



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:30 AM UTC

PDB ID : 1K0G / pdb_00001k0g
Title : THE CRYSTAL STRUCTURE OF AMINODEOXYCHORISMATE SYNTHASE FROM PHOSPHATE GROWN CRYSTALS
Authors : Parsons, J.F.; Jensen, P.Y.; Pachikara, A.S.; Howard, A.J.; Eisenstein, E.; Ladner, J.E.
Deposited on : 2001-09-19
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

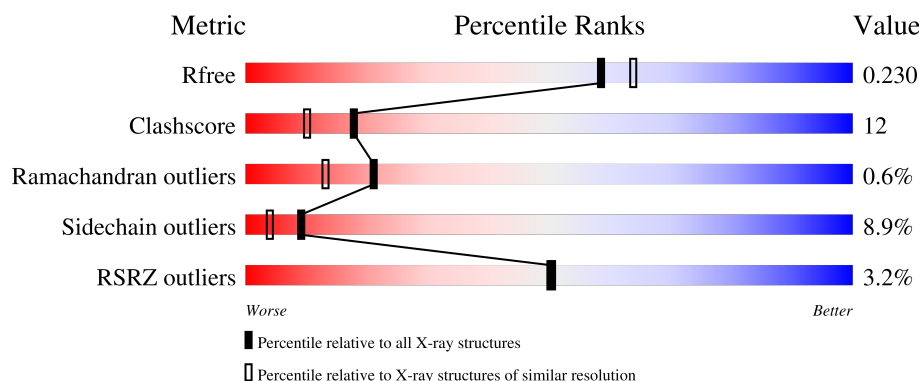
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

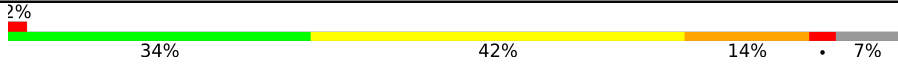
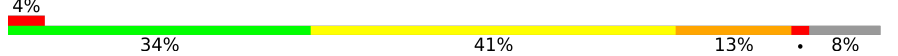
The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	453	
1	B	453	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	701	-	X	-	-
2	PO4	B	702	-	-	X	-

2 Entry composition [i](#)

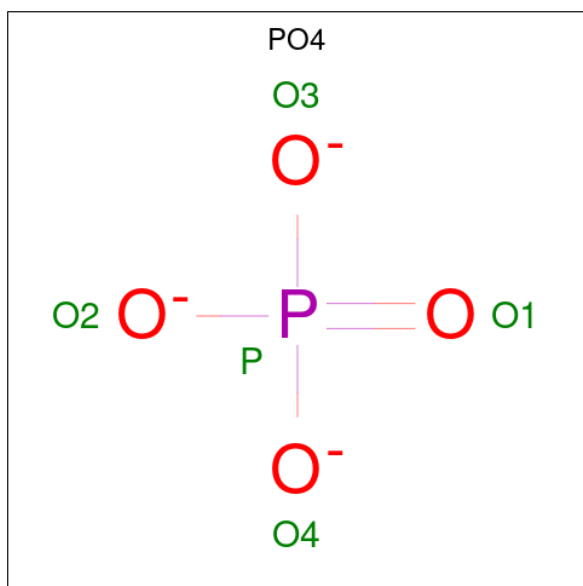
There are 4 unique types of molecules in this entry. The entry contains 7228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 p-aminobenzoate synthase component I.

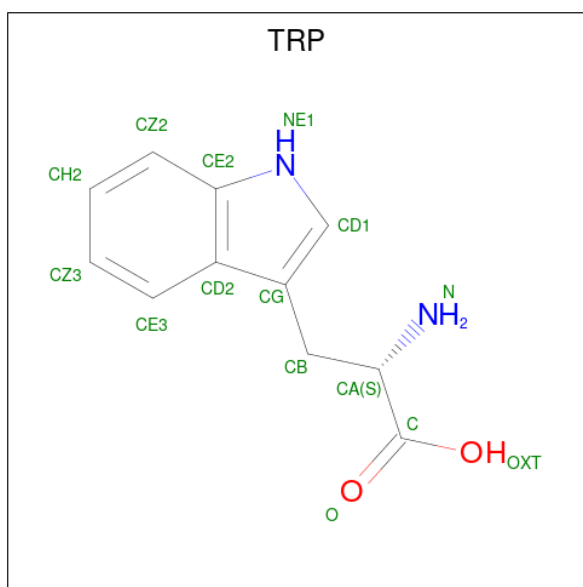
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3340	2106	580	640	14			
1	B	415	Total	C	N	O	S	0	0	0
			3288	2073	571	630	14			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		

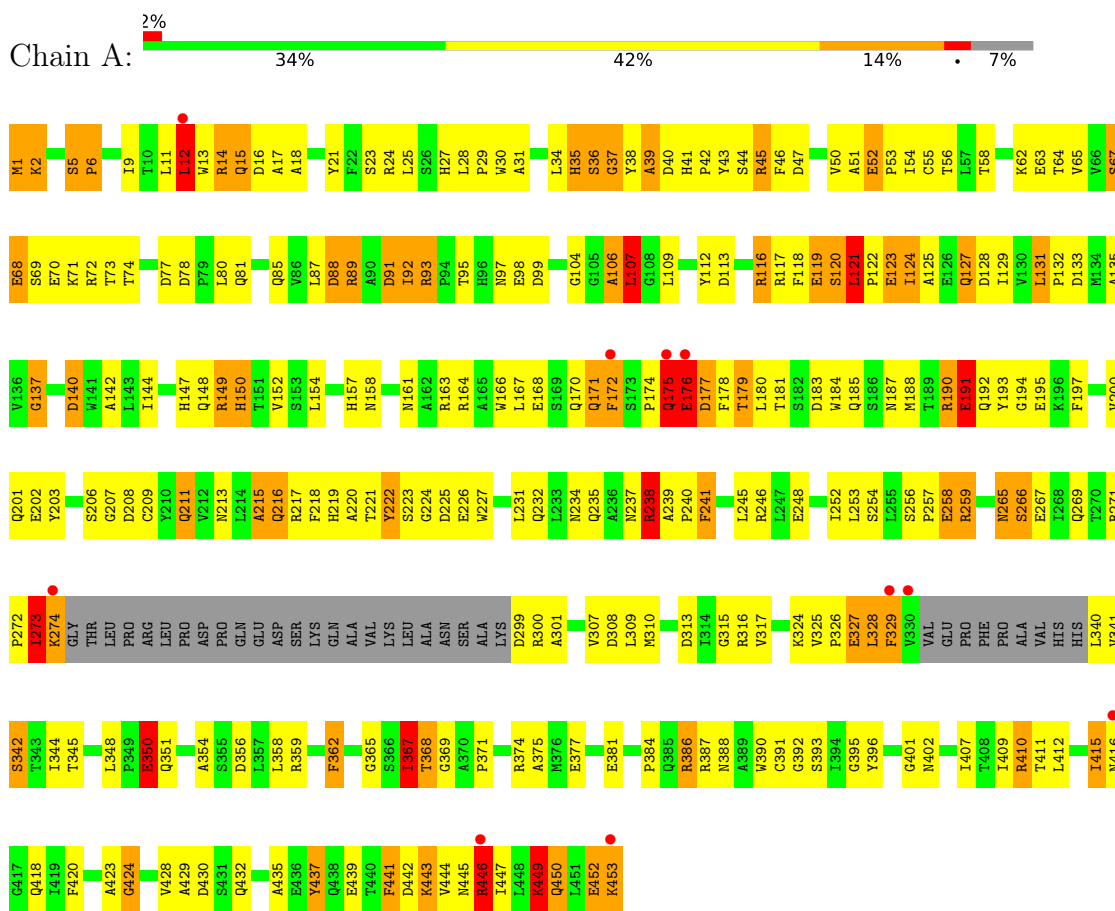
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	286	Total	O	0	0
			286	286		
4	B	274	Total	O	0	0
			274	274		

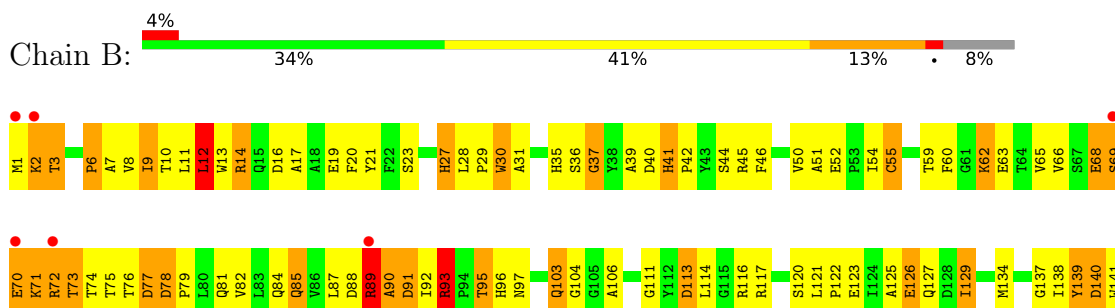
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: p-aminobenzoate synthase component I



• Molecule 1: p-aminobenzoate synthase component I





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.01Å 109.71Å 134.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 10.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	86.2 (10.00-2.05) 89.8 (10.00-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.05Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.172 , 0.238 0.177 , 0.230	Depositor DCC
R_{free} test set	4337 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 107.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7228	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.43	13/3410 (0.4%)	3.02	413/4626 (8.9%)
1	B	1.37	8/3357 (0.2%)	2.91	384/4557 (8.4%)
All	All	1.40	21/6767 (0.3%)	2.97	797/9183 (8.7%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	GLU	CD-OE1	13.36	1.50	1.25
1	A	452	GLU	CD-OE2	9.92	1.44	1.25
1	A	52	GLU	C-O	9.51	1.28	1.23
1	A	52	GLU	CA-C	-7.45	1.48	1.53
1	A	374	ARG	CZ-NH1	6.73	1.42	1.32
1	B	236	ALA	N-CA	-6.61	1.38	1.46
1	A	362	PHE	CA-CB	6.16	1.62	1.53
1	A	348	LEU	CA-C	-5.83	1.46	1.52
1	B	210	TYR	N-CA	-5.83	1.38	1.46
1	B	163	ARG	CD-NE	5.71	1.54	1.46
1	B	243	ALA	C-O	5.67	1.30	1.23
1	B	311	ARG	N-CA	5.62	1.53	1.46
1	A	226	GLU	N-CA	5.51	1.53	1.46
1	A	452	GLU	CG-CD	-5.46	1.38	1.52
1	B	52	GLU	CA-CB	5.41	1.56	1.52
1	A	113	ASP	N-CA	5.39	1.53	1.46
1	A	203	TYR	C-O	-5.38	1.17	1.24
1	A	50	VAL	C-O	5.17	1.29	1.23
1	B	356	ASP	C-O	-5.05	1.18	1.24
1	A	246	ARG	CD-NE	5.04	1.53	1.46
1	B	45	ARG	CD-NE	5.00	1.53	1.46

All (797) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ASP	CA-CB-CG	19.36	131.96	112.60
1	B	445	ASN	CA-CB-CG	19.30	131.90	112.60
1	A	410	ARG	CA-CB-CG	15.73	145.56	114.10
1	B	442	ASP	CA-CB-CG	15.27	127.87	112.60
1	A	45	ARG	NE-CZ-NH2	15.25	132.93	119.20
1	B	241	PHE	CA-CB-CG	-14.97	98.83	113.80
1	A	93	ARG	CA-C-O	14.77	136.09	121.32
1	A	93	ARG	O-C-N	-14.64	109.70	121.12
1	A	185	GLN	CA-CB-CG	13.88	141.86	114.10
1	A	273	ILE	CA-C-N	13.75	146.45	121.70
1	A	273	ILE	C-N-CA	13.75	146.45	121.70
1	B	443	LYS	N-CA-C	-13.42	96.99	113.50
1	A	452	GLU	CA-C-N	13.37	145.77	121.70
1	A	452	GLU	C-N-CA	13.37	145.77	121.70
1	B	328	LEU	CA-C-O	-13.23	98.32	120.80
1	B	78	ASP	O-C-N	13.22	131.78	121.47
1	B	205	HIS	CA-CB-CG	-13.14	100.66	113.80
1	A	119	GLU	CB-CG-CD	13.10	134.87	112.60
1	A	446	ARG	CD-NE-CZ	12.31	141.63	124.40
1	A	238	ARG	CA-CB-CG	11.99	138.08	114.10
1	B	28	LEU	CA-C-O	11.99	130.43	119.76
1	B	208	ASP	CA-CB-CG	-11.67	100.93	112.60
1	B	150	HIS	CA-CB-CG	-11.49	102.31	113.80
1	A	238	ARG	NE-CZ-NH1	11.45	132.95	121.50
1	B	237	ASN	OD1-CG-ND2	11.12	133.72	122.60
1	B	7	ALA	CA-C-O	-10.99	108.84	121.81
1	B	273	ILE	CA-C-O	-10.97	108.40	120.25
1	B	315	GLY	CA-C-O	10.88	132.16	120.40
1	A	176	GLU	CB-CG-CD	10.78	130.93	112.60
1	A	374	ARG	CA-C-O	10.77	132.13	120.82
1	B	421	CYS	CA-C-O	-10.74	108.85	120.24
1	B	404	ASP	CA-CB-CG	-10.71	101.89	112.60
1	A	231	LEU	CA-C-O	10.57	132.04	120.63
1	B	450	GLN	O-C-N	-10.50	110.03	122.11
1	B	450	GLN	OE1-CD-NE2	10.47	133.07	122.60
1	A	180	LEU	CA-C-N	-10.45	107.60	123.17
1	A	180	LEU	C-N-CA	-10.45	107.60	123.17
1	A	80	LEU	CA-C-O	10.36	132.02	119.79
1	B	237	ASN	CA-CB-CG	-10.28	102.32	112.60
1	A	351	GLN	OE1-CD-NE2	10.23	132.83	122.60
1	B	158	ASN	CA-C-N	-10.20	108.67	122.85
1	B	158	ASN	C-N-CA	-10.20	108.67	122.85
1	B	235	GLN	O-C-N	10.14	136.08	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	HIS	CA-CB-CG	-10.13	103.67	113.80
1	B	140	ASP	OD1-CG-OD2	-10.03	98.84	122.90
1	B	63	GLU	CB-CG-CD	10.02	129.63	112.60
1	B	444	VAL	CA-C-O	-9.99	108.69	118.98
1	B	341	VAL	CA-C-O	9.96	128.42	118.96
1	A	362	PHE	CA-CB-CG	-9.92	103.88	113.80
1	A	62	LYS	CA-C-N	-9.88	108.61	122.93
1	A	62	LYS	C-N-CA	-9.88	108.61	122.93
1	B	184	TRP	O-C-N	-9.83	111.41	123.01
1	A	177	ASP	CA-C-N	-9.82	107.55	122.09
1	A	177	ASP	C-N-CA	-9.82	107.55	122.09
1	A	39	ALA	O-C-N	-9.77	111.92	122.96
1	A	407	ILE	CA-C-O	-9.74	109.97	120.59
1	B	402	ASN	CA-CB-CG	-9.74	102.86	112.60
1	B	11	LEU	CA-C-N	-9.73	106.89	120.71
1	B	11	LEU	C-N-CA	-9.73	106.89	120.71
1	A	190	ARG	CA-C-O	9.69	131.09	120.63
1	B	121	LEU	CA-C-O	-9.68	108.89	120.41
1	A	415	ILE	CA-CB-CG1	9.66	126.81	110.40
1	A	52	GLU	CB-CG-CD	-9.59	96.29	112.60
1	B	246	ARG	NE-CZ-NH1	-9.56	111.94	121.50
1	B	440	THR	O-C-N	-9.51	109.94	122.59
1	A	329	PHE	CA-CB-CG	9.50	123.30	113.80
1	B	438	GLN	OE1-CD-NE2	-9.49	113.11	122.60
1	A	52	GLU	CA-C-O	9.47	127.77	120.48
1	A	113	ASP	CA-CB-CG	-9.45	103.15	112.60
1	A	386	ARG	CD-NE-CZ	-9.45	111.17	124.40
1	A	166	TRP	CA-C-O	9.45	130.56	120.55
1	A	45	ARG	NE-CZ-NH1	-9.43	112.07	121.50
1	A	265	ASN	OD1-CG-ND2	-9.41	113.19	122.60
1	A	154	LEU	CA-C-O	9.40	130.66	120.32
1	B	402	ASN	CB-CG-ND2	-9.38	102.34	116.40
1	B	158	ASN	CA-CB-CG	-9.33	103.27	112.60
1	A	401	GLY	CA-C-O	9.31	128.68	119.27
1	B	6	PRO	O-C-N	-9.31	111.60	123.06
1	B	246	ARG	NE-CZ-NH2	9.29	127.56	119.20
1	A	271	ARG	CD-NE-CZ	-9.27	111.43	124.40
1	A	225	ASP	O-C-N	9.26	134.86	122.82
1	B	312	ASN	CA-CB-CG	-9.21	103.39	112.60
1	B	417	GLY	O-C-N	9.18	134.12	122.28
1	A	325	VAL	N-CA-C	-9.16	101.68	109.19
1	A	200	VAL	O-C-N	-9.15	112.99	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ARG	NE-CZ-NH1	-9.14	112.36	121.50
1	A	161	ASN	CA-C-O	9.13	130.10	120.42
1	B	443	LYS	CA-C-O	9.13	129.18	119.14
1	A	208	ASP	CA-CB-CG	-9.11	103.49	112.60
1	B	341	VAL	N-CA-CB	-9.09	102.21	112.21
1	A	42	PRO	O-C-N	9.09	134.66	122.30
1	A	172	PHE	CA-CB-CG	-9.06	104.74	113.80
1	B	417	GLY	CA-C-O	-9.03	109.47	119.04
1	B	215	ALA	CA-C-O	-8.98	110.61	121.11
1	A	2	LYS	CA-C-O	8.96	130.16	120.58
1	A	266	SER	CA-C-N	-8.96	110.86	122.77
1	A	266	SER	C-N-CA	-8.96	110.86	122.77
1	A	87	LEU	CA-C-O	8.93	130.01	120.55
1	A	117	ARG	CA-C-O	8.93	129.80	119.18
1	B	221	THR	CA-CB-OG1	-8.91	96.24	109.60
1	A	384	PRO	CA-C-N	-8.88	107.89	122.81
1	A	384	PRO	C-N-CA	-8.88	107.89	122.81
1	B	304	LEU	CA-C-O	8.87	131.19	121.16
1	A	149	ARG	CD-NE-CZ	-8.86	112.00	124.40
1	B	265	ASN	CA-CB-CG	-8.82	103.78	112.60
1	A	40	ASP	O-C-N	-8.78	110.92	122.59
1	B	88	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	273	ILE	O-C-N	8.75	132.72	122.66
1	A	23	SER	CA-C-O	8.71	130.67	120.92
1	B	407	ILE	CA-C-N	-8.69	109.05	122.08
1	B	407	ILE	C-N-CA	-8.69	109.05	122.08
1	B	242	SER	O-C-N	-8.66	112.98	122.85
1	A	272	PRO	O-C-N	-8.62	112.60	123.03
1	B	164	ARG	NE-CZ-NH2	8.61	126.94	119.20
1	B	322	SER	CA-C-N	-8.58	109.82	121.66
1	B	322	SER	C-N-CA	-8.58	109.82	121.66
1	A	52	GLU	CB-CA-C	-8.58	103.54	111.00
1	B	89	ARG	NH1-CZ-NH2	8.57	130.44	119.30
1	B	116	ARG	CD-NE-CZ	-8.54	112.44	124.40
1	B	356	ASP	CA-CB-CG	-8.51	104.09	112.60
1	A	179	THR	CA-C-N	-8.50	108.83	120.82
1	A	179	THR	C-N-CA	-8.50	108.83	120.82
1	B	122	PRO	O-C-N	-8.50	112.51	122.71
1	A	208	ASP	CA-C-O	-8.48	109.08	119.18
1	B	304	LEU	O-C-N	-8.44	112.53	123.16
1	B	213	ASN	OD1-CG-ND2	-8.43	114.17	122.60
1	B	316	ARG	NE-CZ-NH2	-8.42	111.62	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	GLN	CB-CG-CD	8.41	126.91	112.60
1	B	93	ARG	O-C-N	8.40	128.25	121.20
1	B	186	SER	O-C-N	-8.40	113.28	122.85
1	B	157	HIS	N-CA-C	-8.38	103.06	113.28
1	A	452	GLU	CB-CG-CD	-8.38	98.36	112.60
1	A	219	HIS	CA-CB-CG	8.37	122.17	113.80
1	B	438	GLN	CA-C-O	-8.34	109.95	119.79
1	A	218	PHE	CA-C-O	-8.33	111.33	120.92
1	A	95	THR	CA-C-O	-8.33	112.48	121.56
1	A	211	GLN	CA-C-O	-8.31	110.62	120.43
1	B	147	HIS	CA-CB-CG	-8.31	105.49	113.80
1	B	443	LYS	N-CA-CB	8.29	122.72	110.53
1	B	173	SER	CA-C-N	-8.29	111.47	119.76
1	B	173	SER	C-N-CA	-8.29	111.47	119.76
1	A	299	ASP	CA-CB-CG	-8.27	104.33	112.60
1	A	63	GLU	CA-C-O	8.26	129.47	120.71
1	A	36	SER	CA-C-N	8.26	137.15	120.80
1	A	36	SER	C-N-CA	8.26	137.15	120.80
1	B	316	ARG	CD-NE-CZ	8.23	135.93	124.40
1	B	182	SER	N-CA-CB	8.23	124.13	111.46
1	A	258	GLU	CB-CA-C	-8.22	94.67	109.71
1	A	36	SER	O-C-N	-8.22	111.85	122.37
1	A	443	LYS	CA-C-N	-8.21	112.84	122.36
1	A	443	LYS	C-N-CA	-8.21	112.84	122.36
1	B	167	LEU	CA-C-O	8.20	129.24	120.55
1	B	121	LEU	O-C-N	8.17	129.50	121.57
1	A	116	ARG	NE-CZ-NH2	8.16	126.55	119.20
1	B	11	LEU	CA-C-O	-8.15	111.54	121.89
1	A	188	MET	CA-C-O	8.14	129.85	120.89
1	A	64	THR	O-C-N	8.13	132.71	123.27
1	A	42	PRO	CA-C-N	-8.12	109.66	122.65
1	A	42	PRO	C-N-CA	-8.12	109.66	122.65
1	A	238	ARG	NE-CZ-NH2	-8.11	111.90	119.20
1	A	449	LYS	CA-C-O	-8.11	111.83	120.42
1	B	16	ASP	CA-C-N	-8.10	108.61	120.28
1	B	16	ASP	C-N-CA	-8.10	108.61	120.28
1	A	183	ASP	CA-CB-CG	8.08	120.68	112.60
1	A	222	TYR	CB-CG-CD2	8.06	132.89	120.80
1	B	327	GLU	CA-C-O	-8.04	111.57	120.81
1	A	211	GLN	O-C-N	8.01	132.61	123.48
1	A	15	GLN	CA-CB-CG	8.00	130.09	114.10
1	B	410	ARG	NE-CZ-NH2	-7.98	112.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	PHE	N-CA-C	7.97	121.17	109.62
1	A	55	CYS	CA-C-O	-7.93	110.78	120.54
1	A	239	ALA	CA-C-O	7.92	126.16	119.66
1	A	120	SER	CA-C-N	-7.92	109.59	122.26
1	A	120	SER	C-N-CA	-7.92	109.59	122.26
1	A	217	ARG	NE-CZ-NH1	7.87	129.37	121.50
1	B	350	GLU	O-C-N	-7.86	113.79	122.12
1	A	174	PRO	O-C-N	7.85	132.72	123.06
1	B	76	THR	N-CA-C	-7.85	102.75	112.88
1	A	104	GLY	N-CA-C	-7.85	100.05	112.61
1	A	118	PHE	CA-C-N	7.84	134.81	122.74
1	A	118	PHE	C-N-CA	7.84	134.81	122.74
1	B	178	PHE	O-C-N	7.83	132.82	123.27
1	B	274	LYS	CA-C-N	7.83	135.79	121.70
1	B	274	LYS	C-N-CA	7.83	135.79	121.70
1	A	201	GLN	CA-C-O	-7.78	111.02	119.97
1	B	207	GLY	O-C-N	-7.78	113.34	122.45
1	A	125	ALA	CA-C-O	7.77	130.42	121.87
1	B	140	ASP	CB-CG-OD2	7.77	136.28	118.40
1	A	326	PRO	CA-C-N	7.76	132.41	121.24
1	A	326	PRO	C-N-CA	7.76	132.41	121.24
1	A	31	ALA	O-C-N	-7.73	113.99	123.04
1	B	234	ASN	CA-C-O	7.72	128.92	120.82
1	B	104	GLY	N-CA-C	-7.70	102.64	112.65
1	A	38	TYR	N-CA-C	-7.69	103.84	113.23
1	A	41	HIS	CA-CB-CG	7.69	121.49	113.80
1	B	157	HIS	CA-C-N	-7.69	110.92	121.84
1	B	157	HIS	C-N-CA	-7.69	110.92	121.84
1	A	387	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	A	218	PHE	CA-CB-CG	-7.67	106.13	113.80
1	A	415	ILE	CB-CA-C	-7.66	98.72	111.29
1	A	180	LEU	O-C-N	-7.65	113.46	122.95
1	B	163	ARG	CD-NE-CZ	-7.64	113.71	124.40
1	B	184	TRP	CA-C-O	7.63	129.75	121.05
1	B	182	SER	O-C-N	7.62	131.27	123.26
1	A	174	PRO	CA-C-N	7.62	134.47	122.74
1	A	174	PRO	C-N-CA	7.62	134.47	122.74
1	B	113	ASP	CA-CB-CG	-7.62	104.98	112.60
1	B	89	ARG	NE-CZ-NH2	-7.59	112.36	119.20
1	A	17	ALA	O-C-N	7.58	130.16	122.12
1	B	170	GLN	OE1-CD-NE2	7.57	130.17	122.60
1	A	369	GLY	CA-C-O	7.57	127.30	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ARG	NE-CZ-NH2	7.56	126.00	119.20
1	B	181	THR	N-CA-CB	-7.55	98.84	110.92
1	A	191	GLU	CB-CG-CD	-7.54	99.78	112.60
1	A	53	PRO	O-C-N	-7.53	113.67	123.01
1	B	184	TRP	CA-C-N	-7.49	109.48	122.37
1	B	184	TRP	C-N-CA	-7.49	109.48	122.37
1	A	362	PHE	CA-C-O	-7.49	111.22	119.61
1	A	217	ARG	O-C-N	-7.47	114.41	123.30
1	B	59	THR	O-C-N	-7.47	114.47	123.29
1	B	186	SER	CA-C-O	7.46	130.62	121.81
1	A	125	ALA	O-C-N	-7.45	114.03	122.75
1	B	40	ASP	O-C-N	-7.44	111.65	122.96
1	A	157	HIS	CA-C-O	7.44	128.03	119.18
1	A	119	GLU	CA-C-N	-7.43	112.27	122.30
1	A	119	GLU	C-N-CA	-7.43	112.27	122.30
1	A	21	TYR	O-C-N	-7.42	113.14	122.27
1	B	219	HIS	ND1-CE1-NE2	7.42	115.82	108.40
1	A	386	ARG	NE-CZ-NH1	-7.41	114.09	121.50
1	B	317	VAL	CA-C-O	7.41	125.42	118.90
1	B	317	VAL	CB-CA-C	-7.39	102.82	110.88
1	B	106	ALA	O-C-N	7.39	131.73	123.16
1	A	58	THR	CA-C-O	7.38	128.15	120.40
1	A	375	ALA	O-C-N	-7.37	114.31	122.12
1	B	417	GLY	CA-C-N	-7.37	112.24	122.93
1	B	417	GLY	C-N-CA	-7.37	112.24	122.93
1	A	144	ILE	CA-C-O	-7.36	112.65	120.53
1	A	135	ALA	CA-C-N	-7.35	112.12	122.71
1	A	135	ALA	C-N-CA	-7.35	112.12	122.71
1	A	147	HIS	CA-CB-CG	-7.35	106.45	113.80
1	A	225	ASP	CA-CB-CG	-7.33	105.27	112.60
1	A	342	SER	N-CA-CB	-7.33	98.93	111.69
1	A	265	ASN	CA-CB-CG	-7.32	105.28	112.60
1	B	68	GLU	CA-C-N	7.31	135.51	121.54
1	B	68	GLU	C-N-CA	7.31	135.51	121.54
1	A	437	TYR	CA-C-O	7.28	128.69	120.90
1	A	39	ALA	CA-C-O	7.27	129.83	121.47
1	B	237	ASN	CB-CG-ND2	-7.25	105.52	116.40
1	A	416	ASN	CB-CA-C	-7.24	101.79	111.63
1	B	181	THR	CA-CB-CG2	7.23	122.80	110.50
1	B	73	THR	N-CA-C	7.21	120.16	110.35
1	A	350	GLU	CA-C-O	7.21	128.28	120.20
1	B	77	ASP	CA-C-O	-7.21	113.94	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ALA	CA-C-O	7.19	128.17	120.55
1	A	225	ASP	CA-C-N	-7.18	109.11	120.60
1	A	225	ASP	C-N-CA	-7.18	109.11	120.60
1	B	387	ARG	CA-C-O	-7.17	111.33	119.79
1	B	103	GLN	O-C-N	7.16	132.11	122.59
1	A	315	GLY	O-C-N	-7.14	114.62	122.68
1	A	112	TYR	CA-C-O	-7.13	113.27	120.90
1	A	227	TRP	CA-C-O	7.13	128.16	120.10
1	A	329	PHE	CA-C-N	7.12	134.52	121.70
1	A	329	PHE	C-N-CA	7.12	134.52	121.70
1	B	148	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	A	99	ASP	CA-CB-CG	-7.11	105.49	112.60
1	B	11	LEU	O-C-N	7.11	131.08	122.84
1	B	258	GLU	N-CA-C	7.10	120.10	108.52
1	A	17	ALA	CA-C-N	-7.10	111.21	120.44
1	A	17	ALA	C-N-CA	-7.10	111.21	120.44
1	A	317	VAL	CB-CA-C	-7.10	103.95	110.63
1	A	51	ALA	CA-C-N	-7.09	115.17	122.83
1	A	51	ALA	C-N-CA	-7.09	115.17	122.83
1	B	430	ASP	CA-CB-CG	-7.09	105.51	112.60
1	A	327	GLU	CA-C-N	-7.08	110.46	122.92
1	A	327	GLU	C-N-CA	-7.08	110.46	122.92
1	B	233	LEU	CA-C-O	7.08	128.15	119.79
1	A	307	VAL	O-C-N	7.08	130.90	123.26
1	A	316	ARG	CA-C-N	-7.08	111.62	121.53
1	A	316	ARG	C-N-CA	-7.08	111.62	121.53
1	B	28	LEU	O-C-N	-7.08	113.92	121.42
1	B	302	GLU	CA-CB-CG	-7.07	99.95	114.10
1	A	202	GLU	O-C-N	-7.06	114.80	122.07
1	A	216	GLN	OE1-CD-NE2	7.05	129.65	122.60
1	B	228	GLN	OE1-CD-NE2	-7.03	115.57	122.60
1	B	191	GLU	CA-C-N	-7.02	109.64	120.31
1	B	191	GLU	C-N-CA	-7.02	109.64	120.31
1	B	225	ASP	CA-CB-CG	-7.01	105.59	112.60
1	A	193	TYR	O-C-N	7.01	129.29	122.07
1	A	374	ARG	O-C-N	-7.00	114.86	122.07
1	B	215	ALA	N-CA-C	7.00	120.57	109.50
1	A	122	PRO	CA-C-N	6.98	133.98	123.23
1	A	122	PRO	C-N-CA	6.98	133.98	123.23
1	B	95	THR	CA-C-O	-6.96	113.97	121.56
1	A	125	ALA	CA-C-N	-6.95	111.81	122.09
1	A	125	ALA	C-N-CA	-6.95	111.81	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	VAL	O-C-N	-6.94	113.81	122.97
1	A	207	GLY	CA-C-O	-6.94	110.42	119.44
1	B	219	HIS	CE1-NE2-CD2	-6.93	102.07	109.00
1	A	148	GLN	CG-CD-NE2	6.92	126.78	116.40
1	A	176	GLU	CA-CB-CG	6.91	127.92	114.10
1	A	191	GLU	CA-C-O	6.91	127.94	119.79
1	A	121	LEU	CB-CA-C	6.91	119.34	110.22
1	A	14	ARG	NE-CZ-NH2	-6.90	112.99	119.20
1	A	430	ASP	CA-CB-CG	-6.89	105.70	112.60
1	B	239	ALA	O-C-N	6.89	127.69	121.35
1	A	88	ASP	CA-C-O	6.89	127.72	120.42
1	B	93	ARG	CA-C-O	-6.89	114.27	121.29
1	A	354	ALA	O-C-N	6.88	129.42	122.12
1	A	6	PRO	CA-C-O	-6.87	113.29	121.67
1	A	174	PRO	CA-C-O	-6.86	113.30	121.67
1	B	213	ASN	O-C-N	-6.85	114.71	122.93
1	B	117	ARG	N-CA-C	-6.85	104.93	113.28
1	A	201	GLN	CA-CB-CG	-6.83	100.43	114.10
1	A	446	ARG	CA-C-N	-6.83	111.81	120.56
1	A	446	ARG	C-N-CA	-6.83	111.81	120.56
1	A	253	LEU	CA-C-O	-6.83	112.92	120.70
1	B	416	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	A	386	ARG	O-C-N	6.79	131.16	122.81
1	A	14	ARG	NE-CZ-NH1	6.79	128.28	121.50
1	B	148	GLN	CB-CG-CD	-6.79	101.06	112.60
1	B	238	ARG	CD-NE-CZ	6.78	133.90	124.40
1	A	328	LEU	CA-C-O	6.78	129.77	121.56
1	B	351	GLN	OE1-CD-NE2	6.77	129.37	122.60
1	B	77	ASP	O-C-N	6.75	130.64	122.75
1	A	344	ILE	O-C-N	-6.74	115.89	123.10
1	A	202	GLU	CA-C-O	6.72	127.88	120.82
1	A	70	GLU	CA-C-N	-6.72	112.15	122.09
1	A	70	GLU	C-N-CA	-6.72	112.15	122.09
1	B	435	ALA	CA-C-O	6.71	127.67	120.55
1	B	235	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	381	GLU	CB-CA-C	-6.69	98.45	110.70
1	B	410	ARG	CB-CA-C	-6.68	101.93	111.95
1	B	8	VAL	N-CA-C	6.67	118.09	108.48
1	A	119	GLU	CB-CA-C	-6.67	97.62	109.70
1	A	299	ASP	CA-C-O	-6.67	109.46	120.80
1	A	241	PHE	CA-CB-CG	-6.67	107.13	113.80
1	A	359	ARG	O-C-N	6.64	128.91	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	N-CA-C	6.64	120.35	109.72
1	B	129	ILE	CB-CG1-CD1	-6.64	99.86	113.80
1	A	223	SER	CA-C-N	-6.62	111.92	122.65
1	A	223	SER	C-N-CA	-6.62	111.92	122.65
1	B	91	ASP	CA-CB-CG	-6.62	105.97	112.60
1	B	215	ALA	O-C-N	6.62	131.38	123.24
1	A	37	GLY	O-C-N	6.61	130.40	122.34
1	A	11	LEU	CA-C-N	-6.60	110.78	120.75
1	A	11	LEU	C-N-CA	-6.60	110.78	120.75
1	B	381	GLU	O-C-N	-6.60	114.63	122.15
1	B	189	THR	O-C-N	6.59	130.63	122.86
1	B	207	GLY	CA-C-O	6.58	126.63	119.06
1	B	182	SER	N-CA-C	-6.57	99.00	108.60
1	B	327	GLU	CB-CG-CD	6.57	123.77	112.60
1	B	323	VAL	CA-C-O	-6.55	113.38	120.85
1	B	446	ARG	CA-C-N	6.54	129.34	120.77
1	B	446	ARG	C-N-CA	6.54	129.34	120.77
1	A	429	ALA	CA-C-N	-6.54	112.18	122.65
1	A	429	ALA	C-N-CA	-6.54	112.18	122.65
1	A	348	LEU	O-C-N	-6.52	114.51	121.42
1	B	27	HIS	CA-CB-CG	-6.51	107.28	113.80
1	B	90	ALA	O-C-N	6.50	131.15	122.43
1	B	431	SER	CA-C-O	-6.50	114.33	121.87
1	B	199	GLN	CA-C-N	-6.50	112.37	120.56
1	B	199	GLN	C-N-CA	-6.50	112.37	120.56
1	A	107	LEU	CA-CB-CG	6.49	139.02	116.30
1	B	120	SER	CA-C-O	6.49	127.70	120.43
1	A	377	GLU	CA-C-N	-6.49	109.67	120.30
1	A	377	GLU	C-N-CA	-6.49	109.67	120.30
1	B	213	ASN	CA-C-O	6.48	127.51	120.58
1	A	152	VAL	CA-C-O	-6.48	113.08	120.66
1	B	444	VAL	N-CA-CB	-6.46	103.39	112.12
1	B	203	TYR	CA-C-O	6.45	127.39	120.10
1	A	234	ASN	CA-C-N	6.45	129.76	120.79
1	A	234	ASN	C-N-CA	6.45	129.76	120.79
1	B	95	THR	CA-C-N	6.45	129.99	120.90
1	B	95	THR	C-N-CA	6.45	129.99	120.90
1	A	93	ARG	CD-NE-CZ	-6.45	115.38	124.40
1	A	416	ASN	CA-C-O	-6.44	112.99	120.98
1	B	16	ASP	O-C-N	6.44	130.44	122.20
1	A	191	GLU	N-CA-CB	-6.43	100.39	110.30
1	B	269	GLN	CA-C-O	-6.43	113.60	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ASN	N-CA-C	6.43	118.83	110.53
1	B	381	GLU	CA-C-O	6.43	127.24	120.42
1	A	248	GLU	CB-CG-CD	6.43	123.53	112.60
1	B	89	ARG	CD-NE-CZ	-6.43	115.40	124.40
1	A	121	LEU	O-C-N	-6.43	115.86	121.71
1	B	183	ASP	O-C-N	-6.42	115.28	122.86
1	B	359	ARG	CD-NE-CZ	-6.41	115.42	124.40
1	B	436	GLU	O-C-N	-6.41	115.42	122.09
1	B	181	THR	CA-CB-OG1	-6.41	99.99	109.60
1	A	215	ALA	CA-C-N	-6.41	111.58	123.05
1	A	215	ALA	C-N-CA	-6.41	111.58	123.05
1	A	309	LEU	N-CA-CB	-6.41	99.15	110.42
1	A	91	ASP	CA-C-N	-6.38	114.61	123.10
1	A	91	ASP	C-N-CA	-6.38	114.61	123.10
1	B	392	GLY	O-C-N	-6.37	114.42	122.70
1	A	271	ARG	N-CA-C	6.37	118.86	109.50
1	B	316	ARG	NH1-CZ-NH2	6.37	127.58	119.30
1	B	178	PHE	CA-CB-CG	6.36	120.16	113.80
1	B	393	SER	CB-CA-C	-6.36	96.39	109.94
1	B	265	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	B	362	PHE	N-CA-C	6.32	118.79	109.62
1	A	257	PRO	CA-C-N	-6.29	114.12	122.99
1	A	257	PRO	C-N-CA	-6.29	114.12	122.99
1	A	381	GLU	CG-CD-OE2	-6.29	103.93	118.40
1	B	353	HIS	CA-CB-CG	-6.29	107.51	113.80
1	A	42	PRO	CB-CA-C	-6.29	102.50	111.68
1	A	140	ASP	CA-CB-CG	-6.27	106.33	112.60
1	B	7	ALA	CA-C-N	-6.27	114.41	123.06
1	B	7	ALA	C-N-CA	-6.27	114.41	123.06
1	A	164	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	A	350	GLU	CA-C-N	-6.25	111.06	122.38
1	A	350	GLU	C-N-CA	-6.25	111.06	122.38
1	A	194	GLY	N-CA-C	-6.25	105.23	112.73
1	B	410	ARG	O-C-N	6.25	130.38	122.57
1	A	359	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	B	259	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	B	442	ASP	CA-C-O	6.24	125.83	119.97
1	B	145	VAL	CA-C-O	-6.24	113.86	120.53
1	B	62	LYS	N-CA-C	6.24	120.72	113.18
1	B	93	ARG	CA-C-N	-6.23	114.23	120.21
1	B	93	ARG	C-N-CA	-6.23	114.23	120.21
1	A	183	ASP	O-C-N	6.22	129.94	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLY	O-C-N	-6.21	116.15	122.17
1	A	209	CYS	O-C-N	-6.20	115.97	123.10
1	B	74	THR	CA-CB-OG1	-6.19	100.31	109.60
1	A	310	MET	N-CA-C	-6.19	105.67	113.72
1	B	271	ARG	CD-NE-CZ	-6.18	115.74	124.40
1	A	58	THR	O-C-N	-6.16	114.99	123.12
1	A	98	GLU	CB-CG-CD	6.16	123.07	112.60
1	A	245	LEU	CA-C-O	-6.16	113.54	120.32
1	B	420	PHE	CA-CB-CG	-6.15	107.65	113.80
1	B	313	ASP	CA-C-N	-6.15	111.69	120.42
1	B	313	ASP	C-N-CA	-6.15	111.69	120.42
1	B	52	GLU	CB-CA-C	-6.14	105.66	111.00
1	A	2	LYS	CB-CA-C	6.14	120.93	110.81
1	B	12	LEU	CA-CB-CG	-6.13	94.83	116.30
1	B	236	ALA	CB-CA-C	-6.12	99.30	110.63
1	A	81	GLN	CB-CG-CD	-6.12	102.19	112.60
1	A	187	ASN	N-CA-C	-6.12	105.87	113.15
1	B	153	SER	CA-C-N	-6.11	114.49	123.05
1	B	153	SER	C-N-CA	-6.11	114.49	123.05
1	A	257	PRO	CA-C-O	6.11	124.15	118.29
1	A	435	ALA	CA-C-O	6.11	127.02	120.55
1	A	77	ASP	CA-C-O	-6.10	115.16	121.87
1	B	395	GLY	CA-C-O	6.09	127.74	121.35
1	A	166	TRP	O-C-N	-6.08	115.67	122.12
1	B	436	GLU	CA-C-O	6.08	127.41	120.90
1	A	442	ASP	CA-C-N	-6.07	111.09	120.31
1	A	442	ASP	C-N-CA	-6.07	111.09	120.31
1	A	178	PHE	CG-CD2-CE2	6.06	131.01	120.70
1	B	248	GLU	O-C-N	-6.06	115.13	122.22
1	A	192	GLN	O-C-N	6.05	129.72	122.27
1	A	452	GLU	CA-CB-CG	-6.05	101.99	114.10
1	B	28	LEU	N-CA-C	6.05	117.28	109.65
1	B	142	ALA	O-C-N	6.05	128.86	123.41
1	B	210	TYR	CA-CB-CG	-6.05	103.01	113.90
1	A	432	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	171	GLN	N-CA-CB	-6.04	100.78	110.63
1	A	28	LEU	CA-C-O	6.04	124.61	119.66
1	A	232	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	A	301	ALA	O-C-N	-6.02	115.61	122.84
1	B	184	TRP	CG-CD2-CE3	-6.01	127.89	133.90
1	A	206	SER	CA-C-O	6.01	126.99	119.12
1	A	220	ALA	O-C-N	5.99	129.55	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	LEU	N-CA-CB	-5.98	100.80	109.83
1	B	163	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	A	31	ALA	CA-C-O	5.98	127.50	120.69
1	B	161	ASN	CA-CB-CG	-5.97	106.62	112.60
1	B	181	THR	CB-CA-C	5.95	120.61	111.02
1	A	432	GLN	CB-CG-CD	5.95	122.71	112.60
1	B	125	ALA	O-C-N	5.95	129.57	122.79
1	A	129	ILE	CB-CG1-CD1	5.94	126.27	113.80
1	A	133	ASP	CA-CB-CG	-5.93	106.67	112.60
1	B	314	ILE	CA-C-N	5.93	127.55	120.14
1	B	314	ILE	C-N-CA	5.93	127.55	120.14
1	B	444	VAL	O-C-N	5.91	131.65	121.67
1	A	171	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	B	206	SER	CA-C-N	-5.90	111.47	121.85
1	B	206	SER	C-N-CA	-5.90	111.47	121.85
1	B	414	ALA	CA-C-O	-5.89	113.99	120.30
1	A	41	HIS	O-C-N	-5.88	114.56	121.32
1	A	13	TRP	CE3-CZ3-CH2	5.88	128.75	121.10
1	B	263	CYS	CA-C-O	5.88	126.68	120.33
1	A	163	ARG	N-CA-C	-5.88	104.95	111.36
1	B	374	ARG	O-C-N	5.86	128.11	122.07
1	B	450	GLN	CA-CB-CG	-5.86	102.38	114.10
1	A	316	ARG	CA-C-O	5.86	126.61	119.11
1	A	77	ASP	CB-CG-OD2	5.86	131.87	118.40
1	A	193	TYR	N-CA-C	-5.85	104.81	111.07
1	B	323	VAL	CA-C-N	-5.84	113.50	122.62
1	B	323	VAL	C-N-CA	-5.84	113.50	122.62
1	A	418	GLN	CA-C-N	-5.84	114.82	122.94
1	A	418	GLN	C-N-CA	-5.84	114.82	122.94
1	A	329	PHE	O-C-N	-5.84	116.36	123.30
1	B	214	LEU	CA-C-N	-5.84	113.51	122.62
1	B	214	LEU	C-N-CA	-5.84	113.51	122.62
1	B	199	GLN	CA-CB-CG	5.83	125.76	114.10
1	A	16	ASP	CA-C-N	-5.82	112.41	120.38
1	A	16	ASP	C-N-CA	-5.82	112.41	120.38
1	B	209	CYS	N-CA-C	5.82	118.03	109.24
1	A	168	GLU	CA-CB-CG	-5.82	102.46	114.10
1	A	179	THR	O-C-N	5.82	130.22	123.41
1	A	109	LEU	O-C-N	5.81	130.59	123.21
1	B	411	THR	CA-C-O	-5.81	113.87	120.32
1	A	246	ARG	O-C-N	-5.80	116.14	123.05
1	A	316	ARG	O-C-N	-5.80	113.96	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ILE	O-C-N	-5.79	117.06	123.20
1	A	170	GLN	CA-C-N	-5.79	112.80	122.64
1	A	170	GLN	C-N-CA	-5.79	112.80	122.64
1	B	137	GLY	CA-C-N	5.79	130.31	122.90
1	B	137	GLY	C-N-CA	5.79	130.31	122.90
1	A	424	GLY	CA-C-O	5.79	127.62	121.31
1	A	371	PRO	N-CA-CB	5.78	108.96	102.60
1	A	152	VAL	O-C-N	5.77	130.44	122.88
1	B	349	PRO	CA-C-N	5.77	128.29	120.38
1	B	349	PRO	C-N-CA	5.77	128.29	120.38
1	B	188	MET	CA-C-O	5.77	127.24	120.89
1	A	52	GLU	OE1-CD-OE2	5.77	136.75	122.90
1	A	127	GLN	CA-C-O	-5.77	115.43	122.41
1	B	178	PHE	CA-C-O	-5.77	114.03	120.66
1	B	62	LYS	CA-CB-CG	-5.76	102.57	114.10
1	A	36	SER	CA-C-O	5.76	126.67	119.59
1	A	246	ARG	CD-NE-CZ	-5.76	116.33	124.40
1	B	66	VAL	CA-C-O	5.76	126.87	120.59
1	A	395	GLY	CA-C-O	5.75	127.42	121.38
1	B	41	HIS	CA-CB-CG	5.75	119.55	113.80
1	A	178	PHE	CA-C-N	-5.75	111.83	121.94
1	A	178	PHE	C-N-CA	-5.75	111.83	121.94
1	B	55	CYS	O-C-N	-5.75	116.69	123.41
1	B	383	GLU	CA-C-O	5.74	124.87	119.76
1	A	167	LEU	CA-C-O	-5.74	113.37	119.97
1	A	341	VAL	CA-CB-CG1	-5.73	100.66	110.40
1	B	342	SER	N-CA-CB	-5.72	101.59	111.55
1	A	47	ASP	N-CA-CB	5.72	120.79	110.83
1	A	254	SER	CA-C-O	-5.72	114.19	120.43
1	B	12	LEU	N-CA-C	5.72	118.52	110.23
1	A	401	GLY	O-C-N	-5.71	116.39	122.56
1	B	167	LEU	CA-C-N	-5.71	109.87	121.18
1	B	167	LEU	C-N-CA	-5.71	109.87	121.18
1	B	184	TRP	CE2-CD2-CE3	5.71	124.52	118.80
1	B	259	ARG	NH1-CZ-NH2	5.71	126.72	119.30
1	A	300	ARG	N-CA-C	5.71	117.65	109.14
1	B	201	GLN	CA-CB-CG	-5.71	102.68	114.10
1	A	142	ALA	O-C-N	5.70	129.11	123.46
1	B	75	THR	CA-C-N	-5.70	113.70	122.60
1	B	75	THR	C-N-CA	-5.70	113.70	122.60
1	A	272	PRO	CA-C-O	5.70	127.84	121.34
1	B	85	GLN	O-C-N	5.70	128.25	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	HIS	CA-C-O	5.69	125.95	119.18
1	B	386	ARG	CA-C-O	-5.69	115.52	121.55
1	A	240	PRO	CA-C-O	-5.69	111.01	118.86
1	A	175	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	B	19	GLU	N-CA-C	-5.68	105.16	111.36
1	A	128	ASP	O-C-N	-5.68	115.52	122.34
1	A	197	PHE	CA-C-O	-5.68	114.83	120.90
1	A	17	ALA	N-CA-C	5.67	118.19	111.33
1	A	170	GLN	N-CA-CB	5.67	118.31	109.85
1	A	392	GLY	N-CA-C	-5.67	99.73	113.18
1	B	60	PHE	N-CA-CB	5.67	119.46	110.84
1	B	222	TYR	CA-C-N	-5.67	113.77	122.62
1	B	222	TYR	C-N-CA	-5.67	113.77	122.62
1	B	374	ARG	CA-C-N	-5.67	112.68	120.28
1	B	374	ARG	C-N-CA	-5.67	112.68	120.28
1	B	45	ARG	CA-C-O	-5.66	114.42	120.42
1	B	225	ASP	O-C-N	5.65	129.67	123.22
1	B	418	GLN	CA-C-O	5.65	126.70	120.71
1	A	238	ARG	CD-NE-CZ	5.64	132.30	124.40
1	B	111	GLY	CA-C-N	5.64	128.10	120.38
1	B	111	GLY	C-N-CA	5.64	128.10	120.38
1	A	446	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	A	35	HIS	CA-CB-CG	-5.63	108.17	113.80
1	A	43	TYR	CA-C-O	5.62	126.13	119.56
1	A	89	ARG	NE-CZ-NH2	5.62	124.25	119.20
1	B	27	HIS	O-C-N	-5.62	114.43	122.41
1	B	196	LYS	CB-CG-CD	-5.62	98.38	111.30
1	A	25	LEU	O-C-N	5.61	129.03	122.24
1	B	81	GLN	O-C-N	5.61	128.54	122.15
1	B	9	ILE	CA-CB-CG1	5.61	119.93	110.40
1	B	31	ALA	O-C-N	-5.60	116.48	123.04
1	B	250	GLY	N-CA-C	-5.60	102.62	110.63
1	A	27	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	213	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	B	12	LEU	CA-C-N	-5.59	112.93	120.82
1	B	12	LEU	C-N-CA	-5.59	112.93	120.82
1	B	311	ARG	CD-NE-CZ	-5.59	116.58	124.40
1	B	62	LYS	CA-C-N	-5.58	114.57	122.94
1	B	62	LYS	C-N-CA	-5.58	114.57	122.94
1	B	391	CYS	CA-CB-SG	-5.58	101.57	114.40
1	B	271	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	B	170	GLN	CA-C-N	-5.57	113.90	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	GLN	C-N-CA	-5.57	113.90	122.60
1	A	150	HIS	CA-C-N	-5.57	113.94	122.62
1	A	150	HIS	C-N-CA	-5.57	113.94	122.62
1	A	245	LEU	CA-C-N	-5.56	115.61	122.84
1	A	245	LEU	C-N-CA	-5.56	115.61	122.84
1	A	325	VAL	O-C-N	5.56	125.19	121.69
1	A	273	ILE	CA-C-O	-5.56	114.23	120.95
1	A	207	GLY	N-CA-C	-5.55	106.53	115.08
1	A	117	ARG	O-C-N	-5.55	114.53	122.41
1	A	234	ASN	OD1-CG-ND2	5.54	128.14	122.60
1	A	452	GLU	O-C-N	5.54	128.54	122.11
1	B	65	VAL	CA-C-O	5.54	126.63	120.59
1	A	238	ARG	CB-CA-C	-5.53	104.03	111.89
1	B	268	ILE	CA-C-O	-5.53	114.46	120.71
1	B	183	ASP	N-CA-CB	-5.53	102.21	110.17
1	A	348	LEU	CA-C-O	-5.51	114.86	119.76
1	A	211	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	68	GLU	O-C-N	5.50	129.62	123.40
1	B	45	ARG	CD-NE-CZ	-5.50	116.71	124.40
1	B	45	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	215	ALA	CA-C-O	-5.49	114.91	121.11
1	A	178	PHE	CZ-CE2-CD2	-5.49	110.12	120.00
1	A	317	VAL	N-CA-C	-5.48	108.50	113.71
1	B	219	HIS	CA-C-N	-5.48	112.89	121.87
1	B	219	HIS	C-N-CA	-5.48	112.89	121.87
1	A	315	GLY	CA-C-O	5.48	125.96	119.50
1	A	131	LEU	CB-CA-C	5.47	120.95	110.17
1	A	388	ASN	OD1-CG-ND2	5.47	128.07	122.60
1	A	317	VAL	CA-C-N	-5.47	110.78	121.06
1	A	317	VAL	C-N-CA	-5.47	110.78	121.06
1	B	91	ASP	CA-C-O	5.47	128.33	120.51
1	A	112	TYR	CD1-CE1-CZ	-5.46	109.77	119.60
1	B	39	ALA	CA-C-N	-5.46	114.88	123.13
1	B	39	ALA	C-N-CA	-5.46	114.88	123.13
1	A	369	GLY	N-CA-C	-5.46	103.30	110.29
1	A	6	PRO	CB-CA-C	-5.46	103.83	110.98
1	B	84	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	428	VAL	O-C-N	5.45	129.39	122.57
1	B	341	VAL	O-C-N	-5.45	116.74	122.25
1	B	274	LYS	CA-CB-CG	5.45	125.00	114.10
1	A	171	GLN	CB-CA-C	5.45	118.70	109.50
1	A	15	GLN	OE1-CD-NE2	-5.44	117.16	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	SER	CA-CB-OG	-5.44	100.22	111.10
1	A	135	ALA	O-C-N	5.44	130.10	123.14
1	B	356	ASP	CA-C-O	5.43	126.18	120.42
1	B	359	ARG	CA-C-O	-5.43	115.09	120.90
1	B	402	ASN	N-CA-CB	-5.42	102.61	110.36
1	A	51	ALA	O-C-N	5.42	128.71	123.29
1	A	93	ARG	N-CA-CB	-5.42	104.35	111.23
1	B	159	ASP	CA-C-O	-5.42	114.99	120.84
1	A	259	ARG	CG-CD-NE	-5.41	100.09	112.00
1	B	42	PRO	CA-C-N	-5.41	113.25	122.56
1	B	42	PRO	C-N-CA	-5.41	113.25	122.56
1	B	323	VAL	N-CA-C	5.41	116.03	108.89
1	B	441	PHE	N-CA-CB	5.41	118.80	110.46
1	B	317	VAL	CA-C-N	-5.41	109.88	121.45
1	B	317	VAL	C-N-CA	-5.41	109.88	121.45
1	A	301	ALA	CA-C-N	5.41	129.02	121.02
1	A	301	ALA	C-N-CA	5.41	129.02	121.02
1	B	310	MET	CA-C-O	5.41	125.75	119.32
1	B	393	SER	N-CA-CB	5.40	121.57	111.52
1	A	450	GLN	O-C-N	-5.39	116.40	122.12
1	B	241	PHE	CE1-CZ-CE2	5.39	129.71	120.00
1	B	21	TYR	CA-C-N	-5.39	112.52	120.28
1	B	21	TYR	C-N-CA	-5.39	112.52	120.28
1	B	13	TRP	O-C-N	-5.38	116.27	122.95
1	A	308	ASP	N-CA-C	-5.38	100.48	109.24
1	A	5	SER	CA-CB-OG	-5.37	100.35	111.10
1	B	68	GLU	CB-CG-CD	-5.37	103.46	112.60
1	B	96	HIS	N-CA-CB	5.37	118.23	109.69
1	A	267	GLU	O-C-N	5.37	129.34	123.22
1	B	309	LEU	CA-C-O	-5.37	112.07	119.05
1	A	209	CYS	CA-CB-SG	-5.36	102.06	114.40
1	A	172	PHE	O-C-N	-5.36	115.19	122.48
1	A	211	GLN	CG-CD-NE2	5.36	124.43	116.40
1	B	106	ALA	CA-C-O	-5.36	114.76	120.92
1	B	129	ILE	CA-CB-CG2	5.36	119.61	110.50
1	B	68	GLU	OE1-CD-OE2	5.34	135.73	122.90
1	A	313	ASP	O-C-N	-5.34	116.57	122.07
1	A	345	THR	CA-C-O	-5.34	114.52	120.66
1	B	184	TRP	CZ3-CH2-CZ2	5.34	128.44	121.50
1	A	163	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	B	443	LYS	CA-CB-CG	5.33	124.76	114.10
1	B	347	GLN	CB-CG-CD	-5.33	103.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ILE	N-CA-C	5.32	115.94	108.17
1	B	216	GLN	CB-CA-C	5.32	119.28	109.71
1	A	184	TRP	CA-C-O	-5.31	115.00	121.05
1	A	367	ILE	CA-CB-CG1	5.29	119.40	110.40
1	B	129	ILE	CA-C-O	-5.29	114.88	120.39
1	A	351	GLN	CB-CG-CD	-5.29	103.61	112.60
1	A	359	ARG	NE-CZ-NH1	-5.29	116.22	121.50
1	B	205	HIS	CB-CG-CD2	5.29	138.07	131.20
1	A	137	GLY	CA-C-O	5.28	126.12	120.94
1	A	5	SER	O-C-N	-5.28	116.00	121.60
1	A	2	LYS	N-CA-CB	-5.28	101.82	110.21
1	B	247	LEU	CA-C-N	-5.28	112.68	120.28
1	B	247	LEU	C-N-CA	-5.28	112.68	120.28
1	B	244	PHE	N-CA-CB	5.28	119.05	110.77
1	B	319	VAL	O-C-N	5.27	128.05	122.67
1	A	9	ILE	CA-C-O	-5.27	114.50	120.67
1	A	356	ASP	CA-CB-CG	-5.27	107.33	112.60
1	A	329	PHE	N-CA-CB	-5.26	101.84	110.68
1	A	269	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	158	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	B	422	SER	CA-C-N	-5.26	112.69	121.94
1	B	422	SER	C-N-CA	-5.26	112.69	121.94
1	B	342	SER	O-C-N	-5.25	116.32	123.15
1	A	124	ILE	CB-CG1-CD1	-5.25	102.77	113.80
1	A	368	THR	N-CA-C	-5.25	103.52	111.34
1	A	74	THR	OG1-CB-CG2	-5.24	98.81	109.30
1	A	316	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	B	14	ARG	CA-C-O	-5.24	113.83	120.28
1	B	394	ILE	CA-C-N	-5.24	113.68	120.91
1	B	394	ILE	C-N-CA	-5.24	113.68	120.91
1	B	16	ASP	CB-CA-C	-5.24	102.69	111.13
1	A	252	ILE	CA-C-O	-5.24	114.93	120.48
1	B	425	GLY	O-C-N	5.24	127.25	123.27
1	B	73	THR	CA-C-O	5.23	127.10	121.55
1	A	356	ASP	CA-C-O	5.23	125.96	120.42
1	B	159	ASP	CA-C-N	-5.23	112.21	120.47
1	B	159	ASP	C-N-CA	-5.23	112.21	120.47
1	A	195	GLU	N-CA-C	5.22	116.97	111.28
1	A	167	LEU	O-C-N	5.21	128.68	122.27
1	A	187	ASN	N-CA-CB	5.21	118.48	110.46
1	B	175	GLN	OE1-CD-NE2	5.21	127.81	122.60
1	B	208	ASP	CA-C-O	5.20	126.06	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ARG	CB-CG-CD	-5.20	99.33	111.30
1	B	347	GLN	CA-C-O	-5.19	115.09	120.70
1	B	10	THR	N-CA-C	5.19	117.19	108.73
1	B	51	ALA	N-CA-CB	5.18	120.28	111.57
1	B	217	ARG	CG-CD-NE	-5.18	100.61	112.00
1	B	72	ARG	O-C-N	-5.18	115.71	122.59
1	B	410	ARG	CD-NE-CZ	5.17	131.65	124.40
1	B	180	LEU	N-CA-C	-5.17	102.21	109.96
1	A	25	LEU	CA-C-O	-5.16	113.18	119.32
1	A	85	GLN	CG-CD-NE2	-5.16	108.66	116.40
1	B	221	THR	CA-C-N	-5.16	113.85	122.21
1	B	221	THR	C-N-CA	-5.16	113.85	122.21
1	B	97	ASN	CB-CG-ND2	-5.16	108.67	116.40
1	A	232	GLN	CA-C-N	-5.15	112.98	120.29
1	A	232	GLN	C-N-CA	-5.15	112.98	120.29
1	A	158	ASN	N-CA-CB	5.14	115.28	108.96
1	B	195	GLU	CB-CA-C	-5.14	102.26	110.79
1	B	344	ILE	O-C-N	-5.14	117.65	123.20
1	A	80	LEU	CA-C-N	-5.14	113.00	120.29
1	A	80	LEU	C-N-CA	-5.14	113.00	120.29
1	B	369	GLY	CA-C-O	5.13	127.02	121.02
1	A	411	THR	CA-C-O	-5.13	114.63	120.32
1	B	180	LEU	N-CA-CB	5.13	117.49	109.85
1	A	194	GLY	CA-C-N	-5.12	113.42	120.28
1	A	194	GLY	C-N-CA	-5.12	113.42	120.28
1	A	72	ARG	CA-C-N	5.12	131.02	122.73
1	A	72	ARG	C-N-CA	5.12	131.02	122.73
1	B	215	ALA	CA-C-N	-5.12	113.92	122.92
1	B	215	ALA	C-N-CA	-5.12	113.92	122.92
1	A	415	ILE	CA-C-O	-5.11	114.39	120.78
1	B	440	THR	N-CA-CB	-5.11	101.85	110.49
1	B	106	ALA	CA-C-N	-5.11	112.94	121.94
1	B	106	ALA	C-N-CA	-5.11	112.94	121.94
1	A	258	GLU	CA-C-O	-5.11	114.84	120.36
1	B	189	THR	CA-C-O	-5.11	115.99	121.56
1	B	87	LEU	CA-C-O	5.10	125.95	120.55
1	A	122	PRO	O-C-N	5.10	129.52	122.64
1	A	256	SER	O-C-N	5.09	126.37	121.28
1	A	18	ALA	O-C-N	-5.09	116.83	122.07
1	A	430	ASP	CA-C-N	-5.08	111.72	120.97
1	A	430	ASP	C-N-CA	-5.08	111.72	120.97
1	A	12	LEU	N-CA-C	5.08	117.26	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	TYR	O-C-N	5.08	129.35	123.30
1	B	152	VAL	N-CA-CB	5.08	118.07	111.67
1	B	129	ILE	N-CA-CB	-5.08	105.04	111.64
1	B	439	GLU	CB-CG-CD	5.07	121.22	112.60
1	B	410	ARG	CA-C-N	-5.07	114.93	122.74
1	B	410	ARG	C-N-CA	-5.07	114.93	122.74
1	B	393	SER	O-C-N	5.07	129.06	123.33
1	A	441	PHE	N-CA-C	5.06	116.80	111.28
1	B	253	LEU	CA-C-N	-5.06	116.02	123.00
1	B	253	LEU	C-N-CA	-5.06	116.02	123.00
1	B	149	ARG	CA-CB-CG	-5.06	103.98	114.10
1	B	160	VAL	CA-CB-CG1	5.06	119.00	110.40
1	B	123	GLU	CA-C-N	-5.05	113.15	121.34
1	B	123	GLU	C-N-CA	-5.05	113.15	121.34
1	A	117	ARG	CD-NE-CZ	5.05	131.47	124.40
1	B	418	GLN	CA-C-N	-5.05	115.92	122.94
1	B	418	GLN	C-N-CA	-5.05	115.92	122.94
1	A	116	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	B	311	ARG	CA-C-O	5.05	126.12	120.82
1	A	393	SER	CA-C-N	-5.04	116.10	123.06
1	A	393	SER	C-N-CA	-5.04	116.10	123.06
1	B	23	SER	O-C-N	5.04	127.91	122.11
1	B	421	CYS	O-C-N	-5.04	117.37	123.27
1	A	63	GLU	N-CA-CB	-5.03	102.58	110.69
1	A	67	SER	CA-CB-OG	-5.03	101.03	111.10
1	A	97	ASN	O-C-N	5.03	129.68	123.14
1	B	62	LYS	CA-C-O	5.03	125.55	119.11
1	B	375	ALA	CA-C-O	5.03	125.88	120.55
1	B	17	ALA	N-CA-C	5.03	117.49	111.71
1	B	60	PHE	N-CA-C	-5.03	99.07	108.02
1	B	96	HIS	N-CA-C	-5.02	103.16	110.24
1	A	78	ASP	O-C-N	5.02	125.38	121.47
1	B	350	GLU	CB-CG-CD	5.01	121.13	112.60
1	A	154	LEU	CA-C-N	-5.01	114.72	122.59
1	A	154	LEU	C-N-CA	-5.01	114.72	122.59
1	A	106	ALA	CA-C-N	-5.01	113.12	121.94
1	A	106	ALA	C-N-CA	-5.01	113.12	121.94
1	A	119	GLU	N-CA-CB	5.00	119.46	110.80
1	B	37	GLY	N-CA-C	-5.00	107.19	114.90
1	B	30	TRP	O-C-N	5.00	128.25	122.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3340	0	3255	83	0
1	B	3288	0	3204	89	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
3	A	15	0	9	2	0
3	B	15	0	9	0	0
4	A	286	0	0	8	0
4	B	274	0	0	1	0
All	All	7228	0	6477	162	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 12.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:HB	1:B:221:THR:HG22	1.54	0.90
1:B:444:VAL:HG23	1:B:448:LEU:HD11	1.65	0.78
1:A:15:GLN:HE22	1:B:178:PHE:H	1.32	0.77
1:B:216:GLN:HE21	1:B:440:THR:HG21	1.47	0.77
1:B:85:GLN:O	1:B:89:ARG:HG3	1.85	0.77
1:B:35:HIS:HD2	1:B:37:GLY:H	1.32	0.74
1:A:328:LEU:HD21	4:A:1268:HOH:O	1.87	0.73
1:A:444:VAL:HA	1:A:446:ARG:NH2	2.03	0.73
1:B:235:GLN:HA	1:B:235:GLN:OE1	1.85	0.71
1:A:35:HIS:HD2	1:A:37:GLY:H	1.38	0.70
1:A:191:GLU:HB2	4:A:1238:HOH:O	1.92	0.69
1:A:14:ARG:HA	1:B:228:GLN:HE22	1.57	0.68
1:A:235:GLN:HE22	1:B:449:LYS:HG2	1.57	0.67
1:A:12:LEU:H	1:A:12:LEU:HD22	1.60	0.64
1:A:116:ARG:NH1	1:A:121:LEU:HD13	2.12	0.64
1:B:322:SER:O	1:B:324:LYS:HE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PRO:HB2	1:B:134:MET:HE3	1.82	0.62
1:B:303:ASN:HD22	1:B:303:ASN:H	1.45	0.62
1:B:190:ARG:HD3	1:B:437:TYR:CE2	2.35	0.61
1:B:1:MET:O	1:B:2:LYS:HB3	1.99	0.61
1:B:442:ASP:HA	1:B:445:ASN:HB2	1.82	0.60
1:B:41:HIS:HB2	1:B:44:SER:OG	2.02	0.59
1:B:303:ASN:H	1:B:303:ASN:ND2	2.00	0.59
1:A:273:ILE:O	1:A:274:LYS:NZ	2.29	0.59
1:B:35:HIS:CD2	1:B:37:GLY:H	2.17	0.59
1:A:446:ARG:NH2	1:A:447:ILE:HD12	2.18	0.58
1:B:269:GLN:HE21	1:B:342:SER:CB	2.15	0.58
1:A:1:MET:CG	1:A:93:ARG:HD2	2.33	0.58
1:A:15:GLN:HE22	1:B:178:PHE:N	2.00	0.58
1:B:216:GLN:HE21	1:B:440:THR:CG2	2.14	0.58
1:A:412:LEU:HA	1:A:420:PHE:O	2.04	0.58
1:B:2:LYS:HD3	1:B:95:THR:CG2	2.33	0.57
1:A:35:HIS:CD2	1:A:37:GLY:H	2.22	0.56
1:A:273:ILE:HD12	1:A:342:SER:N	2.21	0.56
1:B:35:HIS:HD2	1:B:37:GLY:N	2.01	0.55
1:B:442:ASP:HA	1:B:445:ASN:H	1.71	0.55
1:B:269:GLN:HE21	1:B:342:SER:HB3	1.70	0.55
1:B:442:ASP:CA	1:B:445:ASN:HB2	2.37	0.55
1:B:273:ILE:HG22	1:B:341:VAL:O	2.07	0.54
1:B:233:LEU:HD11	1:B:451:LEU:HD11	1.89	0.54
1:A:237:ASN:ND2	1:A:446:ARG:HD2	2.22	0.54
1:A:36:SER:HG	3:A:601:TRP:N	2.06	0.54
1:B:367:ILE:HD13	1:B:391:CYS:HB3	1.88	0.54
1:B:68:GLU:HB3	1:B:71:LYS:HZ3	1.73	0.53
1:A:449:LYS:O	1:A:453:LYS:O	2.27	0.53
1:B:126:GLU:HG3	1:B:127:GLN:N	2.22	0.53
1:A:446:ARG:HG2	4:A:1215:HOH:O	2.08	0.53
1:B:2:LYS:HG3	1:B:3:THR:H	1.74	0.52
1:A:116:ARG:HG2	1:A:121:LEU:CD1	2.40	0.52
4:A:1528:HOH:O	1:B:12:LEU:HD22	2.09	0.52
1:B:79:PRO:HB2	1:B:134:MET:CE	2.38	0.52
1:A:15:GLN:H	1:B:228:GLN:NE2	2.08	0.52
1:B:240:PRO:HD2	1:B:257:PRO:HA	1.92	0.52
1:A:177:ASP:O	1:A:224:GLY:HA3	2.08	0.51
1:A:15:GLN:NE2	1:B:178:PHE:H	2.02	0.51
1:A:37:GLY:O	1:A:238:ARG:HA	2.09	0.51
1:A:215:ALA:HA	1:A:424:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:O	1:A:266:SER:HB2	2.11	0.50
1:A:176:GLU:OE1	1:A:177:ASP:O	2.29	0.50
1:A:238:ARG:HH11	1:A:238:ARG:CB	2.24	0.50
1:B:2:LYS:HD3	1:B:95:THR:HG23	1.93	0.50
1:A:175:GLN:O	1:A:175:GLN:OE1	2.30	0.50
1:A:1:MET:SD	1:A:93:ARG:HD2	2.52	0.50
1:A:30:TRP:CE2	1:A:56:THR:HG21	2.47	0.50
1:A:54:ILE:HD13	1:A:140:ASP:OD2	2.12	0.50
1:B:444:VAL:O	1:B:448:LEU:HG	2.12	0.50
1:B:396:TYR:C	1:B:397:LEU:HD12	2.37	0.49
1:A:450:GLN:O	1:A:450:GLN:OE1	2.31	0.49
1:B:68:GLU:HB3	1:B:71:LYS:NZ	2.27	0.49
1:A:92:ILE:O	1:A:93:ARG:HG3	2.12	0.49
1:A:39:ALA:O	1:A:44:SER:OG	2.31	0.48
1:B:50:VAL:HB	1:B:139:TYR:CD2	2.47	0.48
1:A:12:LEU:HD11	1:B:20:PHE:CD1	2.48	0.48
1:A:444:VAL:HA	1:A:446:ARG:HH21	1.78	0.48
1:B:444:VAL:CG2	1:B:448:LEU:HD21	2.42	0.48
1:A:390:TRP:O	1:A:391:CYS:HB2	2.14	0.48
1:B:77:ASP:HB2	1:B:82:VAL:CG2	2.43	0.47
1:B:195:GLU:HG3	4:B:1537:HOH:O	2.14	0.47
1:A:12:LEU:HD21	1:B:20:PHE:HD1	1.79	0.47
1:A:12:LEU:HD21	1:B:20:PHE:CD1	2.49	0.47
1:A:12:LEU:HD13	1:A:12:LEU:N	2.30	0.47
1:B:2:LYS:HD3	1:B:95:THR:HG22	1.96	0.47
1:A:54:ILE:O	1:A:68:GLU:HG3	2.15	0.47
1:B:113:ASP:OD1	2:B:702:PO4:O2	2.33	0.47
1:A:190:ARG:HD3	1:A:437:TYR:CD2	2.50	0.46
1:A:211:GLN:NE2	4:A:1260:HOH:O	2.48	0.46
1:A:238:ARG:HH11	1:A:238:ARG:CA	2.29	0.46
1:A:235:GLN:NE2	1:B:449:LYS:HG2	2.27	0.46
1:B:72:ARG:HG2	1:B:72:ARG:O	2.15	0.46
1:B:190:ARG:HD3	1:B:437:TYR:CD2	2.50	0.46
1:B:129:ILE:HD13	1:B:129:ILE:HG21	1.40	0.46
1:A:350:GLU:O	1:A:350:GLU:HG3	2.05	0.46
1:B:386:ARG:HG2	2:B:702:PO4:O3	2.16	0.46
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.76	0.46
1:A:89:ARG:NH1	4:A:1290:HOH:O	2.48	0.46
1:A:54:ILE:HD13	1:A:140:ASP:CG	2.41	0.45
1:B:68:GLU:O	1:B:70:GLU:N	2.49	0.45
1:A:107:LEU:HD22	1:A:396:TYR:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HB2	1:B:2:LYS:HE3	1.33	0.45
1:B:3:THR:CG2	1:B:93:ARG:H	2.29	0.45
1:B:269:GLN:HE21	1:B:342:SER:HB2	1.81	0.45
1:B:444:VAL:HB	1:B:448:LEU:HD21	1.97	0.45
1:A:441:PHE:O	1:A:445:ASN:N	2.49	0.45
1:B:55:CYS:HB3	1:B:138:ILE:HB	1.99	0.45
1:B:186:SER:HB2	1:B:218:PHE:CE1	2.52	0.45
1:B:265:ASN:O	1:B:266:SER:HB2	2.15	0.45
1:A:106:ALA:HA	1:A:137:GLY:O	2.16	0.45
1:B:2:LYS:HG3	1:B:3:THR:N	2.31	0.45
1:A:88:ASP:O	1:A:93:ARG:NH2	2.48	0.45
1:A:116:ARG:HG2	1:A:121:LEU:HD11	1.98	0.45
1:A:258:GLU:HG2	1:A:409:ILE:HD11	1.99	0.45
1:A:181:THR:N	1:A:221:THR:O	2.45	0.45
1:B:27:HIS:H	1:B:27:HIS:CD2	2.35	0.45
1:A:5:SER:HB2	1:A:6:PRO:HD2	1.98	0.44
1:A:241:PHE:CZ	1:A:259:ARG:HB2	2.53	0.43
1:A:443:LYS:O	1:A:446:ARG:NH2	2.50	0.43
1:B:90:ALA:O	1:B:92:ILE:HG13	2.18	0.43
1:B:166:TRP:O	1:B:170:GLN:HG2	2.18	0.43
1:A:367:ILE:HD12	1:A:368:THR:HG23	2.00	0.43
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.90	0.43
1:A:1:MET:HE1	1:A:91:ASP:OD1	2.19	0.43
1:A:449:LYS:HG3	1:A:452:GLU:OE2	2.19	0.43
1:A:386:ARG:HH11	1:A:386:ARG:HD2	1.21	0.42
1:B:114:LEU:HD21	1:B:134:MET:CE	2.49	0.42
1:A:149:ARG:O	1:A:150:HIS:HB2	2.18	0.42
1:A:258:GLU:HB3	4:A:1515:HOH:O	2.19	0.42
1:A:29:PRO:O	1:A:30:TRP:HB2	2.20	0.42
1:A:35:HIS:HD2	1:A:37:GLY:N	2.13	0.42
1:B:9:ILE:HD13	1:B:9:ILE:HG21	1.88	0.42
1:B:41:HIS:CD2	1:B:274:LYS:HD2	2.54	0.42
1:B:29:PRO:O	1:B:30:TRP:HB2	2.20	0.42
1:A:1:MET:SD	1:A:91:ASP:HA	2.60	0.42
1:A:123:GLU:H	1:A:123:GLU:HG2	1.57	0.42
1:A:123:GLU:HG2	4:A:1549:HOH:O	2.19	0.42
1:B:444:VAL:HB	1:B:448:LEU:CD2	2.49	0.42
1:B:71:LYS:HZ3	1:B:71:LYS:HG2	1.47	0.41
1:A:45:ARG:HH21	1:A:149:ARG:HD3	1.86	0.41
1:B:6:PRO:CD	1:B:103:GLN:HE21	2.32	0.41
1:B:390:TRP:CE2	1:B:422:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PRO:CG	1:B:114:LEU:HD11	2.49	0.41
1:A:127:GLN:O	1:A:127:GLN:HG2	2.20	0.41
1:A:358:LEU:O	1:A:362:PHE:HB2	2.20	0.41
1:B:184:TRP:HA	1:B:220:ALA:HB2	2.02	0.41
1:B:140:ASP:OD1	1:B:141:TRP:HD1	2.04	0.41
1:B:189:THR:OG1	1:B:192:GLN:HG3	2.21	0.41
1:B:303:ASN:ND2	1:B:303:ASN:N	2.68	0.41
1:B:390:TRP:CD2	1:B:422:SER:HB2	2.55	0.41
1:A:181:THR:H	1:A:222:TYR:HA	1.85	0.41
1:B:176:GLU:O	1:B:228:GLN:HG3	2.21	0.41
1:B:179:THR:N	1:B:223:SER:O	2.48	0.41
1:A:124:ILE:HD13	1:A:124:ILE:HG21	1.81	0.41
1:A:237:ASN:HD21	1:A:446:ARG:HD2	1.85	0.40
1:B:450:GLN:HE21	1:B:450:GLN:HB2	1.54	0.40
1:A:34:LEU:HB3	3:A:601:TRP:CE2	2.56	0.40
1:B:306:ILE:HD13	1:B:306:ILE:HG21	1.87	0.40
1:B:423:ALA:HB2	1:B:444:VAL:CG1	2.52	0.40
1:B:36:SER:OG	1:B:46:PHE:O	2.37	0.40
1:B:41:HIS:HD2	1:B:274:LYS:NZ	2.20	0.40
1:B:306:ILE:HD13	1:B:328:LEU:HD12	2.03	0.40
1:A:24:ARG:HD3	1:A:172:PHE:CZ	2.57	0.40
1:A:120:SER:O	1:A:121:LEU:HB3	2.21	0.40
1:A:216:GLN:N	1:A:423:ALA:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/453 (91%)	399 (96%)	15 (4%)	0	100	100
1	B	409/453 (90%)	382 (93%)	22 (5%)	5 (1%)	10	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	823/906 (91%)	781 (95%)	37 (4%)	5 (1%)	21	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	274	LYS
1	B	445	ASN
1	B	446	ARG
1	B	449	LYS

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	362/390 (93%)	331 (91%)	31 (9%)	10	4
1	B	356/390 (91%)	323 (91%)	33 (9%)	8	3
All	All	718/780 (92%)	654 (91%)	64 (9%)	9	4

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	12	LEU
1	A	52	GLU
1	A	67	SER
1	A	69	SER
1	A	71	LYS
1	A	73	THR
1	A	107	LEU
1	A	119	GLU
1	A	121	LEU
1	A	123	GLU
1	A	171	GLN

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	176	GLU
1	A	179	THR
1	A	191	GLU
1	A	238	ARG
1	A	273	ILE
1	A	274	LYS
1	A	324	LYS
1	A	327	GLU
1	A	329	PHE
1	A	350	GLU
1	A	367	ILE
1	A	410	ARG
1	A	415	ILE
1	A	439	GLU
1	A	446	ARG
1	A	449	LYS
1	A	453	LYS
1	B	2	LYS
1	B	3	THR
1	B	12	LEU
1	B	14	ARG
1	B	54	ILE
1	B	62	LYS
1	B	69	SER
1	B	70	GLU
1	B	71	LYS
1	B	73	THR
1	B	78	ASP
1	B	89	ARG
1	B	91	ASP
1	B	93	ARG
1	B	126	GLU
1	B	171	GLN
1	B	179	THR
1	B	183	ASP
1	B	185	GLN
1	B	191	GLU
1	B	199	GLN
1	B	221	THR
1	B	235	GLN
1	B	273	ILE

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Mol	Chain	Res	Type
1	B	302	GLU
1	B	317	VAL
1	B	327	GLU
1	B	350	GLU
1	B	439	GLU
1	B	440	THR
1	B	446	ARG
1	B	448	LEU
1	B	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	27	HIS
1	A	35	HIS
1	A	170	GLN
1	A	171	GLN
1	A	199	GLN
1	A	201	GLN
1	A	205	HIS
1	A	211	GLN
1	A	213	ASN
1	A	232	GLN
1	A	235	GLN
1	A	237	ASN
1	B	15	GLN
1	B	27	HIS
1	B	35	HIS
1	B	41	HIS
1	B	81	GLN
1	B	103	GLN
1	B	148	GLN
1	B	175	GLN
1	B	199	GLN
1	B	201	GLN
1	B	213	ASN
1	B	216	GLN
1	B	228	GLN
1	B	269	GLN
1	B	303	ASN
1	B	450	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	TRP	B	602	-	15,16,16	1.48	3 (20%)	18,22,22	1.72	3 (16%)
3	TRP	A	601	-	15,16,16	1.10	0	18,22,22	1.64	5 (27%)
2	PO4	A	701	-	4,4,4	2.27	2 (50%)	6,6,6	2.75	3 (50%)
2	PO4	B	702	-	4,4,4	0.93	0	6,6,6	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	B	602	-	-	0/8/8/8	0/2/2/2
3	TRP	A	601	-	-	0/8/8/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PO4	P-O1	3.19	1.58	1.50
3	B	602	TRP	CH2-CZ3	3.06	1.45	1.38
2	A	701	PO4	P-O3	-2.63	1.47	1.54
3	B	602	TRP	OXT-C	-2.49	1.22	1.30
3	B	602	TRP	CE2-NE1	-2.40	1.34	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PO4	O4-P-O3	4.09	120.63	107.91
3	B	602	TRP	CA-CB-CG	-3.89	106.11	113.49
2	A	701	PO4	O4-P-O2	-3.83	96.00	107.91
3	A	601	TRP	CG-CD1-NE1	-3.08	106.92	110.31
3	A	601	TRP	CZ3-CH2-CZ2	3.06	124.02	120.24
2	A	701	PO4	O3-P-O2	2.86	116.82	107.91
3	B	602	TRP	CE3-CD2-CE2	-2.83	115.91	118.84
3	A	601	TRP	OXT-C-O	-2.73	117.89	124.08
3	B	602	TRP	CZ3-CH2-CZ2	-2.47	117.19	120.24
3	A	601	TRP	CD2-CG-CD1	2.19	108.40	106.16
3	A	601	TRP	CH2-CZ2-CE2	-2.06	114.48	118.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TRP	2	0
2	B	702	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	420/453 (92%)	-0.61	10 (2%) 59 61	13, 23, 58, 102	0
1	B	415/453 (91%)	-0.54	17 (4%) 41 41	11, 23, 60, 106	0
All	All	835/906 (92%)	-0.57	27 (3%) 50 50	11, 23, 59, 106	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	PHE	5.9
1	B	301	ALA	5.5
1	B	275	GLY	4.6
1	A	453	LYS	3.6
1	B	442	ASP	3.5
1	B	273	ILE	3.5
1	A	176	GLU	3.4
1	B	445	ASN	3.2
1	A	446	ARG	3.1
1	B	446	ARG	3.0
1	B	70	GLU	3.0
1	B	1	MET	3.0
1	A	175	GLN	2.7
1	B	444	VAL	2.7
1	B	181	THR	2.6
1	B	72	ARG	2.6
1	A	274	LYS	2.5
1	A	172	PHE	2.5
1	B	350	GLU	2.4
1	A	416	ASN	2.4
1	B	441	PHE	2.3
1	B	69	SER	2.3
1	B	443	LYS	2.2
1	B	89	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	LYS	2.2
1	A	12	LEU	2.1
1	A	330	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRP	A	601	15/15	0.98	0.03	12,16,18,22	0
3	TRP	B	602	15/15	0.98	0.03	11,16,21,22	0
2	PO4	A	701	5/5	0.99	0.05	19,24,26,32	0
2	PO4	B	702	5/5	0.99	0.03	15,16,19,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.