



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:02 PM EDT

PDB ID : 3REQ / pdb_00003req
Title : METHYLMALONYL-COA MUTASE, SUBSTRATE-FREE STATE (POOR QUALITY STRUCTURE)
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1997-12-04
Resolution : 2.70 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

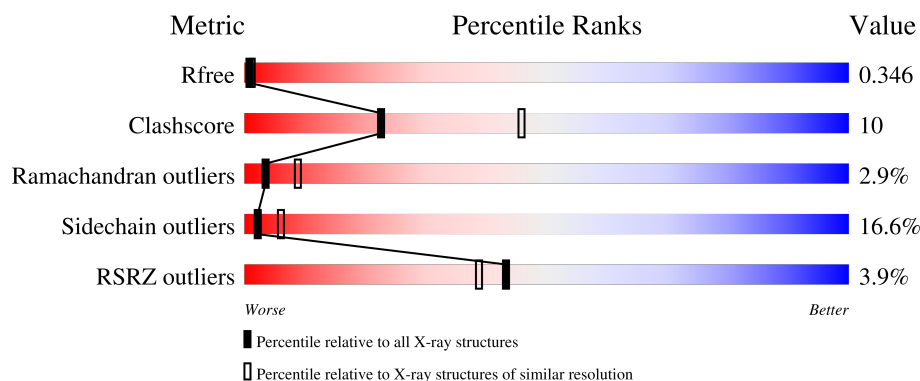
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
2	B	637	

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
3	B12	A	800	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10285 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 METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5552	3508	964	1056	24			

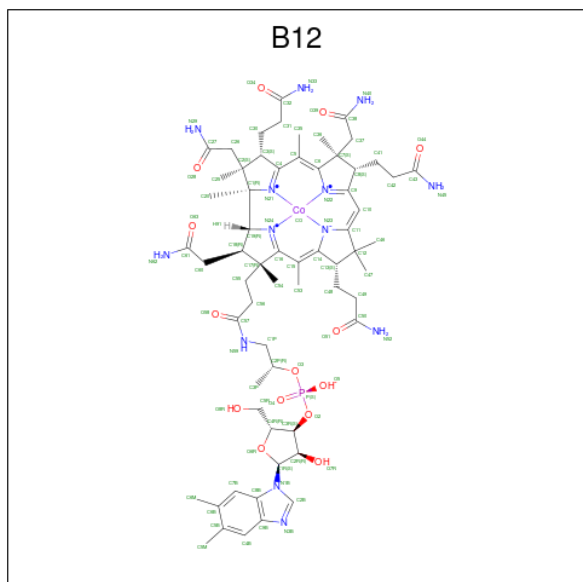
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	620	Total	C	N	O	S	0	0	0
			4624	2918	796	897	13			

There are 3 discrepancies between the modelled and reference sequences:

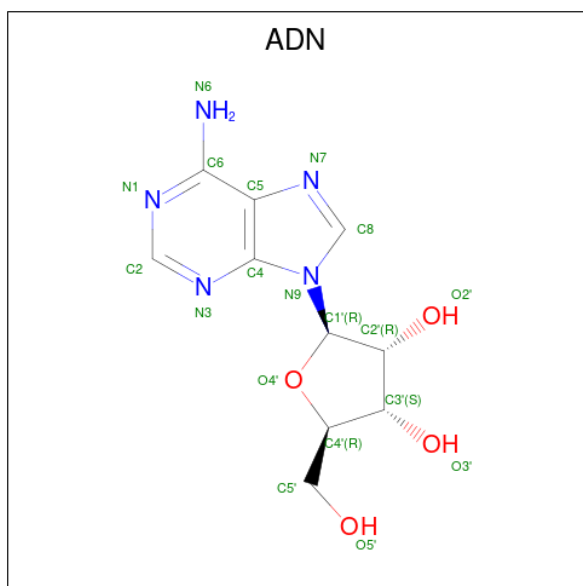
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	conflict	UNP P11652
B	330	GLU	ASP	conflict	UNP P11652
B	331	LEU	VAL	conflict	UNP P11652

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).

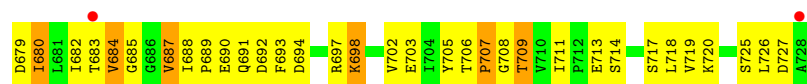


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	
			91	62	1	13	14	1	
								0	0

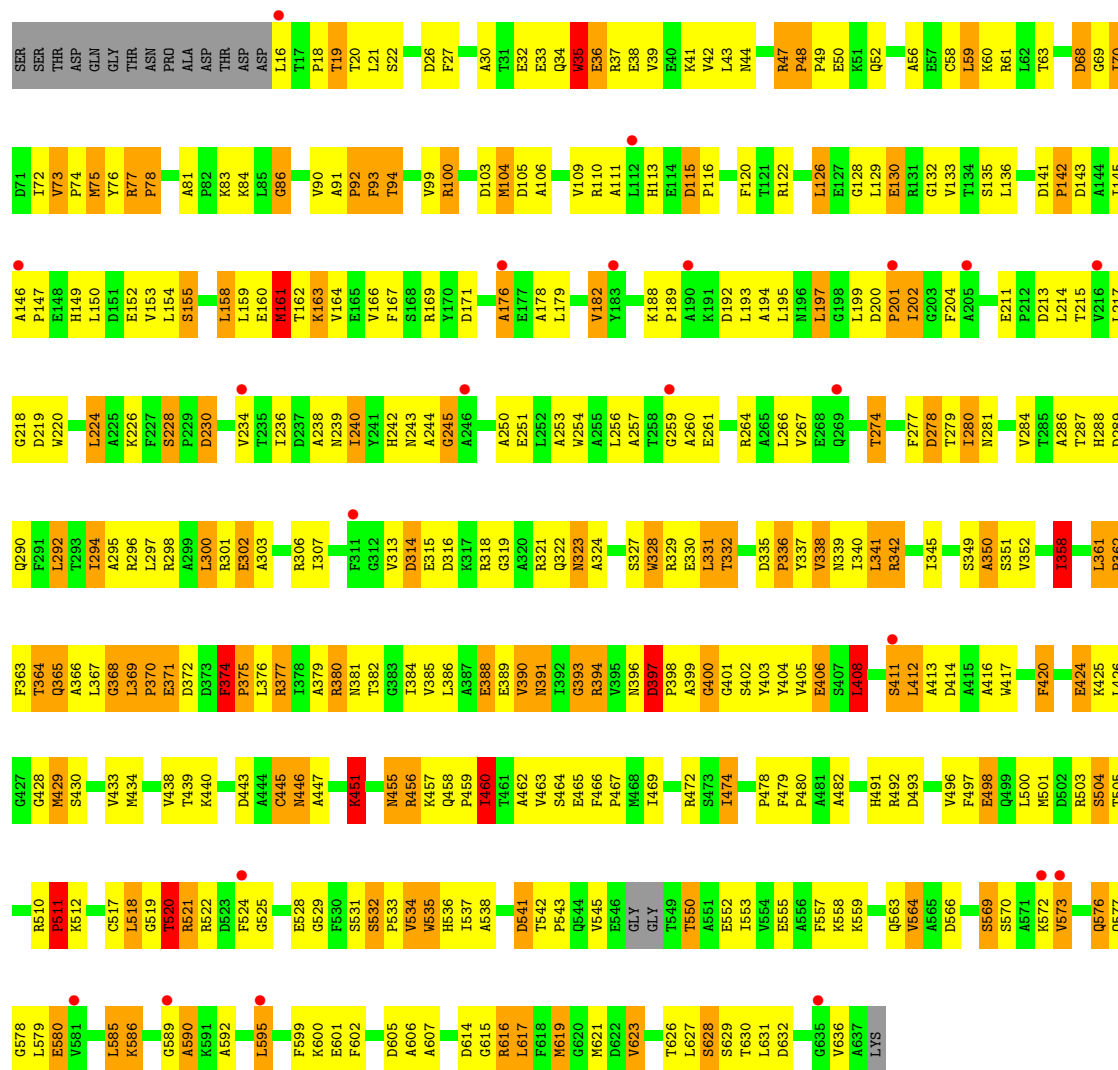
- Molecule 4 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O		
			18	10	5	3	0	0



● Molecule 2: METHYLMALONYL-COA MUTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.91Å 110.91Å 257.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.70) 97.4 (20.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.313 , 0.393 0.277 , 0.346	Depositor DCC
R_{free} test set	2225 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10285	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B12, ADN

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	0.88	1/5667 (0.0%)	2.82	643/7699 (8.4%)
2	B	0.82	1/4714 (0.0%)	2.69	455/6425 (7.1%)
All	All	0.85	2/10381 (0.0%)	2.76	1098/14124 (7.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
2	B	0	8
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	458	GLN	N-CA	-6.06	1.39	1.46
1	A	47	GLY	N-CA	5.40	1.48	1.44

All (1098) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	ARG	CD-NE-CZ	18.90	150.87	124.40
1	A	380	ALA	CA-C-N	16.80	143.29	120.44
1	A	380	ALA	C-N-CA	16.80	143.29	120.44
2	B	457	LYS	CA-C-N	16.59	143.57	123.16
2	B	457	LYS	C-N-CA	16.59	143.57	123.16
2	B	363	PHE	CA-CB-CG	16.32	130.12	113.80
1	A	206	VAL	N-CA-C	14.91	124.63	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	493	ASP	CA-CB-CG	14.81	127.41	112.60
1	A	299	ALA	O-C-N	-14.51	107.00	122.09
1	A	406	SER	CA-C-O	14.43	141.14	120.51
1	A	131	ARG	CD-NE-CZ	14.37	144.52	124.40
2	B	115	ASP	CA-C-O	14.24	131.67	119.71
1	A	23	ARG	CD-NE-CZ	13.91	143.88	124.40
2	B	503	ARG	CD-NE-CZ	13.57	143.40	124.40
1	A	118	ASP	CA-CB-CG	13.39	125.99	112.60
2	B	278	ASP	CA-CB-CG	13.20	125.80	112.60
1	A	529	ARG	CD-NE-CZ	13.15	142.81	124.40
1	A	612	ARG	NE-CZ-NH2	12.98	130.89	119.20
1	A	241	SER	CA-C-O	12.83	134.41	120.43
1	A	381	ARG	CD-NE-CZ	12.36	141.70	124.40
1	A	391	GLN	CB-CG-CD	12.28	133.47	112.60
2	B	147	PRO	CA-C-N	11.99	140.75	120.72
2	B	147	PRO	C-N-CA	11.99	140.75	120.72
1	A	537	ASP	CA-CB-CG	11.88	124.48	112.60
2	B	460	ILE	CB-CA-C	11.43	123.44	110.41
2	B	38	GLU	CA-C-N	11.39	138.99	120.30
2	B	38	GLU	C-N-CA	11.39	138.99	120.30
1	A	319	ASN	CA-CB-CG	11.22	123.82	112.60
1	A	708	GLY	CA-C-O	10.94	129.05	118.77
2	B	394	ARG	CD-NE-CZ	10.80	139.52	124.40
1	A	597	ARG	CD-NE-CZ	10.62	139.26	124.40
2	B	384	ILE	CA-C-O	-10.56	109.97	121.17
2	B	342	ARG	CD-NE-CZ	10.56	139.18	124.40
2	B	239	ASN	CA-CB-CG	10.51	123.11	112.60
1	A	287	PHE	CA-CB-CG	10.50	124.30	113.80
1	A	486	SER	CA-C-N	10.48	135.37	120.28
1	A	486	SER	C-N-CA	10.48	135.37	120.28
2	B	420	PHE	CA-CB-CG	10.46	124.26	113.80
1	A	225	PHE	CA-CB-CG	10.37	124.17	113.80
1	A	452	ARG	CD-NE-CZ	10.34	138.87	124.40
1	A	669	ARG	CD-NE-CZ	10.30	138.82	124.40
2	B	60	LYS	CA-C-N	10.24	135.88	120.31
2	B	60	LYS	C-N-CA	10.24	135.88	120.31
1	A	224	ILE	N-CA-C	-10.21	103.16	113.47
1	A	241	SER	O-C-N	-10.04	111.93	123.27
1	A	73	GLY	CA-C-N	10.04	129.70	119.56
1	A	73	GLY	C-N-CA	10.04	129.70	119.56
1	A	269	ALA	CA-C-N	10.02	132.97	120.34
1	A	269	ALA	C-N-CA	10.02	132.97	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	PRO	CA-C-N	10.00	133.69	120.28
1	A	578	PRO	C-N-CA	10.00	133.69	120.28
1	A	84	TRP	CA-C-N	9.91	136.76	122.09
1	A	84	TRP	C-N-CA	9.91	136.76	122.09
1	A	612	ARG	CD-NE-CZ	9.89	138.24	124.40
1	A	223	GLU	CA-C-N	9.79	133.00	122.14
1	A	223	GLU	C-N-CA	9.79	133.00	122.14
2	B	375	PRO	CA-C-N	9.62	134.13	120.28
2	B	375	PRO	C-N-CA	9.62	134.13	120.28
1	A	357	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	A	170	ALA	CA-C-N	9.54	135.54	120.47
1	A	170	ALA	C-N-CA	9.54	135.54	120.47
1	A	356	THR	CA-C-O	-9.50	110.74	120.90
1	A	88	GLN	CA-C-O	-9.46	109.51	120.49
1	A	340	ASP	CA-C-N	9.43	136.61	120.86
1	A	340	ASP	C-N-CA	9.43	136.61	120.86
1	A	367	SER	O-C-N	-9.32	112.62	123.06
2	B	100	ARG	CD-NE-CZ	9.31	137.43	124.40
2	B	38	GLU	N-CA-C	9.29	122.39	111.71
1	A	465	ILE	CA-C-O	9.28	132.38	120.78
1	A	693	PHE	CA-CB-CG	9.23	123.03	113.80
1	A	406	SER	CA-C-N	9.20	132.96	120.54
1	A	406	SER	C-N-CA	9.20	132.96	120.54
1	A	79	TYR	CA-C-N	9.16	133.48	120.28
1	A	79	TYR	C-N-CA	9.16	133.48	120.28
2	B	72	ILE	CA-C-O	9.14	130.53	120.48
2	B	403	TYR	CA-C-N	9.12	133.46	120.79
2	B	403	TYR	C-N-CA	9.12	133.46	120.79
1	A	128	ASP	CA-CB-CG	9.11	121.71	112.60
1	A	262	ASP	CA-C-O	-9.00	110.91	120.63
1	A	276	ASN	CA-CB-CG	8.98	121.58	112.60
1	A	299	ALA	CA-C-O	8.98	130.51	120.90
1	A	258	TYR	CA-C-N	8.97	132.64	120.44
1	A	258	TYR	C-N-CA	8.97	132.64	120.44
2	B	327	SER	CA-C-N	8.96	133.01	120.29
2	B	327	SER	C-N-CA	8.96	133.01	120.29
1	A	20	ASP	CA-CB-CG	8.94	121.54	112.60
1	A	300	LYS	CA-C-N	8.94	135.63	120.71
1	A	300	LYS	C-N-CA	8.94	135.63	120.71
1	A	354	ALA	CA-C-O	-8.81	111.57	120.82
1	A	243	TYR	CA-C-N	8.81	132.96	120.28
1	A	243	TYR	C-N-CA	8.81	132.96	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	ARG	NH1-CZ-NH2	-8.80	107.86	119.30
2	B	115	ASP	O-C-N	-8.77	114.19	121.38
2	B	337	TYR	CA-C-N	8.76	134.39	121.77
2	B	337	TYR	C-N-CA	8.76	134.39	121.77
1	A	101	PHE	CA-CB-CG	8.76	122.56	113.80
2	B	632	ASP	CA-C-N	8.72	134.34	120.82
2	B	632	ASP	C-N-CA	8.72	134.34	120.82
2	B	632	ASP	CA-CB-CG	8.67	121.27	112.60
2	B	391	ASN	OD1-CG-ND2	-8.64	113.96	122.60
2	B	211	GLU	CA-C-O	8.62	126.32	119.59
2	B	585	LEU	CA-C-O	-8.62	111.59	121.07
1	A	530	ASN	CA-CB-CG	8.56	121.16	112.60
1	A	403	TRP	CA-C-O	-8.55	111.36	120.42
1	A	407	ALA	N-CA-CB	-8.55	97.20	109.94
1	A	303	ALA	O-C-N	-8.47	111.32	122.59
1	A	622	ALA	CA-C-N	8.40	132.22	120.29
1	A	622	ALA	C-N-CA	8.40	132.22	120.29
1	A	46	VAL	CA-C-O	-8.36	111.30	120.67
1	A	294	PHE	CA-C-O	8.35	132.45	120.51
2	B	382	THR	O-C-N	8.35	131.11	122.09
2	B	78	PRO	O-C-N	-8.34	112.08	122.17
1	A	727	ASP	CA-CB-CG	8.33	120.93	112.60
1	A	415	ASP	CA-CB-CG	8.32	120.92	112.60
2	B	171	ASP	CA-CB-CG	8.31	120.92	112.60
1	A	25	PHE	CA-C-N	8.29	131.74	120.54
1	A	25	PHE	C-N-CA	8.29	131.74	120.54
1	A	326	ARG	CA-C-O	8.29	129.44	120.32
2	B	524	PHE	CA-CB-CG	8.29	122.09	113.80
1	A	247	GLU	CA-C-N	8.28	132.90	120.31
1	A	247	GLU	C-N-CA	8.28	132.90	120.31
1	A	41	ALA	CA-C-N	8.24	135.56	121.14
1	A	41	ALA	C-N-CA	8.24	135.56	121.14
1	A	17	VAL	CA-C-O	8.22	125.20	119.20
2	B	512	LYS	O-C-N	-8.17	113.28	123.17
1	A	484	ASP	CA-CB-CG	8.17	120.77	112.60
2	B	457	LYS	CA-C-O	8.15	128.44	119.15
1	A	358	GLY	CA-C-N	8.10	137.02	121.54
1	A	358	GLY	C-N-CA	8.10	137.02	121.54
2	B	367	LEU	N-CA-C	8.10	119.89	111.14
1	A	21	ALA	CA-C-N	8.08	131.45	120.54
1	A	21	ALA	C-N-CA	8.08	131.45	120.54
2	B	56	ALA	O-C-N	-8.07	113.37	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ARG	CB-CG-CD	8.07	129.86	111.30
1	A	177	LEU	CA-C-N	8.05	134.34	120.58
1	A	177	LEU	C-N-CA	8.05	134.34	120.58
2	B	408	LEU	O-C-N	-8.04	112.87	122.11
1	A	231	ASN	N-CA-C	8.03	122.70	113.15
1	A	278	ASP	CA-C-N	8.03	134.83	122.23
1	A	278	ASP	C-N-CA	8.03	134.83	122.23
1	A	608	ASP	CA-CB-CG	8.02	120.61	112.60
2	B	132	GLY	CA-C-O	-7.99	109.93	119.03
1	A	66	GLY	CA-C-N	7.98	130.38	123.04
1	A	66	GLY	C-N-CA	7.98	130.38	123.04
1	A	313	HIS	O-C-N	-7.97	113.86	122.07
1	A	619	THR	O-C-N	-7.95	111.68	122.33
2	B	366	ALA	CA-C-N	7.94	131.24	120.44
2	B	366	ALA	C-N-CA	7.94	131.24	120.44
1	A	60	TRP	CA-C-N	7.91	138.13	122.31
1	A	60	TRP	C-N-CA	7.91	138.13	122.31
1	A	330	GLN	CA-C-O	-7.91	110.55	120.28
2	B	52	GLN	CA-CB-CG	7.91	129.91	114.10
1	A	677	ARG	N-CA-C	7.91	124.99	108.39
2	B	631	LEU	CA-C-N	7.90	131.91	120.38
2	B	631	LEU	C-N-CA	7.90	131.91	120.38
2	B	111	ALA	CA-C-N	7.90	133.27	122.77
2	B	111	ALA	C-N-CA	7.90	133.27	122.77
2	B	289	ASP	CA-CB-CG	-7.89	104.71	112.60
2	B	106	ALA	CA-C-N	7.89	136.62	121.54
2	B	106	ALA	C-N-CA	7.89	136.62	121.54
2	B	380	ARG	CD-NE-CZ	7.89	135.44	124.40
2	B	314	ASP	CA-C-N	7.88	133.22	120.60
2	B	314	ASP	C-N-CA	7.88	133.22	120.60
1	A	577	THR	CA-C-N	7.88	129.69	119.84
1	A	577	THR	C-N-CA	7.88	129.69	119.84
1	A	428	GLU	CA-C-N	7.86	135.70	122.65
1	A	428	GLU	C-N-CA	7.86	135.70	122.65
1	A	495	LYS	N-CA-C	-7.86	103.82	113.41
1	A	726	LEU	N-CA-C	7.86	120.93	111.82
1	A	320	PRO	CA-C-N	7.83	135.17	122.65
1	A	320	PRO	C-N-CA	7.83	135.17	122.65
1	A	597	ARG	NE-CZ-NH1	7.82	129.32	121.50
1	A	40	THR	CA-C-N	7.81	133.09	120.60
1	A	40	THR	C-N-CA	7.81	133.09	120.60
1	A	228	THR	N-CA-CB	7.80	121.30	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	408	LEU	CA-C-N	7.78	131.61	120.79
2	B	408	LEU	C-N-CA	7.78	131.61	120.79
2	B	306	ARG	CD-NE-CZ	7.77	135.28	124.40
2	B	52	GLN	N-CA-CB	7.72	124.27	110.83
2	B	365	GLN	N-CA-C	7.72	122.28	113.01
1	A	277	VAL	O-C-N	-7.72	114.34	121.91
2	B	385	VAL	O-C-N	-7.72	114.35	121.91
1	A	578	PRO	N-CA-CB	7.71	111.34	103.25
1	A	310	LYS	O-C-N	-7.70	112.35	122.59
1	A	593	ALA	N-CA-C	7.70	122.11	112.87
1	A	613	GLY	O-C-N	-7.70	112.69	122.70
1	A	115	VAL	CB-CA-C	-7.67	100.70	111.21
2	B	456	ARG	NE-CZ-NH2	7.67	126.10	119.20
1	A	68	PRO	N-CA-CB	7.64	110.49	103.08
2	B	264	ARG	CD-NE-CZ	7.64	135.10	124.40
2	B	68	ASP	CA-CB-CG	7.64	120.24	112.60
2	B	358	ILE	N-CA-CB	7.62	121.55	111.64
1	A	51	ASN	N-CA-C	7.62	118.30	108.24
1	A	31	LYS	O-C-N	-7.62	112.22	122.43
1	A	614	GLN	CA-C-N	7.62	131.89	120.31
1	A	614	GLN	C-N-CA	7.62	131.89	120.31
1	A	389	PHE	CA-CB-CG	7.61	121.41	113.80
2	B	534	VAL	CA-C-N	7.59	131.07	120.29
2	B	534	VAL	C-N-CA	7.59	131.07	120.29
1	A	392	GLN	CA-C-O	-7.58	111.82	120.24
1	A	215	GLN	CA-C-N	7.58	127.22	119.56
1	A	215	GLN	C-N-CA	7.58	127.22	119.56
2	B	433	VAL	CA-C-N	7.58	130.77	120.38
2	B	433	VAL	C-N-CA	7.58	130.77	120.38
1	A	626	PHE	CA-CB-CG	7.55	121.35	113.80
2	B	242	HIS	CA-C-N	7.55	130.40	120.28
2	B	242	HIS	C-N-CA	7.55	130.40	120.28
2	B	152	GLU	CA-C-O	-7.55	112.89	120.82
2	B	626	THR	CA-C-O	-7.54	112.90	120.82
2	B	286	ALA	CA-C-O	7.54	128.32	120.40
2	B	521	ARG	N-CA-C	7.53	121.39	111.75
1	A	469	LYS	O-C-N	-7.52	114.83	123.33
1	A	437	ILE	CA-C-N	7.52	130.57	120.65
1	A	437	ILE	C-N-CA	7.52	130.57	120.65
2	B	443	ASP	CA-C-N	7.51	130.96	120.29
2	B	443	ASP	C-N-CA	7.51	130.96	120.29
1	A	528	ASP	CA-CB-CG	7.50	120.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	VAL	CA-C-O	7.50	127.84	120.27
2	B	536	HIS	CA-C-N	7.49	131.06	120.42
2	B	536	HIS	C-N-CA	7.49	131.06	120.42
1	A	496	LEU	CA-C-N	7.49	130.06	120.70
1	A	496	LEU	C-N-CA	7.49	130.06	120.70
1	A	352	ALA	CA-C-N	7.48	130.91	120.29
1	A	352	ALA	C-N-CA	7.48	130.91	120.29
2	B	606	ALA	N-CA-C	7.46	120.28	111.71
1	A	678	PRO	CA-C-N	7.45	130.13	120.44
1	A	678	PRO	C-N-CA	7.45	130.13	120.44
1	A	74	PRO	CA-C-N	7.45	134.51	122.81
1	A	74	PRO	C-N-CA	7.45	134.51	122.81
1	A	333	GLY	CA-C-N	7.45	130.87	120.29
1	A	333	GLY	C-N-CA	7.45	130.87	120.29
2	B	462	ALA	CA-C-N	7.45	135.38	121.97
2	B	462	ALA	C-N-CA	7.45	135.38	121.97
1	A	340	ASP	O-C-N	-7.44	113.71	122.86
2	B	382	THR	CA-C-O	-7.42	113.06	120.70
2	B	32	GLU	CA-C-N	7.42	130.82	120.29
2	B	32	GLU	C-N-CA	7.42	130.82	120.29
1	A	673	ASP	CA-CB-CG	7.41	120.01	112.60
2	B	115	ASP	CA-C-N	7.39	127.02	119.19
2	B	115	ASP	C-N-CA	7.39	127.02	119.19
2	B	120	PHE	N-CA-C	-7.39	102.85	112.68
1	A	320	PRO	O-C-N	-7.39	112.67	122.64
1	A	241	SER	N-CA-C	7.38	121.26	109.24
2	B	146	ALA	CA-C-N	7.36	129.04	119.84
2	B	146	ALA	C-N-CA	7.36	129.04	119.84
2	B	34	GLN	OE1-CD-NE2	7.36	129.96	122.60
2	B	176	ALA	CA-C-N	7.36	134.65	121.92
2	B	176	ALA	C-N-CA	7.36	134.65	121.92
1	A	470	TYR	CA-C-N	7.36	131.86	120.75
1	A	470	TYR	C-N-CA	7.36	131.86	120.75
1	A	139	ALA	CA-C-N	7.35	130.50	120.72
1	A	139	ALA	C-N-CA	7.35	130.50	120.72
1	A	182	ALA	CA-C-N	7.33	132.96	120.72
1	A	182	ALA	C-N-CA	7.33	132.96	120.72
2	B	160	GLU	CA-C-N	7.32	130.69	120.29
2	B	160	GLU	C-N-CA	7.32	130.69	120.29
2	B	69	GLY	N-CA-C	7.32	124.71	115.42
2	B	260	ALA	CA-C-N	7.32	130.40	120.38
2	B	260	ALA	C-N-CA	7.32	130.40	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	455	ASN	OD1-CG-ND2	-7.31	115.29	122.60
2	B	105	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	465	ILE	CA-C-N	7.28	133.94	122.51
1	A	465	ILE	C-N-CA	7.28	133.94	122.51
1	A	168	ASN	CA-CB-CG	7.28	119.88	112.60
1	A	469	LYS	CA-C-N	7.28	132.72	122.46
1	A	469	LYS	C-N-CA	7.28	132.72	122.46
2	B	446	ASN	CA-C-N	7.28	133.03	120.58
2	B	446	ASN	C-N-CA	7.28	133.03	120.58
2	B	557	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	206	VAL	CB-CA-C	-7.27	103.19	111.55
2	B	35	TRP	N-CA-C	-7.27	102.75	111.69
1	A	290	ILE	N-CA-CB	7.24	121.36	112.10
1	A	332	SER	O-C-N	-7.23	114.03	122.93
2	B	323	ASN	CA-CB-CG	7.22	119.82	112.60
1	A	295	PHE	CA-C-O	-7.22	112.89	120.55
1	A	410	GLU	CA-CB-CG	7.22	128.53	114.10
1	A	545	VAL	CA-C-N	7.22	127.95	119.94
1	A	545	VAL	C-N-CA	7.22	127.95	119.94
1	A	541	ALA	CA-C-N	7.21	135.31	121.54
1	A	541	ALA	C-N-CA	7.21	135.31	121.54
2	B	152	GLU	CB-CG-CD	7.20	124.84	112.60
2	B	382	THR	CA-C-N	7.19	127.91	120.00
2	B	382	THR	C-N-CA	7.19	127.91	120.00
1	A	61	LEU	N-CA-C	7.19	121.71	113.15
1	A	135	ASP	CA-C-O	7.19	126.66	118.97
1	A	132	VAL	N-CA-C	7.18	122.23	111.89
2	B	543	PRO	N-CA-CB	7.18	110.00	103.33
2	B	159	LEU	N-CA-C	7.16	120.91	111.75
2	B	288	HIS	CA-CB-CG	7.16	120.96	113.80
1	A	344	ASN	CA-CB-CG	7.15	119.75	112.60
1	A	463	PRO	N-CA-CB	7.15	110.76	103.25
1	A	22	ALA	CA-C-N	7.14	129.73	120.44
1	A	22	ALA	C-N-CA	7.14	129.73	120.44
1	A	41	ALA	CA-C-O	7.14	128.13	119.49
2	B	629	SER	O-C-N	-7.14	114.72	122.07
2	B	277	PHE	N-CA-C	7.14	121.68	113.19
1	A	123	ARG	CA-C-N	7.12	130.87	120.11
1	A	123	ARG	C-N-CA	7.12	130.87	120.11
1	A	384	ARG	NE-CZ-NH1	-7.11	114.39	121.50
2	B	167	PHE	CA-CB-CG	7.11	120.91	113.80
2	B	176	ALA	O-C-N	-7.11	112.65	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	577	GLN	N-CA-C	7.10	121.66	112.92
1	A	121	THR	CA-C-O	-7.10	113.26	121.07
2	B	474	ILE	O-C-N	-7.09	114.91	123.00
1	A	725	SER	CA-C-N	7.08	131.08	120.31
1	A	725	SER	C-N-CA	7.08	131.08	120.31
1	A	658	ALA	CA-C-N	7.08	135.80	121.78
1	A	658	ALA	C-N-CA	7.08	135.80	121.78
1	A	720	LYS	CA-C-N	7.08	130.08	120.38
1	A	720	LYS	C-N-CA	7.08	130.08	120.38
2	B	372	ASP	CA-CB-CG	7.08	119.67	112.60
1	A	40	THR	O-C-N	-7.07	113.18	122.59
1	A	392	GLN	N-CA-C	7.07	120.39	111.69
2	B	220	TRP	CA-C-N	7.07	131.89	120.30
2	B	220	TRP	C-N-CA	7.07	131.89	120.30
2	B	467	PRO	N-CA-CB	7.07	109.90	103.33
1	A	252	ALA	CA-C-N	7.06	129.74	120.28
1	A	252	ALA	C-N-CA	7.06	129.74	120.28
2	B	381	ASN	CA-C-N	7.05	130.02	120.44
2	B	381	ASN	C-N-CA	7.05	130.02	120.44
2	B	113	HIS	CA-CB-CG	-7.03	106.77	113.80
1	A	271	GLU	CA-C-N	7.01	133.24	122.23
1	A	271	GLU	C-N-CA	7.01	133.24	122.23
1	A	711	ILE	CA-C-N	7.01	128.60	119.84
1	A	711	ILE	C-N-CA	7.01	128.60	119.84
2	B	342	ARG	O-C-N	-7.01	114.85	122.07
2	B	314	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	278	ASP	O-C-N	-7.00	113.28	122.59
2	B	315	GLU	N-CA-C	6.99	120.91	112.38
2	B	338	VAL	O-C-N	-6.99	115.21	122.20
1	A	622	ALA	O-C-N	-6.98	114.72	122.12
1	A	677	ARG	CA-C-N	6.96	126.57	119.19
1	A	677	ARG	C-N-CA	6.96	126.57	119.19
1	A	419	LYS	CA-C-N	6.96	130.17	120.29
1	A	419	LYS	C-N-CA	6.96	130.17	120.29
1	A	438	GLU	CA-C-N	6.95	131.82	120.63
1	A	438	GLU	C-N-CA	6.95	131.82	120.63
2	B	201	PRO	O-C-N	-6.94	114.25	122.24
2	B	617	LEU	N-CA-CB	6.94	121.48	110.65
2	B	109	VAL	N-CA-CB	6.93	119.84	111.31
2	B	434	MET	N-CA-C	6.93	119.72	111.33
2	B	380	ARG	N-CA-CB	6.93	120.31	110.12
1	A	598	PRO	N-CA-CB	6.93	109.43	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ALA	CA-C-O	6.91	129.63	120.16
1	A	228	THR	CA-C-O	-6.91	113.75	121.00
1	A	100	ALA	CA-C-N	6.90	129.85	120.54
1	A	100	ALA	C-N-CA	6.90	129.85	120.54
1	A	52	GLU	O-C-N	-6.88	113.44	122.39
1	A	348	THR	CA-C-N	6.88	130.77	120.31
1	A	348	THR	C-N-CA	6.88	130.77	120.31
1	A	38	TRP	CA-C-N	-6.88	112.59	122.77
1	A	38	TRP	C-N-CA	-6.88	112.59	122.77
1	A	595	GLY	CA-C-N	6.88	134.67	121.54
1	A	595	GLY	C-N-CA	6.88	134.67	121.54
1	A	382	ILE	CA-C-N	6.87	129.37	120.44
1	A	382	ILE	C-N-CA	6.87	129.37	120.44
1	A	643	GLN	CA-C-N	6.87	129.48	120.28
1	A	643	GLN	C-N-CA	6.87	129.48	120.28
2	B	63	THR	CA-C-O	-6.86	113.23	121.05
2	B	349	SER	CA-C-O	-6.85	113.23	120.63
2	B	501	MET	CA-C-N	6.83	129.99	120.29
2	B	501	MET	C-N-CA	6.83	129.99	120.29
2	B	26	ASP	CA-C-O	6.83	126.93	119.15
2	B	122	ARG	CA-C-O	-6.81	113.61	120.90
2	B	391	ASN	CA-CB-CG	6.81	119.41	112.60
1	A	405	GLY	CA-C-O	-6.80	117.15	122.52
1	A	334	TRP	CA-C-O	-6.78	113.24	120.42
2	B	143	ASP	CA-C-N	6.77	133.49	122.39
2	B	143	ASP	C-N-CA	6.77	133.49	122.39
1	A	328	HIS	CA-CB-CG	6.76	120.56	113.80
1	A	322	SER	CA-C-N	6.75	134.62	122.06
1	A	322	SER	C-N-CA	6.75	134.62	122.06
1	A	281	ALA	N-CA-C	6.75	121.39	112.35
1	A	127	SER	CA-C-N	6.74	132.16	121.44
1	A	127	SER	C-N-CA	6.74	132.16	121.44
2	B	76	TYR	CB-CA-C	6.74	120.89	109.50
2	B	86	GLY	O-C-N	-6.74	114.82	122.64
2	B	403	TYR	CA-C-O	6.72	128.89	121.02
1	A	67	ILE	CA-C-N	6.71	127.30	120.38
1	A	67	ILE	C-N-CA	6.71	127.30	120.38
1	A	321	LYS	CA-C-O	6.71	127.42	119.56
2	B	289	ASP	CA-C-O	6.71	127.90	120.92
1	A	497	VAL	CA-CB-CG1	6.71	121.80	110.40
1	A	635	GLN	OE1-CD-NE2	-6.70	115.90	122.60
2	B	169	ARG	NE-CZ-NH2	6.70	125.23	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	280	ILE	CB-CG1-CD1	6.70	127.86	113.80
1	A	375	PRO	N-CA-CB	6.68	109.56	103.34
2	B	381	ASN	O-C-N	-6.68	112.68	122.43
2	B	535	TRP	O-C-N	-6.67	114.55	122.15
1	A	647	ALA	CA-C-O	6.67	127.52	119.78
1	A	389	PHE	CA-C-O	-6.67	113.48	120.55
2	B	70	ILE	CB-CG1-CD1	6.66	127.79	113.80
1	A	713	GLU	O-C-N	-6.65	115.07	122.12
1	A	245	MET	CA-C-N	6.65	129.85	120.28
1	A	245	MET	C-N-CA	6.65	129.85	120.28
2	B	340	ILE	CA-C-N	6.64	129.17	120.28
2	B	340	ILE	C-N-CA	6.64	129.17	120.28
1	A	357	GLN	CB-CG-CD	6.62	123.86	112.60
1	A	368	LEU	N-CA-C	6.62	119.32	111.71
1	A	405	GLY	N-CA-C	-6.62	104.33	112.33
1	A	673	ASP	O-C-N	-6.61	114.20	122.20
1	A	443	LYS	CA-C-N	6.60	129.42	120.44
1	A	443	LYS	C-N-CA	6.60	129.42	120.44
2	B	336	PRO	O-C-N	-6.60	113.32	122.30
2	B	388	GLU	OE1-CD-OE2	-6.60	107.05	122.90
2	B	239	ASN	CA-C-O	-6.60	113.56	120.55
1	A	82	ARG	CA-C-O	6.58	126.54	120.09
2	B	555	GLU	N-CA-C	6.58	119.45	111.82
1	A	52	GLU	CA-CB-CG	6.58	127.26	114.10
1	A	5	PRO	N-CA-CB	6.58	109.04	103.25
1	A	307	LEU	N-CA-CB	6.58	120.70	110.44
1	A	31	LYS	CA-C-O	6.56	127.45	119.38
1	A	28	LEU	CA-C-O	6.56	127.53	119.79
1	A	513	ASP	CA-C-N	6.55	131.82	120.68
1	A	513	ASP	C-N-CA	6.55	131.82	120.68
2	B	558	LYS	CA-C-N	6.55	129.35	120.44
2	B	558	LYS	C-N-CA	6.55	129.35	120.44
1	A	49	LEU	N-CA-CB	6.55	121.39	110.59
2	B	497	PHE	CA-C-N	6.54	128.94	120.44
2	B	497	PHE	C-N-CA	6.54	128.94	120.44
2	B	77	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	A	617	ILE	O-C-N	-6.53	113.22	121.84
1	A	200	ILE	CB-CG1-CD1	6.53	127.51	113.80
2	B	627	LEU	N-CA-C	6.53	118.40	111.28
1	A	327	THR	N-CA-C	6.53	119.81	109.50
2	B	379	ALA	CA-C-N	6.53	129.03	120.28
2	B	379	ALA	C-N-CA	6.53	129.03	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	566	ASP	CA-CB-CG	6.53	119.12	112.60
1	A	398	ARG	CB-CA-C	6.52	121.06	110.95
2	B	465	GLU	O-C-N	-6.52	114.94	123.28
1	A	66	GLY	O-C-N	-6.52	114.23	122.70
1	A	146	ILE	N-CA-C	6.50	117.25	110.62
2	B	295	ALA	N-CA-C	6.50	119.19	111.33
1	A	487	THR	N-CA-C	6.49	119.17	111.71
1	A	288	TRP	CA-C-N	6.49	128.66	122.36
1	A	288	TRP	C-N-CA	6.49	128.66	122.36
1	A	603	ALA	N-CA-C	6.49	120.03	109.59
1	A	480	VAL	N-CA-C	6.48	116.58	107.37
1	A	303	ALA	CA-C-N	6.47	128.95	120.28
1	A	303	ALA	C-N-CA	6.47	128.95	120.28
2	B	182	VAL	CB-CA-C	-6.47	103.60	111.88
2	B	243	ASN	O-C-N	-6.47	115.26	122.12
1	A	527	PRO	N-CA-C	6.47	122.25	113.84
1	A	31	LYS	CA-C-N	6.47	134.19	121.58
1	A	31	LYS	C-N-CA	6.47	134.19	121.58
1	A	568	GLY	CA-C-N	6.47	128.61	120.72
1	A	568	GLY	C-N-CA	6.47	128.61	120.72
1	A	441	ILE	CA-C-N	6.46	125.89	118.85
1	A	441	ILE	C-N-CA	6.46	125.89	118.85
2	B	200	ASP	CA-C-N	6.46	126.68	119.32
2	B	200	ASP	C-N-CA	6.46	126.68	119.32
1	A	407	ALA	CA-C-O	-6.45	114.00	120.90
1	A	232	MET	CA-C-N	6.45	126.21	119.05
1	A	232	MET	C-N-CA	6.45	126.21	119.05
2	B	578	GLY	CA-C-O	-6.44	112.05	119.65
2	B	578	GLY	N-CA-C	6.44	122.23	113.99
2	B	369	LEU	CA-C-O	6.44	127.72	120.70
2	B	128	GLY	O-C-N	-6.43	114.34	122.70
1	A	526	ASP	CA-C-N	6.43	126.12	119.56
1	A	526	ASP	C-N-CA	6.43	126.12	119.56
1	A	54	VAL	CA-C-N	6.43	129.42	120.29
1	A	54	VAL	C-N-CA	6.43	129.42	120.29
1	A	611	ASP	CA-CB-CG	6.43	119.03	112.60
2	B	370	PRO	N-CA-CB	6.43	109.05	103.27
2	B	628	SER	CA-C-N	6.42	128.78	120.44
2	B	628	SER	C-N-CA	6.42	128.78	120.44
1	A	74	PRO	CB-CA-C	-6.42	102.31	111.68
2	B	142	PRO	CA-C-N	6.42	135.14	122.31
2	B	142	PRO	C-N-CA	6.42	135.14	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	472	ARG	NE-CZ-NH2	6.42	124.97	119.20
1	A	294	PHE	CA-CB-CG	-6.41	107.39	113.80
2	B	388	GLU	CG-CD-OE1	6.41	133.15	118.40
1	A	418	ARG	O-C-N	-6.41	115.17	122.09
1	A	63	THR	N-CA-CB	6.41	119.16	110.38
2	B	328	TRP	O-C-N	-6.41	114.85	122.15
1	A	201	LEU	O-C-N	-6.40	114.45	122.20
2	B	382	THR	CA-CB-OG1	-6.40	100.00	109.60
1	A	573	GLU	N-CA-C	6.40	118.25	111.28
2	B	377	ARG	CA-C-N	6.39	129.50	120.42
2	B	377	ARG	C-N-CA	6.39	129.50	120.42
1	A	558	ARG	CD-NE-CZ	6.39	133.35	124.40
1	A	641	ALA	CA-C-N	6.39	129.67	120.79
1	A	641	ALA	C-N-CA	6.39	129.67	120.79
1	A	637	PRO	CA-C-N	6.39	132.41	122.26
1	A	637	PRO	C-N-CA	6.39	132.41	122.26
2	B	60	LYS	O-C-N	-6.38	115.35	122.12
1	A	525	LYS	CA-C-O	6.38	126.07	119.05
1	A	66	GLY	CA-C-O	6.38	131.66	120.57
1	A	398	ARG	CA-C-N	6.38	131.28	121.71
1	A	398	ARG	C-N-CA	6.38	131.28	121.71
1	A	122	HIS	N-CA-C	6.38	119.04	111.33
2	B	345	ILE	CB-CG1-CD1	6.37	127.17	113.80
1	A	129	ASN	CA-C-O	6.36	125.53	120.19
1	A	677	ARG	N-CA-CB	-6.34	101.89	111.21
2	B	607	ALA	CA-C-N	6.34	131.42	120.58
2	B	607	ALA	C-N-CA	6.34	131.42	120.58
1	A	370	GLU	N-CA-CB	-6.34	101.31	110.56
2	B	466	PHE	CA-C-N	6.33	126.25	119.85
2	B	466	PHE	C-N-CA	6.33	126.25	119.85
2	B	77	ARG	CA-C-N	6.33	126.81	119.47
2	B	77	ARG	C-N-CA	6.33	126.81	119.47
2	B	335	ASP	CA-C-N	6.32	125.95	119.56
2	B	335	ASP	C-N-CA	6.32	125.95	119.56
1	A	439	LYS	N-CA-C	6.32	120.55	112.34
1	A	358	GLY	O-C-N	-6.31	114.50	122.70
2	B	318	ARG	CD-NE-CZ	6.31	133.24	124.40
1	A	213	PRO	CA-C-N	6.31	127.72	119.84
1	A	213	PRO	C-N-CA	6.31	127.72	119.84
2	B	451	LYS	CA-C-O	-6.30	113.87	120.55
2	B	390	VAL	CA-C-O	6.30	127.45	120.46
1	A	241	SER	CA-C-N	6.29	133.75	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	SER	C-N-CA	6.29	133.75	121.41
2	B	48	PRO	CA-C-N	6.29	126.03	119.05
2	B	48	PRO	C-N-CA	6.29	126.03	119.05
1	A	280	PHE	CA-C-N	6.28	127.57	119.78
1	A	280	PHE	C-N-CA	6.28	127.57	119.78
1	A	697	ARG	O-C-N	-6.28	114.99	122.15
1	A	213	PRO	N-CA-CB	6.26	109.15	103.08
1	A	289	GLY	O-C-N	-6.26	116.97	123.48
2	B	397	ASP	CA-C-N	6.26	125.83	119.19
2	B	397	ASP	C-N-CA	6.26	125.83	119.19
1	A	385	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	518	ALA	CA-C-N	6.26	128.95	120.44
1	A	518	ALA	C-N-CA	6.26	128.95	120.44
1	A	41	ALA	N-CA-C	6.25	120.00	112.38
1	A	523	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	105	ASN	CA-C-N	6.25	129.47	120.79
1	A	105	ASN	C-N-CA	6.25	129.47	120.79
1	A	18	PRO	N-CA-CB	6.23	109.80	103.25
1	A	628	VAL	CA-C-O	6.23	127.09	120.48
2	B	394	ARG	CA-C-O	6.23	127.15	119.79
2	B	440	LYS	CA-C-N	6.23	128.41	120.56
2	B	440	LYS	C-N-CA	6.23	128.41	120.56
1	A	121	THR	CA-C-N	6.23	128.92	120.38
1	A	121	THR	C-N-CA	6.23	128.92	120.38
1	A	84	TRP	O-C-N	-6.23	114.31	122.59
1	A	343	ASN	CA-C-N	6.23	131.12	120.72
1	A	343	ASN	C-N-CA	6.23	131.12	120.72
2	B	43	LEU	N-CA-C	6.23	119.04	111.82
1	A	387	GLN	CA-C-N	6.22	128.94	120.54
1	A	387	GLN	C-N-CA	6.22	128.94	120.54
2	B	20	THR	N-CA-CB	6.22	120.60	110.90
2	B	18	PRO	CA-C-O	-6.22	113.85	121.31
2	B	146	ALA	CA-C-O	6.22	127.48	120.70
1	A	322	SER	CA-C-O	6.21	126.87	119.60
2	B	319	GLY	CA-C-O	-6.21	115.73	120.76
1	A	319	ASN	CB-CA-C	6.21	119.17	109.42
1	A	304	ALA	CA-C-N	6.21	128.92	120.54
1	A	304	ALA	C-N-CA	6.21	128.92	120.54
1	A	14	ASN	CA-C-O	6.21	125.96	119.51
1	A	553	GLU	CA-CB-CG	6.20	126.51	114.10
1	A	551	ALA	CA-C-N	6.20	131.99	121.14
1	A	551	ALA	C-N-CA	6.20	131.99	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	364	THR	O-C-N	-6.20	114.63	122.26
1	A	339	GLN	O-C-N	-6.20	115.35	123.16
2	B	350	ALA	CA-C-N	6.20	128.87	120.44
2	B	350	ALA	C-N-CA	6.20	128.87	120.44
2	B	529	GLY	N-CA-C	6.19	121.92	113.99
1	A	81	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	194	GLY	CA-C-O	6.18	127.84	121.35
2	B	384	ILE	N-CA-CB	6.18	117.78	110.55
1	A	332	SER	CA-C-O	6.17	127.91	120.81
2	B	352	VAL	CA-C-N	6.17	133.51	121.41
2	B	352	VAL	C-N-CA	6.17	133.51	121.41
1	A	357	GLN	CA-C-N	6.17	133.50	121.41
1	A	357	GLN	C-N-CA	6.17	133.50	121.41
2	B	238	ALA	CA-C-N	6.17	128.54	120.28
2	B	238	ALA	C-N-CA	6.17	128.54	120.28
2	B	230	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	692	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	171	VAL	CB-CA-C	-6.15	102.62	112.16
1	A	687	VAL	O-C-N	-6.14	114.89	122.57
1	A	171	VAL	CA-C-O	-6.14	114.00	120.57
1	A	659	GLY	N-CA-C	6.14	123.51	115.47
1	A	355	ALA	O-C-N	-6.13	114.44	122.59
1	A	521	ASN	CA-C-N	6.13	127.34	120.66
1	A	521	ASN	C-N-CA	6.13	127.34	120.66
1	A	421	TRP	CA-C-N	6.13	126.91	119.99
1	A	421	TRP	C-N-CA	6.13	126.91	119.99
1	A	590	PHE	CA-C-O	-6.13	113.85	121.02
1	A	44	ILE	N-CA-CB	6.12	119.78	111.21
1	A	597	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	A	345	VAL	CA-C-O	-6.11	114.69	121.17
1	A	492	GLN	CA-C-N	6.11	128.47	120.28
1	A	492	GLN	C-N-CA	6.11	128.47	120.28
1	A	444	MET	CA-C-O	-6.11	114.41	120.70
1	A	28	LEU	CA-C-N	6.11	128.38	120.44
1	A	28	LEU	C-N-CA	6.11	128.38	120.44
2	B	469	ILE	N-CA-C	-6.11	101.67	109.30
1	A	247	GLU	O-C-N	-6.10	114.76	122.27
1	A	633	LEU	O-C-N	-6.10	116.07	122.96
2	B	47	ARG	CD-NE-CZ	6.10	132.94	124.40
2	B	147	PRO	O-C-N	-6.09	114.41	122.64
1	A	297	GLU	CA-C-O	-6.09	112.97	119.97
2	B	385	VAL	CA-C-N	6.09	128.76	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	385	VAL	C-N-CA	6.09	128.76	120.54
1	A	384	ARG	NH1-CZ-NH2	6.06	127.18	119.30
2	B	330	GLU	CA-C-O	-6.06	111.93	119.38
1	A	344	ASN	O-C-N	-6.05	114.32	122.43
2	B	345	ILE	CA-C-O	-6.05	113.94	120.47
2	B	498	GLU	CA-C-N	6.05	128.99	120.28
2	B	498	GLU	C-N-CA	6.05	128.99	120.28
1	A	415	ASP	CA-C-O	-6.04	114.14	120.55
2	B	324	ALA	N-CA-C	6.04	119.37	109.76
1	A	257	ALA	CA-C-O	-6.04	113.95	121.02
1	A	351	GLU	O-C-N	-6.03	115.27	122.15
2	B	39	VAL	CA-C-N	6.03	130.94	120.68
2	B	39	VAL	C-N-CA	6.03	130.94	120.68
2	B	26	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	703	GLU	CA-C-O	6.03	127.49	120.80
1	A	340	ASP	OD1-CG-OD2	-6.02	108.44	122.90
1	A	637	PRO	N-CA-CB	6.01	109.20	103.19
1	A	194	GLY	O-C-N	-6.01	118.15	123.92
1	A	549	SER	CA-C-N	6.01	128.61	120.38
1	A	549	SER	C-N-CA	6.01	128.61	120.38
1	A	664	LEU	CA-C-O	-6.01	114.69	121.00
1	A	48	THR	CA-C-O	6.00	126.29	119.27
1	A	685	GLY	N-CA-C	6.00	121.66	111.04
1	A	20	ASP	N-CA-C	6.00	120.11	113.21
1	A	171	VAL	N-CA-C	5.99	118.54	111.05
1	A	683	THR	O-C-N	5.98	130.97	123.19
1	A	216	PRO	N-CA-CB	5.98	109.25	103.51
2	B	192	ASP	N-CA-C	5.98	120.30	112.89
2	B	478	PRO	N-CA-CB	5.97	108.57	103.19
2	B	63	THR	CA-CB-CG2	5.97	120.65	110.50
1	A	44	ILE	CA-C-O	5.97	127.95	119.95
1	A	441	ILE	CB-CG1-CD1	5.97	126.33	113.80
1	A	524	ASP	N-CA-C	5.97	119.30	112.97
2	B	632	ASP	N-CA-C	5.96	119.39	111.75
2	B	169	ARG	CD-NE-CZ	5.96	132.75	124.40
2	B	341	LEU	CA-C-N	5.96	128.19	120.44
2	B	341	LEU	C-N-CA	5.96	128.19	120.44
1	A	625	GLY	CA-C-N	5.96	129.58	120.82
1	A	625	GLY	C-N-CA	5.96	129.58	120.82
2	B	178	ALA	N-CA-C	-5.96	104.17	112.45
2	B	619	MET	CA-CB-CG	5.96	126.01	114.10
2	B	188	LYS	CA-C-O	5.95	128.31	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	HIS	CA-CB-CG	5.93	119.73	113.80
2	B	129	LEU	O-C-N	-5.93	114.70	122.59
2	B	319	GLY	O-C-N	5.93	127.74	123.35
1	A	576	ASN	N-CA-C	5.92	117.27	107.20
2	B	86	GLY	CA-C-O	5.92	126.32	122.23
2	B	534	VAL	O-C-N	-5.92	115.73	121.83
2	B	600	LYS	O-C-N	-5.92	114.75	122.39
1	A	249	GLY	O-C-N	5.92	130.39	122.70
2	B	522	ARG	CA-C-O	5.92	126.22	119.18
2	B	404	TYR	CB-CG-CD1	5.92	129.67	120.80
1	A	516	THR	O-C-N	-5.91	115.98	122.07
1	A	677	ARG	O-C-N	-5.91	116.05	121.37
2	B	143	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	559	TYR	CA-C-O	5.91	127.78	121.16
1	A	146	ILE	CA-C-N	5.90	128.11	120.44
1	A	146	ILE	C-N-CA	5.90	128.11	120.44
2	B	19	THR	CA-C-N	5.89	130.98	122.44
2	B	19	THR	C-N-CA	5.89	130.98	122.44
2	B	632	ASP	O-C-N	-5.88	115.50	122.20
2	B	447	ALA	CA-C-O	5.88	126.77	120.24
1	A	493	LYS	CA-C-N	5.88	133.01	122.38
1	A	493	LYS	C-N-CA	5.88	133.01	122.38
1	A	347	ARG	NE-CZ-NH2	-5.87	113.91	119.20
2	B	218	GLY	CA-C-N	5.87	128.43	120.38
2	B	218	GLY	C-N-CA	5.87	128.43	120.38
2	B	303	ALA	N-CA-C	5.87	120.30	113.20
2	B	397	ASP	CA-C-O	5.87	128.20	120.16
2	B	465	GLU	CA-C-O	5.87	127.36	120.20
1	A	211	ILE	N-CA-CB	5.87	120.91	111.23
1	A	539	GLY	CA-C-N	5.86	128.41	120.38
1	A	539	GLY	C-N-CA	5.86	128.41	120.38
1	A	119	LEU	CA-C-N	5.86	127.17	119.84
1	A	119	LEU	C-N-CA	5.86	127.17	119.84
2	B	552	GLU	N-CA-C	-5.86	106.47	113.97
1	A	497	VAL	CA-C-N	5.85	128.60	120.29
1	A	497	VAL	C-N-CA	5.85	128.60	120.29
1	A	597	ARG	CA-C-O	5.85	124.97	119.76
1	A	399	VAL	CA-C-N	5.85	129.68	122.37
1	A	399	VAL	C-N-CA	5.85	129.68	122.37
1	A	458	ASP	O-C-N	-5.85	115.38	122.22
1	A	281	ALA	CA-C-N	5.85	125.47	119.56
1	A	281	ALA	C-N-CA	5.85	125.47	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	THR	CA-C-O	-5.85	114.68	120.70
2	B	199	LEU	CA-C-O	5.84	127.71	121.16
2	B	100	ARG	CG-CD-NE	5.84	124.85	112.00
1	A	375	PRO	CA-C-O	5.84	128.31	121.31
2	B	307	ILE	O-C-N	-5.84	116.21	121.87
2	B	411	SER	O-C-N	-5.83	116.03	122.09
1	A	462	GLN	CG-CD-NE2	5.83	125.14	116.40
1	A	11	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	152	LEU	CA-C-N	5.82	132.56	122.56
1	A	152	LEU	C-N-CA	5.82	132.56	122.56
1	A	607	GLN	CA-C-N	5.82	129.98	121.31
1	A	607	GLN	C-N-CA	5.82	129.98	121.31
1	A	62	ASP	N-CA-C	-5.81	104.36	113.02
1	A	245	MET	O-C-N	-5.81	115.98	122.03
2	B	529	GLY	O-C-N	-5.79	116.17	122.54
1	A	575	LYS	CA-CB-CG	5.79	125.68	114.10
1	A	364	HIS	CA-C-O	-5.78	113.96	120.32
1	A	636	THR	CA-C-N	5.78	126.54	120.12
1	A	636	THR	C-N-CA	5.78	126.54	120.12
1	A	509	LYS	N-CA-C	5.78	118.32	111.33
1	A	314	GLN	N-CA-C	5.77	123.10	110.80
2	B	27	PHE	CA-C-N	5.77	125.72	119.78
2	B	27	PHE	C-N-CA	5.77	125.72	119.78
1	A	340	ASP	CB-CG-OD2	5.77	131.67	118.40
1	A	157	PRO	CA-C-O	-5.76	114.18	120.92
1	A	535	CYS	CA-C-N	5.76	127.82	120.56
1	A	535	CYS	C-N-CA	5.76	127.82	120.56
1	A	428	GLU	O-C-N	-5.76	114.51	122.46
1	A	6	ARG	CA-CB-CG	5.75	125.60	114.10
1	A	251	THR	CA-C-N	5.75	128.26	120.38
1	A	251	THR	C-N-CA	5.75	128.26	120.38
2	B	536	HIS	CB-CG-CD2	5.75	138.67	131.20
1	A	347	ARG	NH1-CZ-NH2	5.74	126.77	119.30
2	B	59	LEU	CA-C-N	5.74	128.25	120.38
2	B	59	LEU	C-N-CA	5.74	128.25	120.38
2	B	72	ILE	O-C-N	-5.74	116.85	122.99
2	B	323	ASN	CA-C-N	5.74	129.71	121.50
2	B	323	ASN	C-N-CA	5.74	129.71	121.50
2	B	552	GLU	CA-C-N	5.74	130.16	120.29
2	B	552	GLU	C-N-CA	5.74	130.16	120.29
2	B	580	GLU	CA-C-N	5.74	128.00	120.60
2	B	580	GLU	C-N-CA	5.74	128.00	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	VAL	CA-CB-CG1	5.73	120.14	110.40
2	B	520	THR	CA-C-O	5.73	128.70	120.51
2	B	22	SER	CA-CB-OG	5.73	122.56	111.10
1	A	693	PHE	CA-C-N	5.73	127.95	120.28
1	A	693	PHE	C-N-CA	5.73	127.95	120.28
1	A	391	GLN	OE1-CD-NE2	-5.72	116.88	122.60
2	B	149	HIS	CA-C-N	5.72	128.41	120.29
2	B	149	HIS	C-N-CA	5.72	128.41	120.29
2	B	377	ARG	CD-NE-CZ	-5.72	116.40	124.40
2	B	467	PRO	CB-CA-C	-5.72	103.49	110.98
2	B	328	TRP	CA-C-N	5.71	127.94	120.28
2	B	328	TRP	C-N-CA	5.71	127.94	120.28
1	A	662	LEU	N-CA-C	5.71	119.86	113.01
1	A	600	ILE	CA-C-O	5.71	126.41	120.36
2	B	76	TYR	O-C-N	-5.71	116.54	123.10
2	B	197	LEU	CA-C-O	-5.71	114.43	120.71
1	A	313	HIS	CA-C-N	5.70	132.44	121.54
1	A	313	HIS	C-N-CA	5.70	132.44	121.54
2	B	18	PRO	N-CA-CB	5.70	108.64	103.34
2	B	294	ILE	CA-C-N	5.70	128.19	120.38
2	B	294	ILE	C-N-CA	5.70	128.19	120.38
2	B	518	LEU	N-CA-C	5.70	117.50	108.67
1	A	406	SER	N-CA-CB	5.69	120.10	110.49
1	A	411	GLU	CB-CG-CD	5.68	122.26	112.60
2	B	600	LYS	CA-C-N	5.68	131.97	121.52
2	B	600	LYS	C-N-CA	5.68	131.97	121.52
2	B	279	THR	N-CA-C	-5.68	106.99	114.31
2	B	338	VAL	N-CA-C	-5.68	106.24	113.22
2	B	580	GLU	CA-CB-CG	5.68	125.45	114.10
1	A	358	GLY	CA-C-O	5.68	130.45	120.57
2	B	204	PHE	CA-C-O	5.67	126.95	121.00
2	B	614	ASP	CA-CB-CG	-5.67	106.93	112.60
1	A	70	PHE	O-C-N	-5.67	114.81	122.41
1	A	621	TYR	CA-C-O	-5.67	114.87	120.82
1	A	273	VAL	O-C-N	5.67	127.97	122.25
1	A	361	GLN	CG-CD-OE1	5.66	132.13	120.80
1	A	59	ASP	CA-C-O	5.66	126.33	119.31
2	B	505	THR	CA-C-N	5.66	128.18	120.54
2	B	505	THR	C-N-CA	5.66	128.18	120.54
2	B	115	ASP	N-CA-CB	-5.66	99.84	109.57
1	A	9	SER	CA-C-N	5.65	132.15	121.97
1	A	9	SER	C-N-CA	5.65	132.15	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	327	SER	N-CA-C	5.65	118.75	109.76
1	A	32	ALA	CA-C-N	5.65	129.28	121.26
1	A	32	ALA	C-N-CA	5.65	129.28	121.26
2	B	84	LYS	CA-C-O	-5.65	114.42	120.92
2	B	492	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	A	499	LEU	N-CA-C	5.65	118.21	111.71
2	B	36	GLU	CA-C-N	5.65	127.78	120.44
2	B	36	GLU	C-N-CA	5.65	127.78	120.44
1	A	291	GLY	O-C-N	-5.65	116.83	122.82
1	A	168	ASN	N-CA-C	-5.64	107.04	114.04
1	A	20	ASP	CA-C-N	5.64	132.31	121.54
1	A	20	ASP	C-N-CA	5.64	132.31	121.54
1	A	632	PRO	N-CA-CB	5.64	108.69	103.39
1	A	311	LEU	N-CA-C	5.63	119.66	112.34
1	A	220	ILE	CA-C-N	5.63	128.41	120.42
1	A	220	ILE	C-N-CA	5.63	128.41	120.42
2	B	219	ASP	CA-C-N	5.63	128.09	120.44
2	B	219	ASP	C-N-CA	5.63	128.09	120.44
1	A	346	VAL	CB-CA-C	-5.62	104.77	111.97
1	A	601	LEU	N-CA-CB	5.62	119.38	110.55
1	A	194	GLY	N-CA-C	5.62	118.17	110.69
2	B	35	TRP	N-CA-CB	5.62	118.57	110.20
2	B	445	CYS	N-CA-CB	5.61	119.54	110.40
1	A	342	TYR	CA-C-N	5.60	130.94	121.14
1	A	342	TYR	C-N-CA	5.60	130.94	121.14
1	A	451	ALA	O-C-N	-5.60	116.30	122.07
2	B	296	ARG	NE-CZ-NH2	5.60	124.24	119.20
2	B	240	ILE	CA-C-N	5.60	127.78	120.28
2	B	240	ILE	C-N-CA	5.60	127.78	120.28
1	A	436	ALA	O-C-N	-5.59	116.19	122.12
2	B	403	TYR	O-C-N	-5.59	115.43	122.20
2	B	439	THR	CA-C-N	5.59	128.09	120.54
2	B	439	THR	C-N-CA	5.59	128.09	120.54
1	A	617	ILE	CA-C-O	5.59	126.69	120.71
2	B	377	ARG	NE-CZ-NH1	5.59	127.09	121.50
2	B	457	LYS	O-C-N	-5.58	115.10	122.42
1	A	432	GLY	CA-C-O	-5.58	115.99	120.79
1	A	679	ASP	CA-C-O	-5.58	114.96	120.82
2	B	302	GLU	CA-C-N	5.58	133.10	121.94
2	B	302	GLU	C-N-CA	5.58	133.10	121.94
2	B	480	PRO	N-CA-CB	5.58	108.21	103.19
2	B	536	HIS	O-C-N	-5.58	114.76	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	GLU	CA-CB-CG	-5.57	102.95	114.10
2	B	380	ARG	CA-C-O	-5.57	114.64	120.55
2	B	74	PRO	N-CA-CB	5.57	109.43	103.52
1	A	298	VAL	CA-C-N	5.57	128.06	120.54
1	A	298	VAL	C-N-CA	5.57	128.06	120.54
1	A	442	PRO	N-CA-C	5.57	120.86	113.40
1	A	628	VAL	N-CA-C	5.57	115.97	108.17
1	A	381	ARG	CB-CA-C	-5.57	102.11	110.90
1	A	208	ASN	N-CA-C	5.56	119.31	111.52
1	A	419	LYS	O-C-N	-5.56	115.71	122.22
1	A	265	ASP	CA-CB-CG	5.56	118.16	112.60
2	B	500	LEU	CA-C-O	5.56	125.78	119.27
1	A	633	LEU	CA-C-N	5.54	132.13	121.54
1	A	633	LEU	C-N-CA	5.54	132.13	121.54
1	A	244	HIS	CA-C-N	5.54	127.97	120.65
1	A	244	HIS	C-N-CA	5.54	127.97	120.65
1	A	135	ASP	CA-C-N	5.53	128.77	120.69
1	A	135	ASP	C-N-CA	5.53	128.77	120.69
1	A	285	SER	CA-C-O	5.53	126.67	120.70
1	A	392	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	A	720	LYS	O-C-N	-5.53	116.28	122.03
1	A	129	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	132	VAL	CB-CA-C	-5.53	101.23	111.79
1	A	311	LEU	CA-C-N	5.52	129.36	121.02
1	A	311	LEU	C-N-CA	5.52	129.36	121.02
1	A	11	ASP	CA-C-N	5.52	128.14	120.63
1	A	11	ASP	C-N-CA	5.52	128.14	120.63
2	B	375	PRO	O-C-N	-5.52	116.22	122.18
1	A	250	ALA	CA-C-O	-5.52	114.46	120.81
1	A	212	TYR	CA-C-N	5.51	126.06	120.38
1	A	212	TYR	C-N-CA	5.51	126.06	120.38
1	A	512	LEU	CA-C-N	5.51	128.69	120.31
1	A	512	LEU	C-N-CA	5.51	128.69	120.31
2	B	397	ASP	O-C-N	-5.51	114.99	121.32
2	B	243	ASN	CA-C-O	5.50	126.38	120.55
1	A	698	LYS	N-CA-C	5.50	118.03	111.71
2	B	292	LEU	CB-CA-C	5.49	120.19	110.85
1	A	529	ARG	N-CA-C	-5.49	104.82	112.45
1	A	284	LEU	O-C-N	5.49	129.74	123.27
2	B	482	ALA	CA-C-O	5.49	126.62	120.04
1	A	188	LYS	CA-C-N	5.48	126.69	119.84
1	A	188	LYS	C-N-CA	5.48	126.69	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	GLN	N-CA-C	5.48	117.25	111.28
1	A	436	ALA	CA-C-N	5.48	128.20	120.42
1	A	436	ALA	C-N-CA	5.48	128.20	120.42
1	A	117	PHE	CA-C-O	5.47	127.34	121.16
1	A	582	GLU	CA-C-O	-5.47	115.08	120.82
1	A	63	THR	CA-C-N	-5.47	113.87	122.73
1	A	63	THR	C-N-CA	-5.47	113.87	122.73
2	B	267	VAL	CA-C-N	5.47	128.15	120.28
2	B	267	VAL	C-N-CA	5.47	128.15	120.28
2	B	377	ARG	CG-CD-NE	5.46	124.01	112.00
1	A	678	PRO	N-CA-CB	5.46	109.31	103.52
1	A	52	GLU	N-CA-C	5.45	119.03	112.38
1	A	357	GLN	N-CA-C	5.45	119.55	113.01
2	B	531	SER	CA-C-O	-5.44	113.50	120.31
2	B	251	GLU	CA-C-N	5.44	128.02	120.29
2	B	251	GLU	C-N-CA	5.44	128.02	120.29
2	B	120	PHE	CA-CB-CG	-5.44	108.36	113.80
2	B	532	SER	CA-C-O	5.43	123.62	118.63
2	B	511	PRO	N-CA-CB	5.42	108.94	103.25
1	A	256	MET	CB-CG-SD	-5.42	96.43	112.70
1	A	528	ASP	CA-C-O	5.42	125.99	119.59
1	A	527	PRO	CA-C-N	5.42	131.05	122.60
1	A	527	PRO	C-N-CA	5.42	131.05	122.60
2	B	398	PRO	CA-C-N	5.42	127.81	120.44
2	B	398	PRO	C-N-CA	5.42	127.81	120.44
2	B	563	GLN	CA-C-N	5.42	131.77	122.67
2	B	563	GLN	C-N-CA	5.42	131.77	122.67
1	A	128	ASP	CA-C-O	5.41	124.91	118.79
1	A	82	ARG	CD-NE-CZ	5.41	131.98	124.40
1	A	224	ILE	CA-C-O	5.41	123.85	118.98
1	A	292	MET	N-CA-C	5.41	119.75	113.20
2	B	496	VAL	O-C-N	-5.41	116.41	121.87
2	B	558	LYS	CA-C-O	5.41	126.25	120.24
1	A	105	ASN	O-C-N	-5.41	116.39	122.12
2	B	615	GLY	CA-C-N	-5.41	113.35	123.03
2	B	615	GLY	C-N-CA	-5.41	113.35	123.03
1	A	485	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	638	GLU	N-CA-C	-5.40	106.70	113.72
2	B	280	ILE	CA-C-O	5.40	127.34	120.75
1	A	621	TYR	O-C-N	-5.40	116.51	122.07
1	A	135	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	361	GLN	CB-CA-C	5.38	118.44	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	318	ARG	CA-CB-CG	5.38	124.87	114.10
2	B	460	ILE	N-CA-CB	-5.38	105.34	112.34
1	A	347	ARG	O-C-N	-5.38	116.50	122.09
2	B	406	GLU	CA-C-O	-5.38	114.73	121.02
2	B	424	GLU	CA-C-N	5.38	132.07	122.06
2	B	424	GLU	C-N-CA	5.38	132.07	122.06
1	A	214	PRO	CA-C-N	5.38	128.93	120.97
1	A	214	PRO	C-N-CA	5.38	128.93	120.97
1	A	684	VAL	CA-CB-CG1	5.38	119.54	110.40
2	B	213	ASP	CA-CB-CG	-5.37	107.23	112.60
2	B	202	ILE	CA-C-N	5.36	125.90	120.00
2	B	202	ILE	C-N-CA	5.36	125.90	120.00
2	B	243	ASN	CA-CB-CG	5.36	117.96	112.60
2	B	75	MET	N-CA-C	5.36	117.13	108.34
2	B	503	ARG	CA-C-O	-5.36	114.87	120.55
2	B	492	ARG	CD-NE-CZ	5.35	131.89	124.40
1	A	150	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	335	SER	N-CA-C	5.34	119.06	112.54
1	A	347	ARG	CG-CD-NE	-5.34	100.24	112.00
1	A	331	THR	CA-CB-OG1	-5.34	101.60	109.60
1	A	364	HIS	CG-CD2-NE2	5.34	112.54	107.20
2	B	37	ARG	CA-C-O	-5.34	115.22	120.82
1	A	77	THR	N-CA-C	-5.33	106.90	113.41
1	A	180	VAL	CA-C-N	5.33	127.74	120.54
1	A	180	VAL	C-N-CA	5.33	127.74	120.54
1	A	74	PRO	N-CA-C	5.33	120.52	113.86
1	A	401	ASP	CA-C-O	5.33	127.46	120.16
2	B	338	VAL	CA-C-N	5.33	130.46	121.14
2	B	338	VAL	C-N-CA	5.33	130.46	121.14
1	A	137	GLY	N-CA-C	5.33	121.25	113.48
1	A	454	GLN	CG-CD-NE2	5.33	124.39	116.40
2	B	413	ALA	CA-C-O	-5.32	115.41	121.00
1	A	351	GLU	CB-CG-CD	5.32	121.64	112.60
2	B	160	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	520	GLY	CA-C-N	5.32	130.26	122.98
1	A	520	GLY	C-N-CA	5.32	130.26	122.98
2	B	126	LEU	O-C-N	-5.32	116.56	122.09
1	A	697	ARG	CA-C-N	5.31	127.93	120.28
1	A	697	ARG	C-N-CA	5.31	127.93	120.28
2	B	563	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	325	LEU	CA-C-O	-5.31	115.40	120.92
2	B	316	ASP	CA-C-N	5.30	132.55	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	316	ASP	C-N-CA	5.30	132.55	121.94
1	A	385	ASN	CA-C-N	5.30	127.65	120.44
1	A	385	ASN	C-N-CA	5.30	127.65	120.44
2	B	414	ASP	CA-C-N	5.30	127.69	120.54
2	B	414	ASP	C-N-CA	5.30	127.69	120.54
2	B	351	SER	CA-C-N	5.30	129.43	120.64
2	B	351	SER	C-N-CA	5.30	129.43	120.64
1	A	202	LYS	CA-C-N	5.29	129.55	120.71
1	A	202	LYS	C-N-CA	5.29	129.55	120.71
1	A	281	ALA	CA-C-O	5.29	123.87	118.79
2	B	236	ILE	CB-CA-C	-5.29	105.52	111.23
1	A	325	LEU	CA-CB-CG	5.29	134.80	116.30
1	A	316	GLY	CA-C-N	5.28	126.44	119.84
1	A	316	GLY	C-N-CA	5.28	126.44	119.84
1	A	224	ILE	O-C-N	-5.28	115.28	122.03
1	A	422	GLY	O-C-N	-5.28	116.91	122.13
1	A	449	ALA	O-C-N	-5.27	115.54	122.39
2	B	374	PHE	CA-C-N	5.27	124.72	119.24
2	B	374	PHE	C-N-CA	5.27	124.72	119.24
1	A	497	VAL	CB-CA-C	5.26	118.39	111.81
2	B	280	ILE	N-CA-C	5.26	115.94	107.73
2	B	576	GLN	CB-CG-CD	5.26	121.55	112.60
2	B	376	LEU	O-C-N	-5.26	116.06	122.22
1	A	258	TYR	N-CA-C	5.26	117.92	111.82
2	B	92	PRO	N-CA-CB	5.25	108.38	102.60
2	B	342	ARG	CA-C-N	5.25	125.78	120.00
2	B	342	ARG	C-N-CA	5.25	125.78	120.00
2	B	329	ARG	CA-CB-CG	5.24	124.58	114.10
1	A	319	ASN	N-CA-CB	-5.24	101.74	110.02
1	A	357	GLN	O-C-N	-5.24	115.23	122.46
1	A	479	ASP	N-CA-C	5.24	116.84	108.41
1	A	582	GLU	CB-CG-CD	5.24	121.50	112.60
2	B	220	TRP	O-C-N	-5.24	116.44	122.09
2	B	389	GLU	CA-CB-CG	5.23	124.57	114.10
1	A	179	VAL	CA-C-N	5.23	127.62	120.77
1	A	179	VAL	C-N-CA	5.23	127.62	120.77
2	B	300	LEU	CA-C-N	5.23	127.60	120.54
2	B	300	LEU	C-N-CA	5.23	127.60	120.54
2	B	306	ARG	CA-C-O	-5.23	115.30	120.90
1	A	46	VAL	CA-C-N	-5.23	117.25	122.69
1	A	46	VAL	C-N-CA	-5.23	117.25	122.69
2	B	176	ALA	N-CA-C	5.22	119.28	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ASN	O-C-N	-5.22	116.72	122.72
1	A	380	ALA	O-C-N	-5.22	116.11	122.22
2	B	103	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	538	ALA	CA-C-N	5.22	128.68	121.26
2	B	538	ALA	C-N-CA	5.22	128.68	121.26
1	A	588	GLU	O-C-N	-5.22	115.65	122.59
1	A	613	GLY	CA-C-N	5.21	128.64	120.82
1	A	613	GLY	C-N-CA	5.21	128.64	120.82
1	A	309	ALA	N-CA-CB	-5.21	101.68	110.49
1	A	149	MET	CA-CB-CG	-5.20	103.69	114.10
1	A	305	ARG	CA-C-O	-5.20	115.33	120.90
1	A	374	LEU	CA-C-O	5.20	125.29	120.50
1	A	133	ALA	N-CA-C	5.20	121.88	110.80
1	A	638	GLU	CA-CB-CG	5.20	124.49	114.10
2	B	161	MET	CB-CA-C	-5.20	102.02	110.85
1	A	238	ILE	N-CA-C	5.19	114.71	108.06
1	A	524	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	588	GLU	CA-C-N	5.19	129.44	121.19
1	A	588	GLU	C-N-CA	5.19	129.44	121.19
1	A	511	ALA	N-CA-C	-5.18	106.11	112.90
2	B	417	TRP	CA-C-N	5.18	128.60	120.82
2	B	417	TRP	C-N-CA	5.18	128.60	120.82
1	A	719	VAL	CA-C-O	-5.18	115.56	120.95
2	B	48	PRO	N-CA-CB	5.18	108.11	103.08
2	B	302	GLU	O-C-N	-5.18	115.93	122.20
1	A	321	LYS	O-C-N	-5.17	116.13	122.34
1	A	495	LYS	CA-C-O	5.17	125.25	119.41
1	A	76	ALA	N-CA-C	5.17	119.64	113.23
2	B	555	GLU	CA-C-N	5.17	130.18	121.14
2	B	555	GLU	C-N-CA	5.17	130.18	121.14
2	B	465	GLU	CG-CD-OE1	5.16	130.28	118.40
1	A	596	ARG	N-CA-CB	5.16	119.21	110.49
2	B	541	ASP	O-C-N	-5.16	116.97	122.85
2	B	159	LEU	CA-C-N	5.15	127.61	120.29
2	B	159	LEU	C-N-CA	5.15	127.61	120.29
2	B	106	ALA	CA-C-O	5.15	126.28	120.92
2	B	389	GLU	CB-CG-CD	5.15	121.36	112.60
2	B	331	LEU	N-CA-CB	5.15	117.54	109.97
1	A	654	VAL	N-CA-C	5.15	116.10	108.23
2	B	44	ASN	O-C-N	-5.15	115.27	122.37
2	B	361	LEU	CA-C-O	5.14	124.03	119.71
2	B	393	GLY	CA-C-N	5.14	129.43	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	393	GLY	C-N-CA	5.14	129.43	120.68
1	A	182	ALA	O-C-N	-5.14	116.29	122.15
1	A	508	VAL	N-CA-C	5.14	115.28	110.30
1	A	565	THR	CA-C-O	5.14	126.78	120.92
1	A	584	ARG	CA-C-N	5.14	127.42	120.44
1	A	584	ARG	C-N-CA	5.14	127.42	120.44
2	B	73	VAL	CA-C-N	5.14	124.63	119.19
2	B	73	VAL	C-N-CA	5.14	124.63	119.19
2	B	368	GLY	CA-C-O	-5.14	115.96	121.35
1	A	301	LEU	CA-C-O	-5.13	115.06	120.55
2	B	510	ARG	CA-C-O	5.13	124.33	119.76
1	A	300	LYS	CA-CB-CG	-5.13	103.84	114.10
2	B	619	MET	CB-CA-C	5.13	120.62	110.42
1	A	27	GLU	CA-C-N	5.12	129.39	120.68
1	A	27	GLU	C-N-CA	5.12	129.39	120.68
1	A	122	HIS	O-C-N	-5.12	116.69	122.12
1	A	608	ASP	CA-C-O	5.12	126.60	121.07
1	A	718	LEU	CA-C-N	5.12	127.48	120.46
1	A	718	LEU	C-N-CA	5.12	127.48	120.46
2	B	332	THR	N-CA-CB	5.12	119.50	111.20
1	A	445	ARG	CD-NE-CZ	5.12	131.56	124.40
1	A	592	GLN	O-C-N	-5.12	115.79	122.59
1	A	637	PRO	N-CA-C	5.11	120.33	114.20
2	B	155	SER	CA-C-N	5.11	128.08	120.31
2	B	155	SER	C-N-CA	5.11	128.08	120.31
2	B	528	GLU	CA-C-N	5.11	129.53	120.74
2	B	528	GLU	C-N-CA	5.11	129.53	120.74
2	B	491	HIS	N-CA-C	5.11	117.30	109.07
1	A	240	ILE	N-CA-C	5.11	114.64	106.88
1	A	684	VAL	CB-CA-C	5.10	117.31	110.42
1	A	45	PRO	N-CA-C	-5.10	103.18	111.14
1	A	34	THR	N-CA-CB	5.10	117.57	109.51
1	A	59	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	480	VAL	CB-CA-C	-5.10	106.39	111.80
2	B	200	ASP	CA-C-O	5.10	127.15	120.16
1	A	690	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	481	LEU	CA-C-N	5.09	129.90	122.41
1	A	481	LEU	C-N-CA	5.09	129.90	122.41
2	B	307	ILE	N-CA-C	5.09	115.82	110.62
2	B	425	LYS	CA-C-N	5.09	130.20	122.87
2	B	425	LYS	C-N-CA	5.09	130.20	122.87
2	B	456	ARG	CG-CD-NE	5.09	123.20	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	VAL	CA-C-O	-5.09	114.42	120.78
2	B	364	THR	CA-C-O	5.09	125.95	119.95
1	A	180	VAL	CA-C-O	-5.08	116.13	121.41
1	A	538	ALA	CA-C-O	-5.08	115.17	120.55
2	B	403	TYR	CB-CG-CD1	5.08	128.42	120.80
1	A	261	ALA	O-C-N	-5.08	116.84	122.07
1	A	401	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	669	ARG	CA-CB-CG	5.07	124.24	114.10
2	B	491	HIS	CA-CB-CG	-5.07	108.73	113.80
2	B	512	LYS	CB-CA-C	5.07	121.22	110.07
2	B	398	PRO	O-C-N	-5.06	115.44	122.27
1	A	448	GLU	O-C-N	-5.05	116.67	122.08
2	B	389	GLU	CA-C-O	5.05	124.95	119.24
2	B	349	SER	O-C-N	-5.05	116.77	122.12
1	A	550	ASP	N-CA-C	5.05	117.44	111.33
1	A	154	ALA	N-CA-C	-5.04	102.40	109.96
1	A	376	THR	CA-CB-OG1	5.04	117.16	109.60
1	A	452	ARG	NH1-CZ-NH2	5.04	125.86	119.30
1	A	685	GLY	O-C-N	-5.04	118.74	123.48
2	B	600	LYS	CA-C-O	5.04	125.53	119.43
2	B	250	ALA	O-C-N	-5.04	116.85	122.09
1	A	369	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	404	SER	CA-C-O	5.03	127.71	120.51
1	A	453	THR	O-C-N	5.03	127.53	122.09
2	B	532	SER	O-C-N	-5.03	115.77	120.55
1	A	123	ARG	CB-CG-CD	5.03	122.87	111.30
2	B	94	THR	CA-CB-OG1	-5.03	102.06	109.60
2	B	519	GLY	CA-C-O	-5.02	116.18	122.61
2	B	614	ASP	N-CA-C	5.02	119.26	113.18
2	B	570	SER	N-CA-CB	-5.02	102.73	110.56
1	A	452	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	A	707	PRO	N-CA-CB	5.01	108.51	103.25
2	B	158	LEU	CA-C-N	5.01	127.70	120.38
2	B	158	LEU	C-N-CA	5.01	127.70	120.38
1	A	59	ASP	N-CA-CB	-5.01	102.23	110.40
1	A	385	ASN	N-CA-CB	5.01	118.33	110.46
2	B	412	LEU	N-CA-C	5.01	116.74	111.28
1	A	173	PRO	N-CA-CB	5.00	108.33	102.88
1	A	207	ARG	NE-CZ-NH1	-5.00	116.50	121.50
1	A	677	ARG	CA-CB-CG	5.00	124.10	114.10
2	B	189	PRO	N-CA-CB	5.00	108.50	103.25

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	LEU	Mainchain
1	A	215	GLN	Mainchain
1	A	264	VAL	Mainchain
1	A	277	VAL	Mainchain
1	A	30	ALA	Mainchain
1	A	339	GLN	Mainchain
1	A	340	ASP	Mainchain
1	A	438	GLU	Mainchain
1	A	621	TYR	Mainchain
1	A	640	THR	Mainchain
1	A	687	VAL	Mainchain
1	A	74	PRO	Mainchain
2	B	336	PRO	Mainchain
2	B	338	VAL	Mainchain
2	B	35	TRP	Mainchain
2	B	362	PRO	Mainchain
2	B	451	LYS	Mainchain
2	B	535	TRP	Mainchain
2	B	599	PHE	Mainchain
2	B	86	GLY	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5552	0	5449	109	0
2	B	4624	0	4439	107	0
3	A	91	0	88	22	0
4	A	18	0	10	0	0
All	All	10285	0	9986	212	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 10.

All (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:SER:HB2	2:B:400:GLY:O	1.34	1.22
3:A:800:B12:H362	3:A:800:B12:H351	1.35	1.06
3:A:800:B12:H353	3:A:800:B12:H302	1.37	1.06
1:A:406:SER:CB	2:B:400:GLY:O	2.02	1.05
3:A:800:B12:H312	3:A:800:B12:C25	1.90	1.01
1:A:406:SER:N	2:B:401:GLY:O	2.04	0.91
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.55	0.87
1:A:405:GLY:C	2:B:401:GLY:O	2.18	0.86
1:A:406:SER:HA	2:B:400:GLY:O	1.76	0.85
3:A:800:B12:H312	3:A:800:B12:H251	1.58	0.85
1:A:706:THR:HB	1:A:707:PRO:HD2	1.61	0.83
1:A:316:GLY:H	1:A:317:PRO:HD3	1.43	0.81
3:A:800:B12:O28	3:A:800:B12:H3	1.80	0.79
3:A:800:B12:H312	3:A:800:B12:H253	1.65	0.78
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.69	0.75
1:A:305:ARG:HG2	1:A:325:LEU:HB3	1.69	0.75
3:A:800:B12:H302	3:A:800:B12:C35	2.15	0.74
1:A:224:ILE:HG12	1:A:532:LEU:HD22	1.70	0.74
1:A:665:VAL:HG13	1:A:682:ILE:HG21	1.70	0.73
3:A:800:B12:H482	3:A:800:B12:H533	1.72	0.72
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.71	0.72
2:B:361:LEU:HD22	2:B:365:GLN:HG2	1.71	0.71
1:A:173:PRO:HB2	1:A:545:VAL:HG22	1.71	0.71
1:A:406:SER:CA	2:B:400:GLY:O	2.37	0.71
3:A:800:B12:H531	3:A:800:B12:H552	1.73	0.71
1:A:205:MET:HG2	1:A:437:ILE:HD11	1.73	0.70
2:B:331:LEU:HD13	2:B:365:GLN:HB3	1.75	0.68
1:A:406:SER:HB2	2:B:400:GLY:C	2.18	0.68
3:A:800:B12:H353	3:A:800:B12:C30	2.21	0.68
1:A:601:LEU:HA	1:A:629:ASP:HB2	1.75	0.68
2:B:202:ILE:HD13	2:B:429:MET:HB3	1.76	0.67
1:A:406:SER:CB	2:B:399:ALA:O	2.42	0.67
1:A:101:PHE:HA	1:A:104:ARG:HD2	1.76	0.67
2:B:284:VAL:HG11	2:B:322:GLN:HE21	1.60	0.67
2:B:332:THR:HG21	2:B:460:ILE:HD11	1.76	0.66
1:A:406:SER:N	2:B:401:GLY:C	2.53	0.66
2:B:391:ASN:ND2	2:B:394:ARG:HE	1.93	0.66
2:B:386:LEU:HD23	2:B:390:VAL:HG21	1.78	0.65
1:A:172:LEU:HB2	1:A:173:PRO:HD3	1.78	0.65
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.45	0.65
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.78	0.65
1:A:15:ALA:HB1	2:B:92:PRO:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:800:B12:H362	3:A:800:B12:C35	2.21	0.63
2:B:550:THR:HG21	2:B:580:GLU:HG2	1.80	0.63
1:A:405:GLY:CA	2:B:401:GLY:O	2.46	0.63
2:B:91:ALA:HA	2:B:92:PRO:C	2.22	0.63
2:B:104:MET:HG3	2:B:388:GLU:HG2	1.81	0.63
1:A:171:VAL:HG11	1:A:198:ASN:HD22	1.65	0.62
1:A:406:SER:HB3	2:B:399:ALA:O	2.00	0.61
1:A:63:THR:HG21	1:A:69:PRO:HD2	1.82	0.61
1:A:316:GLY:N	1:A:317:PRO:HD3	2.15	0.60
3:A:800:B12:O7R	3:A:800:B12:C2B	2.49	0.60
2:B:254:TRP:HA	2:B:257:ALA:HB3	1.82	0.60
1:A:172:LEU:HD11	1:A:220:ILE:HG12	1.83	0.60
3:A:800:B12:O7R	3:A:800:B12:H2B	2.01	0.60
2:B:92:PRO:O	2:B:93:PHE:HB2	2.01	0.60
2:B:202:ILE:HG21	2:B:429:MET:HG3	1.85	0.58
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.84	0.58
1:A:405:GLY:HA3	2:B:401:GLY:O	2.04	0.58
1:A:437:ILE:HG13	1:A:442:PRO:HG2	1.85	0.58
2:B:460:ILE:HG23	2:B:464:SER:H	1.69	0.58
3:A:800:B12:H351	3:A:800:B12:C36	2.17	0.58
2:B:150:LEU:HD21	2:B:166:VAL:HG11	1.85	0.58
1:A:406:SER:HB3	2:B:401:GLY:C	2.29	0.57
1:A:665:VAL:HB	1:A:666:PRO:HD3	1.86	0.57
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.86	0.57
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.86	0.57
1:A:494:ALA:HA	1:A:497:VAL:HB	1.87	0.57
1:A:240:ILE:HD11	1:A:284:LEU:HD22	1.86	0.56
2:B:234:VAL:HB	2:B:280:ILE:HG12	1.86	0.56
1:A:406:SER:HB3	2:B:402:SER:N	2.21	0.56
3:A:800:B12:C25	3:A:800:B12:C31	2.72	0.56
3:A:800:B12:H2B	3:A:800:B12:O2	2.06	0.56
1:A:64:TYR:HB3	2:B:35:TRP:HB2	1.88	0.55
2:B:534:VAL:HA	2:B:537:ILE:HD12	1.88	0.54
2:B:424:GLU:HA	2:B:428:GLY:HA2	1.89	0.54
1:A:587:VAL:HG11	1:A:625:GLY:HA3	1.89	0.53
2:B:617:LEU:HD22	2:B:621:MET:HE1	1.89	0.53
1:A:665:VAL:HB	1:A:666:PRO:CD	2.38	0.53
1:A:123:ARG:HD2	1:A:209:THR:HA	1.89	0.53
1:A:705:TYR:HB3	1:A:709:THR:HG21	1.90	0.53
2:B:390:VAL:O	2:B:391:ASN:HB2	2.08	0.53
1:A:406:SER:CB	2:B:400:GLY:C	2.81	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:PHE:HB3	2:B:605:ASP:HB2	1.91	0.52
1:A:672:LEU:HD22	1:A:680:ILE:HD12	1.91	0.52
1:A:406:SER:HA	2:B:401:GLY:HA3	1.91	0.52
2:B:460:ILE:HD12	2:B:463:VAL:HB	1.91	0.52
1:A:281:ALA:N	1:A:282:PRO:HD2	2.25	0.52
2:B:595:LEU:HD23	2:B:616:ARG:HG2	1.90	0.52
1:A:58:MET:HE2	1:A:414:TRP:HB2	1.91	0.51
1:A:264:VAL:HG21	1:A:311:LEU:HD22	1.92	0.51
2:B:154:LEU:HD21	2:B:164:VAL:HG11	1.91	0.51
1:A:522:PRO:O	1:A:523:ASP:HB2	2.09	0.51
3:A:800:B12:H541	3:A:800:B12:H621	1.75	0.51
1:A:503:ARG:NH1	1:A:508:VAL:HG11	2.26	0.51
1:A:344:ASN:HA	1:A:347:ARG:HB2	1.93	0.51
3:A:800:B12:H541	3:A:800:B12:N62	2.25	0.51
2:B:374:PHE:HB3	2:B:375:PRO:CD	2.34	0.51
2:B:166:VAL:HG13	2:B:179:LEU:HD22	1.92	0.50
2:B:81:ALA:HA	2:B:406:GLU:HB3	1.93	0.50
2:B:364:THR:HG22	2:B:474:ILE:HG21	1.93	0.50
1:A:299:ALA:O	1:A:300:LYS:C	2.54	0.50
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.59	0.49
1:A:515:ILE:HG23	1:A:552:LEU:HG	1.94	0.49
2:B:534:VAL:HG13	2:B:623:VAL:HG12	1.93	0.49
2:B:253:ALA:HB2	2:B:416:ALA:HA	1.94	0.49
1:A:202:LYS:HA	1:A:205:MET:HG3	1.93	0.49
2:B:399:ALA:HB1	2:B:405:VAL:HG11	1.93	0.49
1:A:122:HIS:HA	1:A:167:MET:HE1	1.95	0.49
1:A:67:ILE:HG21	2:B:30:ALA:HB2	1.95	0.49
1:A:330:GLN:HG3	1:A:364:HIS:HB3	1.95	0.49
2:B:201:PRO:HB2	2:B:214:LEU:HD12	1.95	0.49
1:A:563:ILE:HG21	1:A:630:VAL:HB	1.94	0.48
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.95	0.48
1:A:574:VAL:O	1:A:575:LYS:HB2	2.13	0.48
1:A:338:ALA:HB3	1:A:339:GLN:NE2	2.30	0.47
1:A:503:ARG:HD2	1:A:508:VAL:HG21	1.97	0.47
2:B:328:TRP:HA	2:B:331:LEU:HG	1.96	0.46
2:B:274:THR:HA	2:B:313:VAL:HG13	1.98	0.46
2:B:292:LEU:HD23	2:B:408:LEU:HD21	1.97	0.46
1:A:605:MET:HE3	1:A:664:LEU:HD13	1.98	0.46
2:B:518:LEU:HB2	2:B:569:SER:HB2	1.96	0.46
2:B:100:ARG:HD3	2:B:393:GLY:O	2.15	0.46
2:B:532:SER:HB2	2:B:533:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:PRO:CB	2:B:49:PRO:HD2	2.46	0.45
2:B:572:LYS:HE2	2:B:573:VAL:HG22	1.99	0.45
1:A:149:MET:HE3	1:A:153:PHE:HE2	1.80	0.45
2:B:564:VAL:HG11	2:B:630:THR:HG23	1.98	0.45
1:A:172:LEU:HD23	1:A:224:ILE:HD11	1.99	0.45
2:B:399:ALA:O	2:B:400:GLY:C	2.60	0.45
1:A:441:ILE:HB	1:A:442:PRO:CD	2.47	0.45
2:B:361:LEU:HD23	2:B:362:PRO:HD2	1.99	0.44
1:A:65:ALA:HA	1:A:72:HIS:HB2	1.98	0.44
1:A:499:LEU:HD11	1:A:542:MET:HG2	1.98	0.44
1:A:531:LEU:HD22	1:A:552:LEU:HD21	1.99	0.44
3:A:800:B12:C2B	3:A:800:B12:O2	2.65	0.44
2:B:163:LYS:HE2	2:B:194:ALA:HB1	1.98	0.44
1:A:338:ALA:HB3	1:A:339:GLN:HE21	1.81	0.44
1:A:359:HIS:CE1	1:A:401:ASP:H	2.35	0.44
1:A:503:ARG:HH11	1:A:508:VAL:HG11	1.81	0.44
2:B:281:ASN:ND2	2:B:323:ASN:HD21	2.15	0.44
2:B:396:ASN:O	2:B:397:ASP:C	2.61	0.44
2:B:77:ARG:HB3	2:B:78:PRO:HD2	1.99	0.44
2:B:115:ASP:HA	2:B:116:PRO:HD2	1.83	0.44
1:A:119:LEU:N	1:A:120:PRO:HD2	2.32	0.44
1:A:500:ARG:HG3	1:A:503:ARG:HH21	1.83	0.44
2:B:553:ILE:HG22	2:B:585:LEU:HD21	1.99	0.44
2:B:517:CYS:HB2	2:B:545:VAL:O	2.18	0.44
2:B:94:THR:OG1	2:B:302:GLU:HG3	2.18	0.44
1:A:167:MET:HE3	1:A:174:ILE:HG13	2.00	0.44
1:A:605:MET:HB2	1:A:664:LEU:HD13	2.00	0.43
2:B:278:ASP:HA	2:B:321:ARG:HH22	1.83	0.43
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.48	0.43
2:B:110:ARG:HA	2:B:135:SER:O	2.17	0.43
1:A:77:THR:OG1	2:B:42:VAL:HG11	2.19	0.43
1:A:392:GLN:HB3	2:B:459:PRO:HG2	2.00	0.43
1:A:29:ALA:HA	2:B:99:VAL:HG11	2.00	0.43
1:A:302:ARG:O	1:A:305:ARG:HB2	2.18	0.43
2:B:298:ARG:HH11	2:B:405:VAL:HG12	1.84	0.43
2:B:585:LEU:O	2:B:586:LYS:C	2.61	0.43
1:A:227:TYR:HB2	1:A:530:ASN:HD21	1.84	0.42
1:A:652:VAL:HG11	1:A:668:LEU:HD21	2.01	0.42
2:B:245:GLY:HA3	2:B:446:ASN:HD21	1.85	0.42
2:B:504:SER:HB3	2:B:511:PRO:HG2	2.01	0.42
1:A:4:LEU:HB3	1:A:5:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:O	2:B:402:SER:HA	2.20	0.42
1:A:205:MET:SD	1:A:245:MET:HE2	2.59	0.42
3:A:800:B12:H262	3:A:800:B12:H91	1.70	0.42
1:A:394:SER:HB2	1:A:396:THR:HG23	2.02	0.42
2:B:532:SER:HB2	2:B:533:PRO:HD3	2.01	0.42
1:A:613:GLY:HA2	1:A:616:VAL:HG22	2.00	0.42
2:B:455:ASN:O	2:B:456:ARG:HB2	2.19	0.42
1:A:172:LEU:HB2	1:A:173:PRO:CD	2.47	0.41
3:A:800:B12:H472	3:A:800:B12:H10	1.88	0.41
2:B:47:ARG:HA	2:B:48:PRO:HD3	1.88	0.41
2:B:589:GLY:O	2:B:590:ALA:C	2.63	0.41
1:A:50:PHE:HE2	1:A:411:GLU:HG2	1.85	0.41
1:A:176:ALA:HB1	1:A:536:ILE:HG13	2.02	0.41
1:A:613:GLY:O	1:A:614:GLN:C	2.62	0.41
2:B:48:PRO:HB3	2:B:49:PRO:HD2	2.02	0.41
2:B:176:ALA:HB1	2:B:197:LEU:HD13	2.02	0.41
1:A:307:LEU:O	1:A:311:LEU:HD12	2.21	0.41
2:B:339:ASN:HA	2:B:342:ARG:HB2	2.02	0.41
1:A:386:THR:HA	2:B:341:LEU:HD13	2.01	0.41
3:A:800:B12:C35	3:A:800:B12:C36	2.90	0.41
2:B:126:LEU:HG	2:B:130:GLU:OE2	2.20	0.41
2:B:332:THR:CG2	2:B:460:ILE:HD11	2.49	0.41
1:A:179:VAL:HG11	1:A:536:ILE:HD13	2.02	0.41
1:A:228:THR:O	1:A:229:SER:C	2.62	0.41
1:A:305:ARG:HG2	1:A:325:LEU:HG	2.02	0.41
1:A:414:TRP:HE3	1:A:414:TRP:HA	1.84	0.41
2:B:377:ARG:HG3	2:B:380:ARG:NH2	2.36	0.41
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.69	0.41
2:B:58:CYS:O	2:B:59:LEU:C	2.64	0.41
1:A:58:MET:HG2	1:A:60:TRP:CH2	2.56	0.41
1:A:199:ASP:HB3	1:A:202:LYS:HZ2	1.85	0.41
1:A:406:SER:HB2	2:B:399:ALA:O	2.21	0.41
1:A:414:TRP:HA	1:A:414:TRP:CE3	2.55	0.41
2:B:33:GLU:HA	2:B:36:GLU:HB2	2.02	0.41
1:A:463:PRO:HB3	1:A:469:LYS:HD2	2.02	0.41
1:A:661:HIS:NE2	1:A:689:PRO:HD2	2.36	0.41
1:A:172:LEU:HD21	1:A:220:ILE:HG23	2.01	0.40
1:A:176:ALA:HB2	1:A:532:LEU:HD12	2.03	0.40
2:B:350:ALA:HB3	2:B:358:ILE:HD13	2.02	0.40
1:A:408:TYR:CE1	1:A:412:LEU:HD11	2.56	0.40
2:B:195:LEU:HD11	2:B:224:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ARG:O	1:A:456:ARG:HG3	2.21	0.40
2:B:158:LEU:HD12	2:B:161:MET:HE2	2.03	0.40
1:A:277:VAL:HG22	1:A:281:ALA:HB2	2.03	0.40
1:A:471:ARG:HE	1:A:471:ARG:HB2	1.77	0.40
2:B:297:LEU:HD23	2:B:322:GLN:NE2	2.37	0.40
2:B:368:GLY:HA2	2:B:479:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	723/727 (99%)	615 (85%)	87 (12%)	21 (3%)	3	9
2	B	616/637 (97%)	521 (85%)	77 (12%)	18 (3%)	3	9
All	All	1339/1364 (98%)	1136 (85%)	164 (12%)	39 (3%)	3	9

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474	HIS
1	A	523	ASP
1	A	596	ARG
2	B	93	PHE
1	A	56	LYS
1	A	205	MET
1	A	486	SER
2	B	400	GLY
2	B	525	GLY
2	B	586	LYS
1	A	43	GLN
1	A	230	ALA

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Mol	Chain	Res	Type
1	A	359	HIS
1	A	475	GLU
1	A	542	MET
2	B	50	GLU
2	B	240	ILE
2	B	245	GLY
2	B	371	GLU
2	B	576	GLN
1	A	192	LEU
1	A	229	SER
1	A	404	SER
1	A	575	LYS
2	B	244	ALA
1	A	10	VAL
1	A	84	TRP
1	A	406	SER
2	B	259	GLY
2	B	520	THR
1	A	130	PRO
2	B	145	ILE
2	B	228	SER
2	B	590	ALA
2	B	374	PHE
1	A	189	PRO
1	A	680	ILE
2	B	397	ASP
2	B	511	PRO

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	568/590 (96%)	467 (82%)	101 (18%)	2	5
2	B	458/509 (90%)	389 (85%)	69 (15%)	3	7
All	All	1026/1099 (93%)	856 (83%)	170 (17%)	2	6

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	9	SER
1	A	24	ARG
1	A	26	GLU
1	A	78	MET
1	A	87	ARG
1	A	103	ARG
1	A	113	LEU
1	A	114	SER
1	A	123	ARG
1	A	128	ASP
1	A	138	MET
1	A	149	MET
1	A	162	SER
1	A	164	SER
1	A	168	ASN
1	A	171	VAL
1	A	190	GLU
1	A	202	LYS
1	A	205	MET
1	A	207	ARG
1	A	209	THR
1	A	217	SER
1	A	222	SER
1	A	232	MET
1	A	236	ASN
1	A	237	SER
1	A	245	MET
1	A	256	MET
1	A	265	ASP
1	A	273	VAL
1	A	275	LEU
1	A	276	ASN
1	A	283	ARG
1	A	310	LYS
1	A	312	VAL
1	A	313	HIS
1	A	321	LYS
1	A	323	MET
1	A	325	LEU
1	A	336	LEU
1	A	348	THR

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Mol	Chain	Res	Type
1	A	365	THR
1	A	368	LEU
1	A	370	GLU
1	A	381	ARG
1	A	400	ILE
1	A	414	TRP
1	A	419	LYS
1	A	423	HIS
1	A	427	VAL
1	A	428	GLU
1	A	430	VAL
1	A	433	MET
1	A	438	GLU
1	A	441	ILE
1	A	444	MET
1	A	445	ARG
1	A	456	ARG
1	A	478	LEU
1	A	481	LEU
1	A	482	LYS
1	A	488	VAL
1	A	489	LEU
1	A	497	VAL
1	A	508	VAL
1	A	515	ILE
1	A	528	ASP
1	A	533	LYS
1	A	534	LEU
1	A	535	CYS
1	A	537	ASP
1	A	545	VAL
1	A	549	SER
1	A	552	LEU
1	A	554	LYS
1	A	560	THR
1	A	562	GLN
1	A	564	ARG
1	A	566	ILE
1	A	577	THR
1	A	585	GLU
1	A	597	ARG
1	A	602	LEU

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Mol	Chain	Res	Type
1	A	604	LYS
1	A	628	VAL
1	A	635	GLN
1	A	636	THR
1	A	639	GLU
1	A	651	VAL
1	A	674	LYS
1	A	677	ARG
1	A	684	VAL
1	A	688	ILE
1	A	691	GLN
1	A	694	ASP
1	A	698	LYS
1	A	702	VAL
1	A	709	THR
1	A	714	SER
1	A	717	SER
2	B	16	LEU
2	B	19	THR
2	B	21	LEU
2	B	41	LYS
2	B	61	ARG
2	B	68	ASP
2	B	70	ILE
2	B	73	VAL
2	B	75	MET
2	B	83	LYS
2	B	90	VAL
2	B	104	MET
2	B	130	GLU
2	B	136	LEU
2	B	153	VAL
2	B	155	SER
2	B	161	MET
2	B	162	THR
2	B	163	LYS
2	B	182	VAL
2	B	193	LEU
2	B	215	THR
2	B	217	LEU
2	B	224	LEU
2	B	226	LYS

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Mol	Chain	Res	Type
2	B	228	SER
2	B	230	ASP
2	B	256	LEU
2	B	261	GLU
2	B	266	LEU
2	B	274	THR
2	B	287	THR
2	B	294	ILE
2	B	300	LEU
2	B	301	ARG
2	B	314	ASP
2	B	358	ILE
2	B	369	LEU
2	B	371	GLU
2	B	408	LEU
2	B	411	SER
2	B	412	LEU
2	B	420	PHE
2	B	426	LEU
2	B	429	MET
2	B	430	SER
2	B	438	VAL
2	B	445	CYS
2	B	451	LYS
2	B	460	ILE
2	B	498	GLU
2	B	504	SER
2	B	520	THR
2	B	521	ARG
2	B	541	ASP
2	B	542	THR
2	B	550	THR
2	B	559	LYS
2	B	564	VAL
2	B	569	SER
2	B	573	VAL
2	B	579	LEU
2	B	595	LEU
2	B	601	GLU
2	B	616	ARG
2	B	619	MET
2	B	623	VAL

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Mol	Chain	Res	Type
2	B	628	SER
2	B	636	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	197	GLN
1	A	198	ASN
1	A	215	GLN
1	A	339	GLN
1	A	385	ASN
1	A	425	GLN
1	A	485	ASN
1	A	635	GLN
1	A	643	GLN
2	B	113	HIS
2	B	290	GLN
2	B	322	GLN
2	B	323	ASN
2	B	391	ASN
2	B	446	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ADN	A	801	-	20,20,21	0.53	0	28,30,31	1.87	9 (32%)
3	B12	A	800	1	94,101,101	0.94	3 (3%)	149,166,166	1.87	37 (24%)

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
4	ADN	A	801	-	-	3/4/20/22	0/3/3/3
3	B12	A	800	1	-	19/56/223/223	0/3/11/11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	C14-N23	2.71	1.38	1.35
3	A	800	B12	C55-C56	2.57	1.58	1.53
3	A	800	B12	C56-C57	2.14	1.55	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C54-C17-C18	-5.47	105.14	112.99
3	A	800	B12	C56-C57-N59	-5.29	106.70	116.34
4	A	801	ADN	O2'-C2'-C3'	-5.25	94.99	111.82
3	A	800	B12	C25-C2-C1	5.15	121.45	113.75
3	A	800	B12	C55-C56-C57	-4.52	101.18	111.25
3	A	800	B12	C13-C14-C15	-3.85	118.45	124.32
3	A	800	B12	C53-C15-C16	3.74	126.71	120.36
3	A	800	B12	O34-C32-C31	-3.65	110.03	121.04
3	A	800	B12	O34-C32-N33	3.63	132.23	122.53
3	A	800	B12	O58-C57-N59	3.59	130.08	123.03
4	A	801	ADN	C2'-C1'-N9	3.41	121.78	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	ADN	C2'-C3'-C4'	-3.41	97.33	102.36
3	A	800	B12	C53-C15-C14	-3.38	111.71	118.42
3	A	800	B12	C36-C7-C8	3.30	118.14	112.05
4	A	801	ADN	O3'-C3'-C2'	-3.30	101.24	111.82
3	A	800	B12	C7-C6-N22	3.24	113.84	107.94
3	A	800	B12	C2P-C1P-N59	3.16	117.57	112.92
3	A	800	B12	C30-C31-C32	-2.92	102.62	112.55
3	A	800	B12	C26-C2-C3	-2.92	102.33	107.42
3	A	800	B12	C7-C6-C5	-2.81	123.69	128.07
3	A	800	B12	C26-C2-C1	-2.78	105.71	110.00
3	A	800	B12	C4B-C9B-C8B	-2.78	117.61	120.16
3	A	800	B12	C4B-C5B-C6B	2.75	123.72	119.69
3	A	800	B12	O8R-C5R-C4R	-2.74	102.00	111.33
3	A	800	B12	C31-C30-C3	-2.72	106.95	114.65
3	A	800	B12	C17-C16-C15	2.71	130.55	126.26
3	A	800	B12	C15-C14-N23	2.70	129.51	126.26
4	A	801	ADN	O4'-C1'-N9	-2.58	103.14	108.09
3	A	800	B12	C7B-C6B-C5B	-2.57	115.92	119.69
3	A	800	B12	C55-C17-C16	2.53	121.55	116.59
3	A	800	B12	C19-N24-C16	2.49	110.01	107.29
3	A	800	B12	C19-C1-N21	2.43	104.64	102.14
3	A	800	B12	C7B-C8B-C9B	2.42	125.38	122.47
3	A	800	B12	C17-C16-N24	-2.41	107.49	111.17
3	A	800	B12	C17-C18-C19	-2.39	98.74	102.36
3	A	800	B12	C36-C7-C37	2.38	114.78	110.74
3	A	800	B12	C4R-O6R-C1R	2.35	114.65	109.47
4	A	801	ADN	O4'-C1'-C2'	-2.30	101.70	106.62
3	A	800	B12	C2-C1-C19	-2.25	115.12	118.61
4	A	801	ADN	C5'-C4'-C3'	2.24	118.05	115.70
3	A	800	B12	C46-C12-C11	2.17	117.83	110.08
3	A	800	B12	C13-C14-N23	2.15	112.01	109.09
3	A	800	B12	C18-C19-N24	2.15	105.55	102.33
4	A	801	ADN	O3'-C3'-C4'	-2.11	105.30	110.47
4	A	801	ADN	N3-C4-N9	2.02	130.60	127.17
3	A	800	B12	C3-C4-C5	-2.01	120.46	123.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2P-O3-P-O4
3	A	800	B12	C2P-O3-P-O2

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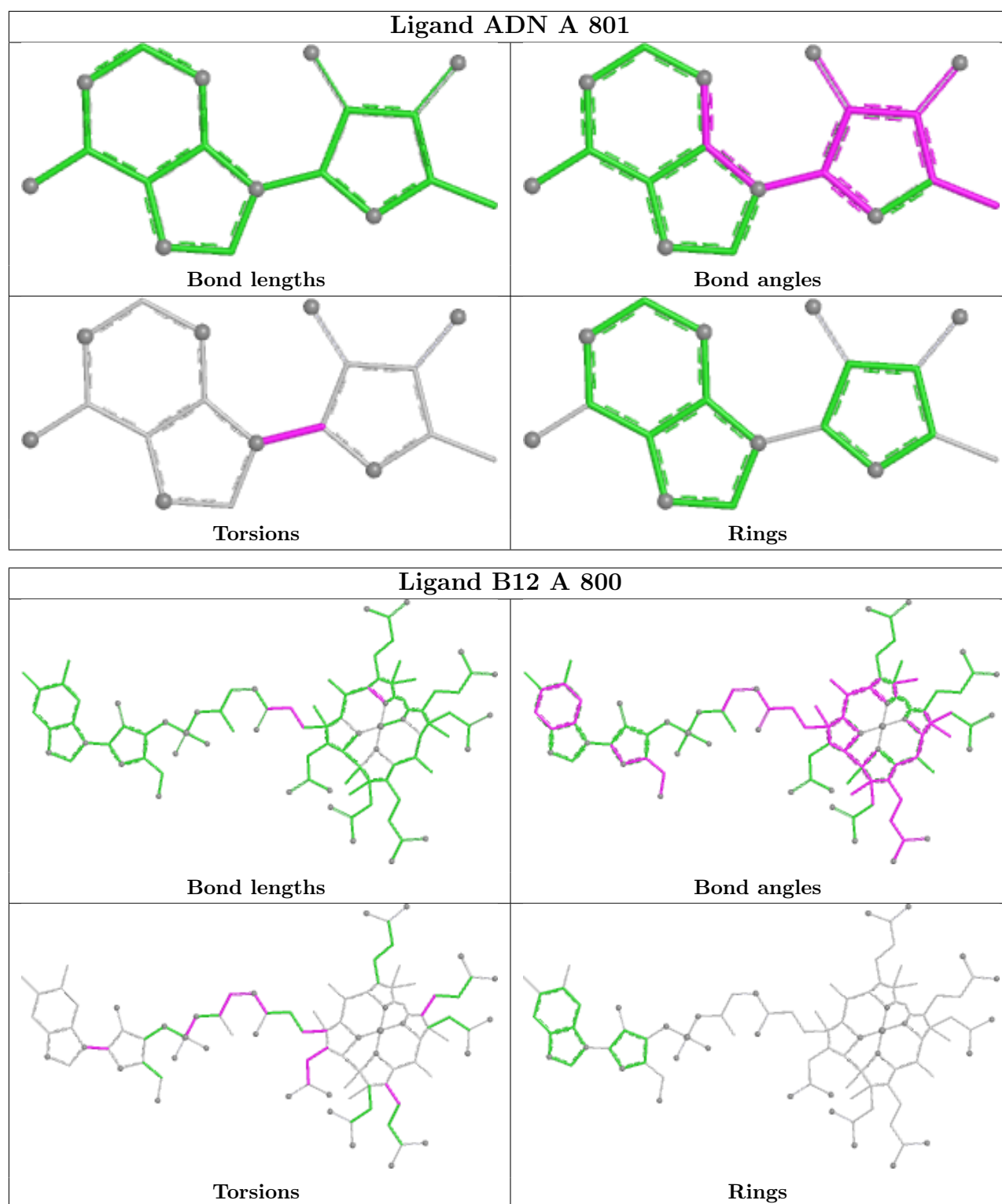
Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2P-C1P-N59-C57
3	A	800	B12	C18-C17-C55-C56
3	A	800	B12	C16-C17-C55-C56
3	A	800	B12	C17-C18-C60-C61
3	A	800	B12	C2R-C1R-N1B-C8B
3	A	800	B12	C2R-C1R-N1B-C2B
3	A	800	B12	C42-C41-C8-C9
4	A	801	ADN	C2'-C1'-N9-C4
4	A	801	ADN	C2'-C1'-N9-C8
3	A	800	B12	N59-C1P-C2P-O3
3	A	800	B12	O58-C57-N59-C1P
3	A	800	B12	C42-C41-C8-C7
3	A	800	B12	C18-C60-C61-O63
3	A	800	B12	C18-C60-C61-N62
3	A	800	B12	O6R-C1R-N1B-C8B
3	A	800	B12	C2-C3-C30-C31
4	A	801	ADN	O4'-C1'-N9-C8
3	A	800	B12	C2P-O3-P-O5
3	A	800	B12	O6R-C1R-N1B-C2B
3	A	800	B12	C56-C57-N59-C1P

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	B12	22	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.43	30 (4%) 41 37	27, 71, 94, 102	0
2	B	620/637 (97%)	0.48	22 (3%) 47 43	29, 72, 94, 109	0
All	All	1345/1364 (98%)	0.45	52 (3%) 43 39	27, 71, 94, 109	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	581	VAL	4.1
2	B	311	PHE	3.9
1	A	235	TRP	3.5
1	A	544	THR	3.1
1	A	543	ALA	3.1
2	B	201	PRO	3.1
2	B	183	TYR	2.9
2	B	589	GLY	2.8
1	A	675	LEU	2.7
1	A	676	GLY	2.6
1	A	683	THR	2.6
1	A	519	ALA	2.6
1	A	210	TYR	2.6
2	B	205	ALA	2.5
1	A	161	MET	2.5
1	A	71	VAL	2.5
1	A	552	LEU	2.4
2	B	176	ALA	2.4
2	B	259	GLY	2.4
1	A	529	ARG	2.4
1	A	517	TRP	2.4
1	A	176	ALA	2.4
2	B	190	ALA	2.4
1	A	126	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	94	THR	2.3
1	A	166	THR	2.3
2	B	216	VAL	2.3
1	A	494	ALA	2.3
1	A	511	ALA	2.3
1	A	555	VAL	2.3
1	A	728	ALA	2.3
2	B	635	GLY	2.3
2	B	573	VAL	2.3
2	B	112	LEU	2.2
1	A	541	ALA	2.2
2	B	146	ALA	2.2
1	A	406	SER	2.2
2	B	595	LEU	2.2
2	B	246	ALA	2.2
2	B	411	SER	2.2
1	A	281	ALA	2.1
1	A	267	ILE	2.1
2	B	524	PHE	2.1
2	B	269	GLN	2.1
1	A	441	ILE	2.1
1	A	127	SER	2.1
2	B	572	LYS	2.0
2	B	16	LEU	2.0
2	B	234	VAL	2.0
1	A	538	ALA	2.0
1	A	645	VAL	2.0
1	A	665	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

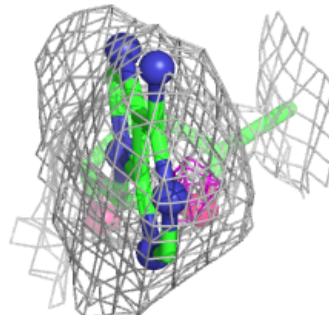
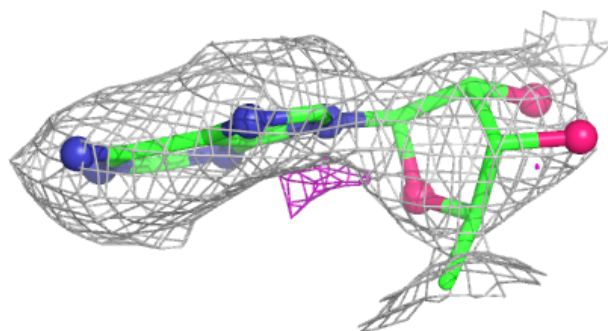
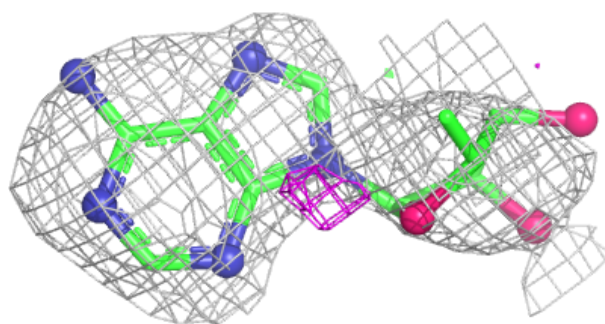
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADN	A	801	18/19	0.83	0.13	56,79,82,83	0
3	B12	A	800	91/91	0.94	0.10	26,48,67,75	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.

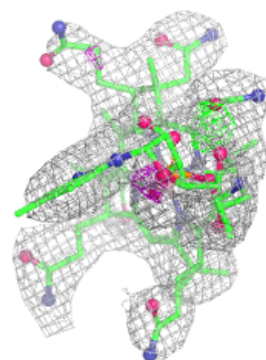
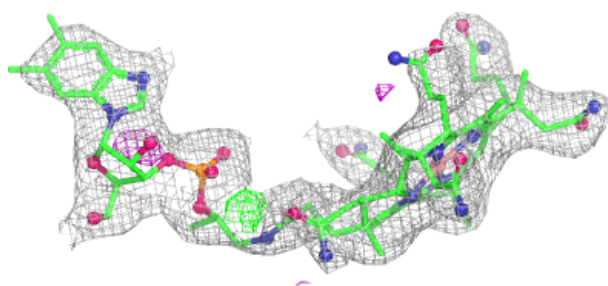
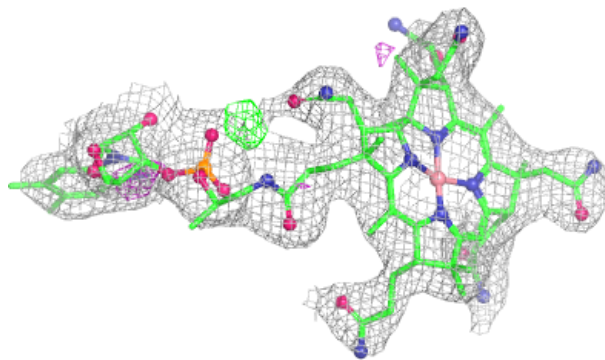
Electron density around ADN A 801:

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 800:

$2mF_o-DF_c$ (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.