	127.10	123.40
3	C	2801	2CP	CP5-NP2-CP6	-2.85	117.42	122.55
3	A	1801	2CP	CP9-CPA-CP7	-2.77	104.04	108.77
4	C	2800	B12	C9B-C8B-N1B	2.77	106.53	105.30
3	C	2801	2CP	CP9-CPA-CP7	-2.74	104.10	108.77
4	A	1800	B12	C7-C6-N22	2.73	112.90	107.94
4	C	2800	B12	C4B-C5B-C6B	2.71	123.67	119.69
4	C	2800	B12	C13-C14-C15	-2.71	120.20	124.32
4	A	1800	B12	C36-C7-C8	2.68	117.00	112.05
4	C	2800	B12	C18-C19-N24	2.68	106.36	102.33
3	C	2801	2CP	CP9-CPA-CPB	2.66	112.61	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	2CP	OS5-CS4-OS4	-2.64	118.10	124.08
4	C	2800	B12	C55-C56-C57	-2.60	105.45	111.25
3	A	1801	2CP	CP8-CPA-CP9	-2.57	104.07	109.20
4	A	1800	B12	C8B-C9B-N3B	-2.57	107.22	110.00
4	A	1800	B12	C7-C8-C9	2.56	104.14	100.89
3	A	1801	2CP	O33-P3-O32	2.52	117.23	107.80
4	A	1800	B12	C15-C16-N24	2.49	125.97	122.42
4	A	1800	B12	C16-C15-C14	-2.47	117.49	121.26
4	C	2800	B12	C1-C19-C18	-2.46	117.91	121.90
4	A	1800	B12	C20-C1-C19	2.40	111.66	109.35
4	C	2800	B12	O28-C27-N29	-2.37	116.20	122.53
3	A	1801	2CP	OS5-CS4-CS2	2.37	122.73	115.05
4	A	1800	B12	C7B-C8B-C9B	2.35	125.29	122.47
4	C	2800	B12	C2P-C1P-N59	-2.34	109.48	112.92
4	C	2800	B12	C8B-C9B-N3B	-2.34	107.47	110.00
4	A	1800	B12	C48-C13-C12	-2.32	109.89	116.52
4	A	1800	B12	C5M-C5B-C6B	-2.31	116.04	120.76
4	A	1800	B12	O8R-C5R-C4R	-2.29	103.54	111.33
4	A	1800	B12	C2-C1-C19	-2.24	115.14	118.61
3	A	1801	2CP	OP2-CP6-CP7	-2.24	114.65	120.89
4	A	1800	B12	C47-C12-C46	-2.23	105.72	109.41
4	A	1800	B12	O28-C27-N29	-2.22	116.62	122.53
4	C	2800	B12	C9B-C4B-C5B	-2.21	116.74	120.83
3	C	2801	2CP	C4-N9-C8	-2.16	103.47	105.74
3	A	1801	2CP	O4'-C1'-N9	2.14	112.21	108.09
3	A	1801	2CP	OP2-CP6-NP2	2.13	127.49	122.98
3	C	2801	2CP	OP2-CP6-CP7	-2.09	115.07	120.89
4	A	1800	B12	C31-C30-C3	-2.07	108.79	114.65
4	A	1800	B12	C9-C10-C11	2.05	128.89	125.97
4	C	2800	B12	C53-C15-C16	2.05	123.84	120.36
4	C	2800	B12	O2-C3R-C2R	2.01	118.90	111.68
3	C	2801	2CP	CP7-CP6-NP2	2.01	120.30	116.48
4	A	1800	B12	O6R-C1R-N1B	-2.01	104.23	108.09

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	2CP	P1-O6-P2-O7
3	A	1801	2CP	S-CS1-CS2-CS3
3	A	1801	2CP	S-CS1-CS2-CS4
3	C	2801	2CP	P1-O6-P2-O7

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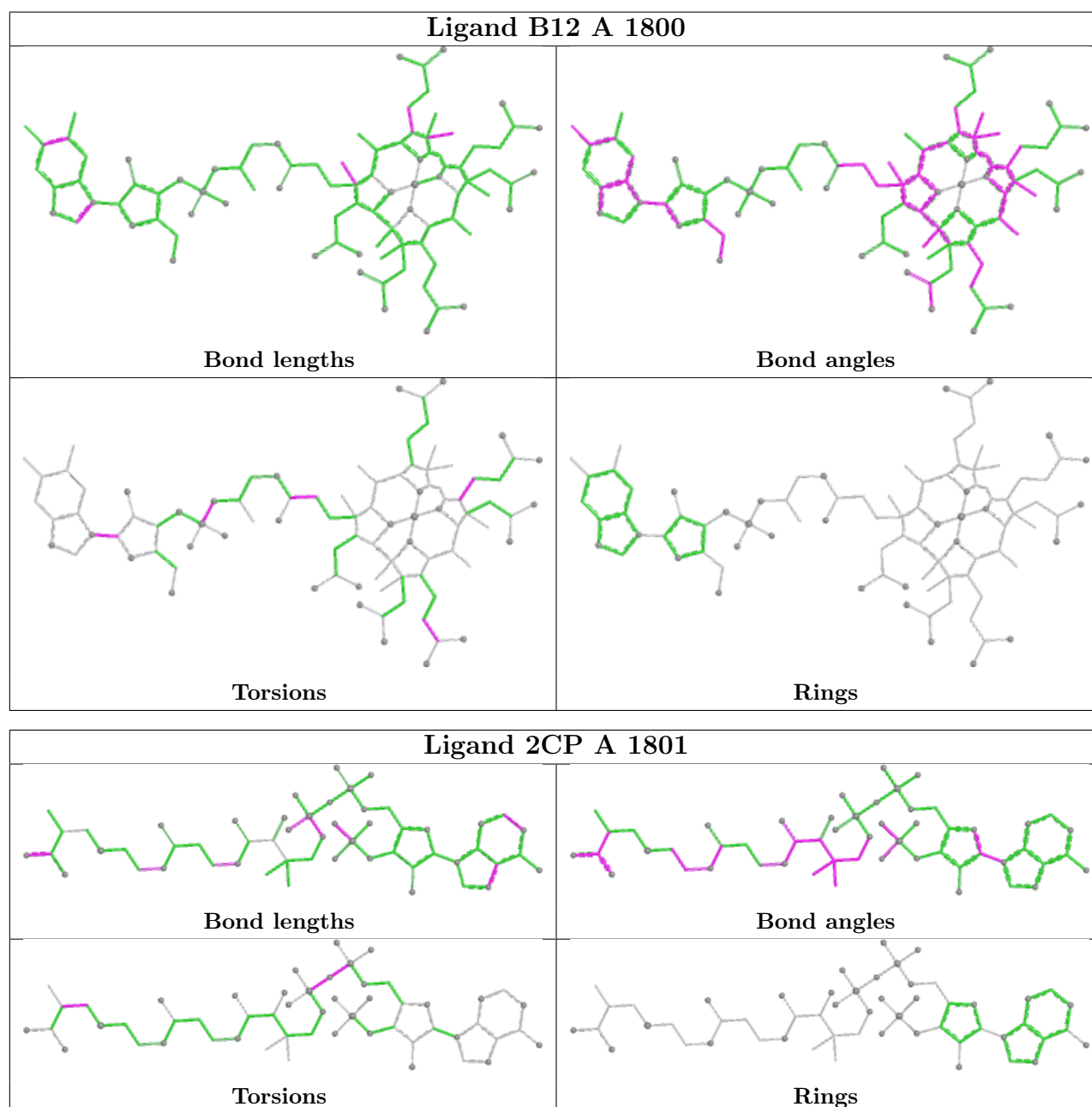
Mol	Chain	Res	Type	Atoms
3	C	2801	2CP	S-CS1-CS2-CS3
3	C	2801	2CP	S-CS1-CS2-CS4
4	A	1800	B12	C42-C41-C8-C9
4	A	1800	B12	C2R-C1R-N1B-C2B
4	C	2800	B12	C2R-C1R-N1B-C2B
5	B	3001	GOL	O1-C1-C2-C3
5	B	3002	GOL	C1-C2-C3-O3
5	D	3003	GOL	O1-C1-C2-C3
5	D	3003	GOL	C1-C2-C3-O3
5	B	3001	GOL	O1-C1-C2-O2
4	C	2800	B12	C42-C41-C8-C9
4	C	2800	B12	C16-C17-C55-C56
4	A	1800	B12	C2R-C1R-N1B-C8B
4	C	2800	B12	C2R-C1R-N1B-C8B
5	B	3002	GOL	O2-C2-C3-O3
5	D	3003	GOL	O1-C1-C2-O2
4	C	2800	B12	C30-C31-C32-N33
4	C	2800	B12	C30-C31-C32-O34
5	D	3003	GOL	O2-C2-C3-O3
4	A	1800	B12	O6R-C1R-N1B-C8B
4	C	2800	B12	O6R-C1R-N1B-C8B
3	A	1801	2CP	P2-O6-P1-O12
3	C	2801	2CP	P2-O6-P1-O12
5	B	3001	GOL	O2-C2-C3-O3
4	A	1800	B12	C30-C31-C32-N33
4	C	2800	B12	C38-C37-C7-C36
4	A	1800	B12	C2P-O3-P-O5
4	C	2800	B12	C2P-O3-P-O5
4	A	1800	B12	C30-C31-C32-O34
4	A	1800	B12	C55-C56-C57-O58
4	C	2800	B12	C55-C56-C57-O58

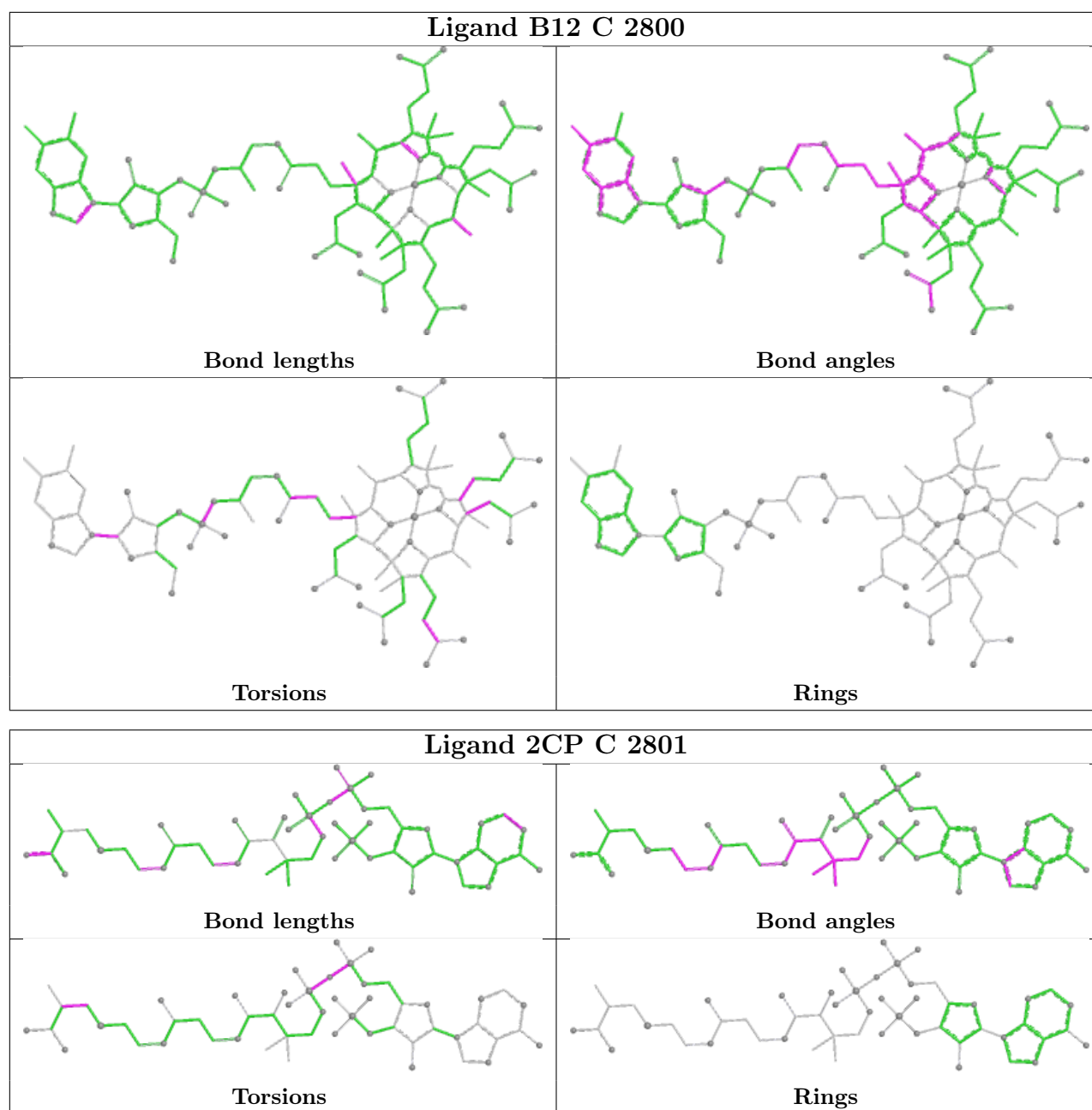
There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3002	GOL	2	0
4	A	1800	B12	9	0
3	A	1801	2CP	2	0
5	D	3004	GOL	2	0
4	C	2800	B12	7	0
3	C	2801	2CP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	725/727 (99%)	-0.41	5 (0%) 84 82	9, 19, 38, 65	0
1	C	725/727 (99%)	-0.44	6 (0%) 82 80	7, 19, 38, 66	0
2	B	623/637 (97%)	0.01	9 (1%) 73 71	14, 29, 49, 80	0
2	D	623/637 (97%)	-0.03	8 (1%) 75 73	13, 29, 49, 79	0
All	All	2696/2728 (98%)	-0.23	28 (1%) 79 77	7, 24, 45, 80	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	PRO	6.6
2	D	19	THR	5.2
2	B	16	LEU	5.1
2	B	19	THR	4.9
1	C	728	ALA	4.8
2	D	16	LEU	4.7
2	D	18	PRO	3.6
2	B	17	THR	3.2
2	B	20	THR	3.1
2	D	638	LYS	2.9
2	D	30	ALA	2.8
1	A	576	ASN	2.7
2	B	638	LYS	2.6
1	A	574	VAL	2.5
1	A	728	ALA	2.5
2	D	20	THR	2.4
1	C	215	GLN	2.3
1	A	9	SER	2.2
2	D	17	THR	2.2
1	A	23	ARG	2.2
1	C	475	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	57	GLU	2.1
1	C	576	ASN	2.1
1	C	429	LYS	2.1
1	C	524	ASP	2.1
2	D	484	ALA	2.1
2	B	610	GLU	2.1
2	B	270	GLY	2.1

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](#)

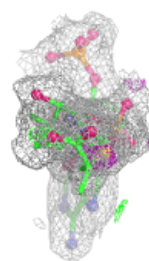
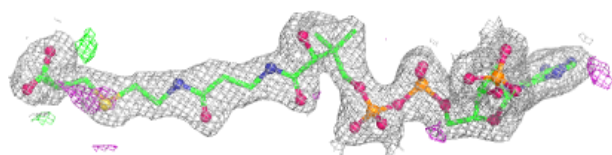
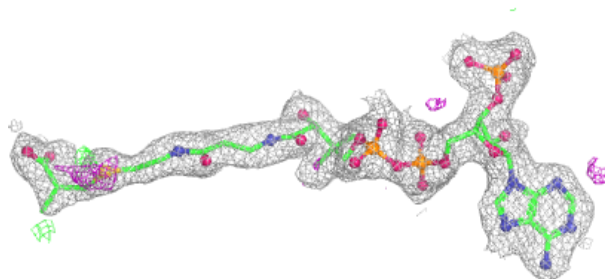
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	D	3004	3/6	0.56	0.40	65,65,65,66	0
5	GOL	B	3002	6/6	0.79	0.25	64,67,68,69	0
5	GOL	B	3001	6/6	0.83	0.16	57,59,60,60	0
5	GOL	D	3003	6/6	0.88	0.13	59,60,60,61	0
3	2CP	C	2801	54/54	0.98	0.06	6,13,31,33	0
4	B12	C	2800	91/91	0.98	0.05	4,13,19,24	0
3	2CP	A	1801	54/54	0.98	0.06	8,14,29,31	0
4	B12	A	1800	91/91	0.99	0.05	4,12,18,23	0

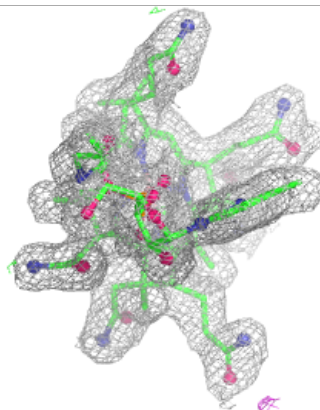
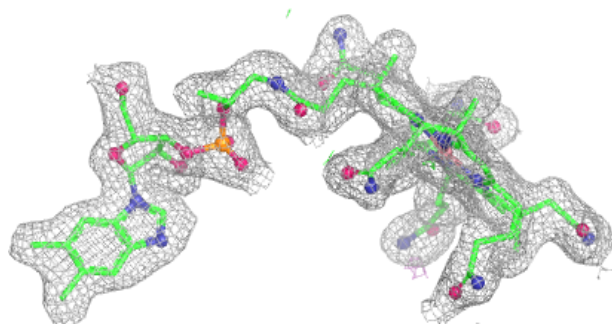
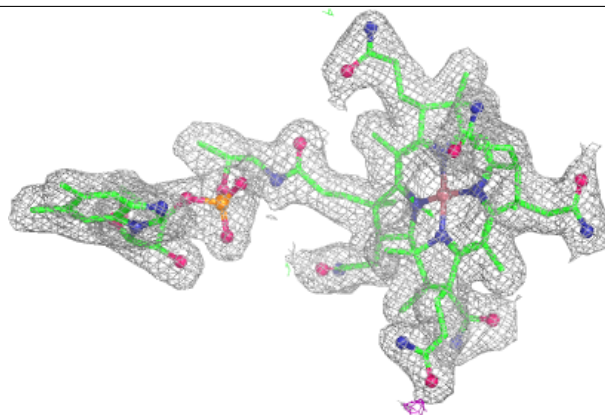
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2CP C 2801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

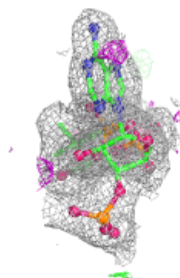
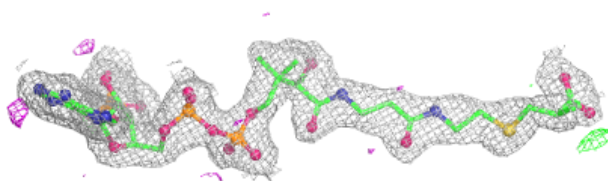
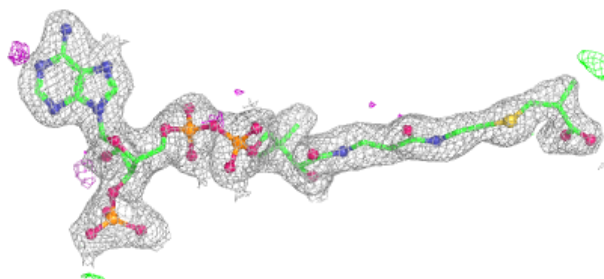
**Electron density around B12 C 2800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

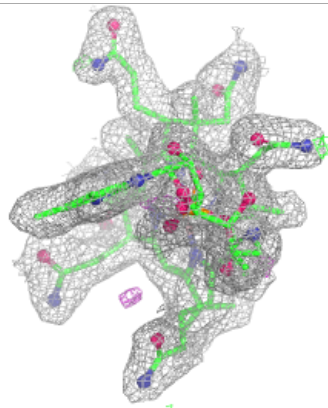
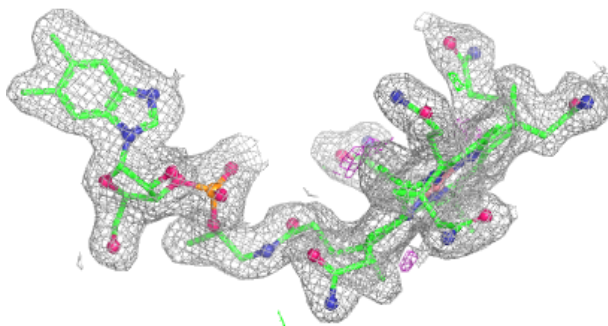
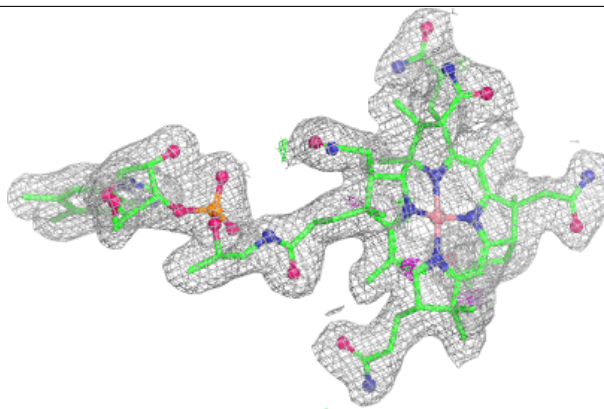


Electron density around 2CP A 1801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B12 A 1800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.