



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 08:56 am BST

PDB ID : 1E1C
Title : METHYLMALONYL-COA MUTASE H244A Mutant
Authors : Evans, P.R.; Thoma, N.H.
Deposited on : 2000-04-30
Resolution : 2.62 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

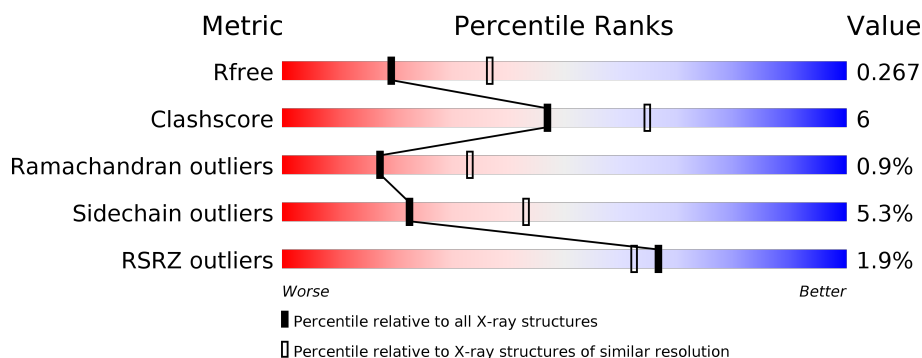
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 on 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	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>35%</div> <div>7%</div> </div> </div>
1	C	727	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>36%</div> <div>7%</div> </div> </div>
2	B	637	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>34%</div> <div></div> </div> </div>
2	D	637	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>35%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22307 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 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5558	3511	958	1065	24			
1	C	727	Total	C	N	O	S	0	0	0
			5558	3511	958	1065	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	HIS	engineered mutation	UNP P11652
C	244	ALA	HIS	engineered mutation	UNP P11652

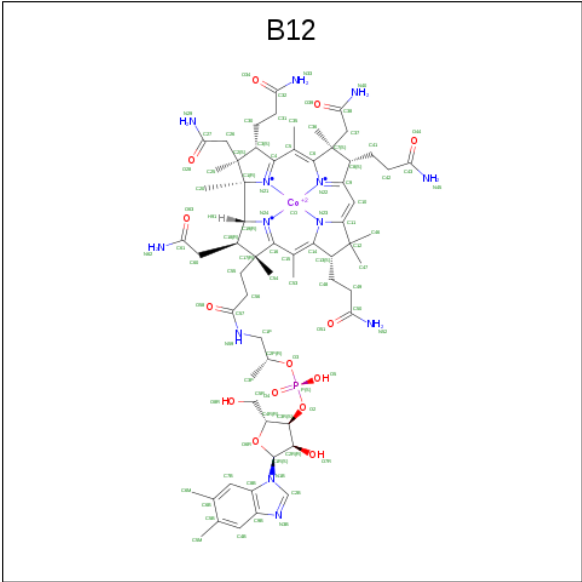
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			
2	D	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			

There are 6 discrepancies between the modelled and reference sequences:

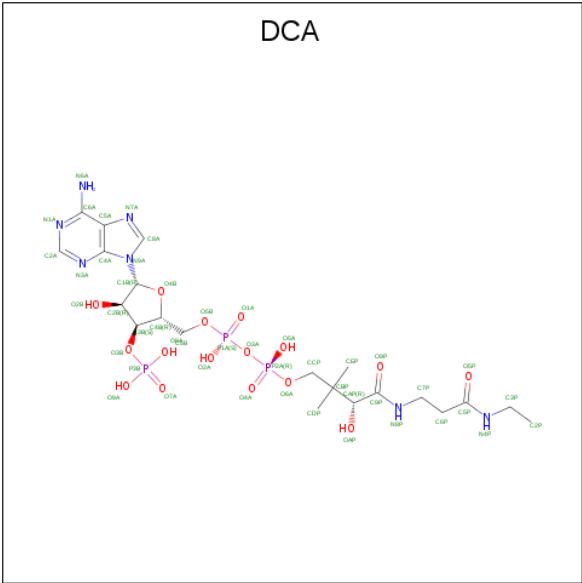
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



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

- Molecule 4 is DESULFO-COENZYME A (three-letter code: DCA) (formula: $C_{21}H_{36}N_7O_{16}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	47	21	7	16	3	0	0
4	C	1	47	21	7	16	3	0	0

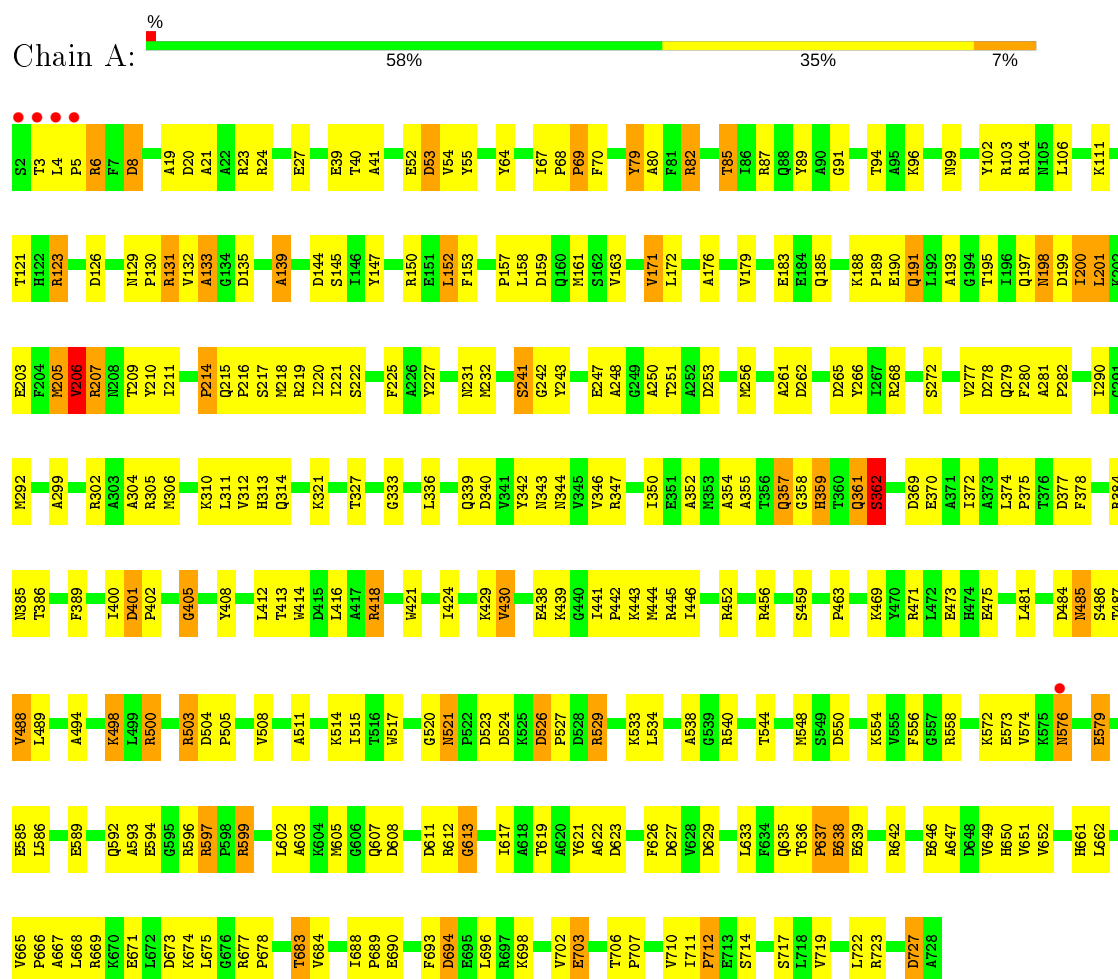
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	454	Total 454	O 454	0	0
5	B	316	Total 316	O 316	0	0
5	C	490	Total 490	O 490	0	0
5	D	265	Total 265	O 265	0	0

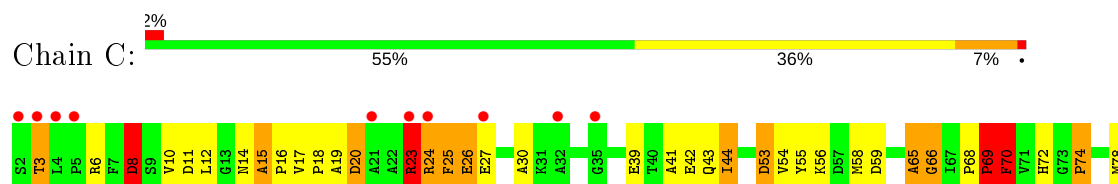
3 Residue-property plots

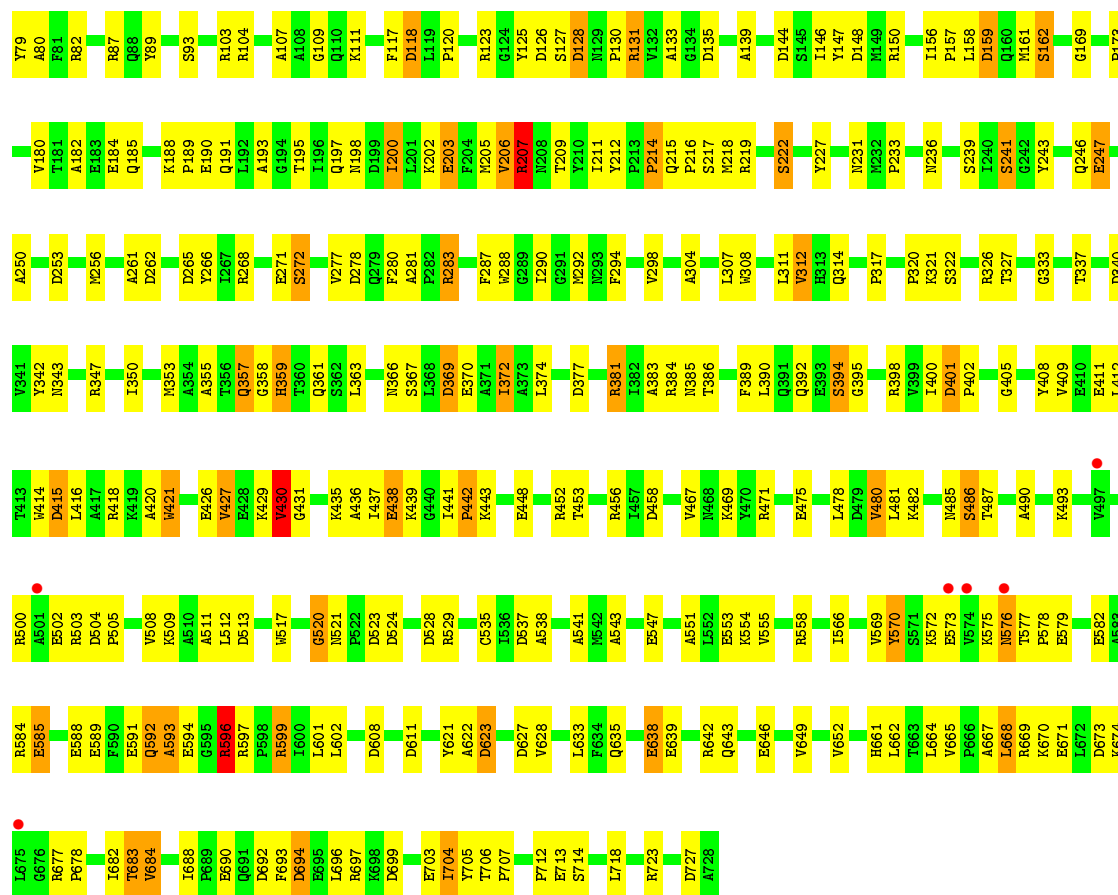
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

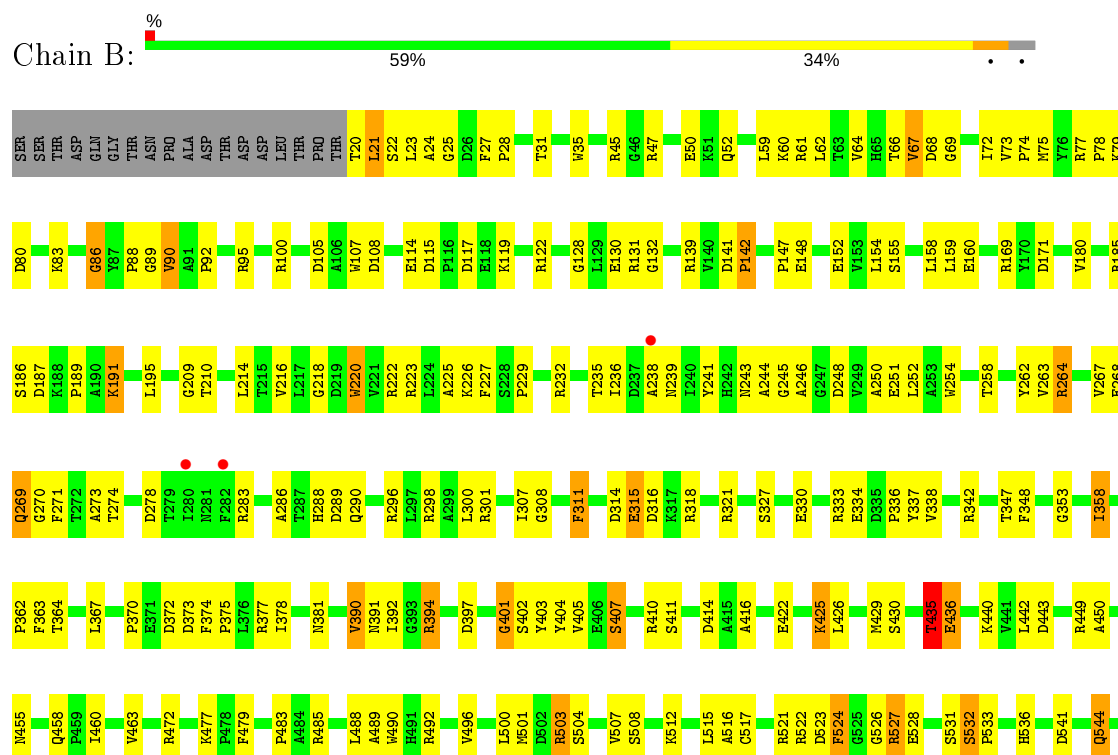


• Molecule 1: METHYLMALONYL-COA MUTASE ALPHA CHAIN



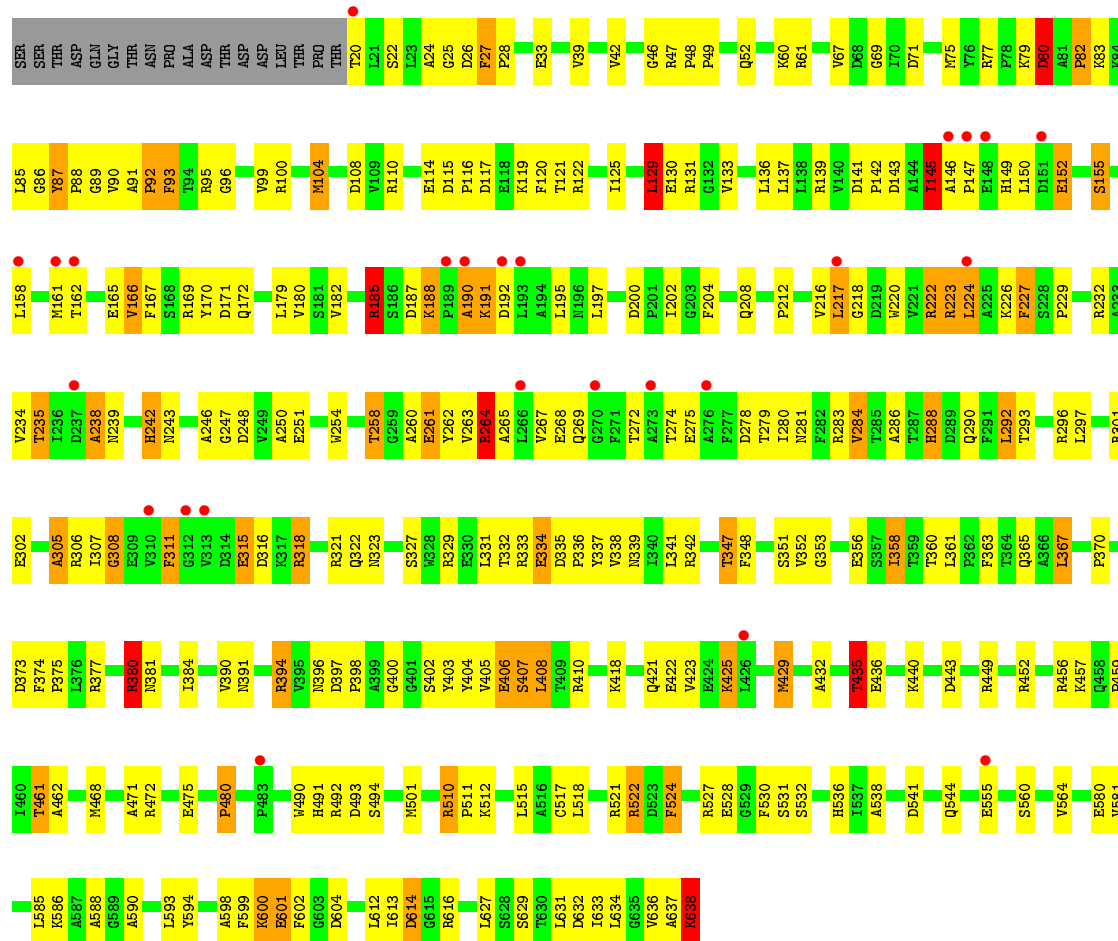


- Molecule 2: METHYLMALONYL-COA MUTASE BETA CHAIN





• Molecule 2: METHYLMALONYL-COA MUTASE BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.40Å 161.83Å 166.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 2.62 29.23 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.20-2.62) 97.5 (29.23-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.283 0.200 , 0.267	Depositor DCC
R_{free} test set	5001 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 87.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22307	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7263e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, DCA

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	0.81	0/5673	2.54	364/7710 (4.7%)
1	C	0.80	1/5673 (0.0%)	2.59	414/7710 (5.4%)
2	B	0.76	1/4785 (0.0%)	2.54	291/6499 (4.5%)
2	D	0.72	1/4785 (0.0%)	2.53	310/6499 (4.8%)
All	All	0.78	3/20916 (0.0%)	2.55	1379/28418 (4.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	87	TYR	CA-CB	6.49	1.68	1.53
2	B	270	GLY	N-CA	-6.09	1.36	1.46
1	C	593	ALA	N-CA	-5.01	1.36	1.46

All (1379) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ARG	CD-NE-CZ	33.57	170.60	123.60
2	D	510	ARG	NE-CZ-NH2	24.63	132.62	120.30
1	C	131	ARG	CD-NE-CZ	24.52	157.93	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	ARG	CD-NE-CZ	24.48	157.87	123.60
2	B	77	ARG	CD-NE-CZ	24.16	157.42	123.60
1	A	384	ARG	CD-NE-CZ	23.80	156.91	123.60
1	C	456	ARG	NE-CZ-NH1	23.43	132.01	120.30
1	C	596	ARG	NE-CZ-NH2	-23.04	108.78	120.30
1	C	384	ARG	CD-NE-CZ	21.54	153.75	123.60
1	A	485	ASN	CA-CB-CG	21.12	159.87	113.40
1	A	268	ARG	NE-CZ-NH2	-21.06	109.77	120.30
2	B	47	ARG	NE-CZ-NH1	20.85	130.72	120.30
2	D	223	ARG	NE-CZ-NH1	20.51	130.55	120.30
1	A	103	ARG	CD-NE-CZ	18.85	150.00	123.60
1	C	642	ARG	CD-NE-CZ	18.74	149.84	123.60
1	C	596	ARG	NE-CZ-NH1	18.39	129.50	120.30
1	C	123	ARG	NE-CZ-NH1	17.19	128.89	120.30
2	D	87	TYR	CB-CG-CD1	17.07	131.24	121.00
2	B	223	ARG	NE-CZ-NH2	-16.75	111.92	120.30
1	C	24	ARG	NE-CZ-NH2	-16.55	112.02	120.30
2	D	139	ARG	NE-CZ-NH2	-16.37	112.12	120.30
1	C	723	ARG	NE-CZ-NH1	16.28	128.44	120.30
1	C	723	ARG	NE-CZ-NH2	-16.18	112.21	120.30
2	D	403	TYR	CB-CG-CD1	15.96	130.57	121.00
1	A	597	ARG	NE-CZ-NH1	15.83	128.21	120.30
2	B	394	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	A	723	ARG	NE-CZ-NH1	15.37	127.98	120.30
2	B	521	ARG	NE-CZ-NH1	15.27	127.93	120.30
2	B	115	ASP	CB-CG-OD1	15.08	131.87	118.30
1	C	131	ARG	NE-CZ-NH2	-14.83	112.88	120.30
1	A	219	ARG	NE-CZ-NH2	-14.52	113.04	120.30
1	C	558	ARG	NE-CZ-NH2	-14.46	113.07	120.30
1	A	79	TYR	CB-CG-CD2	-14.18	112.49	121.00
1	C	23	ARG	NE-CZ-NH1	14.08	127.34	120.30
2	D	223	ARG	CD-NE-CZ	14.05	143.27	123.60
1	C	123	ARG	CD-NE-CZ	13.98	143.17	123.60
1	A	23	ARG	NE-CZ-NH1	13.93	127.27	120.30
1	A	596	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	A	347	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	C	694	ASP	CB-CG-OD1	13.26	130.23	118.30
1	A	20	ASP	CB-CG-OD1	13.20	130.18	118.30
2	B	269	GLN	C-N-CA	13.19	149.99	122.30
1	C	456	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	A	82	ARG	CD-NE-CZ	13.10	141.94	123.60
1	A	131	ARG	CD-NE-CZ	13.03	141.84	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	485	ASN	CA-CB-CG	13.01	142.03	113.40
2	D	77	ARG	CD-NE-CZ	12.96	141.74	123.60
2	B	403	TYR	CB-CG-CD2	-12.89	113.27	121.00
1	C	219	ARG	NE-CZ-NH2	-12.88	113.86	120.30
2	B	47	ARG	CD-NE-CZ	12.86	141.60	123.60
1	C	131	ARG	NE-CZ-NH1	12.77	126.69	120.30
2	D	117	ASP	CB-CG-OD1	12.71	129.74	118.30
1	A	131	ARG	NE-CZ-NH1	12.68	126.64	120.30
2	B	100	ARG	NE-CZ-NH2	-12.64	113.98	120.30
2	D	403	TYR	CB-CG-CD2	-12.56	113.46	121.00
1	C	268	ARG	NE-CZ-NH2	-12.47	114.06	120.30
2	B	342	ARG	NE-CZ-NH1	-12.44	114.08	120.30
1	C	53	ASP	CB-CG-OD1	12.41	129.47	118.30
2	D	232	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	C	430	VAL	CA-CB-CG1	12.30	129.35	110.90
2	B	117	ASP	CB-CG-OD1	12.29	129.36	118.30
2	D	278	ASP	CA-C-N	12.19	144.01	117.20
1	C	504	ASP	CB-CG-OD1	12.15	129.24	118.30
2	B	131	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	D	521	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	B	20	THR	CA-C-N	12.12	143.86	117.20
2	D	139	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	A	305	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	A	597	ARG	CD-NE-CZ	11.97	140.36	123.60
2	B	47	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	C	79	TYR	CB-CG-CD2	-11.87	113.88	121.00
1	C	485	ASN	N-CA-CB	11.79	131.82	110.60
2	D	342	ARG	NE-CZ-NH2	11.78	126.19	120.30
2	D	316	ASP	CB-CG-OD1	11.76	128.89	118.30
2	B	296	ARG	NE-CZ-NH1	11.73	126.16	120.30
2	D	232	ARG	CA-CB-CG	11.70	139.15	113.40
2	D	47	ARG	NE-CZ-NH1	11.65	126.12	120.30
2	B	435	THR	CA-CB-CG2	11.62	128.67	112.40
2	D	522	ARG	NE-CZ-NH1	11.62	126.11	120.30
2	B	403	TYR	CB-CG-CD1	11.61	127.97	121.00
2	D	223	ARG	NE-CZ-NH2	-11.43	114.58	120.30
1	C	41	ALA	C-N-CA	11.42	150.25	121.70
2	B	414	ASP	CB-CG-OD2	11.32	128.49	118.30
2	D	452	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	C	123	ARG	NE-CZ-NH2	-11.30	114.65	120.30
2	B	410	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	A	377	ASP	CB-CG-OD1	11.21	128.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	NH1-CZ-NH2	11.20	131.72	119.40
2	D	95	ARG	CG-CD-NE	11.19	135.29	111.80
1	A	612	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	150	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	123	ARG	CD-NE-CZ	11.10	139.14	123.60
2	D	47	ARG	CD-NE-CZ	11.10	139.14	123.60
1	A	20	ASP	CB-CG-OD2	-11.02	108.38	118.30
1	C	41	ALA	O-C-N	-10.89	105.28	122.70
2	D	321	ARG	NE-CZ-NH2	-10.87	114.86	120.30
1	C	597	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	A	131	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	C	340	ASP	CB-CG-OD1	10.79	128.01	118.30
2	B	232	ARG	CD-NE-CZ	10.77	138.68	123.60
1	C	398	ARG	NE-CZ-NH2	-10.75	114.93	120.30
2	B	316	ASP	CB-CG-OD1	10.67	127.90	118.30
1	C	456	ARG	CD-NE-CZ	10.64	138.50	123.60
2	D	87	TYR	CG-CD2-CE2	10.62	129.80	121.30
1	A	302	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	638	GLU	CB-CG-CD	10.58	142.76	114.20
2	B	492	ARG	CD-NE-CZ	10.56	138.38	123.60
2	B	232	ARG	NE-CZ-NH1	10.51	125.56	120.30
1	C	333	GLY	CA-C-O	10.49	139.48	120.60
2	D	380	ARG	CD-NE-CZ	10.45	138.23	123.60
2	D	492	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	A	41	ALA	C-N-CA	10.31	147.48	121.70
2	D	435	THR	CA-CB-CG2	10.25	126.75	112.40
2	B	77	ARG	NE-CZ-NH1	10.25	125.42	120.30
2	B	472	ARG	NE-CZ-NH2	-10.21	115.20	120.30
2	B	169	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	C	147	TYR	CB-CG-CD1	10.19	127.11	121.00
2	B	410	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	A	627	ASP	N-CA-CB	10.17	128.91	110.60
2	D	600	LYS	O-C-N	-10.17	106.42	122.70
1	A	219	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	C	670	LYS	CA-CB-CG	-10.11	91.16	113.40
1	C	326	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	A	79	TYR	CB-CG-CD1	10.06	127.03	121.00
1	A	623	ASP	CB-CG-OD1	10.04	127.33	118.30
1	A	278	ASP	CB-CG-OD1	10.04	127.33	118.30
1	C	314	GLN	C-N-CA	10.00	146.69	121.70
1	A	405	GLY	CA-C-N	9.97	139.15	117.20
2	D	115	ASP	CB-CG-OD1	9.91	127.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	86	GLY	CA-C-O	9.91	138.44	120.60
2	D	217	LEU	CA-CB-CG	9.90	138.07	115.30
2	B	524	PHE	CB-CG-CD1	9.88	127.72	120.80
2	D	122	ARG	NE-CZ-NH2	-9.87	115.36	120.30
2	D	600	LYS	C-N-CA	9.87	146.37	121.70
1	C	207	ARG	NE-CZ-NH2	-9.84	115.38	120.30
2	D	169	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	123	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	C	589	GLU	CB-CG-CD	9.83	140.75	114.20
1	C	104	ARG	CD-NE-CZ	9.83	137.36	123.60
2	D	544	GLN	CA-CB-CG	9.82	135.00	113.40
1	C	381	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	A	23	ARG	CD-NE-CZ	9.80	137.33	123.60
1	A	485	ASN	N-CA-CB	9.79	128.21	110.60
1	C	469	LYS	O-C-N	-9.75	107.09	122.70
1	C	611	ASP	CB-CG-OD1	9.75	127.08	118.30
1	A	23	ARG	NE-CZ-NH2	-9.72	115.44	120.30
2	D	527	ARG	NE-CZ-NH2	-9.70	115.45	120.30
2	B	95	ARG	NE-CZ-NH2	-9.67	115.46	120.30
2	D	61	ARG	CD-NE-CZ	9.64	137.10	123.60
2	D	262	TYR	CB-CG-CD1	9.60	126.76	121.00
1	C	642	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	A	232	MET	CA-CB-CG	9.52	129.48	113.30
1	C	683	THR	N-CA-CB	9.52	128.39	110.30
1	C	272	SER	CA-C-N	9.45	138.00	117.20
2	D	394	ARG	CD-NE-CZ	9.43	136.81	123.60
1	A	611	ASP	CB-CG-OD1	9.43	126.79	118.30
2	B	72	ILE	CB-CG1-CD1	9.37	140.13	113.90
2	B	614	ASP	CB-CG-OD1	9.30	126.67	118.30
1	C	8	ASP	C-N-CA	9.29	144.94	121.70
1	A	183	GLU	OE1-CD-OE2	9.29	134.45	123.30
2	B	243	ASN	C-N-CA	9.26	144.85	121.70
1	A	41	ALA	O-C-N	-9.26	107.89	122.70
2	D	418	LYS	CA-C-N	9.25	137.54	117.20
2	B	318	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	B	422	GLU	O-C-N	-9.16	108.05	122.70
1	C	24	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	A	678	PRO	C-N-CA	9.12	144.51	121.70
2	D	296	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	529	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	C	128	ASP	CB-CG-OD1	9.06	126.46	118.30
2	B	289	ASP	CB-CG-OD1	9.06	126.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ALA	CA-C-N	9.06	137.13	117.20
1	C	439	LYS	C-N-CA	9.03	141.27	122.30
2	D	170	TYR	CB-CG-CD2	-9.03	115.58	121.00
2	D	190	ALA	CA-C-N	9.00	137.00	117.20
1	C	430	VAL	O-C-N	-8.99	107.91	123.20
2	B	139	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	B	601	GLU	C-N-CA	8.96	144.09	121.70
1	A	265	ASP	CB-CG-OD1	8.95	126.36	118.30
1	C	570	TYR	CB-CG-CD2	8.94	126.36	121.00
1	A	347	ARG	CD-NE-CZ	8.93	136.10	123.60
1	C	627	ASP	N-CA-CB	8.91	126.65	110.60
2	B	522	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	C	278	ASP	CA-C-N	8.87	136.71	117.20
2	B	67	VAL	C-N-CA	8.84	143.81	121.70
2	D	170	TYR	CB-CG-CD1	8.84	126.30	121.00
1	A	622	ALA	O-C-N	-8.82	108.59	122.70
2	B	422	GLU	CA-C-N	8.78	136.52	117.20
1	C	59	ASP	CB-CG-OD1	8.78	126.20	118.30
2	D	95	ARG	NE-CZ-NH1	8.73	124.67	120.30
2	B	225	ALA	C-N-CA	8.71	143.49	121.70
1	C	705	TYR	CB-CG-CD1	-8.70	115.78	121.00
1	A	210	TYR	CG-CD1-CE1	8.70	128.26	121.30
1	C	133	ALA	C-N-CA	8.70	140.57	122.30
1	C	408	TYR	CB-CG-CD2	-8.69	115.79	121.00
2	B	602	PHE	C-N-CA	8.68	140.52	122.30
1	A	313	HIS	O-C-N	-8.67	108.83	122.70
2	B	337	TYR	CA-C-N	8.65	136.22	117.20
1	C	41	ALA	CA-C-N	8.65	136.22	117.20
2	B	286	ALA	N-CA-CB	8.64	122.20	110.10
1	C	570	TYR	CB-CG-CD1	-8.64	115.82	121.00
2	D	524	PHE	CB-CG-CD1	8.63	126.84	120.80
2	D	457	LYS	C-N-CA	8.62	143.24	121.70
1	A	693	PHE	CB-CG-CD1	8.61	126.83	120.80
1	C	80	ALA	CA-C-N	8.61	136.14	117.20
2	D	501	MET	CA-CB-CG	8.59	127.91	113.30
2	B	479	PHE	CB-CG-CD2	-8.56	114.81	120.80
1	C	377	ASP	CB-CG-OD2	-8.56	110.60	118.30
2	B	318	ARG	NE-CZ-NH2	-8.55	116.02	120.30
2	D	86	GLY	O-C-N	-8.54	109.03	122.70
1	C	79	TYR	CB-CG-CD1	8.49	126.09	121.00
1	A	596	ARG	NE-CZ-NH1	8.48	124.54	120.30
2	D	278	ASP	CA-C-O	-8.46	102.33	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	ASP	CB-CG-OD1	8.45	125.91	118.30
2	D	614	ASP	CB-CG-OD1	8.45	125.91	118.30
2	D	616	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	282	PRO	O-C-N	-8.44	109.19	122.70
1	A	646	GLU	CA-C-N	8.41	135.70	117.20
2	B	229	PRO	C-N-CA	8.41	142.73	121.70
1	C	408	TYR	CB-CG-CD1	8.39	126.03	121.00
1	C	246	GLN	CA-C-N	8.38	135.65	117.20
1	C	243	TYR	CB-CG-CD1	8.37	126.02	121.00
2	B	394	ARG	NH1-CZ-NH2	8.37	128.61	119.40
1	A	342	TYR	CB-CG-CD1	-8.37	115.98	121.00
1	A	253	ASP	CB-CG-OD1	8.36	125.82	118.30
1	A	694	ASP	CB-CG-OD1	8.35	125.82	118.30
2	B	20	THR	CA-C-O	-8.33	102.61	120.10
2	B	95	ARG	CG-CD-NE	8.32	129.26	111.80
1	C	298	VAL	O-C-N	-8.32	109.39	122.70
2	D	347	THR	O-C-N	-8.32	109.39	122.70
2	B	278	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	C	627	ASP	CB-CG-OD1	8.28	125.75	118.30
1	A	53	ASP	CB-CG-OD1	8.27	125.74	118.30
1	C	623	ASP	CB-CG-OD1	8.27	125.74	118.30
1	C	642	ARG	NE-CZ-NH2	-8.27	116.17	120.30
2	D	490	TRP	O-C-N	-8.25	109.50	122.70
2	B	449	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	C	520	GLY	O-C-N	-8.25	109.50	122.70
2	D	527	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	256	MET	CG-SD-CE	-8.23	87.03	100.20
2	D	187	ASP	CA-CB-CG	8.21	131.47	113.40
1	C	523	ASP	N-CA-CB	8.20	125.36	110.60
2	D	238	ALA	O-C-N	-8.19	109.59	122.70
1	C	93	SER	N-CA-CB	-8.18	98.23	110.50
2	B	289	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	A	268	ARG	NE-CZ-NH1	8.15	124.38	120.30
2	B	90	VAL	CA-CB-CG2	8.15	123.12	110.90
2	D	457	LYS	O-C-N	-8.14	109.67	122.70
2	D	425	LYS	O-C-N	-8.13	109.68	122.70
1	C	599	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	261	ALA	CB-CA-C	8.12	122.29	110.10
1	A	727	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	485	ASN	CB-CA-C	-8.12	94.16	110.40
1	C	582	GLU	OE1-CD-OE2	-8.12	113.56	123.30
1	C	669	ARG	NE-CZ-NH1	8.11	124.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	LYS	CB-CG-CD	8.11	132.68	111.60
2	B	362	PRO	N-CA-CB	8.10	113.02	103.30
1	C	418	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	C	674	LYS	O-C-N	-8.08	109.77	122.70
2	D	243	ASN	C-N-CA	8.08	141.89	121.70
1	C	278	ASP	CB-CG-OD2	-8.06	111.05	118.30
2	D	335	ASP	CB-CG-OD1	8.05	125.55	118.30
2	B	108	ASP	N-CA-CB	-8.05	96.11	110.60
2	D	243	ASN	O-C-N	-8.03	109.85	122.70
2	D	510	ARG	NH1-CZ-NH2	-8.03	110.57	119.40
1	C	82	ARG	CD-NE-CZ	8.02	134.83	123.60
2	B	274	THR	CA-C-N	8.02	134.84	117.20
1	A	540	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	A	504	ASP	CB-CG-OD1	7.99	125.49	118.30
2	B	238	ALA	O-C-N	-7.99	109.92	122.70
1	A	429	LYS	C-N-CA	7.98	141.65	121.70
1	C	633	LEU	O-C-N	-7.98	109.93	122.70
2	D	301	ARG	CA-C-N	7.98	134.75	117.20
2	D	600	LYS	CA-C-N	7.98	134.75	117.20
2	D	493	ASP	CB-CG-OD2	7.97	125.48	118.30
2	D	162	THR	CA-CB-CG2	7.96	123.54	112.40
1	A	456	ARG	CD-NE-CZ	7.95	134.73	123.60
1	C	693	PHE	CB-CG-CD1	7.95	126.36	120.80
2	D	337	TYR	CA-C-N	7.93	134.65	117.20
1	A	159	ASP	CB-CG-OD1	7.93	125.44	118.30
2	B	25	GLY	O-C-N	-7.92	110.03	122.70
1	C	369	ASP	O-C-N	-7.92	110.03	122.70
2	D	315	GLU	O-C-N	-7.92	110.03	122.70
2	D	449	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	C	705	TYR	CB-CG-CD2	7.91	125.74	121.00
1	C	678	PRO	C-N-CA	7.90	141.44	121.70
1	A	639	GLU	CA-CB-CG	7.89	130.77	113.40
2	B	443	ASP	CB-CG-OD1	7.88	125.40	118.30
1	C	420	ALA	O-C-N	-7.87	110.11	122.70
2	B	372	ASP	CB-CG-OD2	-7.86	111.23	118.30
2	D	380	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	A	231	ASN	O-C-N	-7.83	110.17	122.70
2	B	45	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	C	504	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	484	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	485	ASN	OD1-CG-ND2	7.79	139.81	121.90
2	D	410	ARG	CA-C-N	7.77	134.29	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	VAL	CA-CB-CG1	7.76	122.55	110.90
1	C	633	LEU	CA-C-O	7.76	136.40	120.10
1	A	357	GLN	C-N-CA	7.74	138.55	122.30
1	A	727	ASP	CA-CB-CG	7.69	130.31	113.40
1	C	597	ARG	CD-NE-CZ	7.68	134.35	123.60
2	B	187	ASP	CA-CB-CG	7.67	130.28	113.40
2	B	271	PHE	CB-CG-CD2	-7.67	115.43	120.80
2	B	492	ARG	CG-CD-NE	7.67	127.91	111.80
2	B	67	VAL	O-C-N	-7.67	110.43	122.70
1	C	611	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	A	161	MET	CA-CB-CG	7.64	126.30	113.30
1	A	608	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	633	LEU	O-C-N	-7.64	110.47	122.70
2	D	443	ASP	CB-CG-OD1	7.64	125.18	118.30
2	D	89	GLY	C-N-CA	7.64	140.81	121.70
2	B	235	THR	N-CA-CB	7.64	124.81	110.30
1	A	207	ARG	CG-CD-NE	7.64	127.83	111.80
1	C	262	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	282	PRO	CA-C-N	7.61	133.95	117.20
1	A	683	THR	N-CA-CB	7.61	124.76	110.30
2	D	631	LEU	CB-CA-C	7.61	124.66	110.20
1	C	541	ALA	C-N-CA	7.61	140.72	121.70
1	A	405	GLY	O-C-N	-7.60	110.54	122.70
1	C	123	ARG	C-N-CA	7.59	138.25	122.30
2	D	342	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	C	147	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	A	589	GLU	CB-CG-CD	7.58	134.66	114.20
1	C	184	GLU	C-N-CA	7.57	140.62	121.70
1	C	412	LEU	O-C-N	-7.56	110.60	122.70
2	D	286	ALA	N-CA-CB	7.56	120.68	110.10
1	A	669	ARG	NE-CZ-NH2	7.55	124.07	120.30
1	A	439	LYS	O-C-N	-7.54	110.38	123.20
1	A	185	GLN	C-N-CA	7.54	138.13	122.30
2	B	633	ILE	CA-C-N	7.54	133.78	117.20
2	B	634	LEU	C-N-CA	7.53	138.11	122.30
1	C	547	GLU	OE1-CD-OE2	-7.52	114.27	123.30
1	A	402	PRO	O-C-N	-7.51	110.69	122.70
1	A	592	GLN	CB-CA-C	-7.50	95.40	110.40
1	A	69	PRO	O-C-N	-7.50	110.71	122.70
1	A	503	ARG	CD-NE-CZ	7.49	134.09	123.60
1	A	262	ASP	CB-CG-OD1	7.48	125.04	118.30
2	B	100	ARG	NH1-CZ-NH2	7.48	127.63	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	GLY	O-C-N	-7.48	110.73	122.70
1	C	298	VAL	CA-C-N	7.48	133.65	117.20
1	A	452	ARG	CD-NE-CZ	7.47	134.06	123.60
2	D	425	LYS	CA-CB-CG	7.47	129.83	113.40
2	D	224	LEU	CA-CB-CG	7.46	132.46	115.30
2	B	274	THR	O-C-N	-7.45	110.78	122.70
1	C	150	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	205	MET	CA-C-N	7.43	133.56	117.20
1	C	314	GLN	O-C-N	-7.43	110.81	122.70
1	C	623	ASP	O-C-N	-7.43	110.81	122.70
1	A	690	GLU	O-C-N	-7.43	110.82	122.70
2	D	380	ARG	NE-CZ-NH1	7.41	124.00	120.30
2	B	25	GLY	CA-C-N	7.40	133.49	117.20
2	B	147	PRO	N-CA-CB	7.40	112.18	103.30
1	C	11	ASP	CB-CG-OD2	-7.40	111.64	118.30
2	B	64	VAL	CA-CB-CG1	7.38	121.97	110.90
2	B	214	LEU	CA-CB-CG	7.37	132.24	115.30
1	C	485	ASN	CB-CA-C	-7.36	95.68	110.40
2	D	449	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	592	GLN	CB-CG-CD	7.34	130.70	111.60
1	A	144	ASP	CB-CG-OD1	-7.34	111.69	118.30
2	B	353	GLY	C-N-CA	7.34	137.71	122.30
2	B	633	ILE	O-C-N	-7.34	110.96	122.70
1	C	144	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	430	VAL	CA-CB-CG1	7.33	121.89	110.90
1	A	362	SER	N-CA-CB	7.33	121.49	110.50
1	A	727	ASP	C-N-CA	7.32	140.01	121.70
2	B	105	ASP	C-N-CA	7.32	140.00	121.70
2	B	298	ARG	CG-CD-NE	7.31	127.15	111.80
2	B	521	ARG	O-C-N	-7.31	111.01	122.70
1	A	574	VAL	CA-CB-CG2	7.29	121.84	110.90
1	C	314	GLN	CA-C-N	7.28	133.20	117.20
1	C	528	ASP	C-N-CA	7.27	139.88	121.70
1	C	576	ASN	CA-CB-CG	7.27	129.39	113.40
2	B	139	ARG	N-CA-CB	7.27	123.68	110.60
1	A	408	TYR	CA-CB-CG	7.26	127.19	113.40
2	B	239	ASN	C-N-CA	7.26	139.85	121.70
1	C	415	ASP	CB-CG-OD2	7.25	124.82	118.30
1	A	429	LYS	O-C-N	-7.24	111.11	122.70
2	B	86	GLY	O-C-N	-7.24	111.12	122.70
1	C	59	ASP	N-CA-CB	-7.23	97.58	110.60
2	B	268	GLU	CA-C-N	7.23	133.11	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	GLN	CB-CA-C	7.22	124.83	110.40
2	D	293	THR	O-C-N	-7.22	111.16	122.70
1	C	674	LYS	C-N-CA	7.21	139.74	121.70
1	A	629	ASP	N-CA-CB	7.21	123.58	110.60
2	B	148	GLU	CA-C-N	7.21	133.06	117.20
2	D	316	ASP	CB-CG-OD2	-7.19	111.83	118.30
2	D	541	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	C	452	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	214	PRO	O-C-N	-7.18	111.21	122.70
2	B	503	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	B	429	MET	CA-CB-CG	7.16	125.47	113.30
1	C	80	ALA	O-C-N	-7.15	111.26	122.70
2	D	318	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	248	ALA	CA-C-N	7.13	130.47	116.20
2	B	227	PHE	N-CA-CB	-7.13	97.76	110.60
1	C	159	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C	584	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	A	305	ARG	NE-CZ-NH2	-7.13	116.73	120.30
2	B	594	TYR	CB-CG-CD1	7.12	125.28	121.00
1	C	261	ALA	O-C-N	-7.12	111.30	122.70
2	D	22	SER	CB-CA-C	-7.12	96.56	110.10
2	D	397	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	261	ALA	O-C-N	-7.12	111.31	122.70
1	C	190	GLU	O-C-N	-7.12	111.31	122.70
2	B	490	TRP	O-C-N	-7.11	111.33	122.70
1	A	340	ASP	CB-CG-OD1	7.11	124.69	118.30
1	A	277	VAL	O-C-N	-7.10	111.34	122.70
2	B	342	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	C	727	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	304	ALA	O-C-N	-7.09	111.35	122.70
2	D	79	LYS	CA-C-N	7.09	132.80	117.20
1	A	520	GLY	O-C-N	-7.09	111.35	122.70
1	C	262	ASP	O-C-N	-7.09	111.15	123.20
1	C	343	ASN	O-C-N	-7.09	111.36	122.70
2	D	492	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	C	443	LYS	CA-C-N	7.08	132.78	117.20
1	A	82	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	C	209	THR	CA-CB-CG2	7.07	122.29	112.40
2	D	104	MET	CA-C-N	7.07	132.75	117.20
1	A	674	LYS	CA-CB-CG	7.06	128.94	113.40
2	B	521	ARG	CA-CB-CG	7.06	128.94	113.40
1	A	693	PHE	CB-CG-CD2	-7.06	115.86	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ILE	C-N-CA	7.05	139.33	121.70
2	B	50	GLU	CA-CB-CG	7.05	128.91	113.40
2	D	472	ARG	CD-NE-CZ	7.04	133.46	123.60
2	B	458	GLN	N-CA-CB	7.04	123.28	110.60
1	C	207	ARG	CG-CD-NE	7.04	126.58	111.80
2	B	88	PRO	N-CA-CB	7.04	111.74	103.30
2	D	229	PRO	C-N-CA	7.04	139.29	121.70
1	A	661	HIS	O-C-N	-7.03	111.45	122.70
2	B	160	GLU	C-N-CA	7.03	139.28	121.70
2	B	564	VAL	CG1-CB-CG2	-7.03	99.65	110.90
2	B	278	ASP	CB-CG-OD1	7.03	124.63	118.30
1	C	70	PHE	CB-CG-CD1	7.03	125.72	120.80
1	A	438	GLU	CA-C-N	7.02	132.64	117.20
1	C	150	ARG	CD-NE-CZ	7.01	133.42	123.60
1	C	246	GLN	O-C-N	-7.01	111.49	122.70
1	A	629	ASP	CB-CG-OD2	-7.00	112.00	118.30
2	B	68	ASP	CB-CG-OD2	7.00	124.60	118.30
2	D	510	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	C	608	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	C	667	ALA	O-C-N	-6.97	111.55	122.70
1	C	321	LYS	O-C-N	-6.96	111.56	122.70
1	A	262	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	343	ASN	O-C-N	-6.96	111.57	122.70
2	D	232	ARG	NH1-CZ-NH2	-6.94	111.76	119.40
1	C	211	ILE	C-N-CA	6.94	139.04	121.70
1	C	337	THR	CA-CB-CG2	6.93	122.11	112.40
1	C	674	LYS	CA-C-N	6.93	132.45	117.20
1	C	471	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	D	380	ARG	NH1-CZ-NH2	-6.93	111.78	119.40
1	A	6	ARG	NE-CZ-NH1	6.91	123.76	120.30
2	D	27	PHE	CB-CG-CD2	-6.91	115.96	120.80
1	C	320	PRO	N-CA-CB	6.91	111.59	103.30
2	B	100	ARG	CD-NE-CZ	6.91	133.27	123.60
1	A	150	ARG	NH1-CZ-NH2	6.90	126.99	119.40
1	C	247	GLU	OE1-CD-OE2	6.90	131.58	123.30
1	A	377	ASP	CB-CG-OD2	-6.90	112.09	118.30
2	D	191	LYS	O-C-N	-6.89	111.68	122.70
1	C	594	GLU	N-CA-CB	-6.88	98.21	110.60
2	D	337	TYR	O-C-N	-6.88	111.69	122.70
2	B	128	GLY	CA-C-N	6.88	132.34	117.20
2	D	538	ALA	CA-C-N	6.88	129.96	116.20
2	B	578	GLY	CA-C-O	6.88	132.98	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	TYR	CB-CG-CD1	6.88	125.12	121.00
1	A	469	LYS	O-C-N	-6.87	111.70	122.70
1	C	662	LEU	CB-CG-CD1	-6.87	99.32	111.00
1	C	321	LYS	CA-C-N	6.87	132.30	117.20
2	D	632	ASP	O-C-N	-6.87	111.71	122.70
1	C	326	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	D	408	LEU	CA-C-N	6.86	132.30	117.20
1	A	439	LYS	C-N-CA	6.86	136.71	122.30
2	B	191	LYS	C-N-CA	6.86	138.85	121.70
2	B	115	ASP	CB-CG-OD2	-6.86	112.13	118.30
2	D	638	LYS	CA-CB-CG	6.86	128.48	113.40
1	C	430	VAL	CA-C-N	6.85	129.90	116.20
1	C	594	GLU	CA-CB-CG	6.85	128.47	113.40
2	B	449	ARG	CD-NE-CZ	6.84	133.17	123.60
1	C	420	ALA	CA-C-N	6.84	132.24	117.20
1	C	677	ARG	CA-CB-CG	6.83	128.42	113.40
2	D	218	GLY	C-N-CA	6.83	138.77	121.70
1	A	471	ARG	CA-CB-CG	6.83	128.41	113.40
2	D	302	GLU	OE1-CD-OE2	-6.82	115.12	123.30
2	B	189	PRO	N-CA-CB	6.81	111.47	103.30
2	D	425	LYS	C-N-CA	6.81	138.72	121.70
1	A	214	PRO	O-C-N	-6.79	111.84	122.70
1	A	597	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	B	278	ASP	CA-C-N	6.78	132.12	117.20
1	A	343	ASN	CA-C-N	6.77	132.10	117.20
1	C	342	TYR	O-C-N	-6.77	111.86	122.70
1	A	385	ASN	CA-C-N	6.77	132.09	117.20
2	B	254	TRP	CA-C-N	6.77	132.09	117.20
1	C	384	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	227	TYR	CB-CG-CD1	6.76	125.06	121.00
2	B	66	THR	O-C-N	-6.75	111.89	122.70
2	B	296	ARG	CD-NE-CZ	6.75	133.06	123.60
2	B	223	ARG	CG-CD-NE	6.74	125.96	111.80
1	A	163	VAL	CG1-CB-CG2	-6.74	100.11	110.90
2	D	333	ARG	NE-CZ-NH2	6.74	123.67	120.30
2	B	223	ARG	NH1-CZ-NH2	6.74	126.81	119.40
2	B	131	ARG	NE-CZ-NH2	-6.73	116.93	120.30
2	B	599	PHE	O-C-N	-6.73	111.93	122.70
1	C	3	THR	N-CA-CB	6.73	123.09	110.30
1	A	210	TYR	CB-CG-CD2	6.71	125.03	121.00
1	A	265	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	513	ASP	CB-CG-OD1	6.71	124.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	589	GLU	O-C-N	-6.71	111.96	122.70
1	A	321	LYS	CA-C-N	6.70	131.94	117.20
1	C	401	ASP	CA-C-O	6.70	134.16	120.10
1	C	30	ALA	CB-CA-C	6.69	120.14	110.10
1	C	17	VAL	N-CA-CB	6.69	126.22	111.50
1	C	480	VAL	CB-CA-C	-6.69	98.70	111.40
1	A	574	VAL	CB-CA-C	6.68	124.09	111.40
1	C	623	ASP	CA-C-N	6.68	131.89	117.20
1	C	628	VAL	CG1-CB-CG2	-6.67	100.22	110.90
2	B	78	PRO	N-CA-CB	6.67	111.30	103.30
1	A	54	VAL	CA-C-N	6.66	131.85	117.20
1	C	692	ASP	CA-C-N	6.66	131.85	117.20
2	D	301	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	B	283	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	B	107	TRP	CA-C-N	-6.65	102.56	117.20
2	B	89	GLY	C-N-CA	6.65	138.33	121.70
1	A	248	ALA	N-CA-CB	6.65	119.41	110.10
1	A	312	VAL	O-C-N	-6.65	112.06	122.70
2	B	191	LYS	O-C-N	-6.64	112.07	122.70
2	B	531	SER	CA-C-O	6.63	134.03	120.10
1	A	198	ASN	N-CA-CB	-6.63	98.66	110.60
2	D	80	ASP	CA-C-N	6.62	131.76	117.20
1	C	231	ASN	O-C-N	-6.61	112.13	122.70
2	D	25	GLY	O-C-N	-6.61	112.13	122.70
1	C	427	VAL	CA-C-N	6.61	131.73	117.20
2	D	633	ILE	O-C-N	-6.61	112.13	122.70
1	C	69	PRO	O-C-N	-6.60	112.13	122.70
1	C	385	ASN	CA-C-N	6.60	131.72	117.20
2	D	25	GLY	CA-C-N	6.60	131.73	117.20
1	C	6	ARG	NE-CZ-NH2	-6.60	117.00	120.30
2	D	456	ARG	O-C-N	-6.60	112.14	122.70
2	B	78	PRO	O-C-N	-6.59	112.15	122.70
2	B	611	LYS	CA-C-N	6.59	131.70	117.20
1	C	184	GLU	O-C-N	-6.58	112.16	122.70
1	C	529	ARG	N-CA-CB	-6.58	98.75	110.60
2	D	348	PHE	CB-CG-CD1	6.58	125.41	120.80
1	C	703	GLU	CA-CB-CG	6.58	127.88	113.40
1	C	118	ASP	CB-CG-OD1	6.58	124.22	118.30
2	B	218	GLY	C-N-CA	6.57	138.13	121.70
1	C	513	ASP	CA-CB-CG	6.57	127.84	113.40
2	B	404	TYR	CA-CB-CG	6.56	125.86	113.40
1	C	70	PHE	O-C-N	-6.56	112.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	ALA	CB-CA-C	6.56	119.94	110.10
1	A	626	PHE	N-CA-CB	-6.56	98.80	110.60
2	B	229	PRO	O-C-N	-6.55	112.21	122.70
2	D	190	ALA	O-C-N	-6.55	112.22	122.70
2	D	71	ASP	CB-CG-OD1	6.55	124.19	118.30
1	C	209	THR	N-CA-CB	6.55	122.74	110.30
2	D	311	PHE	C-N-CA	6.55	136.05	122.30
1	C	158	LEU	O-C-N	-6.54	112.23	122.70
2	B	90	VAL	CG1-CB-CG2	-6.54	100.43	110.90
1	A	369	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	312	VAL	O-C-N	-6.54	112.23	122.70
2	B	220	TRP	N-CA-CB	-6.53	98.84	110.60
1	A	416	LEU	O-C-N	-6.53	112.25	122.70
2	B	524	PHE	CB-CG-CD2	-6.53	116.23	120.80
2	B	500	LEU	CA-C-N	6.53	131.56	117.20
2	B	262	TYR	CB-CG-CD1	6.52	124.92	121.00
2	D	327	SER	CA-C-O	6.52	133.80	120.10
1	A	52	GLU	C-N-CA	6.52	138.01	121.70
2	B	503	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	D	33	GLU	CA-C-N	6.52	131.55	117.20
2	B	243	ASN	O-C-N	-6.50	112.29	122.70
2	B	66	THR	CA-C-N	6.50	131.50	117.20
1	A	727	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	120	PRO	O-C-N	-6.49	112.31	122.70
1	A	384	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	438	GLU	CB-CG-CD	6.48	131.71	114.20
1	A	523	ASP	N-CA-CB	6.48	122.26	110.60
1	C	207	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	678	PRO	N-CA-CB	6.46	111.06	103.30
1	A	405	GLY	CA-C-O	-6.46	108.97	120.60
1	A	103	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	C	678	PRO	O-C-N	-6.46	112.36	122.70
1	C	281	ALA	N-CA-CB	6.46	119.14	110.10
1	A	53	ASP	N-CA-CB	6.46	122.22	110.60
1	A	313	HIS	C-N-CA	6.46	137.84	121.70
1	A	6	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	C	243	TYR	CB-CG-CD2	-6.45	117.13	121.00
2	B	358	ILE	CG1-CB-CG2	-6.45	97.21	111.40
1	C	502	GLU	CA-C-N	6.45	131.39	117.20
2	D	410	ARG	O-C-N	-6.44	112.39	122.70
1	C	409	VAL	CA-C-N	6.44	131.36	117.20
2	B	185	ARG	CA-C-N	6.43	131.34	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	265	ALA	CA-C-N	6.42	131.33	117.20
2	B	403	TYR	O-C-N	-6.41	112.44	122.70
2	D	390	VAL	O-C-N	-6.41	112.45	122.70
2	D	510	ARG	CD-NE-CZ	6.41	132.57	123.60
1	A	79	TYR	C-N-CA	6.40	137.71	121.70
2	B	79	LYS	O-C-N	-6.40	112.46	122.70
1	A	52	GLU	CA-C-N	6.40	131.27	117.20
2	D	96	GLY	CA-C-O	6.40	132.12	120.60
1	C	294	PHE	CB-CG-CD1	6.40	125.28	120.80
1	A	418	ARG	CA-C-N	6.39	131.27	117.20
2	B	158	LEU	O-C-N	-6.39	112.47	122.70
2	B	185	ARG	NE-CZ-NH1	6.39	123.50	120.30
2	D	342	ARG	CB-CG-CD	6.39	128.22	111.60
2	B	86	GLY	C-N-CA	6.39	137.68	121.70
2	D	248	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	458	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	342	TYR	O-C-N	-6.38	112.49	122.70
1	C	292	MET	O-C-N	-6.38	112.50	122.70
2	D	171	ASP	O-C-N	-6.38	112.50	122.70
2	D	191	LYS	C-N-CA	6.38	137.64	121.70
2	D	116	PRO	N-CA-CB	6.37	110.95	103.30
1	C	370	GLU	O-C-N	-6.37	112.51	122.70
2	D	67	VAL	O-C-N	-6.37	112.50	122.70
1	A	222	SER	O-C-N	-6.37	112.51	122.70
2	B	268	GLU	O-C-N	-6.37	112.51	122.70
2	B	564	VAL	CA-CB-CG2	6.37	120.45	110.90
1	A	55	TYR	O-C-N	-6.36	112.52	122.70
2	B	600	LYS	CA-C-N	6.36	131.19	117.20
1	C	381	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	D	307	ILE	O-C-N	-6.36	112.39	123.20
2	D	238	ALA	C-N-CA	6.35	137.58	121.70
1	A	579	GLU	N-CA-CB	6.35	122.03	110.60
1	C	43	GLN	C-N-CA	6.35	137.57	121.70
2	D	229	PRO	O-C-N	-6.35	112.55	122.70
2	D	429	MET	CB-CG-SD	6.35	131.44	112.40
1	C	579	GLU	CA-C-N	6.34	131.15	117.20
2	B	296	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	D	522	ARG	CD-NE-CZ	6.33	132.46	123.60
1	A	677	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	343	ASN	C-N-CA	6.32	137.50	121.70
1	C	588	GLU	CA-C-N	6.32	131.10	117.20
2	D	435	THR	O-C-N	-6.31	112.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	PRO	N-CA-CB	6.31	110.87	103.30
1	A	593	ALA	O-C-N	-6.31	112.60	122.70
1	C	272	SER	O-C-N	-6.31	112.61	122.70
2	D	338	VAL	CA-C-N	6.30	131.07	117.20
1	C	712	PRO	N-CA-CB	6.30	110.86	103.30
1	A	333	GLY	CA-C-O	6.29	131.93	120.60
1	A	504	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	A	723	ARG	NH1-CZ-NH2	-6.29	112.48	119.40
2	B	337	TYR	O-C-N	-6.29	112.64	122.70
1	A	52	GLU	O-C-N	-6.29	112.64	122.70
2	B	315	GLU	C-N-CA	6.28	137.41	121.70
2	D	46	GLY	C-N-CA	6.28	137.41	121.70
2	D	521	ARG	NH1-CZ-NH2	-6.28	112.50	119.40
2	B	75	MET	O-C-N	-6.27	112.66	122.70
1	A	696	LEU	CA-C-N	6.27	131.00	117.20
1	A	207	ARG	N-CA-C	6.27	127.93	111.00
2	B	523	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	B	21	LEU	O-C-N	-6.27	112.67	122.70
2	D	204	PHE	CB-CG-CD1	-6.26	116.42	120.80
2	B	515	LEU	C-N-CA	6.26	137.34	121.70
2	D	404	TYR	CB-CG-CD2	6.25	124.75	121.00
2	D	87	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	D	602	PHE	C-N-CA	6.25	135.43	122.30
1	C	372	ILE	CA-C-N	6.25	130.95	117.20
1	A	439	LYS	CA-C-N	6.24	128.68	116.20
1	A	689	PRO	O-C-N	-6.24	112.72	122.70
2	B	338	VAL	O-C-N	-6.24	112.72	122.70
2	B	507	VAL	N-CA-CB	-6.24	97.78	111.50
1	C	599	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	B	508	SER	CA-C-N	6.23	130.91	117.20
1	A	278	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	B	378	ILE	O-C-N	-6.23	112.73	122.70
1	A	400	ILE	C-N-CA	6.23	137.27	121.70
1	A	443	LYS	O-C-N	-6.23	112.74	122.70
2	D	336	PRO	N-CA-CB	6.23	110.77	103.30
1	C	704	ILE	O-C-N	-6.23	112.74	122.70
1	A	459	SER	C-N-CA	6.22	135.36	122.30
2	B	430	SER	C-N-CA	6.22	137.25	121.70
2	D	169	ARG	CA-CB-CG	6.22	127.08	113.40
2	D	292	LEU	CA-C-N	6.22	130.88	117.20
2	D	352	VAL	C-N-CA	6.22	135.35	122.30
2	B	512	LYS	CB-CA-C	-6.21	97.97	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	622	ALA	O-C-N	-6.21	112.77	122.70
2	D	242	HIS	CA-C-N	6.21	130.86	117.20
2	D	394	ARG	NE-CZ-NH2	-6.21	117.20	120.30
2	D	408	LEU	O-C-N	-6.21	112.77	122.70
2	B	187	ASP	C-N-CA	6.20	137.21	121.70
1	C	219	ARG	CD-NE-CZ	-6.20	114.92	123.60
1	C	253	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	107	TRP	N-CA-CB	6.20	121.76	110.60
1	C	471	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	D	541	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	89	TYR	CB-CG-CD1	6.20	124.72	121.00
2	B	381	ASN	CB-CA-C	6.20	122.79	110.40
2	D	599	PHE	CA-C-N	6.19	130.82	117.20
1	C	146	ILE	O-C-N	-6.18	112.81	122.70
1	C	572	LYS	N-CA-CB	6.18	121.73	110.60
2	D	262	TYR	CB-CG-CD2	-6.18	117.29	121.00
2	D	223	ARG	CB-CG-CD	6.18	127.66	111.60
2	B	59	LEU	O-C-N	-6.18	112.82	122.70
1	A	498	LYS	CB-CG-CD	6.17	127.65	111.60
2	B	479	PHE	CB-CG-CD1	6.17	125.12	120.80
1	C	195	THR	CA-CB-CG2	6.17	121.03	112.40
2	D	404	TYR	CA-CB-CG	6.17	125.11	113.40
2	B	273	ALA	N-CA-CB	6.16	118.72	110.10
1	C	277	VAL	O-C-N	-6.16	112.84	122.70
2	D	79	LYS	O-C-N	-6.16	112.84	122.70
1	C	182	ALA	C-N-CA	6.16	137.09	121.70
1	C	551	ALA	CA-C-N	6.16	130.75	117.20
1	C	661	HIS	CA-C-N	6.16	130.75	117.20
1	A	438	GLU	O-C-N	-6.15	112.86	122.70
1	C	579	GLU	O-C-N	-6.15	112.86	122.70
1	A	558	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	D	588	ALA	CA-C-N	6.14	128.49	116.20
1	A	8	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	D	274	THR	O-C-N	-6.14	112.88	122.70
2	B	483	PRO	CA-C-N	6.14	130.70	117.20
2	D	239	ASN	C-N-CA	6.14	137.04	121.70
2	D	150	LEU	C-N-CA	6.14	137.04	121.70
1	C	385	ASN	O-C-N	-6.13	112.89	122.70
2	D	629	SER	O-C-N	-6.13	112.89	122.70
2	B	327	SER	CA-C-O	6.13	132.97	120.10
2	B	472	ARG	CD-NE-CZ	6.13	132.18	123.60
1	A	529	ARG	N-CA-CB	-6.13	99.57	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	646	GLU	C-N-CA	6.12	137.00	121.70
1	C	572	LYS	CB-CA-C	-6.12	98.16	110.40
1	C	327	THR	N-CA-C	6.11	127.50	111.00
1	C	367	SER	CA-C-O	6.11	132.94	120.10
1	C	130	PRO	N-CA-CB	6.11	110.63	103.30
1	A	190	GLU	O-C-N	-6.10	112.94	122.70
1	A	638	GLU	O-C-N	-6.10	112.94	122.70
2	D	75	MET	C-N-CA	6.10	136.94	121.70
2	D	147	PRO	C-N-CA	6.09	136.94	121.70
1	A	494	ALA	O-C-N	-6.09	112.95	122.70
1	A	133	ALA	C-N-CA	6.09	135.09	122.30
2	B	504	SER	O-C-N	-6.09	112.96	122.70
2	D	110	ARG	CD-NE-CZ	6.09	132.12	123.60
1	C	646	GLU	CA-C-N	6.07	130.56	117.20
1	C	19	ALA	C-N-CA	6.07	136.86	121.70
2	D	490	TRP	N-CA-CB	-6.06	99.69	110.60
1	A	241	SER	N-CA-C	6.06	127.37	111.00
1	A	369	ASP	O-C-N	-6.06	113.00	122.70
2	B	348	PHE	CB-CG-CD2	6.05	125.04	120.80
2	B	407	SER	O-C-N	-6.05	113.01	122.70
1	A	675	LEU	O-C-N	-6.05	112.91	123.20
1	C	8	ASP	O-C-N	-6.04	113.03	122.70
2	B	629	SER	CA-C-N	6.04	130.49	117.20
1	C	25	PHE	N-CA-CB	6.04	121.48	110.60
2	D	316	ASP	CA-C-N	6.04	130.49	117.20
1	A	195	THR	CA-CB-CG2	6.04	120.86	112.40
1	A	272	SER	CA-C-N	6.04	130.48	117.20
2	D	421	GLN	CG-CD-OE1	6.04	133.68	121.60
1	A	70	PHE	CB-CG-CD1	6.04	125.03	120.80
1	C	684	VAL	CA-CB-CG2	6.04	119.95	110.90
2	D	329	ARG	C-N-CA	6.03	136.78	121.70
1	C	118	ASP	N-CA-CB	6.03	121.45	110.60
1	A	576	ASN	CA-CB-CG	6.02	126.65	113.40
1	C	467	VAL	CG1-CB-CG2	-6.02	101.26	110.90
1	A	64	TYR	CB-CG-CD2	6.02	124.61	121.00
2	D	425	LYS	CB-CG-CD	6.02	127.25	111.60
2	D	239	ASN	O-C-N	-6.02	113.08	122.70
2	B	544	GLN	CA-CB-CG	6.01	126.63	113.40
2	D	165	GLU	N-CA-CB	6.00	121.41	110.60
2	B	422	GLU	OE1-CD-OE2	-6.00	116.10	123.30
2	D	629	SER	CA-C-N	6.00	130.40	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	613	ILE	CA-C-O	5.99	132.68	120.10
1	A	102	TYR	CA-CB-CG	5.99	124.78	113.40
2	B	171	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	D	92	PRO	N-CA-C	5.99	127.68	112.10
1	A	145	SER	O-C-N	-5.99	113.12	122.70
1	A	147	TYR	CB-CG-CD1	5.99	124.59	121.00
2	D	338	VAL	O-C-N	-5.98	113.13	122.70
1	C	693	PHE	N-CA-C	5.98	127.16	111.00
1	A	459	SER	O-C-N	-5.98	113.04	123.20
1	A	550	ASP	O-C-N	-5.98	113.14	122.70
1	C	169	GLY	CA-C-O	5.98	131.36	120.60
2	D	24	ALA	O-C-N	-5.98	113.04	123.20
2	B	422	GLU	CA-CB-CG	5.98	126.55	113.40
2	B	496	VAL	O-C-N	-5.97	113.14	122.70
2	B	69	GLY	N-CA-C	5.97	128.02	113.10
2	B	521	ARG	CA-C-N	5.96	130.32	117.20
2	B	455	ASN	O-C-N	-5.96	113.17	122.70
2	D	334	GLU	OE1-CD-OE2	5.96	130.45	123.30
1	C	133	ALA	O-C-N	-5.96	113.08	123.20
1	C	696	LEU	CA-C-N	5.95	130.29	117.20
1	A	573	GLU	CA-C-N	5.95	130.28	117.20
2	B	154	LEU	O-C-N	-5.95	113.18	122.70
1	C	42	GLU	CB-CA-C	-5.95	98.51	110.40
1	C	411	GLU	OE1-CD-OE2	-5.95	116.17	123.30
2	D	530	PHE	CB-CG-CD1	-5.95	116.64	120.80
1	A	573	GLU	CA-C-O	-5.94	107.63	120.10
1	C	395	GLY	CA-C-O	-5.94	109.91	120.60
1	A	121	THR	CA-C-N	5.93	130.25	117.20
1	A	205	MET	CA-CB-CG	5.93	123.38	113.30
2	D	129	LEU	N-CA-CB	5.93	122.26	110.40
1	A	91	GLY	O-C-N	-5.93	113.22	122.70
1	C	599	ARG	N-CA-CB	-5.93	99.93	110.60
1	A	179	VAL	O-C-N	-5.93	113.22	122.70
1	A	321	LYS	O-C-N	-5.93	113.22	122.70
1	C	206	VAL	CG1-CB-CG2	-5.93	101.42	110.90
2	B	536	HIS	CA-C-N	5.92	130.23	117.20
1	C	43	GLN	CA-C-O	5.92	132.53	120.10
1	A	106	LEU	O-C-N	-5.92	113.23	122.70
2	D	429	MET	CA-CB-CG	5.92	123.36	113.30
1	C	287	PHE	CB-CG-CD1	5.91	124.94	120.80
1	A	40	THR	CA-CB-CG2	5.91	120.67	112.40
2	B	148	GLU	OE1-CD-OE2	5.91	130.39	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	THR	N-CA-C	5.91	126.95	111.00
2	B	489	ALA	CB-CA-C	5.91	118.96	110.10
2	D	268	GLU	CA-C-N	5.91	130.19	117.20
1	A	347	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	D	585	LEU	CB-CA-C	5.90	121.42	110.20
1	A	475	GLU	CA-CB-CG	5.90	126.37	113.40
1	C	416	LEU	O-C-N	-5.89	113.27	122.70
2	B	31	THR	O-C-N	-5.89	113.28	122.70
1	C	582	GLU	CG-CD-OE2	5.89	130.08	118.30
2	B	330	GLU	CB-CA-C	5.89	122.17	110.40
2	B	426	LEU	CB-CA-C	-5.89	99.02	110.20
1	A	651	VAL	N-CA-CB	-5.88	98.56	111.50
1	C	592	GLN	N-CA-CB	5.88	121.19	110.60
2	D	261	GLU	C-N-CA	5.88	136.40	121.70
1	A	135	ASP	CB-CG-OD1	5.88	123.59	118.30
2	B	187	ASP	O-C-N	-5.88	113.30	122.70
1	C	694	ASP	CB-CA-C	5.88	122.15	110.40
2	D	87	TYR	CD1-CG-CD2	-5.87	111.44	117.90
2	D	315	GLU	CA-C-N	5.87	130.11	117.20
1	A	375	PRO	N-CA-CB	5.87	110.34	103.30
1	A	126	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	201	LEU	O-C-N	-5.87	113.32	122.70
1	A	268	ARG	NH1-CZ-NH2	5.87	125.85	119.40
1	C	541	ALA	O-C-N	-5.86	113.32	122.70
2	D	229	PRO	N-CA-CB	5.86	110.33	103.30
1	A	488	VAL	C-N-CA	5.86	136.34	121.70
1	A	665	VAL	CA-CB-CG2	-5.86	102.12	110.90
2	B	269	GLN	O-C-N	-5.86	113.25	123.20
1	C	261	ALA	CA-C-N	5.85	130.07	117.20
2	B	574	TYR	CB-CG-CD1	5.85	124.51	121.00
1	C	6	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	B	521	ARG	NH1-CZ-NH2	-5.84	112.97	119.40
1	C	26	GLU	O-C-N	-5.84	113.35	122.70
2	D	235	THR	CA-CB-CG2	5.84	120.58	112.40
1	C	311	LEU	CA-C-N	5.84	130.05	117.20
2	B	268	GLU	CA-CB-CG	5.84	126.25	113.40
1	C	250	ALA	CB-CA-C	-5.84	101.34	110.10
2	D	274	THR	CA-C-N	5.84	130.05	117.20
1	C	20	ASP	CB-CG-OD1	5.84	123.55	118.30
1	C	475	GLU	CA-CB-CG	5.83	126.23	113.40
2	B	241	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	C	157	PRO	N-CA-CB	5.83	110.29	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	26	ASP	N-CA-CB	5.83	121.09	110.60
1	C	673	ASP	O-C-N	-5.83	113.38	122.70
1	A	661	HIS	CA-C-N	5.82	130.01	117.20
1	A	352	ALA	O-C-N	-5.82	113.38	122.70
2	B	159	LEU	CA-C-N	5.82	130.01	117.20
2	B	373	ASP	CB-CG-OD1	5.82	123.54	118.30
2	D	564	VAL	CG1-CB-CG2	-5.82	101.59	110.90
2	D	22	SER	N-CA-CB	-5.82	101.78	110.50
2	B	460	ILE	N-CA-CB	5.81	124.17	110.80
2	D	93	PHE	O-C-N	-5.81	113.40	122.70
1	C	646	GLU	CA-CB-CG	5.81	126.18	113.40
2	D	261	GLU	O-C-N	-5.81	113.41	122.70
2	B	531	SER	N-CA-C	5.81	126.68	111.00
1	C	350	ILE	O-C-N	-5.81	113.41	122.70
1	A	19	ALA	C-N-CA	5.80	136.21	121.70
2	B	394	ARG	O-C-N	-5.80	113.42	122.70
1	C	405	GLY	CA-C-N	5.80	129.96	117.20
1	A	206	VAL	CB-CA-C	-5.80	100.39	111.40
1	C	125	TYR	CB-CG-CD2	-5.79	117.52	121.00
1	A	265	ASP	N-CA-CB	5.79	121.02	110.60
2	B	604	ASP	CA-C-N	5.79	129.93	117.20
2	D	580	GLU	CA-CB-CG	5.79	126.13	113.40
1	C	111	LYS	CB-CG-CD	5.78	126.64	111.60
1	A	556	PHE	CA-CB-CG	5.77	127.76	113.90
2	D	521	ARG	O-C-N	-5.77	113.46	122.70
1	C	505	PRO	N-CA-CB	5.77	110.23	103.30
2	D	269	GLN	O-C-N	-5.77	113.39	123.20
2	B	390	VAL	O-C-N	-5.77	113.47	122.70
2	D	286	ALA	N-CA-C	-5.77	95.43	111.00
2	B	522	ARG	C-N-CA	5.77	136.11	121.70
2	B	283	ARG	N-CA-CB	5.76	120.98	110.60
1	A	209	THR	CA-CB-CG2	5.76	120.47	112.40
1	C	241	SER	N-CA-C	5.76	126.56	111.00
2	B	425	LYS	CA-CB-CG	5.76	126.07	113.40
2	D	301	ARG	O-C-N	-5.76	113.48	122.70
2	B	337	TYR	C-N-CA	5.76	136.09	121.70
2	D	306	ARG	CA-C-O	-5.75	108.02	120.10
1	A	211	ILE	O-C-N	-5.75	113.51	122.70
2	D	49	PRO	N-CA-CB	5.75	110.19	103.30
1	A	605	MET	CG-SD-CE	5.74	109.39	100.20
2	B	342	ARG	CB-CG-CD	5.74	126.53	111.60
2	D	223	ARG	C-N-CA	5.74	136.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	339	ASN	O-C-N	-5.74	113.52	122.70
2	B	20	THR	O-C-N	-5.74	113.52	122.70
1	C	703	GLU	C-N-CA	5.74	136.04	121.70
2	D	407	SER	O-C-N	-5.74	113.52	122.70
1	C	89	TYR	CB-CG-CD1	5.73	124.44	121.00
1	A	702	VAL	CA-CB-CG2	5.73	119.50	110.90
2	B	604	ASP	O-C-N	-5.73	113.53	122.70
1	C	278	ASP	N-CA-CB	5.73	120.92	110.60
1	A	52	GLU	CA-CB-CG	5.73	126.00	113.40
2	D	258	THR	CA-C-N	5.73	127.65	116.20
1	A	262	ASP	CA-C-N	5.72	127.64	116.20
2	D	48	PRO	N-CA-CB	5.72	110.17	103.30
1	C	54	VAL	CA-CB-CG2	5.72	119.48	110.90
1	A	666	PRO	N-CA-CB	5.72	110.16	103.30
2	B	425	LYS	CA-C-N	5.72	129.78	117.20
2	D	104	MET	CA-C-O	-5.72	108.09	120.10
1	A	354	ALA	O-C-N	5.71	131.84	122.70
1	A	673	ASP	CB-CG-OD2	-5.71	113.16	118.30
2	D	192	ASP	CA-CB-CG	-5.71	100.84	113.40
2	B	311	PHE	O-C-N	-5.70	113.50	123.20
1	C	627	ASP	N-CA-C	-5.70	95.60	111.00
2	D	373	ASP	CA-CB-CG	5.70	125.95	113.40
1	C	727	ASP	CA-CB-CG	5.70	125.94	113.40
2	B	270	GLY	N-CA-C	5.70	127.34	113.10
2	D	492	ARG	CD-NE-CZ	5.70	131.57	123.60
2	D	536	HIS	O-C-N	-5.70	113.59	122.70
2	D	398	PRO	O-C-N	-5.69	113.59	122.70
1	A	344	ASN	CA-C-N	5.69	129.71	117.20
2	B	333	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	A	152	LEU	CA-CB-CG	5.68	128.37	115.30
2	B	316	ASP	CA-CB-CG	5.68	125.90	113.40
1	C	690	GLU	C-N-CA	5.68	135.90	121.70
1	A	199	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	714	SER	C-N-CA	5.68	135.89	121.70
1	A	130	PRO	N-CA-CB	5.67	110.11	103.30
1	A	41	ALA	N-CA-CB	5.67	118.03	110.10
1	C	394	SER	O-C-N	-5.66	113.57	123.20
2	D	172	GLN	C-N-CA	5.66	134.19	122.30
1	A	517	TRP	CA-CB-CG	-5.66	102.95	113.70
2	B	363	PHE	C-N-CA	5.66	135.85	121.70
1	C	429	LYS	O-C-N	-5.66	113.65	122.70
1	C	621	TYR	CB-CG-CD1	5.66	124.39	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	621	TYR	CB-CG-CD1	5.66	124.39	121.00
1	A	698	LYS	C-N-CA	5.66	135.84	121.70
2	D	278	ASP	O-C-N	-5.66	113.65	122.70
1	C	79	TYR	O-C-N	-5.65	113.66	122.70
1	A	111	LYS	CA-C-N	5.65	127.50	116.20
2	B	633	ILE	C-N-CA	5.65	135.82	121.70
1	A	646	GLU	O-C-N	-5.64	113.67	122.70
1	C	66	GLY	N-CA-C	5.64	127.21	113.10
1	C	369	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	577	THR	CA-CB-CG2	5.64	120.30	112.40
2	D	418	LYS	O-C-N	-5.64	113.67	122.70
1	A	619	THR	O-C-N	-5.64	113.67	122.70
1	C	74	PRO	N-CA-CB	5.64	110.07	103.30
2	D	305	ALA	C-N-CA	5.64	135.81	121.70
2	D	338	VAL	C-N-CA	5.64	135.80	121.70
2	B	594	TYR	CB-CG-CD2	-5.64	117.62	121.00
2	B	336	PRO	N-CA-CB	5.64	110.06	103.30
2	B	338	VAL	CA-C-N	5.63	129.59	117.20
1	C	78	MET	O-C-N	-5.63	113.69	122.70
2	D	283	ARG	CB-CG-CD	5.63	126.24	111.60
1	C	256	MET	CB-CA-C	-5.63	99.14	110.40
1	C	347	ARG	O-C-N	-5.63	113.70	122.70
2	D	89	GLY	N-CA-C	5.63	127.17	113.10
2	D	137	LEU	CA-C-N	-5.63	104.82	117.20
1	A	666	PRO	O-C-N	-5.62	113.71	122.70
1	C	517	TRP	CA-CB-CG	-5.62	103.03	113.70
1	A	642	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	D	114	GLU	CA-CB-CG	5.62	125.76	113.40
2	D	75	MET	N-CA-CB	-5.61	100.50	110.60
2	D	521	ARG	CA-C-N	5.61	129.55	117.20
1	C	23	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
2	D	435	THR	CA-C-O	5.61	131.88	120.10
1	C	353	MET	O-C-N	-5.60	113.73	122.70
2	D	601	GLU	C-N-CA	5.60	135.70	121.70
2	D	120	PHE	CA-C-N	5.60	129.52	117.20
2	D	218	GLY	O-C-N	-5.60	113.74	122.70
2	B	248	ASP	CB-CG-OD2	-5.60	113.26	118.30
2	B	477	LYS	CA-CB-CG	5.59	125.71	113.40
1	A	412	LEU	O-C-N	-5.59	113.75	122.70
1	C	8	ASP	N-CA-C	5.59	126.09	111.00
1	C	189	PRO	N-CA-CB	5.59	110.01	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	24	ALA	C-N-CA	5.59	134.04	122.30
2	D	406	GLU	CG-CD-OE1	5.59	129.48	118.30
1	A	281	ALA	N-CA-CB	5.59	117.92	110.10
2	D	521	ARG	CB-CA-C	5.58	121.57	110.40
1	C	283	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	248	ALA	C-N-CA	5.58	134.02	122.30
2	D	264	ARG	NE-CZ-NH1	-5.58	117.51	120.30
2	B	531	SER	CA-C-N	-5.58	104.93	117.20
1	C	65	ALA	N-CA-CB	5.57	117.90	110.10
1	A	292	MET	O-C-N	-5.57	113.79	122.70
2	B	86	GLY	CA-C-O	5.57	130.62	120.60
1	C	173	PRO	N-CA-CB	5.57	109.98	103.30
2	D	311	PHE	CA-CB-CG	5.56	127.25	113.90
1	A	225	PHE	CB-CG-CD1	5.56	124.69	120.80
1	C	694	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	C	677	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	271	GLU	OE1-CD-OE2	-5.56	116.63	123.30
2	B	79	LYS	CA-C-N	5.55	129.42	117.20
2	B	311	PHE	CA-C-N	5.55	127.31	116.20
2	D	188	LYS	N-CA-C	-5.55	96.00	111.00
1	C	82	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	C	327	THR	N-CA-CB	-5.55	99.75	110.30
1	A	176	ALA	O-C-N	-5.55	113.82	122.70
1	A	214	PRO	CA-C-N	5.55	129.41	117.20
2	B	52	GLN	OE1-CD-NE2	5.54	134.65	121.90
1	C	357	GLN	O-C-N	-5.54	113.78	123.20
2	D	632	ASP	CA-C-N	5.54	129.39	117.20
2	B	245	GLY	CA-C-O	-5.54	110.63	120.60
2	B	404	TYR	CB-CG-CD1	5.54	124.32	121.00
2	D	515	LEU	CB-CG-CD2	5.54	120.41	111.00
1	C	333	GLY	O-C-N	-5.53	113.85	122.70
1	A	621	TYR	CB-CG-CD2	-5.53	117.69	121.00
1	A	639	GLU	N-CA-CB	-5.52	100.66	110.60
1	C	699	ASP	CA-C-N	5.52	127.25	116.20
2	D	200	ASP	CB-CA-C	5.52	121.44	110.40
2	D	318	ARG	CG-CD-NE	-5.52	100.20	111.80
1	A	139	ALA	C-N-CA	5.52	133.88	122.30
1	A	161	MET	CB-CG-SD	5.51	128.94	112.40
1	C	578	PRO	N-CA-CB	5.51	109.92	103.30
2	D	335	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	B	314	ASP	CB-CG-OD1	5.51	123.26	118.30
2	D	367	LEU	CB-CA-C	-5.51	99.73	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	GLU	CA-C-N	5.51	129.32	117.20
1	C	638	GLU	CA-C-N	5.51	129.32	117.20
1	A	674	LYS	CA-C-N	5.51	129.31	117.20
1	C	326	ARG	CD-NE-CZ	5.51	131.31	123.60
1	A	642	ARG	CG-CD-NE	5.50	123.36	111.80
2	B	414	ASP	OD1-CG-OD2	-5.50	112.84	123.30
1	C	58	MET	O-C-N	-5.50	113.90	122.70
1	A	612	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
2	B	370	PRO	CA-C-O	5.50	133.39	120.20
1	A	39	GLU	CA-CB-CG	5.49	125.49	113.40
1	A	131	ARG	CG-CD-NE	5.49	123.34	111.80
2	B	436	GLU	CA-CB-CG	5.49	125.48	113.40
1	C	594	GLU	CB-CG-CD	5.49	129.03	114.20
2	D	69	GLY	CA-C-O	-5.49	110.72	120.60
1	C	66	GLY	C-N-CA	5.48	135.40	121.70
2	D	131	ARG	CD-NE-CZ	5.48	131.27	123.60
1	A	572	LYS	CA-CB-CG	5.48	125.46	113.40
1	C	27	GLU	O-C-N	-5.48	113.93	122.70
2	D	422	GLU	CA-C-N	5.48	129.25	117.20
1	C	400	ILE	C-N-CA	5.48	135.40	121.70
2	B	251	GLU	CB-CG-CD	5.47	128.98	114.20
2	B	370	PRO	N-CA-CB	5.47	109.87	103.30
1	A	131	ARG	O-C-N	-5.47	113.94	122.70
1	A	261	ALA	CA-C-N	5.47	129.24	117.20
2	B	377	ARG	NE-CZ-NH1	-5.47	117.56	120.30
2	D	493	ASP	O-C-N	-5.47	113.95	122.70
1	C	117	PHE	CA-CB-CG	5.47	127.02	113.90
2	D	115	ASP	OD1-CG-OD2	-5.47	112.91	123.30
2	B	512	LYS	CA-CB-CG	5.46	125.42	113.40
1	C	558	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	C	131	ARG	O-C-N	-5.46	113.96	122.70
1	A	378	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	A	280	PHE	CB-CA-C	5.46	121.31	110.40
2	D	490	TRP	CA-CB-CG	5.45	124.06	113.70
2	D	494	SER	N-CA-CB	-5.45	102.32	110.50
2	D	522	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	C	342	TYR	CB-CG-CD2	5.45	124.27	121.00
1	C	443	LYS	CA-CB-CG	5.45	125.39	113.40
1	C	621	TYR	C-N-CA	5.45	135.32	121.70
2	B	238	ALA	C-N-CA	5.45	135.32	121.70
1	C	594	GLU	CB-CA-C	5.45	121.29	110.40
2	D	247	GLY	N-CA-C	-5.44	99.49	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MET	O-C-N	-5.44	113.99	122.70
1	C	39	GLU	CA-CB-CG	5.44	125.37	113.40
1	A	333	GLY	O-C-N	-5.44	114.00	122.70
1	A	662	LEU	CA-C-O	-5.44	108.67	120.10
1	A	27	GLU	C-N-CA	5.44	135.29	121.70
1	A	443	LYS	CA-C-N	5.44	129.16	117.20
2	B	407	SER	CA-C-N	5.44	129.16	117.20
1	C	103	ARG	CA-CB-CG	-5.43	101.44	113.40
2	B	77	ARG	CA-C-O	5.43	131.51	120.10
1	C	236	ASN	CB-CG-ND2	-5.43	103.66	116.70
2	D	612	LEU	O-C-N	-5.43	114.01	122.70
2	D	536	HIS	CA-C-N	5.43	129.15	117.20
1	C	363	LEU	N-CA-CB	-5.43	99.55	110.40
1	C	577	THR	N-CA-CB	-5.43	99.99	110.30
2	D	363	PHE	C-N-CA	5.42	135.26	121.70
1	C	104	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	C	268	ARG	CG-CD-NE	-5.42	100.41	111.80
1	C	304	ALA	O-C-N	-5.42	114.03	122.70
2	D	288	HIS	CA-CB-CG	5.42	122.82	113.60
2	D	130	GLU	C-N-CA	5.42	135.25	121.70
2	D	418	LYS	CA-C-O	-5.42	108.72	120.10
1	C	621	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	123	ARG	C-N-CA	5.42	133.67	122.30
2	D	480	PRO	N-CA-CB	5.42	109.80	103.30
1	C	203	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	C	370	GLU	CA-C-N	5.41	129.10	117.20
1	C	535	CYS	O-C-N	-5.41	114.04	122.70
1	A	158	LEU	O-C-N	-5.41	114.05	122.70
1	C	421	TRP	O-C-N	-5.41	114.01	123.20
1	A	203	GLU	O-C-N	-5.41	114.05	122.70
2	D	332	THR	O-C-N	5.41	131.35	122.70
2	D	560	SER	O-C-N	-5.41	114.01	123.20
1	C	623	ASP	C-N-CA	5.40	135.20	121.70
2	B	298	ARG	CB-CG-CD	5.40	125.64	111.60
1	A	54	VAL	CA-C-O	-5.40	108.77	120.10
1	A	70	PHE	O-C-N	-5.40	114.07	122.70
2	B	114	GLU	OE1-CD-OE2	5.40	129.78	123.30
2	B	95	ARG	CA-C-N	5.39	126.99	116.20
1	C	661	HIS	O-C-N	-5.39	114.07	122.70
1	C	128	ASP	CA-C-N	5.39	129.06	117.20
2	B	443	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	723	ARG	O-C-N	-5.39	114.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ALA	O-C-N	-5.39	114.08	122.70
2	D	87	TYR	CZ-CE2-CD2	-5.38	114.95	119.80
1	C	288	TRP	CB-CA-C	-5.38	99.64	110.40
1	A	135	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	180	VAL	CB-CA-C	5.38	121.62	111.40
1	A	70	PHE	CA-C-O	5.38	131.39	120.10
1	A	696	LEU	O-C-N	-5.38	114.10	122.70
2	D	169	ARG	CG-CD-NE	5.38	123.09	111.80
1	A	401	ASP	CB-CA-C	5.37	121.15	110.40
2	B	397	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	398	ARG	CA-CB-CG	5.37	125.22	113.40
2	D	95	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	B	132	GLY	N-CA-C	5.37	126.53	113.10
1	C	278	ASP	O-C-N	-5.37	114.11	122.70
1	A	85	THR	CA-C-N	5.37	129.01	117.20
1	A	667	ALA	O-C-N	-5.37	114.12	122.70
2	B	79	LYS	C-N-CA	5.37	135.11	121.70
2	D	80	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	594	GLU	CA-CB-CG	5.36	125.20	113.40
1	A	572	LYS	CB-CA-C	-5.36	99.68	110.40
1	A	667	ALA	N-CA-CB	-5.36	102.60	110.10
2	D	351	SER	N-CA-CB	5.36	118.54	110.50
2	D	491	HIS	N-CA-CB	5.35	120.24	110.60
1	A	372	ILE	CA-C-N	5.35	128.98	117.20
1	C	44	ILE	CA-C-O	5.35	131.34	120.10
1	C	55	TYR	O-C-N	-5.35	114.14	122.70
1	C	592	GLN	CB-CA-C	-5.35	99.70	110.40
1	A	99	ASN	O-C-N	-5.35	114.14	122.70
1	A	714	SER	O-C-N	-5.35	114.14	122.70
1	C	266	TYR	O-C-N	-5.35	114.14	122.70
1	C	427	VAL	CA-C-O	-5.35	108.87	120.10
2	D	93	PHE	C-N-CA	5.35	135.07	121.70
1	A	342	TYR	CB-CG-CD2	5.35	124.21	121.00
2	B	528	GLU	C-N-CA	5.35	133.53	122.30
1	A	639	GLU	CB-CA-C	5.34	121.09	110.40
2	B	62	LEU	O-C-N	-5.34	114.15	122.70
1	A	157	PRO	N-CA-CB	5.34	109.71	103.30
1	A	306	MET	CA-C-O	-5.34	108.89	120.10
2	D	512	LYS	CB-CA-C	-5.34	99.73	110.40
2	D	360	THR	N-CA-CB	-5.33	100.17	110.30
1	C	485	ASN	CB-CG-OD1	-5.33	110.94	121.60
1	A	104	ARG	CD-NE-CZ	5.33	131.06	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	500	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	540	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	207	ARG	C-N-CA	5.32	135.01	121.70
1	A	54	VAL	CA-CB-CG2	5.32	118.88	110.90
1	A	635	GLN	CA-CB-CG	5.32	125.10	113.40
2	D	634	LEU	C-N-CA	5.32	133.47	122.30
2	D	226	LYS	CA-CB-CG	5.32	125.10	113.40
1	A	702	VAL	CB-CA-C	-5.32	101.30	111.40
2	D	69	GLY	CA-C-N	5.32	128.89	117.20
2	D	284	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	191	GLN	CA-C-N	5.31	128.89	117.20
1	A	357	GLN	O-C-N	-5.31	114.17	123.20
1	C	521	ASN	N-CA-C	5.31	125.34	111.00
1	C	311	LEU	O-C-N	-5.31	114.20	122.70
1	A	438	GLU	CB-CG-CD	5.31	128.54	114.20
2	D	358	ILE	CB-CG1-CD1	5.31	128.76	113.90
2	D	531	SER	CA-C-O	5.31	131.25	120.10
2	D	52	GLN	CA-CB-CG	5.31	125.07	113.40
1	A	210	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
2	B	516	ALA	C-N-CA	-5.30	108.44	121.70
1	A	637	PRO	N-CA-CB	5.30	109.66	103.30
1	C	127	SER	CA-C-N	5.30	128.86	117.20
1	C	553	GLU	C-N-CA	5.29	134.92	121.70
2	D	39	VAL	CA-C-N	5.29	128.84	117.20
1	C	585	GLU	OE1-CD-OE2	5.29	129.64	123.30
1	C	12	LEU	CA-C-N	5.29	126.77	116.20
1	C	597	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	D	627	LEU	CB-CA-C	5.28	120.24	110.20
2	B	577	GLN	OE1-CD-NE2	5.28	134.05	121.90
2	B	600	LYS	O-C-N	-5.28	114.25	122.70
1	A	135	ASP	OD1-CG-OD2	-5.28	113.27	123.30
1	A	203	GLU	OE1-CD-OE2	-5.28	116.96	123.30
2	B	523	ASP	O-C-N	5.28	131.15	122.70
2	D	185	ARG	C-N-CA	5.28	134.90	121.70
1	A	206	VAL	CG1-CB-CG2	-5.28	102.46	110.90
1	A	521	ASN	CB-CG-OD1	-5.28	111.04	121.60
1	C	554	LYS	N-CA-CB	5.28	120.10	110.60
1	A	80	ALA	C-N-CA	5.28	134.89	121.70
1	A	626	PHE	CB-CG-CD1	-5.28	117.11	120.80
1	C	312	VAL	CA-CB-CG1	5.28	118.81	110.90
1	C	453	THR	O-C-N	-5.28	114.26	122.70
1	A	361	GLN	CA-CB-CG	5.27	125.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	469	LYS	CA-C-N	5.27	128.80	117.20
1	A	339	GLN	CA-CB-CG	5.27	124.99	113.40
1	A	554	LYS	N-CA-CB	5.27	120.09	110.60
1	C	579	GLU	CA-CB-CG	5.27	124.99	113.40
1	A	171	VAL	CA-CB-CG1	5.27	118.80	110.90
2	D	356	GLU	CB-CA-C	5.26	120.93	110.40
1	A	279	GLN	CA-C-O	-5.26	109.05	120.10
1	C	265	ASP	CA-C-N	5.26	128.77	117.20
2	D	122	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	89	TYR	CA-CB-CG	5.25	123.38	113.40
1	A	677	ARG	CA-CB-CG	5.25	124.95	113.40
2	B	450	ALA	CA-C-N	5.25	128.75	117.20
1	C	469	LYS	CB-CG-CD	-5.25	97.95	111.60
1	C	156	ILE	CA-CB-CG1	5.25	120.98	111.00
2	D	306	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	B	160	GLU	CB-CG-CD	5.25	128.37	114.20
2	B	296	ARG	CA-C-N	5.25	128.75	117.20
1	C	185	GLN	N-CA-CB	5.25	120.05	110.60
1	A	386	THR	O-C-N	-5.25	114.31	122.70
1	C	278	ASP	CA-C-O	-5.25	109.08	120.10
2	B	210	THR	N-CA-CB	5.24	120.26	110.30
1	A	484	ASP	OD1-CG-OD2	-5.24	113.34	123.30
1	C	684	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	C	109	GLY	N-CA-C	5.24	126.20	113.10
1	C	87	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	442	PRO	N-CA-CB	5.23	109.58	103.30
1	A	673	ASP	O-C-N	-5.23	114.33	122.70
1	A	304	ALA	CA-C-N	5.23	128.70	117.20
1	C	537	ASP	CB-CG-OD1	5.23	123.01	118.30
2	D	604	ASP	CA-C-N	5.23	128.70	117.20
1	A	500	ARG	CD-NE-CZ	5.23	130.92	123.60
2	B	632	ASP	O-C-N	-5.23	114.33	122.70
1	C	342	TYR	CB-CG-CD1	-5.23	117.86	121.00
2	D	49	PRO	N-CA-C	5.22	125.69	112.10
1	A	67	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	A	126	ASP	O-C-N	-5.22	114.34	122.70
1	A	242	GLY	O-C-N	-5.22	114.34	122.70
2	B	463	VAL	O-C-N	5.22	131.06	122.70
1	C	39	GLU	CB-CA-C	5.22	120.85	110.40
1	C	437	ILE	O-C-N	-5.22	114.34	122.70
2	B	148	GLU	CA-C-O	-5.22	109.14	120.10
2	D	594	TYR	N-CA-CB	5.22	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ARG	CA-C-N	5.22	128.68	117.20
2	B	130	GLU	C-N-CA	5.22	134.75	121.70
1	C	107	ALA	O-C-N	-5.22	114.35	122.70
1	A	266	TYR	CA-C-N	5.22	128.68	117.20
1	A	385	ASN	O-C-N	-5.22	114.35	122.70
1	C	150	ARG	NH1-CZ-NH2	5.22	125.14	119.40
2	D	208	GLN	C-N-CA	5.21	133.25	122.30
2	D	555	GLU	N-CA-CB	5.21	119.98	110.60
1	C	394	SER	CA-C-O	5.21	131.04	120.10
1	A	131	ARG	N-CA-CB	-5.21	101.23	110.60
1	A	251	THR	O-C-N	-5.21	114.37	122.70
1	A	529	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	C	131	ARG	C-N-CA	5.20	134.71	121.70
1	C	126	ASP	CA-C-O	5.20	131.02	120.10
1	C	218	MET	CB-CA-C	5.20	120.80	110.40
1	C	524	ASP	O-C-N	-5.20	114.38	122.70
1	C	261	ALA	CB-CA-C	5.20	117.89	110.10
1	C	150	ARG	CG-CD-NE	-5.19	100.89	111.80
1	A	526	ASP	CA-C-O	5.19	131.00	120.10
2	D	104	MET	CB-CA-C	5.19	120.77	110.40
1	A	231	ASN	CB-CA-C	-5.19	100.03	110.40
2	D	515	LEU	CA-C-O	5.19	130.99	120.10
1	A	243	TYR	CG-CD2-CE2	5.18	125.45	121.30
2	B	67	VAL	N-CA-CB	-5.18	100.09	111.50
1	C	206	VAL	CB-CA-C	-5.18	101.55	111.40
2	B	209	GLY	C-N-CA	5.18	134.65	121.70
2	D	254	TRP	CB-CA-C	5.18	120.76	110.40
2	B	501	MET	CA-CB-CG	5.18	122.10	113.30
2	B	321	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	23	ARG	O-C-N	-5.17	114.43	122.70
1	C	148	ASP	N-CA-CB	-5.17	101.30	110.60
1	C	203	GLU	CG-CD-OE1	5.17	128.63	118.30
1	C	697	ARG	C-N-CA	5.17	134.62	121.70
2	B	92	PRO	O-C-N	-5.17	114.44	122.70
2	D	616	ARG	N-CA-CB	-5.17	101.30	110.60
2	D	407	SER	CA-C-N	5.16	128.56	117.20
1	A	206	VAL	CA-CB-CG1	5.16	118.64	110.90
2	B	526	GLY	O-C-N	-5.16	114.44	122.70
1	C	222	SER	O-C-N	-5.16	114.44	122.70
1	C	430	VAL	N-CA-CB	-5.16	100.15	111.50
2	D	472	ARG	CB-CG-CD	5.16	125.01	111.60
1	A	421	TRP	O-C-N	-5.16	114.43	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	427	VAL	CA-CB-CG1	5.16	118.64	110.90
2	B	416	ALA	O-C-N	-5.16	114.45	122.70
2	D	613	ILE	C-N-CA	5.16	134.59	121.70
1	A	231	ASN	N-CA-C	5.15	124.92	111.00
1	C	585	GLU	CA-C-N	5.15	128.54	117.20
2	B	552	GLU	CA-C-N	5.14	128.52	117.20
1	A	623	ASP	CA-CB-CG	5.14	124.71	113.40
1	A	703	GLU	CA-CB-CG	5.14	124.70	113.40
2	B	35	TRP	CB-CG-CD1	5.14	133.68	127.00
1	C	123	ARG	O-C-N	-5.14	114.47	123.20
2	B	128	GLY	CA-C-O	-5.13	111.36	120.60
2	D	137	LEU	CA-C-O	5.13	130.88	120.10
2	D	283	ARG	CG-CD-NE	5.13	122.58	111.80
1	C	272	SER	CA-C-O	-5.13	109.32	120.10
2	B	435	THR	CA-CB-OG1	-5.13	98.23	109.00
2	D	528	GLU	O-C-N	-5.13	114.48	123.20
1	A	389	PHE	CA-C-N	5.13	128.48	117.20
1	C	322	SER	O-C-N	-5.13	114.50	122.70
1	C	438	GLU	CB-CA-C	5.13	120.65	110.40
2	B	315	GLU	CA-CB-CG	5.12	124.67	113.40
1	A	652	VAL	N-CA-CB	5.12	122.77	111.50
1	A	193	ALA	C-N-CA	-5.12	111.55	122.30
1	A	221	ILE	CA-CB-CG1	5.12	120.72	111.00
2	B	401	GLY	O-C-N	-5.12	114.51	122.70
2	D	422	GLU	O-C-N	-5.12	114.52	122.70
1	A	207	ARG	NE-CZ-NH2	-5.11	117.74	120.30
2	D	145	ILE	CA-CB-CG2	5.11	121.13	110.90
2	D	197	LEU	CA-CB-CG	5.11	127.06	115.30
2	B	308	GLY	O-C-N	-5.11	114.52	122.70
1	C	8	ASP	CA-C-N	5.11	128.45	117.20
1	A	8	ASP	CB-CG-OD1	5.11	122.90	118.30
2	D	306	ARG	N-CA-CB	5.11	119.80	110.60
1	C	723	ARG	O-C-N	-5.11	114.53	122.70
1	C	664	LEU	CB-CA-C	-5.11	100.50	110.20
2	D	461	THR	O-C-N	-5.11	114.53	122.70
1	A	19	ALA	CA-C-N	5.11	128.43	117.20
2	D	308	GLY	N-CA-C	5.11	125.86	113.10
2	D	515	LEU	CA-CB-CG	5.11	127.04	115.30
1	C	665	VAL	CA-CB-CG2	-5.10	103.25	110.90
1	A	402	PRO	C-N-CA	5.10	134.44	121.70
2	B	23	LEU	O-C-N	-5.10	114.54	122.70
1	A	189	PRO	O-C-N	-5.09	114.55	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	LYS	CA-C-N	5.09	126.39	116.20
2	D	147	PRO	N-CA-CB	5.09	109.41	103.30
2	D	286	ALA	CB-CA-C	5.09	117.74	110.10
2	D	456	ARG	C-N-CA	5.09	134.44	121.70
1	C	246	GLN	N-CA-CB	5.09	119.77	110.60
1	C	24	ARG	CG-CD-NE	5.09	122.49	111.80
1	C	233	PRO	N-CA-CB	5.09	109.41	103.30
2	B	485	ARG	CD-NE-CZ	5.09	130.72	123.60
2	B	550	THR	N-CA-CB	5.09	119.97	110.30
1	C	280	PHE	CB-CG-CD1	5.09	124.36	120.80
2	D	307	ILE	CA-C-N	5.09	126.38	116.20
1	A	574	VAL	CG1-CB-CG2	-5.09	102.76	110.90
2	B	159	LEU	O-C-N	-5.09	114.56	122.70
1	C	150	ARG	CB-CA-C	-5.09	100.23	110.40
1	C	23	ARG	CA-C-N	5.08	128.39	117.20
2	B	35	TRP	CB-CA-C	5.08	120.57	110.40
2	B	602	PHE	CB-CA-C	-5.08	100.23	110.40
1	C	10	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	C	161	MET	CG-SD-CE	-5.08	92.07	100.20
1	A	613	GLY	O-C-N	-5.08	114.57	122.70
1	C	308	TRP	O-C-N	-5.08	114.57	122.70
2	D	222	ARG	CA-CB-CG	5.08	124.57	113.40
1	C	366	ASN	C-N-CA	5.08	134.39	121.70
2	D	152	GLU	CA-CB-CG	-5.08	102.23	113.40
1	A	87	ARG	CD-NE-CZ	5.08	130.71	123.60
1	C	54	VAL	CA-C-N	5.08	128.37	117.20
1	C	639	GLU	CB-CA-C	-5.08	100.25	110.40
2	D	337	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	603	ALA	CB-CA-C	-5.07	102.49	110.10
1	C	347	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	150	ARG	CB-CA-C	-5.07	100.26	110.40
1	C	601	LEU	N-CA-CB	5.07	120.53	110.40
1	A	675	LEU	C-N-CA	5.06	132.93	122.30
2	B	307	ILE	C-N-CA	5.06	132.93	122.30
2	B	222	ARG	CD-NE-CZ	5.06	130.69	123.60
2	D	185	ARG	O-C-N	-5.06	114.61	122.70
1	A	524	ASP	CA-C-N	5.06	128.32	117.20
1	C	575	LYS	C-N-CA	5.06	134.34	121.70
1	A	498	LYS	O-C-N	-5.05	114.61	122.70
2	B	273	ALA	CA-C-N	5.05	128.32	117.20
2	B	528	GLU	O-C-N	-5.05	114.61	123.20
2	B	541	ASP	N-CA-CB	5.05	119.70	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	717	SER	CA-C-N	5.05	128.32	117.20
2	B	411	SER	CA-CB-OG	-5.05	97.56	111.20
1	C	30	ALA	CA-C-N	5.05	128.32	117.20
1	C	678	PRO	CA-C-O	5.05	132.33	120.20
1	A	347	ARG	CA-CB-CG	5.05	124.50	113.40
2	B	158	LEU	CA-C-N	5.05	128.30	117.20
2	B	264	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	C	367	SER	O-C-N	-5.05	114.63	122.70
1	A	712	PRO	N-CA-CB	5.04	109.35	103.30
1	C	485	ASN	CA-C-N	5.04	128.28	117.20
1	C	599	ARG	CA-CB-CG	5.04	124.48	113.40
1	A	197	GLN	CA-CB-CG	-5.03	102.33	113.40
1	C	361	GLN	CA-CB-CG	5.03	124.47	113.40
1	C	212	TYR	CB-CA-C	-5.03	100.34	110.40
1	A	139	ALA	N-CA-CB	-5.03	103.06	110.10
2	D	108	ASP	CB-CA-C	5.02	120.45	110.40
1	A	8	ASP	C-N-CA	5.02	134.26	121.70
1	A	55	TYR	C-N-CA	5.02	134.26	121.70
1	C	189	PRO	O-C-N	-5.02	114.67	122.70
1	C	169	GLY	O-C-N	-5.02	114.67	122.70
1	C	521	ASN	CA-C-O	5.02	130.64	120.10
1	C	509	LYS	O-C-N	-5.02	114.67	122.70
1	C	490	ALA	CA-C-N	5.01	128.23	117.20
1	A	96	LYS	CA-CB-CG	-5.01	102.38	113.40
1	C	268	ARG	NH1-CZ-NH2	5.01	124.91	119.40
2	B	573	VAL	CA-C-N	5.01	128.21	117.20
2	D	636	VAL	CB-CA-C	5.01	120.91	111.40
1	C	409	VAL	O-C-N	-5.00	114.69	122.70
2	D	301	ARG	NE-CZ-NH2	-5.00	117.80	120.30
2	B	61	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	A	343	ASN	C-N-CA	5.00	134.21	121.70
2	D	82	PRO	N-CA-CB	5.00	109.30	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	GLY	Mainchain
2	B	401	GLY	Mainchain
1	C	593	ALA	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	5558	0	5437	68	0
1	C	5558	0	5436	66	0
2	B	4695	0	4607	40	0
2	D	4695	0	4609	78	0
3	A	91	0	88	18	0
3	C	91	0	88	13	0
4	A	47	0	32	0	0
4	C	47	0	32	0	0
5	A	454	0	0	3	0
5	B	316	0	0	1	0
5	C	490	0	0	4	0
5	D	265	0	0	0	0
All	All	22307	0	20329	256	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 6.

All (256) 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)
3:C:800:B12:H421	3:C:800:B12:C36	1.80	1.11
3:C:800:B12:H363	3:C:800:B12:C42	1.77	1.10
3:C:800:B12:H531	3:C:800:B12:H552	1.26	1.10
3:A:800:B12:H363	3:A:800:B12:H421	1.07	1.05
3:A:800:B12:H421	3:A:800:B12:C36	1.90	1.01
3:A:800:B12:H363	3:A:800:B12:C42	1.96	0.95
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.17	0.92
3:C:800:B12:H421	3:C:800:B12:H363	0.89	0.86
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.25	0.85
1:C:374:LEU:HB2	1:C:481:LEU:HD23	1.67	0.77
3:A:800:B12:H531	3:A:800:B12:H552	1.67	0.77
1:A:188:LYS:H	1:A:191:GLN:NE2	1.83	0.77
1:C:188:LYS:H	1:C:191:GLN:NE2	1.85	0.75
1:C:247:GLU:HB3	3:C:800:B12:H532	1.68	0.75
1:A:374:LEU:HB2	1:A:481:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:ARG:HD2	1:C:508:VAL:HG21	1.70	0.74
3:C:800:B12:H531	3:C:800:B12:C55	2.11	0.73
1:C:357:GLN:HE22	2:D:290:GLN:NE2	1.86	0.73
1:C:188:LYS:H	1:C:191:GLN:HE21	1.37	0.72
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.70	0.72
2:D:202:ILE:HD12	2:D:258:THR:HG23	1.71	0.72
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.72	0.72
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.70	0.72
2:D:297:LEU:HD12	2:D:353:GLY:HA3	1.72	0.71
1:A:133:ALA:HB1	1:A:489:LEU:HD21	1.72	0.71
1:A:650:HIS:HB3	1:A:722:LEU:HD21	1.73	0.70
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.74	0.69
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.73	0.69
2:D:284:VAL:HG11	2:D:322:GLN:HE21	1.57	0.68
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.75	0.68
1:A:357:GLN:HE22	2:B:290:GLN:NE2	1.92	0.67
1:C:652:VAL:HG11	1:C:668:LEU:HD11	1.78	0.65
2:B:246:ALA:HB1	2:B:250:ALA:HB3	1.79	0.65
3:C:800:B12:H353	3:C:800:B12:H302	1.77	0.65
1:A:94:THR:HG22	1:A:488:VAL:HG13	1.78	0.65
3:C:800:B12:H372	3:C:800:B12:H351	1.79	0.64
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.78	0.64
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.80	0.63
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.80	0.63
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.81	0.63
2:D:121:THR:HG21	2:D:145:ILE:HD11	1.81	0.62
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.79	0.62
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.80	0.62
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.45	0.62
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.82	0.61
2:D:391:ASN:HB3	2:D:394:ARG:HD2	1.81	0.61
1:A:683:THR:HG22	1:A:703:GLU:HB2	1.81	0.61
2:D:292:LEU:HD23	2:D:408:LEU:HD21	1.82	0.60
2:D:82:PRO:HD2	2:D:406:GLU:HG3	1.83	0.60
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.84	0.60
1:A:188:LYS:H	1:A:191:GLN:HE21	1.50	0.60
1:A:247:GLU:HB3	3:A:800:B12:H532	1.84	0.59
1:C:638:GLU:HA	1:C:671:GLU:HG3	1.83	0.59
3:A:800:B12:H2B	3:A:800:B12:O7R	2.00	0.59
1:A:684:VAL:HG12	1:A:688:ILE:HD11	1.84	0.59
2:B:220:TRP:CE3	2:B:220:TRP:HA	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:LEU:HA	2:D:322:GLN:HE22	1.67	0.58
3:A:800:B12:H372	3:A:800:B12:H351	1.85	0.58
2:D:402:SER:HB3	2:D:405:VAL:HB	1.85	0.58
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.84	0.58
3:A:800:B12:C55	3:A:800:B12:H531	2.35	0.57
1:A:617:ILE:HD13	1:A:711:ILE:HG12	1.86	0.57
1:C:24:ARG:HH22	2:D:315:GLU:HG3	1.69	0.57
1:C:392:GLN:HB3	2:D:459:PRO:HG2	1.87	0.57
1:A:599:ARG:HG2	1:A:649:VAL:HA	1.86	0.57
1:A:359:HIS:HE1	1:A:401:ASP:H	1.52	0.57
1:C:359:HIS:HE1	1:C:401:ASP:H	1.51	0.57
2:D:179:LEU:HG	2:D:195:LEU:HD12	1.87	0.56
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.51	0.56
2:B:552:GLU:HA	2:B:555:GLU:HG2	1.87	0.56
2:D:100:ARG:HD2	2:D:396:ASN:HA	1.87	0.56
2:D:80:ASP:HB3	2:D:407:SER:HB2	1.87	0.56
1:A:359:HIS:CE1	1:A:401:ASP:H	2.24	0.56
2:D:220:TRP:HA	2:D:220:TRP:CE3	2.40	0.55
1:C:372:ILE:HD13	1:C:478:LEU:HD23	1.87	0.55
2:D:27:PHE:HB3	2:D:28:PRO:HD2	1.87	0.55
1:C:359:HIS:CE1	1:C:401:ASP:H	2.24	0.55
1:A:579:GLU:HB3	1:A:712:PRO:HB2	1.89	0.55
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.37	0.55
2:D:281:ASN:ND2	2:D:323:ASN:HD21	2.04	0.55
2:D:423:VAL:HG13	2:D:432:ALA:HB2	1.89	0.54
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.88	0.54
2:D:141:ASP:HB3	2:D:142:PRO:HD2	1.89	0.54
2:D:284:VAL:HG21	2:D:297:LEU:HD22	1.89	0.54
1:C:65:ALA:HB2	1:C:72:HIS:HB2	1.90	0.53
3:A:800:B12:C2B	3:A:800:B12:O7R	2.56	0.53
1:A:21:ALA:HA	2:B:90:VAL:HG11	1.90	0.53
2:D:238:ALA:HB1	2:D:251:GLU:HG3	1.91	0.53
1:A:599:ARG:HH21	1:A:647:ALA:HB1	1.74	0.53
1:A:311:LEU:HD11	1:A:424:ILE:HD13	1.91	0.52
1:C:448:GLU:HG2	1:C:569:VAL:HG21	1.90	0.52
1:A:710:VAL:HG12	1:A:712:PRO:HD2	1.90	0.52
1:C:599:ARG:HG3	1:C:649:VAL:HA	1.92	0.52
1:A:24:ARG:HH22	2:B:315:GLU:HG3	1.73	0.52
1:C:386:THR:HA	2:D:341:LEU:HD13	1.92	0.52
2:D:305:ALA:HA	2:D:318:ARG:HB3	1.90	0.51
2:D:92:PRO:O	2:D:93:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:ALA:HB3	2:D:149:HIS:ND1	2.26	0.51
2:D:331:LEU:HD11	2:D:361:LEU:HD12	1.93	0.51
1:A:706:THR:HB	1:A:707:PRO:CD	2.41	0.51
1:A:139:ALA:HB1	3:A:800:B12:H362	1.93	0.51
1:C:20:ASP:OD2	1:C:24:ARG:HD2	2.11	0.51
1:A:498:LYS:HG3	1:C:23:ARG:NH2	2.26	0.51
2:D:158:LEU:HD12	2:D:161:MET:SD	2.51	0.50
2:D:598:ALA:HB3	2:D:601:GLU:HG3	1.93	0.50
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.91	0.50
2:D:166:VAL:HG22	2:D:179:LEU:HD22	1.94	0.49
2:D:370:PRO:HB3	2:D:375:PRO:HG2	1.93	0.49
2:D:91:ALA:HB1	2:D:92:PRO:HA	1.94	0.49
2:D:331:LEU:HD13	2:D:365:GLN:HB3	1.94	0.49
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.95	0.49
3:C:800:B12:H552	3:C:800:B12:C53	2.16	0.49
2:D:91:ALA:HA	2:D:92:PRO:C	2.32	0.49
1:A:215:GLN:HB3	1:A:216:PRO:CD	2.42	0.49
1:C:390:LEU:HA	1:C:394:SER:HB3	1.95	0.49
1:C:706:THR:HB	1:C:707:PRO:CD	2.43	0.49
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.59	0.49
1:A:4:LEU:N	1:A:5:PRO:HD3	2.27	0.49
3:C:800:B12:O7R	3:C:800:B12:O5	2.26	0.48
1:A:8:ASP:HB2	2:B:425:LYS:HE2	1.94	0.48
2:D:129:LEU:HD11	2:D:136:LEU:HD21	1.94	0.48
2:D:264:ARG:HG3	2:D:311:PHE:HZ	1.79	0.48
1:A:123:ARG:HD3	1:A:607:GLN:OE1	2.14	0.48
1:C:8:ASP:HB2	2:D:425:LYS:HE2	1.94	0.48
1:A:310:LYS:HE2	2:B:21:LEU:HD11	1.95	0.48
3:A:800:B12:H492	3:A:800:B12:C47	2.43	0.48
3:A:800:B12:H551	3:A:800:B12:C61	2.44	0.48
1:C:381:ARG:CD	2:D:468:MET:HE1	2.44	0.48
1:A:586:LEU:HB3	1:A:719:VAL:HG11	1.96	0.47
2:B:152:GLU:O	2:B:155:SER:HB2	2.13	0.47
2:B:391:ASN:ND2	2:B:394:ARG:HE	2.11	0.47
1:C:512:LEU:HD21	1:C:543:ALA:HB1	1.96	0.47
1:C:139:ALA:HB1	3:C:800:B12:H362	1.96	0.47
2:D:143:ASP:HA	2:D:480:PRO:HB2	1.95	0.47
1:A:358:GLY:O	1:A:359:HIS:HB2	2.14	0.47
1:A:5:PRO:HD2	2:B:311:PHE:CE1	2.49	0.47
1:C:203:GLU:OE1	1:C:207:ARG:HB3	2.15	0.47
1:A:511:ALA:HB1	1:A:538:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:ILE:HG23	2:D:136:LEU:HD11	1.96	0.47
2:B:364:THR:HA	2:B:367:LEU:HD12	1.96	0.47
1:C:369:ASP:HB3	1:C:478:LEU:HD21	1.96	0.47
1:A:613:GLY:HA2	3:A:800:B12:H3P1	1.97	0.47
1:A:201:LEU:HG	1:A:218:MET:HE1	1.96	0.46
2:B:252:LEU:HD11	2:B:300:LEU:HA	1.96	0.46
2:B:390:VAL:HG12	2:B:392:ILE:HG23	1.97	0.46
2:D:133:VAL:HG23	2:D:380:ARG:HD3	1.97	0.46
1:C:431:GLY:HA3	1:C:435:LYS:HD2	1.97	0.46
1:A:172:LEU:HD11	1:A:220:ILE:HG23	1.97	0.46
2:D:88:PRO:HG2	2:D:99:VAL:HG22	1.98	0.46
1:C:128:ASP:HB3	1:C:493:LYS:HG2	1.98	0.46
2:D:435:THR:HG22	2:D:436:GLU:H	1.81	0.46
2:D:637:ALA:O	2:D:638:LYS:HB3	2.15	0.46
2:B:435:THR:HG22	2:B:436:GLU:H	1.80	0.46
1:A:521:ASN:O	1:A:529:ARG:HD3	2.16	0.46
3:A:800:B12:H302	3:A:800:B12:H353	1.97	0.46
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.98	0.45
1:C:599:ARG:CG	1:C:649:VAL:HA	2.46	0.45
1:C:602:LEU:HD22	3:C:800:B12:HM52	1.99	0.45
1:A:636:THR:HB	1:A:637:PRO:HD2	1.98	0.45
1:C:283:ARG:HD3	1:C:283:ARG:HA	1.87	0.45
2:B:73:VAL:HB	2:B:74:PRO:CD	2.43	0.45
1:A:79:TYR:HA	1:A:82:ARG:O	2.17	0.45
1:C:358:GLY:O	1:C:359:HIS:HB2	2.15	0.45
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.52	0.45
2:B:402:SER:HB3	2:B:405:VAL:HB	1.99	0.45
1:C:68:PRO:HA	1:C:69:PRO:HA	1.78	0.45
1:A:529:ARG:HA	1:A:534:LEU:HD11	1.97	0.45
2:B:86:GLY:HA3	5:B:2047:HOH:O	2.16	0.44
1:A:500:ARG:HD3	5:A:2340:HOH:O	2.16	0.44
2:B:263:VAL:O	2:B:267:VAL:HG23	2.17	0.44
1:C:44:ILE:HD13	1:C:415:ASP:HB3	1.99	0.44
1:A:515:ILE:HD11	1:A:538:ALA:HB2	1.99	0.44
1:A:706:THR:HB	1:A:707:PRO:HD2	1.98	0.44
2:B:80:ASP:HB3	2:B:407:SER:HB2	1.99	0.44
1:C:197:GLN:HG3	1:C:239:SER:HB3	2.00	0.44
1:A:636:THR:HB	1:A:637:PRO:CD	2.48	0.44
2:D:586:LYS:HD2	2:D:590:ALA:HB3	1.99	0.44
2:B:503:ARG:NE	2:B:638:LYS:HB3	2.33	0.44
1:A:503:ARG:HD2	1:A:508:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:ALA:O	2:D:227:PHE:HA	2.17	0.44
2:D:381:ASN:HA	2:D:384:ILE:HB	2.00	0.44
2:B:236:ILE:HG23	2:B:258:THR:HG21	2.00	0.44
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.53	0.44
1:C:591:GLU:HA	1:C:596:ARG:O	2.18	0.44
1:C:162:SER:HA	1:C:193:ALA:O	2.18	0.43
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.99	0.43
1:C:684:VAL:O	1:C:704:ILE:HA	2.19	0.43
2:D:510:ARG:HA	2:D:511:PRO:HD3	1.93	0.43
1:C:520:GLY:N	1:C:555:VAL:HG21	2.34	0.43
1:A:544:THR:O	1:A:548:MET:HG3	2.18	0.43
3:A:800:B12:H492	3:A:800:B12:H473	2.00	0.43
5:C:2490:HOH:O	2:D:42:VAL:HG21	2.19	0.43
1:A:514:LYS:HD3	1:A:534:LEU:HD22	2.00	0.43
2:B:191:LYS:HD2	2:B:226:LYS:O	2.19	0.43
2:B:532:SER:CB	2:B:533:PRO:HD3	2.46	0.43
2:D:461:THR:O	2:D:462:ALA:HB3	2.19	0.43
1:A:85:THR:HB	1:A:362:SER:HB3	2.01	0.43
1:A:69:PRO:HG3	2:B:24:ALA:HA	2.01	0.43
3:C:800:B12:H362	3:C:800:B12:H351	2.00	0.43
2:D:242:HIS:HB2	2:D:251:GLU:OE1	2.17	0.43
3:A:800:B12:H473	5:A:2443:HOH:O	2.19	0.42
1:C:118:ASP:HB2	5:C:2125:HOH:O	2.18	0.42
1:A:205:MET:HG3	1:A:442:PRO:HB2	2.01	0.42
2:D:275:GLU:O	2:D:279:THR:HG22	2.19	0.42
2:D:518:LEU:HD21	2:D:581:VAL:HG11	2.00	0.42
1:A:602:LEU:HD22	3:A:800:B12:HM52	2.01	0.42
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.48	0.42
1:C:389:PHE:HA	2:D:461:THR:OG1	2.19	0.42
1:A:336:LEU:HD21	5:A:2255:HOH:O	2.19	0.42
2:D:264:ARG:HG3	2:D:311:PHE:CZ	2.55	0.42
1:A:129:ASN:HB3	1:A:132:VAL:HG22	2.02	0.42
2:B:527:ARG:HB3	2:B:568:CYS:HB3	2.01	0.42
1:A:336:LEU:HD12	1:A:370:GLU:HB3	2.02	0.42
1:A:299:ALA:HB1	1:A:413:THR:HA	2.01	0.42
1:C:215:GLN:HB3	1:C:216:PRO:CD	2.50	0.42
2:D:182:VAL:HG23	2:D:185:ARG:HH21	1.84	0.42
1:A:602:LEU:CD2	3:A:800:B12:HM52	2.49	0.42
2:D:260:ALA:O	2:D:261:GLU:C	2.58	0.42
1:A:68:PRO:HA	1:A:69:PRO:HA	1.72	0.41
1:C:570:TYR:HB3	1:C:623:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:GLN:OE1	1:C:643:GLN:NE2	2.53	0.41
2:D:152:GLU:O	2:D:155:SER:HB3	2.20	0.41
1:A:638:GLU:HA	1:A:671:GLU:HG3	2.02	0.41
1:A:346:VAL:O	1:A:350:ILE:HG12	2.21	0.41
1:A:526:ASP:HA	1:A:527:PRO:HD2	1.93	0.41
1:C:15:ALA:HA	1:C:16:PRO:HD2	1.86	0.41
2:D:166:VAL:O	2:D:167:PHE:HB3	2.21	0.41
1:C:312:VAL:HG12	1:C:317:PRO:HG3	2.02	0.41
1:C:401:ASP:HA	1:C:402:PRO:HD2	1.83	0.41
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.50	0.41
1:C:511:ALA:HB1	1:C:538:ALA:HA	2.03	0.41
5:C:2253:HOH:O	2:D:377:ARG:HD2	2.20	0.41
1:C:566:ILE:HD12	1:C:569:VAL:HG21	2.03	0.41
2:D:234:VAL:HB	2:D:280:ILE:HG23	2.02	0.41
1:A:152:LEU:HD23	1:A:153:PHE:CE2	2.55	0.41
1:C:18:PRO:HB2	1:C:20:ASP:OD1	2.21	0.41
1:C:596:ARG:HD3	5:C:2401:HOH:O	2.21	0.41
1:C:14:ASN:O	1:C:15:ALA:C	2.59	0.41
1:C:307:LEU:HD22	1:C:421:TRP:CE3	2.56	0.41
1:C:66:GLY:HA2	1:C:74:PRO:O	2.20	0.41
2:D:468:MET:CE	2:D:471:ALA:HA	2.50	0.41
2:D:517:CYS:HB3	2:D:524:PHE:CD1	2.56	0.41
1:A:171:VAL:HG21	1:A:198:ASN:ND2	2.35	0.41
2:B:244:ALA:HB1	2:B:442:LEU:HD13	2.02	0.41
1:C:426:GLU:O	1:C:427:VAL:C	2.59	0.41
2:D:315:GLU:O	2:D:318:ARG:HG3	2.21	0.41
2:D:90:VAL:HG12	2:D:91:ALA:O	2.20	0.41
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.18	0.41
1:A:6:ARG:HD3	2:B:264:ARG:NH1	2.36	0.40
2:B:442:LEU:HD12	2:B:488:LEU:HD22	2.03	0.40
2:D:263:VAL:O	2:D:267:VAL:HG23	2.20	0.40
2:D:91:ALA:HA	2:D:93:PHE:N	2.36	0.40
2:B:220:TRP:HE3	2:B:220:TRP:HA	1.83	0.40
1:C:372:ILE:CG2	1:C:480:VAL:HG11	2.51	0.40
2:B:577:GLN:O	2:B:581:VAL:HG23	2.20	0.40
1:A:414:TRP:CZ2	1:A:418:ARG:HD3	2.56	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	725/727 (100%)	671 (93%)	51 (7%)	3 (0%)	34	55
1	C	725/727 (100%)	652 (90%)	62 (9%)	11 (2%)	10	19
2	B	617/637 (97%)	566 (92%)	47 (8%)	4 (1%)	25	45
2	D	617/637 (97%)	554 (90%)	56 (9%)	7 (1%)	14	27
All	All	2684/2728 (98%)	2443 (91%)	216 (8%)	25 (1%)	17	33

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	LYS
2	B	578	GLY
1	C	3	THR
1	C	8	ASP
1	C	573	GLU
2	D	435	THR
1	A	214	PRO
2	B	269	GLN
2	D	80	ASP
1	A	359	HIS
1	C	70	PHE
2	D	227	PHE
2	B	435	THR
1	C	214	PRO
1	C	359	HIS
1	C	430	VAL
2	D	185	ARG
2	D	400	GLY
2	D	600	LYS
1	C	206	VAL
1	C	486	SER
2	B	603	GLY

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Mol	Chain	Res	Type
1	A	206	VAL
2	D	308	GLY
1	C	15	ALA

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	570/589 (97%)	544 (95%)	26 (5%)	27	50
1	C	570/589 (97%)	542 (95%)	28 (5%)	25	46
2	B	474/509 (93%)	452 (95%)	22 (5%)	27	50
2	D	474/509 (93%)	440 (93%)	34 (7%)	14	27
All	All	2088/2196 (95%)	1978 (95%)	110 (5%)	22	43

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	53	ASP
1	A	131	ARG
1	A	200	ILE
1	A	206	VAL
1	A	207	ARG
1	A	241	SER
1	A	361	GLN
1	A	362	SER
1	A	430	VAL
1	A	441	ILE
1	A	444	MET
1	A	445	ARG
1	A	463	PRO
1	A	473	GLU
1	A	485	ASN
1	A	486	SER
1	A	487	THR

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Mol	Chain	Res	Type
1	A	533	LYS
1	A	576	ASN
1	A	585	GLU
1	A	597	ARG
1	A	599	ARG
1	A	668	LEU
1	A	694	ASP
1	A	727	ASP
2	B	22	SER
2	B	60	LYS
2	B	67	VAL
2	B	83	LYS
2	B	119	LYS
2	B	122	ARG
2	B	142	PRO
2	B	180	VAL
2	B	186	SER
2	B	195	LEU
2	B	216	VAL
2	B	288	HIS
2	B	334	GLU
2	B	440	LYS
2	B	527	ARG
2	B	532	SER
2	B	544	GLN
2	B	552	GLU
2	B	560	SER
2	B	586	LYS
2	B	614	ASP
2	B	617	LEU
1	C	23	ARG
1	C	26	GLU
1	C	53	ASP
1	C	69	PRO
1	C	70	PHE
1	C	131	ARG
1	C	159	ASP
1	C	162	SER
1	C	198	ASN
1	C	200	ILE
1	C	202	LYS
1	C	207	ARG

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Mol	Chain	Res	Type
1	C	222	SER
1	C	241	SER
1	C	272	SER
1	C	414	TRP
1	C	430	VAL
1	C	438	GLU
1	C	482	LYS
1	C	486	SER
1	C	487	THR
1	C	576	ASN
1	C	585	GLU
1	C	592	GLN
1	C	596	ARG
1	C	668	LEU
1	C	694	ASP
1	C	713	GLU
2	D	20	THR
2	D	60	LYS
2	D	83	LYS
2	D	85	LEU
2	D	104	MET
2	D	119	LYS
2	D	129	LEU
2	D	145	ILE
2	D	155	SER
2	D	166	VAL
2	D	180	VAL
2	D	188	LYS
2	D	191	LYS
2	D	212	PRO
2	D	216	VAL
2	D	217	LEU
2	D	222	ARG
2	D	223	ARG
2	D	224	LEU
2	D	235	THR
2	D	264	ARG
2	D	272	THR
2	D	288	HIS
2	D	334	GLU
2	D	367	LEU
2	D	380	ARG

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Mol	Chain	Res	Type
2	D	429	MET
2	D	440	LYS
2	D	475	GLU
2	D	522	ARG
2	D	532	SER
2	D	593	LEU
2	D	614	ASP
2	D	638	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	198	ASN
1	A	359	HIS
1	A	385	ASN
1	A	485	ASN
1	A	492	GLN
1	A	635	GLN
1	A	643	GLN
2	B	290	GLN
2	B	322	GLN
2	B	323	ASN
2	B	391	ASN
1	C	191	GLN
1	C	198	ASN
1	C	359	HIS
1	C	385	ASN
1	C	492	GLN
1	C	635	GLN
1	C	643	GLN
2	D	290	GLN
2	D	322	GLN
2	D	323	ASN
2	D	391	ASN
2	D	421	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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$
3	B12	C	800	1,5	80,101,101	1.29	7 (8%)	101,166,166	2.27	33 (32%)
4	DCA	A	801	-	41,49,49	0.85	0	51,74,74	1.74	15 (29%)
4	DCA	C	801	-	41,49,49	0.91	1 (2%)	51,74,74	1.72	10 (19%)
3	B12	A	800	1	80,101,101	1.49	7 (8%)	101,166,166	2.32	32 (31%)

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
3	B12	C	800	1,5	-	8/51/223/223	0/3/11/11
4	DCA	A	801	-	-	3/43/63/63	0/3/3/3
4	DCA	C	801	-	-	2/43/63/63	0/3/3/3
3	B12	A	800	1	-	9/51/223/223	0/3/11/11

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	CO-N23	-7.94	1.56	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	CO-N23	-5.48	1.68	1.94
3	A	800	B12	CO-N21	4.77	2.00	1.89
3	C	800	B12	CO-N22	-4.38	1.73	1.94
3	C	800	B12	C54-C17	3.44	1.61	1.55
3	A	800	B12	CO-N24	-2.85	1.82	1.89
3	A	800	B12	C54-C17	2.65	1.59	1.55
3	A	800	B12	CO-N22	-2.56	1.82	1.94
3	C	800	B12	C2-C3	-2.43	1.54	1.58
3	A	800	B12	C11-C10	-2.28	1.37	1.40
4	C	801	DCA	C8A-N7A	-2.26	1.30	1.34
3	A	800	B12	C6B-C5B	2.26	1.46	1.40
3	C	800	B12	C11-C10	-2.13	1.37	1.40
3	C	800	B12	C6B-C5B	2.06	1.46	1.40
3	C	800	B12	O8R-C5R	2.01	1.50	1.42

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C55-C17-C18	8.38	127.33	111.14
3	C	800	B12	C16-C15-C14	-8.31	111.31	124.27
3	A	800	B12	C16-C15-C14	-7.93	111.90	124.27
4	A	801	DCA	CDP-CBP-CAP	-6.14	98.17	108.82
4	C	801	DCA	C2P-C3P-N4P	5.98	132.15	111.52
3	A	800	B12	C55-C17-C18	5.77	122.28	111.14
3	C	800	B12	C6-C5-C4	-5.20	116.16	124.27
3	A	800	B12	C13-C14-C15	-4.92	113.84	131.68
3	A	800	B12	C55-C17-C16	4.90	126.23	109.92
3	A	800	B12	C7B-C8B-C9B	4.84	125.33	120.54
3	C	800	B12	O5-P-O3	4.82	125.81	106.78
3	C	800	B12	C26-C2-C1	-4.62	102.85	110.02
3	A	800	B12	C1-C19-N24	-4.39	101.30	106.24
4	C	801	DCA	C5A-C6A-N6A	4.36	126.97	120.35
3	A	800	B12	C1P-N59-C57	-4.35	113.22	122.69
3	A	800	B12	C47-C12-C46	-4.28	100.75	109.73
3	A	800	B12	C8-C9-N22	4.23	116.41	111.12
3	A	800	B12	C54-C17-C18	-4.21	106.77	112.98
4	A	801	DCA	C5A-C6A-N6A	4.20	126.73	120.35
3	C	800	B12	C30-C3-C2	4.11	127.85	119.13
3	A	800	B12	C54-C17-C55	-3.95	102.74	109.26
3	A	800	B12	C25-C2-C1	3.92	119.62	113.80
3	A	800	B12	C2-C1-C19	-3.86	112.50	118.60
3	C	800	B12	C54-C17-C18	-3.84	107.32	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C13-C14-C15	-3.76	118.03	131.68
3	A	800	B12	C4B-C9B-C8B	-3.71	117.30	121.10
3	A	800	B12	C26-C2-C1	-3.69	104.28	110.02
3	C	800	B12	C8-C9-N22	3.61	115.64	111.12
4	A	801	DCA	O2B-C2B-C3B	3.44	120.94	111.17
3	A	800	B12	C20-C1-C2	3.37	118.89	113.32
4	C	801	DCA	C1B-N9A-C4A	3.31	132.46	126.64
3	C	800	B12	C55-C17-C16	3.20	120.59	109.92
3	C	800	B12	C5M-C5B-C6B	-3.18	114.21	120.74
3	C	800	B12	C7B-C8B-C9B	3.15	123.66	120.54
3	A	800	B12	C25-C2-C3	-3.13	110.80	115.58
3	A	800	B12	C49-C50-N52	3.13	126.24	116.51
3	C	800	B12	C20-C1-C19	3.12	112.36	109.36
3	C	800	B12	C54-C17-C55	-3.11	104.12	109.26
4	A	801	DCA	O5P-C5P-N4P	-3.10	117.16	123.01
3	A	800	B12	C5M-C5B-C6B	-3.03	114.53	120.74
4	C	801	DCA	C5A-C6A-N1A	-2.97	113.62	120.35
3	A	800	B12	C41-C42-C43	2.97	122.65	112.59
3	A	800	B12	C6-C5-C4	-2.87	119.80	124.27
4	A	801	DCA	C2P-C3P-N4P	2.84	121.33	111.52
3	C	800	B12	C47-C12-C46	-2.82	103.81	109.73
4	C	801	DCA	CDP-CBP-CCP	2.81	112.82	108.23
3	C	800	B12	C2-C1-C19	-2.81	114.17	118.60
3	C	800	B12	C3-C4-C5	-2.75	121.70	131.68
3	A	800	B12	C6M-C6B-C5B	2.74	126.34	120.74
3	C	800	B12	C48-C13-C12	-2.72	109.02	116.59
3	A	800	B12	O63-C61-C60	2.68	126.51	120.87
3	C	800	B12	C18-C60-C61	-2.67	107.30	113.97
4	A	801	DCA	C1B-N9A-C4A	2.65	131.30	126.64
3	A	800	B12	O34-C32-C31	-2.65	113.29	121.07
4	C	801	DCA	C6P-C5P-N4P	2.65	120.88	116.42
3	C	800	B12	C2R-C3R-C4R	2.64	107.90	103.22
4	C	801	DCA	O5P-C5P-N4P	-2.63	118.05	123.01
3	C	800	B12	O8R-C5R-C4R	-2.63	102.27	111.29
3	A	800	B12	O63-C61-N62	-2.57	115.49	122.50
3	C	800	B12	C25-C2-C1	2.54	117.57	113.80
3	C	800	B12	C5B-C4B-C9B	-2.51	117.66	121.22
3	A	800	B12	C3-C4-C5	-2.51	122.57	131.68
4	A	801	DCA	O9A-P3B-O7A	2.50	120.45	110.68
3	A	800	B12	C48-C13-C12	-2.41	109.88	116.59
4	A	801	DCA	CAP-C9P-N8P	2.37	121.29	116.58
4	C	801	DCA	O2B-C2B-C3B	2.36	117.88	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C4B-C9B-N3B	2.34	137.14	130.88
4	A	801	DCA	CEP-CBP-CCP	2.33	112.04	108.23
4	C	801	DCA	CDP-CBP-CAP	-2.33	104.78	108.82
3	C	800	B12	C41-C8-C7	-2.30	107.86	114.08
3	A	800	B12	C9-C10-C11	-2.29	122.91	130.91
3	C	800	B12	C17-C18-C19	2.26	105.82	102.37
4	A	801	DCA	C4A-C5A-N7A	2.25	111.75	109.40
3	A	800	B12	C7B-C6B-C5B	-2.25	116.13	119.91
4	A	801	DCA	CDP-CBP-CCP	2.24	111.89	108.23
3	C	800	B12	C1-C19-C18	-2.24	118.23	121.93
3	C	800	B12	C5R-C4R-C3R	-2.22	107.78	114.85
3	A	800	B12	O5-P-O3	2.20	115.47	106.78
4	A	801	DCA	CEP-CBP-CDP	2.19	113.63	109.17
3	C	800	B12	C6M-C6B-C5B	-2.18	116.26	120.74
3	A	800	B12	C2R-C3R-C4R	2.18	107.08	103.22
3	C	800	B12	C26-C2-C3	2.16	111.45	107.47
3	C	800	B12	C56-C55-C17	-2.11	111.42	115.50
4	A	801	DCA	O9P-C9P-N8P	-2.09	118.51	122.99
4	A	801	DCA	C6P-C7P-N8P	2.07	116.08	111.90
4	C	801	DCA	C4A-C5A-N7A	2.06	111.55	109.40
3	C	800	B12	O6R-C1R-C2R	-2.04	103.94	106.93
3	C	800	B12	C36-C7-C37	2.03	114.29	110.83
4	A	801	DCA	C5A-C6A-N1A	-2.02	115.78	120.35
3	C	800	B12	C1-C19-N24	-2.00	103.98	106.24

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	800	B12	C16-C17-C55-C56
3	A	800	B12	C30-C31-C32-O34
3	A	800	B12	C30-C31-C32-N33
3	A	800	B12	C2P-O3-P-O2
3	A	800	B12	C42-C41-C8-C7
3	C	800	B12	C41-C42-C43-O44
3	C	800	B12	C41-C42-C43-N45
3	A	800	B12	C41-C42-C43-O44
3	A	800	B12	C41-C42-C43-N45
4	C	801	DCA	P2A-O3A-P1A-O1A
3	A	800	B12	C3-C30-C31-C32
4	A	801	DCA	P1A-O3A-P2A-O6A
4	A	801	DCA	P2A-O3A-P1A-O2A

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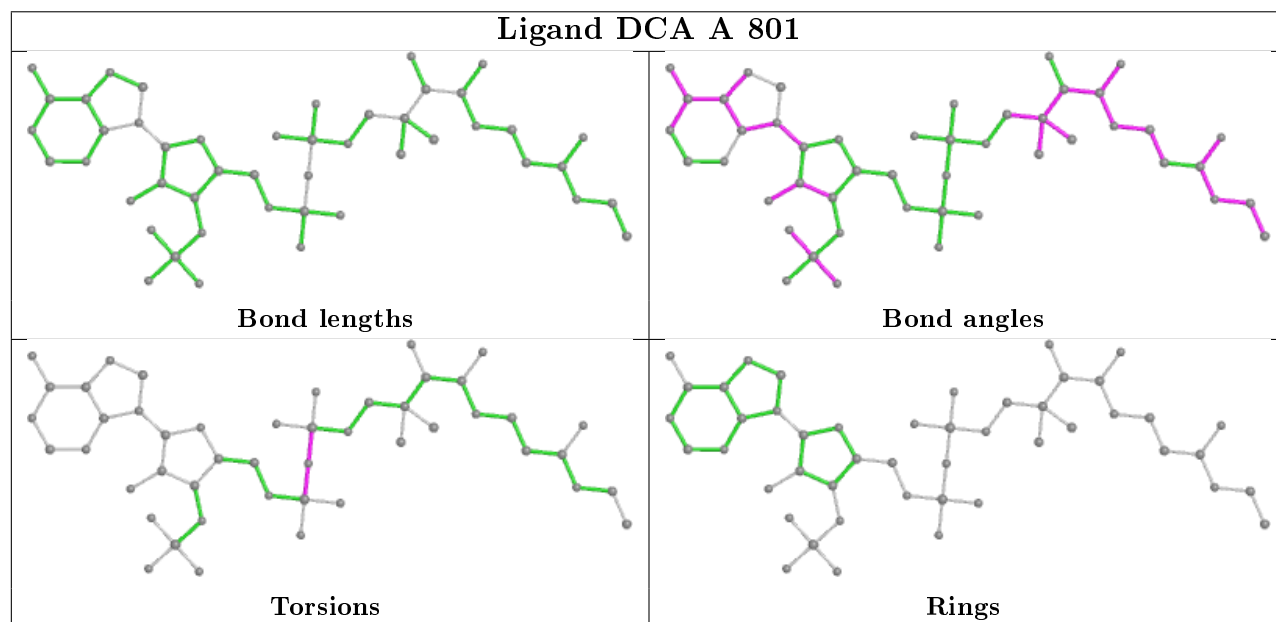
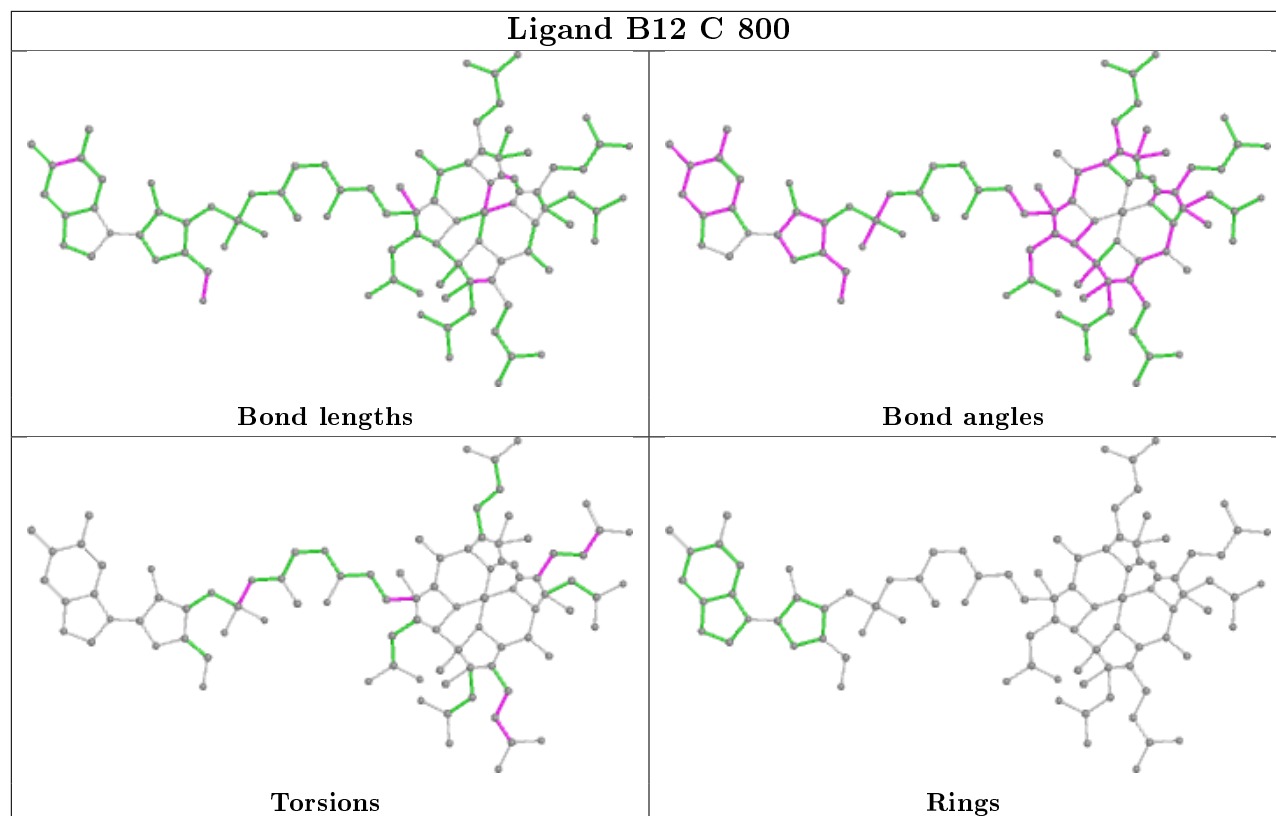
Mol	Chain	Res	Type	Atoms
3	C	800	B12	C2P-O3-P-O2
3	C	800	B12	C42-C41-C8-C7
3	C	800	B12	C3-C30-C31-C32
4	C	801	DCA	P2A-O3A-P1A-O2A
3	C	800	B12	C30-C31-C32-N33
4	A	801	DCA	P2A-O3A-P1A-O1A
3	A	800	B12	C55-C56-C57-O58
3	C	800	B12	C30-C31-C32-O34
3	A	800	B12	C55-C56-C57-N59

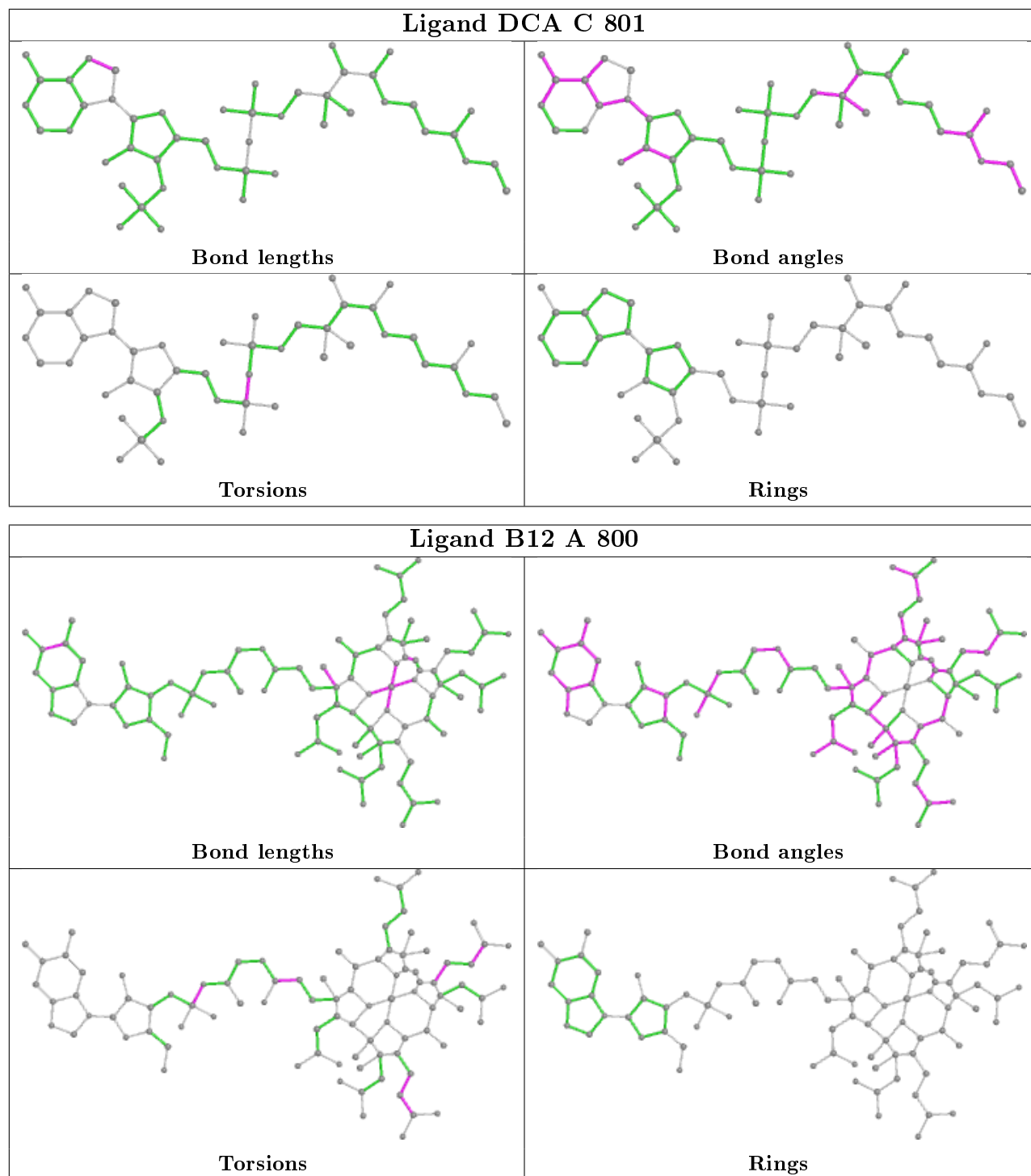
There are no ring outliers.

2 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	800	B12	13	0
3	A	800	B12	18	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	727/727 (100%)	-0.53	5 (0%) 87 85	17, 36, 64, 145	0
1	C	727/727 (100%)	-0.34	16 (2%) 62 57	20, 41, 74, 145	0
2	B	619/637 (97%)	-0.37	4 (0%) 89 88	21, 49, 74, 103	0
2	D	619/637 (97%)	0.02	25 (4%) 38 32	27, 58, 88, 112	0
All	All	2692/2728 (98%)	-0.32	50 (1%) 66 62	17, 45, 80, 145	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	9.6
1	C	3	THR	5.2
1	C	2	SER	5.0
1	A	3	THR	4.5
2	D	266	LEU	4.1
1	C	576	ASN	3.6
1	C	27	GLU	3.6
1	C	497	VAL	3.5
2	D	483	PRO	3.3
2	B	603	GLY	3.2
2	D	270	GLY	3.2
2	D	273	ALA	3.2
1	C	23	ARG	3.2
1	C	574	VAL	3.2
2	D	162	THR	3.1
2	D	158	LEU	3.0
2	D	193	LEU	3.0
2	D	151	ASP	2.9
2	D	192	ASP	2.9
2	D	310	VAL	2.9
2	D	147	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	576	ASN	2.6
2	D	146	ALA	2.6
2	D	161	MET	2.4
1	A	4	LEU	2.4
1	C	4	LEU	2.4
2	D	426	LEU	2.4
2	D	276	ALA	2.3
2	D	148	GLU	2.3
2	D	312	GLY	2.3
2	B	280	ILE	2.2
2	D	555	GLU	2.2
1	C	21	ALA	2.2
1	C	32	ALA	2.2
1	C	675	LEU	2.2
2	D	237	ASP	2.2
1	C	5	PRO	2.2
2	D	224	LEU	2.2
2	B	238	ALA	2.2
1	C	501	ALA	2.1
2	D	190	ALA	2.1
2	B	282	PHE	2.1
2	D	189	PRO	2.1
1	C	24	ARG	2.1
1	C	573	GLU	2.1
2	D	313	VAL	2.1
2	D	20	THR	2.0
1	A	5	PRO	2.0
1	C	35	GLY	2.0
2	D	217	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

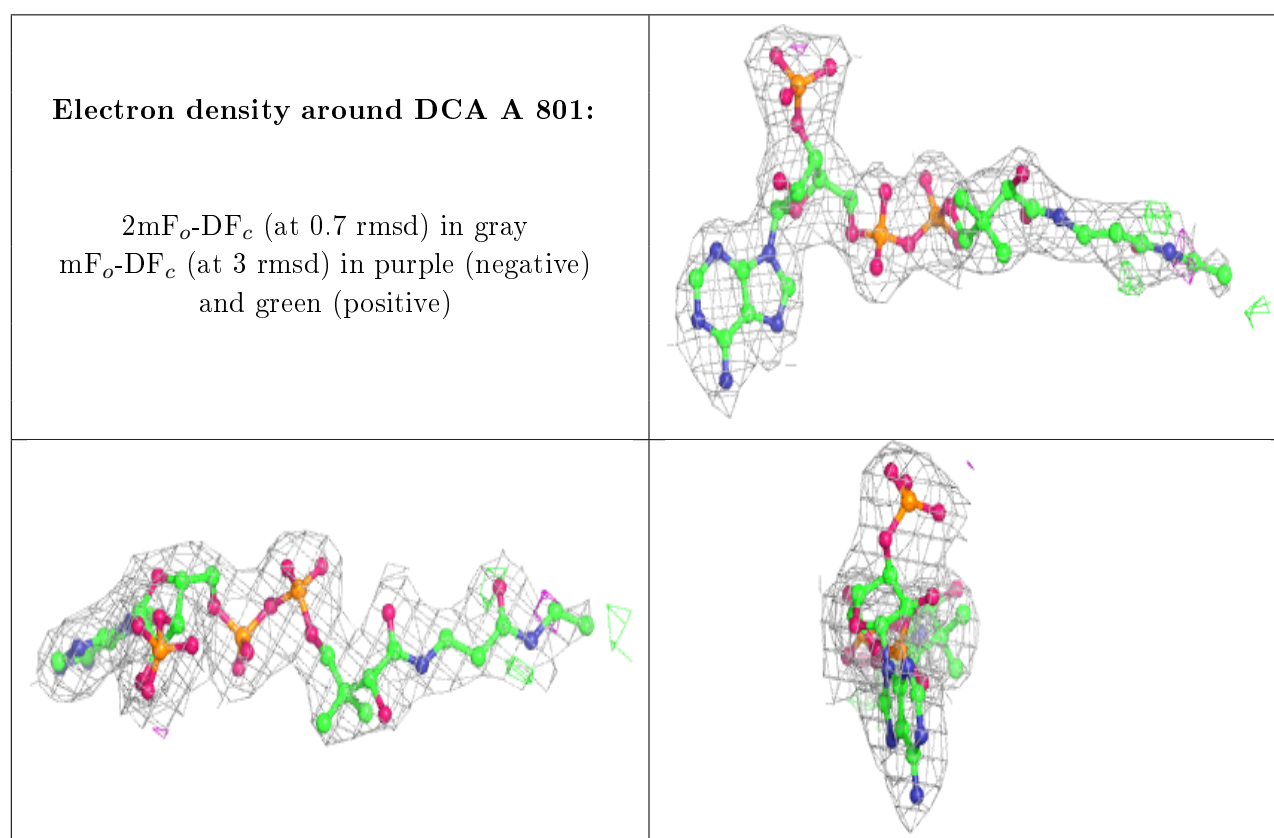
There are no carbohydrates in this entry.

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.

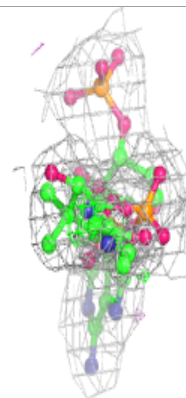
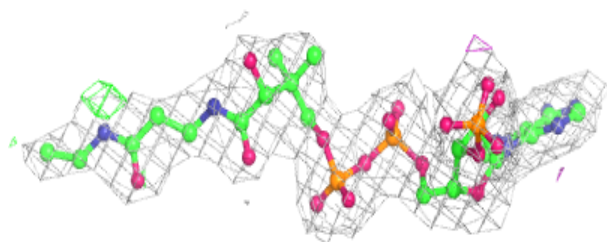
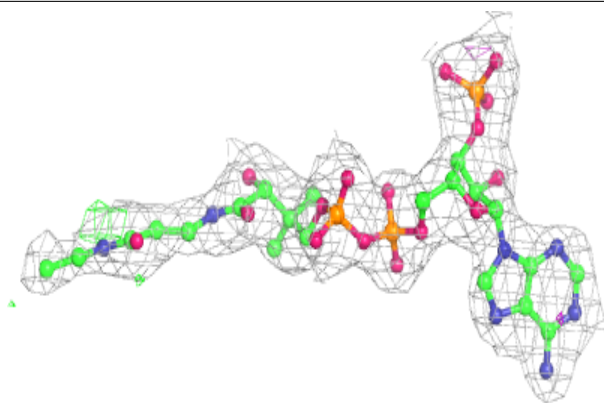
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DCA	A	801	47/47	0.97	0.10	19,29,35,39	0
4	DCA	C	801	47/47	0.97	0.12	21,28,32,35	0
3	B12	C	800	91/91	0.98	0.14	18,28,39,41	0
3	B12	A	800	91/91	0.98	0.15	13,27,35,38	0

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.

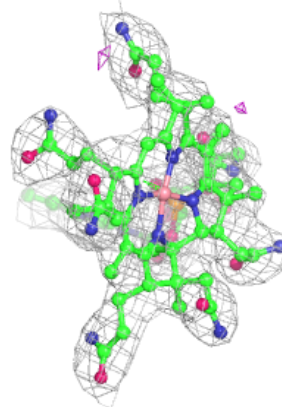
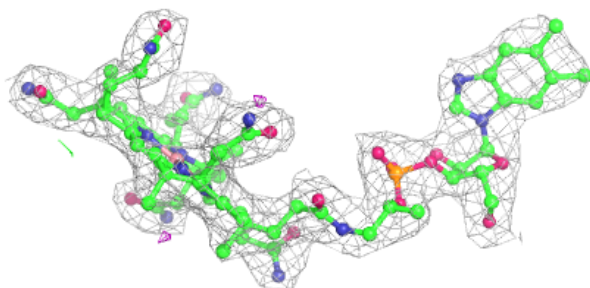
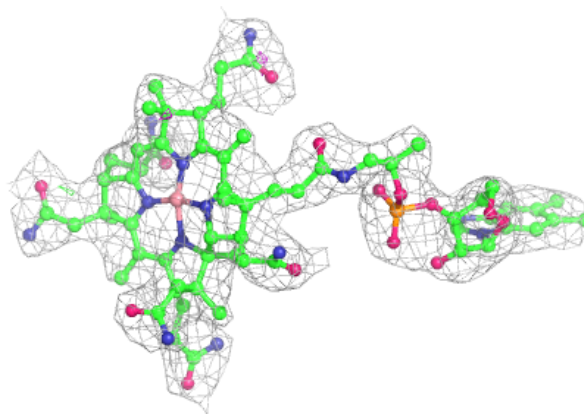


Electron density around DCA C 801:

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

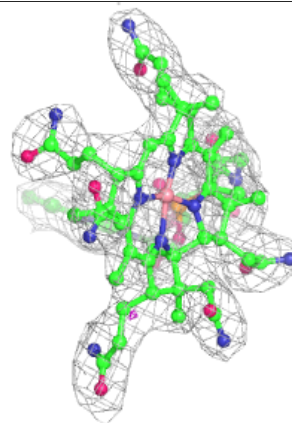
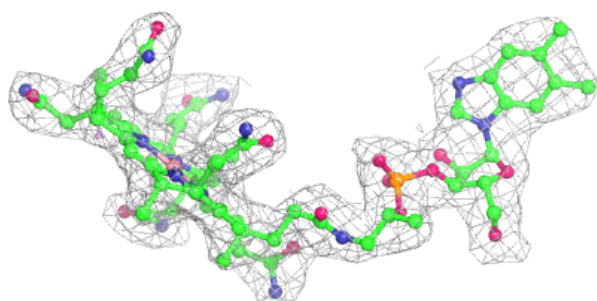
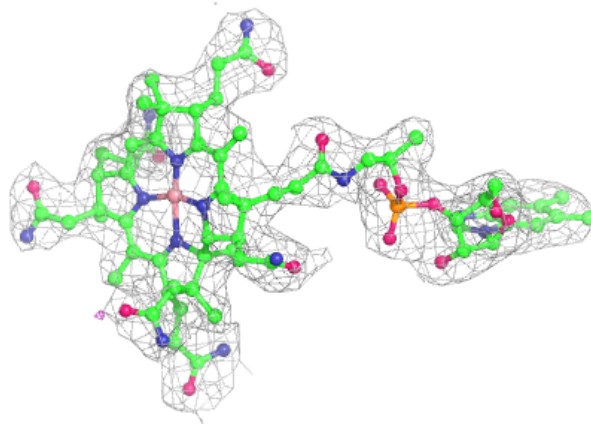
**Electron density around B12 C 800:**

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.