



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:11 PM UTC

PDB ID : 1NAW / pdb_00001naw
Title : ENOLPYRUVYL TRANSFERASE
Authors : Schoenbrunn, E.; Sack, S.; Eschenburg, S.; Perrakis, A.; Krekel, F.; Amrhein, N.; Mandelkow, E.
Deposited on : 1996-07-23
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

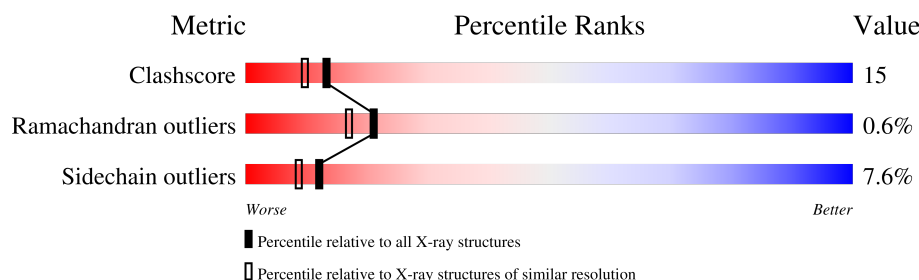
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	419	
1	B	419	

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	HAI	A	480	-	-	X	-

2 Entry composition [i](#)

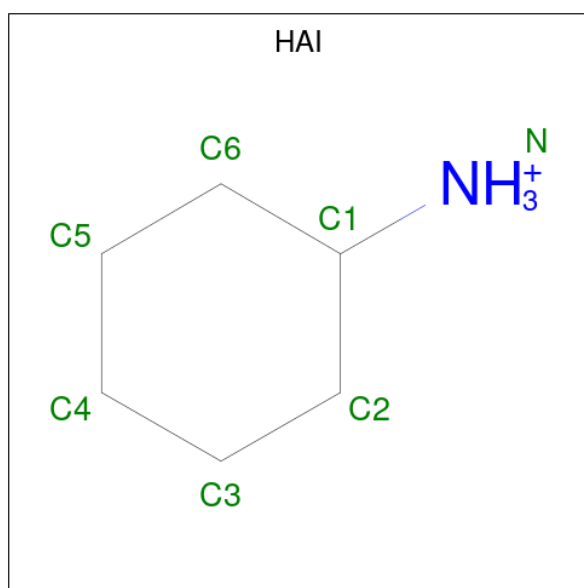
There are 3 unique types of molecules in this entry. The entry contains 6776 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-ACETYLGLUCOSAMINE 1-CARBOXYVINYL-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3142	1976	555	597	14			
1	B	419	Total	C	N	O	S	0	0	0
			3142	1976	555	597	14			

- Molecule 2 is CYCLOHEXYLAMMONIUM ION (CCD ID: HAI) (formula: C₆H₁₄N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			7	6	1		
2	A	1	Total	C	N	0	0
			7	6	1		

- Molecule 3 is water.

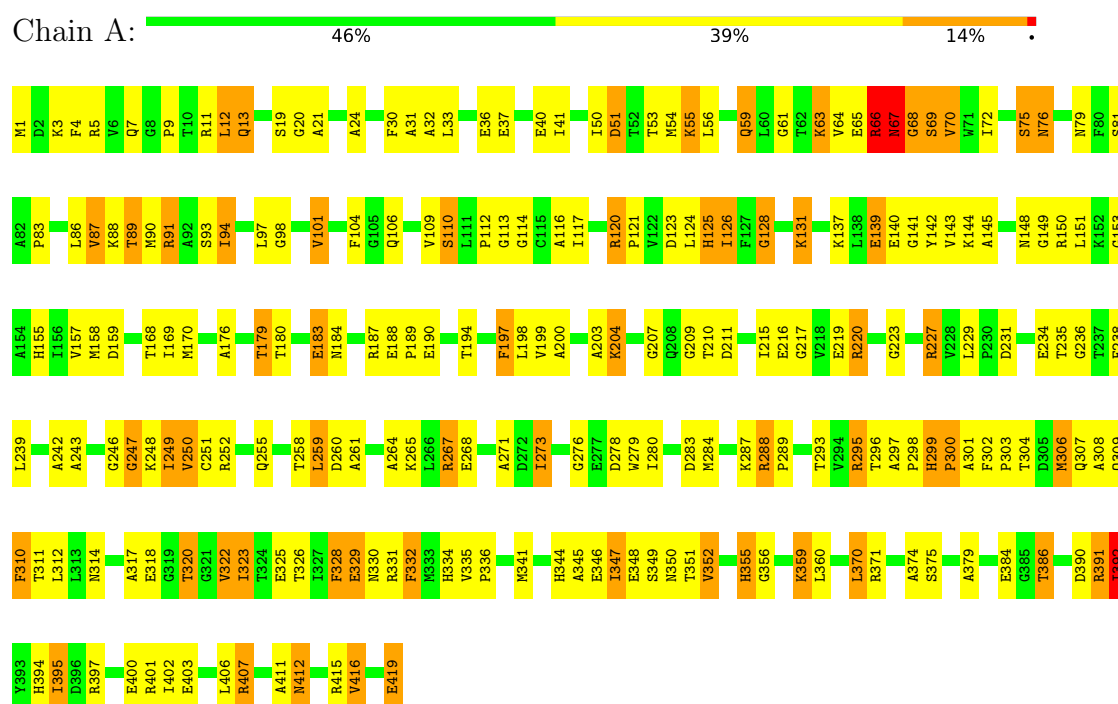
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total 242	O 242	0	0
3	B	236	Total 236	O 236	0	0

3 Residue-property plots

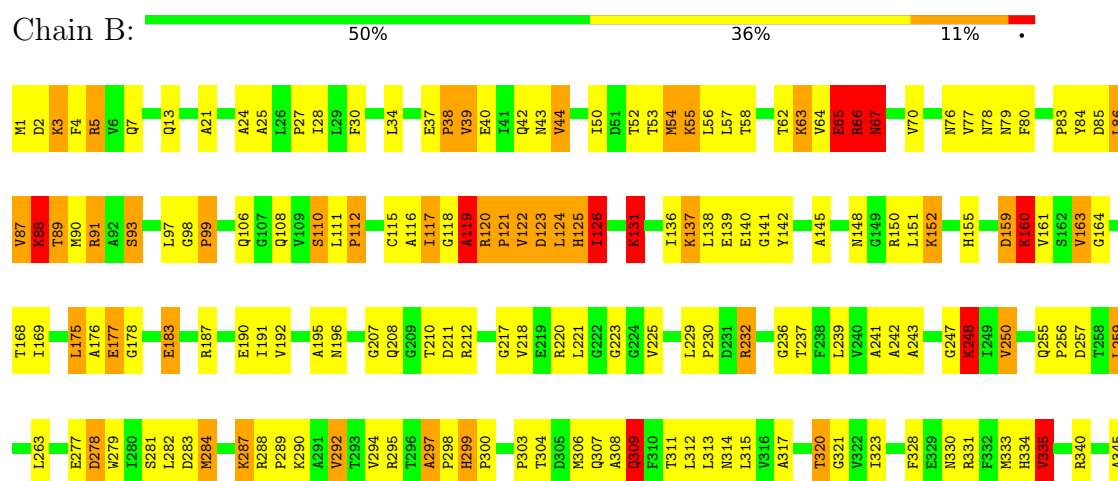
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: UDP-N-ACETYLGUCOSAMINE 1-CARBOXYVINYL-TRANSFERASE



• Molecule 1: UDP-N-ACETYLGUCOSAMINE 1-CARBOXYVINYL-TRANSFERASE



E346	I347	E348	S349	N350	T351		C384	R385	G386		K359	L360		L370	R371	A372		S375		L378	A379	G380		E384	G385	T386	T387	V388	V389	D390	R391	L392	Y393	H394	I395	D396	R397		E403		L406	R407		M412	I413	E414	R415	V416	K417	G418	E419
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.90Å 155.90Å 83.85Å 90.00° 91.65° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.9 (10.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.197 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6776	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.07	2/3187 (0.1%)	2.60	247/4319 (5.7%)
1	B	1.10	0/3187	2.65	260/4319 (6.0%)
All	All	1.09	2/6374 (0.0%)	2.63	507/8638 (5.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ASN	N-CA	-5.37	1.39	1.46
1	A	67	ASN	C-N	-5.10	1.26	1.33

All (507) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	CD-NE-CZ	23.10	156.74	124.40
1	B	67	ASN	CA-CB-CG	-19.89	92.71	112.60
1	A	220	ARG	CD-NE-CZ	19.70	151.97	124.40
1	A	67	ASN	CA-CB-CG	-17.00	95.60	112.60
1	B	91	ARG	CD-NE-CZ	15.88	146.63	124.40
1	B	350	ASN	OD1-CG-ND2	-15.07	107.53	122.60
1	B	340	ARG	CD-NE-CZ	14.43	144.59	124.40
1	B	414	GLU	CB-CG-CD	14.29	136.89	112.60
1	A	88	LYS	CA-C-N	13.65	141.05	120.31
1	A	88	LYS	C-N-CA	13.65	141.05	120.31
1	A	12	LEU	CA-C-O	13.24	134.89	120.32
1	B	66	ARG	CA-C-N	12.96	146.29	121.54
1	B	66	ARG	C-N-CA	12.96	146.29	121.54
1	B	120	ARG	N-CA-CB	12.80	124.59	109.74
1	A	391	ARG	CD-NE-CZ	12.36	141.70	124.40
1	B	212	ARG	NE-CZ-NH1	11.47	132.97	121.50
1	B	412	ASN	CB-CG-ND2	11.40	133.49	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	NE-CZ-NH2	11.28	129.35	119.20
1	A	350	ASN	OD1-CG-ND2	-10.76	111.84	122.60
1	B	196	ASN	OD1-CG-ND2	-10.72	111.88	122.60
1	B	292	VAL	N-CA-CB	-10.72	94.44	112.44
1	A	113	GLY	N-CA-C	10.58	127.42	112.82
1	B	91	ARG	CA-CB-CG	10.55	135.20	114.10
1	B	187	ARG	NE-CZ-NH2	-10.40	109.84	119.20
1	B	307	GLN	OE1-CD-NE2	-10.32	112.28	122.60
1	B	123	ASP	CB-CA-C	10.17	131.78	110.32
1	B	232	ARG	CD-NE-CZ	10.14	138.59	124.40
1	B	391	ARG	NE-CZ-NH2	-9.90	110.29	119.20
1	A	267	ARG	NH1-CZ-NH2	9.82	132.06	119.30
1	A	391	ARG	NE-CZ-NH2	-9.75	110.43	119.20
1	A	391	ARG	NE-CZ-NH1	9.72	131.22	121.50
1	A	416	VAL	CA-C-O	9.56	130.99	120.48
1	B	331	ARG	CD-NE-CZ	9.54	137.76	124.40
1	A	397	ARG	CD-NE-CZ	-9.48	111.12	124.40
1	B	248	LYS	CA-CB-CG	9.48	133.06	114.10
1	A	227	ARG	NE-CZ-NH1	-9.31	112.19	121.50
1	A	76	ASN	CA-CB-CG	9.29	121.89	112.60
1	A	93	SER	O-C-N	-9.23	110.38	122.39
1	B	190	GLU	CA-C-N	9.22	132.36	120.56
1	B	190	GLU	C-N-CA	9.22	132.36	120.56
1	A	59	GLN	CB-CG-CD	9.17	128.19	112.60
1	A	267	ARG	NE-CZ-NH2	-9.09	111.02	119.20
1	A	67	ASN	N-CA-C	9.08	130.14	110.80
1	A	89	THR	CB-CA-C	-8.99	93.42	110.67
1	B	24	ALA	N-CA-C	-8.97	100.75	112.68
1	B	44	VAL	CB-CA-C	8.97	121.09	110.78
1	B	93	SER	O-C-N	-8.90	110.82	122.39
1	A	68	GLY	N-CA-C	-8.86	92.19	113.18
1	B	386	THR	CA-C-O	8.79	129.97	120.38
1	A	249	ILE	CA-C-O	8.79	130.33	121.63
1	B	335	VAL	N-CA-CB	8.75	123.46	111.21
1	B	88	LYS	CA-C-N	8.72	136.41	121.14
1	B	88	LYS	C-N-CA	8.72	136.41	121.14
1	B	13	GLN	OE1-CD-NE2	8.68	131.28	122.60
1	B	299	HIS	CA-CB-CG	-8.64	105.16	113.80
1	A	131	LYS	CA-C-O	8.63	129.85	120.10
1	A	55	LYS	CG-CD-CE	8.54	130.94	111.30
1	B	391	ARG	CA-C-N	8.45	134.62	121.19
1	B	391	ARG	C-N-CA	8.45	134.62	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ASN	CA-C-O	-8.26	108.71	120.51
1	B	212	ARG	CD-NE-CZ	8.15	135.82	124.40
1	A	184	ASN	CA-C-O	8.15	131.08	120.98
1	B	256	PRO	O-C-N	-8.13	112.89	122.24
1	A	140	GLU	CA-C-O	8.10	129.78	120.96
1	B	120	ARG	N-CA-C	-8.05	99.57	110.36
1	A	329	GLU	N-CA-C	-8.02	97.57	110.32
1	B	108	GLN	OE1-CD-NE2	8.00	130.60	122.60
1	A	13	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	A	328	PHE	CA-CB-CG	-7.95	105.85	113.80
1	A	65	GLU	CA-CB-CG	7.94	129.99	114.10
1	B	236	GLY	O-C-N	-7.91	114.59	122.19
1	B	392	ILE	CA-CB-CG2	7.90	123.93	110.50
1	B	412	ASN	CB-CG-OD1	-7.90	105.01	120.80
1	A	13	GLN	N-CA-CB	-7.89	96.84	111.52
1	A	220	ARG	CG-CD-NE	7.89	129.35	112.00
1	A	234	GLU	N-CA-C	-7.88	102.77	111.36
1	A	407	ARG	CD-NE-CZ	7.88	135.43	124.40
1	B	123	ASP	CB-CG-OD1	7.88	136.52	118.40
1	A	271	ALA	CA-C-O	7.88	129.98	121.16
1	B	380	GLY	CA-C-O	7.84	128.49	120.80
1	B	379	ALA	CA-C-O	-7.81	112.62	120.82
1	A	125	HIS	CA-CB-CG	7.81	121.61	113.80
1	B	89	THR	N-CA-CB	-7.76	97.74	110.40
1	B	4	PHE	CA-CB-CG	7.72	121.52	113.80
1	B	351	THR	CA-CB-CG2	7.71	123.61	110.50
1	A	32	ALA	CA-C-N	7.66	133.52	120.72
1	A	32	ALA	C-N-CA	7.66	133.52	120.72
1	B	91	ARG	CB-CG-CD	7.58	128.72	111.30
1	B	50	ILE	CA-C-N	7.56	130.26	120.44
1	B	50	ILE	C-N-CA	7.56	130.26	120.44
1	A	320	THR	O-C-N	7.55	132.20	123.29
1	B	141	GLY	N-CA-C	7.54	122.97	114.67
1	A	330	ASN	CA-CB-CG	7.54	120.14	112.60
1	B	66	ARG	O-C-N	-7.53	112.58	122.59
1	B	66	ARG	NH1-CZ-NH2	7.47	129.01	119.30
1	A	309	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	A	350	ASN	O-C-N	-7.43	112.71	122.59
1	A	267	ARG	CD-NE-CZ	-7.43	114.00	124.40
1	A	318	GLU	CA-C-O	-7.40	112.14	120.43
1	A	149	GLY	CA-C-O	-7.37	113.90	120.53
1	B	145	ALA	CA-C-O	-7.34	112.78	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	LYS	CB-CG-CD	7.33	128.17	111.30
1	B	93	SER	CA-C-O	7.33	128.36	119.49
1	B	236	GLY	CA-C-N	7.31	129.94	120.44
1	B	236	GLY	C-N-CA	7.31	129.94	120.44
1	A	67	ASN	O-C-N	-7.31	112.87	122.59
1	B	212	ARG	NE-CZ-NH2	-7.30	112.63	119.20
1	B	177	GLU	CB-CG-CD	7.26	124.94	112.60
1	A	69	SER	CB-CA-C	-7.23	97.87	109.80
1	B	292	VAL	CB-CA-C	7.22	121.52	110.55
1	A	219	GLU	CA-C-O	-7.21	112.24	120.24
1	A	159	ASP	CA-C-N	7.20	134.40	122.73
1	A	159	ASP	C-N-CA	7.20	134.40	122.73
1	B	90	MET	CA-C-N	7.20	129.93	120.28
1	B	90	MET	C-N-CA	7.20	129.93	120.28
1	B	241	ALA	CA-C-N	7.19	130.21	120.44
1	B	241	ALA	C-N-CA	7.19	130.21	120.44
1	A	331	ARG	NE-CZ-NH1	7.18	128.68	121.50
1	A	66	ARG	CA-C-N	7.17	135.23	121.54
1	A	66	ARG	C-N-CA	7.17	135.23	121.54
1	A	352	VAL	CB-CA-C	-7.15	99.89	110.33
1	B	241	ALA	O-C-N	-7.15	114.54	122.12
1	B	148	ASN	CA-CB-CG	-7.15	105.45	112.60
1	A	170	MET	O-C-N	7.15	129.43	122.07
1	B	54	MET	CA-C-N	7.14	129.73	120.44
1	B	54	MET	C-N-CA	7.14	129.73	120.44
1	A	24	ALA	N-CA-C	-7.13	103.44	112.93
1	B	187	ARG	NE-CZ-NH1	7.12	128.62	121.50
1	A	150	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	A	242	ALA	N-CA-C	-7.09	102.97	111.69
1	B	112	PRO	CB-CA-C	7.08	120.83	110.85
1	B	220	ARG	NE-CZ-NH2	-7.05	112.86	119.20
1	A	299	HIS	CA-CB-CG	-7.00	106.80	113.80
1	B	90	MET	N-CA-C	6.97	120.11	108.13
1	A	347	ILE	CB-CA-C	-6.96	102.55	110.96
1	B	66	ARG	CA-C-O	6.96	130.46	120.51
1	A	392	ILE	CA-CB-CG2	6.94	122.30	110.50
1	B	331	ARG	CG-CD-NE	6.93	127.24	112.00
1	A	310	PHE	CA-C-N	6.92	129.86	120.44
1	A	310	PHE	C-N-CA	6.92	129.86	120.44
1	A	194	THR	CA-C-N	6.91	129.54	120.28
1	A	194	THR	C-N-CA	6.91	129.54	120.28
1	B	21	ALA	CA-C-O	6.91	128.76	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	PRO	N-CA-C	6.91	130.05	112.10
1	B	27	PRO	CA-C-N	6.90	130.22	120.42
1	B	27	PRO	C-N-CA	6.90	130.22	120.42
1	B	79	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	288	ARG	NE-CZ-NH2	6.86	125.37	119.20
1	A	242	ALA	N-CA-CB	6.85	120.41	110.20
1	B	192	VAL	CA-C-O	-6.82	113.94	121.17
1	B	163	VAL	N-CA-CB	6.81	120.80	110.58
1	B	412	ASN	N-CA-CB	6.80	121.96	110.46
1	A	407	ARG	NH1-CZ-NH2	-6.78	110.49	119.30
1	B	295	ARG	CA-C-O	-6.78	113.28	120.40
1	A	370	LEU	CA-C-O	-6.77	112.19	119.97
1	B	397	ARG	NH1-CZ-NH2	6.71	128.02	119.30
1	A	59	GLN	CG-CD-NE2	6.69	126.43	116.40
1	B	320	THR	CA-CB-OG1	-6.65	99.62	109.60
1	B	90	MET	N-CA-CB	-6.65	99.61	110.59
1	B	76	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	A	419	GLU	CA-C-O	6.64	132.09	120.80
1	B	283	ASP	CA-C-O	-6.64	112.95	120.32
1	B	239	LEU	CA-C-N	6.62	129.04	120.56
1	B	239	LEU	C-N-CA	6.62	129.04	120.56
1	B	242	ALA	CA-C-N	6.62	129.81	120.28
1	B	242	ALA	C-N-CA	6.62	129.81	120.28
1	A	66	ARG	N-CA-C	6.61	118.81	108.96
1	A	379	ALA	CA-C-N	6.61	127.31	119.98
1	A	379	ALA	C-N-CA	6.61	127.31	119.98
1	A	322	VAL	CB-CA-C	-6.61	100.78	110.62
1	B	218	VAL	O-C-N	-6.59	115.92	122.97
1	A	211	ASP	CB-CG-OD1	6.59	133.55	118.40
1	A	139	GLU	CA-C-O	-6.58	113.43	121.06
1	A	400	GLU	CA-CB-CG	6.57	127.24	114.10
1	A	190	GLU	CA-C-N	6.56	128.96	120.56
1	A	190	GLU	C-N-CA	6.56	128.96	120.56
1	B	412	ASN	CA-C-N	-6.56	112.88	122.58
1	B	412	ASN	C-N-CA	-6.56	112.88	122.58
1	A	261	ALA	CA-C-O	-6.55	113.47	120.42
1	A	250	VAL	CA-C-O	6.55	126.89	120.27
1	B	309	GLN	CG-CD-NE2	6.54	126.21	116.40
1	B	120	ARG	CA-CB-CG	6.53	127.17	114.10
1	A	318	GLU	O-C-N	6.52	130.63	123.13
1	B	212	ARG	CB-CG-CD	-6.51	96.33	111.30
1	A	51	ASP	O-C-N	-6.50	115.37	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	SER	CA-CB-OG	-6.50	98.10	111.10
1	B	25	ALA	CA-C-O	-6.50	114.00	120.82
1	A	332	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	278	ASP	CA-CB-CG	-6.48	106.12	112.60
1	B	160	LYS	CA-CB-CG	6.47	127.05	114.10
1	B	78	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	323	ILE	CA-C-O	-6.45	113.61	120.39
1	B	169	ILE	N-CA-C	6.45	116.61	110.42
1	B	247	GLY	N-CA-C	6.44	123.13	112.30
1	A	120	ARG	N-CA-C	-6.44	101.19	110.08
1	A	183	GLU	CB-CG-CD	6.44	123.55	112.60
1	A	352	VAL	N-CA-CB	6.42	120.89	111.52
1	B	395	ILE	CA-C-O	-6.42	114.37	121.17
1	B	307	GLN	CA-C-O	-6.41	114.27	121.00
1	A	314	ASN	CA-CB-CG	-6.38	106.22	112.60
1	A	401	ARG	CA-C-O	6.38	129.63	120.51
1	A	81	SER	O-C-N	-6.37	115.81	123.27
1	A	295	ARG	NE-CZ-NH1	-6.37	115.13	121.50
1	A	151	LEU	N-CA-C	-6.37	102.13	110.53
1	B	220	ARG	O-C-N	6.36	130.51	123.33
1	A	59	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	B	151	LEU	CA-C-N	-6.33	112.47	122.73
1	B	151	LEU	C-N-CA	-6.33	112.47	122.73
1	A	149	GLY	O-C-N	6.33	129.39	123.19
1	B	62	THR	CA-C-N	-6.30	114.40	122.77
1	B	62	THR	C-N-CA	-6.30	114.40	122.77
1	A	68	GLY	CA-C-O	6.29	131.51	120.57
1	A	117	ILE	O-C-N	6.28	129.72	123.00
1	A	69	SER	O-C-N	6.27	130.12	123.03
1	A	328	PHE	CB-CA-C	-6.25	98.91	109.72
1	A	128	GLY	N-CA-C	-6.24	104.94	112.49
1	B	196	ASN	CB-CG-OD1	6.23	133.26	120.80
1	A	236	GLY	CA-C-N	6.22	128.52	120.44
1	A	236	GLY	C-N-CA	6.22	128.52	120.44
1	B	163	VAL	CA-CB-CG2	6.22	120.97	110.40
1	A	90	MET	N-CA-C	6.20	118.80	108.13
1	B	52	THR	CA-C-N	6.20	129.10	120.29
1	B	52	THR	C-N-CA	6.20	129.10	120.29
1	B	328	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	239	LEU	CA-C-O	-6.19	114.32	120.82
1	B	255	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	B	350	ASN	CB-CG-ND2	6.18	125.68	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	SER	CA-CB-OG	6.18	123.47	111.10
1	B	123	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	7	GLN	CG-CD-NE2	6.16	125.64	116.40
1	B	131	LYS	CB-CG-CD	6.16	125.46	111.30
1	A	252	ARG	NE-CZ-NH2	-6.15	113.66	119.20
1	B	28	ILE	CA-C-N	6.15	128.44	120.44
1	B	28	ILE	C-N-CA	6.15	128.44	120.44
1	A	20	GLY	CA-C-O	-6.14	114.08	122.31
1	A	90	MET	N-CA-CB	-6.14	100.46	110.59
1	A	239	LEU	N-CA-C	-6.14	104.50	111.07
1	A	350	ASN	CB-CG-ND2	6.13	125.59	116.40
1	B	99	PRO	CA-C-N	6.13	128.41	120.44
1	B	99	PRO	C-N-CA	6.13	128.41	120.44
1	B	323	ILE	O-C-N	6.12	129.69	123.20
1	A	323	ILE	O-C-N	6.11	129.85	123.26
1	B	164	GLY	CA-C-N	6.11	128.46	120.28
1	B	164	GLY	C-N-CA	6.11	128.46	120.28
1	B	55	LYS	CA-CB-CG	6.10	126.31	114.10
1	A	220	ARG	NH1-CZ-NH2	-6.10	111.37	119.30
1	A	106	GLN	OE1-CD-NE2	6.09	128.69	122.60
1	B	138	LEU	CA-C-O	6.09	127.66	120.66
1	B	328	PHE	N-CA-C	6.08	120.18	109.96
1	A	199	VAL	CA-C-N	6.08	128.43	120.28
1	A	199	VAL	C-N-CA	6.08	128.43	120.28
1	B	123	ASP	N-CA-CB	-6.07	100.00	110.32
1	A	40	GLU	CA-CB-CG	-6.07	101.96	114.10
1	A	386	THR	CA-C-O	6.04	126.97	120.38
1	B	207	GLY	CA-C-O	-6.04	112.30	119.06
1	B	304	THR	O-C-N	-6.02	115.33	122.20
1	A	341	MET	CA-C-N	6.02	130.13	122.00
1	A	341	MET	C-N-CA	6.02	130.13	122.00
1	A	81	SER	CA-C-N	6.02	129.68	121.74
1	A	81	SER	C-N-CA	6.02	129.68	121.74
1	A	33	LEU	N-CA-C	-6.01	105.20	112.54
1	A	371	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	A	235	THR	O-C-N	-6.01	115.88	122.07
1	A	223	GLY	CA-C-N	-6.00	114.04	121.83
1	A	223	GLY	C-N-CA	-6.00	114.04	121.83
1	A	415	ARG	CD-NE-CZ	5.98	132.77	124.40
1	B	66	ARG	N-CA-CB	-5.97	100.40	110.49
1	A	66	ARG	CB-CA-C	-5.96	97.55	111.09
1	B	78	ASN	CA-CB-CG	5.96	118.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ARG	NH1-CZ-NH2	5.95	127.04	119.30
1	A	81	SER	CB-CA-C	5.94	119.65	110.14
1	A	288	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	B	331	ARG	NH1-CZ-NH2	-5.94	111.58	119.30
1	A	255	GLN	OE1-CD-NE2	5.93	128.53	122.60
1	A	56	LEU	CA-C-N	5.92	128.49	120.38
1	A	56	LEU	C-N-CA	5.92	128.49	120.38
1	B	5	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	B	303	PRO	N-CA-C	5.91	120.17	110.55
1	B	287	LYS	CA-CB-CG	5.90	125.90	114.10
1	B	106	GLN	CA-C-O	5.90	127.38	120.89
1	B	70	VAL	N-CA-CB	5.87	119.80	111.82
1	A	128	GLY	CA-C-O	-5.87	114.33	120.90
1	A	350	ASN	CA-C-O	5.85	128.88	120.51
1	B	282	LEU	CA-C-N	-5.85	113.73	122.74
1	B	282	LEU	C-N-CA	-5.85	113.73	122.74
1	B	159	ASP	OD1-CG-OD2	-5.85	108.86	122.90
1	A	30	PHE	CA-C-N	5.85	130.49	120.72
1	A	30	PHE	C-N-CA	5.85	130.49	120.72
1	B	178	GLY	CA-C-O	5.83	130.00	122.59
1	B	187	ARG	CG-CD-NE	5.83	124.83	112.00
1	B	257	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	360	LEU	O-C-N	5.83	129.60	122.84
1	A	124	LEU	O-C-N	-5.82	115.11	122.27
1	A	412	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	61	GLY	CA-C-O	5.80	125.23	118.96
1	B	122	VAL	N-CA-C	5.80	120.54	113.00
1	B	284	MET	CA-C-N	5.80	130.82	122.35
1	B	284	MET	C-N-CA	5.80	130.82	122.35
1	B	391	ARG	O-C-N	-5.80	115.36	122.55
1	A	37	GLU	CA-C-O	5.79	127.30	120.87
1	A	50	ILE	CA-C-N	5.79	127.97	120.44
1	A	50	ILE	C-N-CA	5.79	127.97	120.44
1	B	290	LYS	CA-CB-CG	-5.79	102.53	114.10
1	B	259	LEU	CB-CA-C	-5.78	102.14	111.28
1	A	249	ILE	CA-CB-CG1	5.78	120.23	110.40
1	B	91	ARG	CG-CD-NE	5.78	124.72	112.00
1	B	287	LYS	CG-CD-CE	5.78	124.59	111.30
1	B	312	LEU	O-C-N	-5.78	116.12	122.07
1	B	418	GLY	N-CA-C	-5.77	103.56	112.85
1	B	66	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	B	161	VAL	CA-C-O	-5.76	113.94	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLY	N-CA-C	-5.75	107.38	115.32
1	B	66	ARG	CG-CD-NE	-5.75	99.35	112.00
1	A	104	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	139	GLU	CB-CG-CD	-5.73	102.86	112.60
1	A	158	MET	CA-C-O	-5.72	113.85	120.49
1	A	351	THR	CB-CA-C	-5.72	97.48	110.07
1	A	302	PHE	CB-CA-C	5.72	118.60	109.62
1	B	359	LYS	CA-C-O	5.71	127.39	120.99
1	A	345	ALA	O-C-N	5.71	129.78	123.33
1	B	183	GLU	CB-CG-CD	-5.71	102.90	112.60
1	A	273	ILE	N-CA-C	5.70	116.08	108.11
1	A	112	PRO	CA-C-N	5.69	127.81	120.64
1	A	112	PRO	C-N-CA	5.69	127.81	120.64
1	B	119	ALA	CA-C-O	5.68	128.64	120.51
1	A	407	ARG	CA-C-O	5.68	126.51	120.10
1	A	209	GLY	CA-C-N	5.67	133.20	123.05
1	A	209	GLY	C-N-CA	5.67	133.20	123.05
1	A	238	PHE	CA-CB-CG	-5.67	108.13	113.80
1	B	70	VAL	N-CA-C	-5.67	99.38	107.77
1	A	246	GLY	CA-C-N	5.64	129.61	121.54
1	A	246	GLY	C-N-CA	5.64	129.61	121.54
1	A	252	ARG	CG-CD-NE	-5.64	99.58	112.00
1	B	124	LEU	CA-C-O	5.64	126.45	119.79
1	B	125	HIS	CA-C-N	5.64	127.75	120.70
1	B	125	HIS	C-N-CA	5.64	127.75	120.70
1	B	123	ASP	OD1-CG-OD2	-5.63	109.38	122.90
1	A	374	ALA	CA-C-O	-5.63	114.58	120.55
1	A	94	ILE	CA-C-O	5.63	126.59	120.57
1	B	148	ASN	CA-C-O	-5.63	114.34	120.36
1	A	411	ALA	O-C-N	5.61	129.48	122.86
1	A	141	GLY	CA-C-O	-5.59	112.81	119.07
1	A	400	GLU	CB-CG-CD	5.58	122.09	112.60
1	B	346	GLU	N-CA-C	-5.58	100.30	109.40
1	B	76	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	112	PRO	O-C-N	-5.57	116.73	123.03
1	A	359	LYS	CA-C-O	5.57	127.52	121.06
1	B	340	ARG	NE-CZ-NH1	5.55	127.06	121.50
1	A	11	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	B	415	ARG	N-CA-CB	5.54	119.31	110.16
1	B	77	VAL	CA-CB-CG2	-5.53	100.99	110.40
1	B	396	ASP	CA-C-O	5.53	126.61	120.63
1	B	39	VAL	CA-CB-CG1	5.53	119.80	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ILE	O-C-N	-5.53	116.29	121.87
1	A	159	ASP	O-C-N	-5.53	114.83	122.46
1	B	84	TYR	CA-C-N	5.52	127.95	120.38
1	B	84	TYR	C-N-CA	5.52	127.95	120.38
1	A	251	CYS	CA-C-O	5.52	126.28	120.54
1	A	296	THR	N-CA-CB	5.52	118.68	110.29
1	B	43	ASN	CA-C-N	-5.52	117.28	123.02
1	B	43	ASN	C-N-CA	-5.52	117.28	123.02
1	A	312	LEU	CA-C-N	5.51	127.61	120.44
1	A	312	LEU	C-N-CA	5.51	127.61	120.44
1	B	191	ILE	CA-C-O	5.50	127.16	121.05
1	B	3	LYS	CA-C-N	-5.49	115.24	122.99
1	B	3	LYS	C-N-CA	-5.49	115.24	122.99
1	B	250	VAL	N-CA-CB	5.49	118.78	111.64
1	A	179	THR	O-C-N	5.49	129.47	123.27
1	B	211	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	250	VAL	CA-C-N	5.48	129.96	122.84
1	A	250	VAL	C-N-CA	5.48	129.96	122.84
1	A	114	GLY	N-CA-C	5.47	119.06	110.91
1	A	259	LEU	N-CA-C	5.46	119.73	112.30
1	B	321	GLY	N-CA-C	-5.46	101.46	110.80
1	A	54	MET	CA-C-N	5.46	127.59	120.28
1	A	54	MET	C-N-CA	5.46	127.59	120.28
1	A	13	GLN	CB-CG-CD	5.46	121.88	112.60
1	B	320	THR	O-C-N	5.45	130.31	123.23
1	B	55	LYS	CA-C-N	5.44	127.51	120.44
1	B	55	LYS	C-N-CA	5.44	127.51	120.44
1	A	93	SER	CB-CA-C	5.44	121.79	110.32
1	B	289	PRO	O-C-N	-5.44	116.37	123.00
1	A	93	SER	CA-C-N	5.43	129.05	120.47
1	A	93	SER	C-N-CA	5.43	129.05	120.47
1	B	97	LEU	N-CA-C	5.43	117.65	111.02
1	A	79	ASN	N-CA-C	-5.43	98.36	108.02
1	A	189	PRO	CA-C-N	5.42	128.08	120.28
1	A	189	PRO	C-N-CA	5.42	128.08	120.28
1	A	187	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	329	GLU	CB-CG-CD	-5.41	103.41	112.60
1	B	308	ALA	CA-C-N	5.40	127.96	120.29
1	B	308	ALA	C-N-CA	5.40	127.96	120.29
1	B	208	GLN	N-CA-CB	5.40	117.98	109.83
1	A	406	LEU	CA-C-O	-5.39	115.15	120.70
1	A	283	ASP	CA-CB-CG	5.39	117.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	GLY	O-C-N	-5.39	116.94	122.17
1	B	125	HIS	CA-CB-CG	5.38	119.19	113.80
1	B	163	VAL	CA-C-O	-5.38	115.14	120.85
1	B	288	ARG	CA-CB-CG	5.38	124.87	114.10
1	B	38	PRO	CA-C-N	-5.38	114.13	122.69
1	B	38	PRO	C-N-CA	-5.38	114.13	122.69
1	B	58	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	308	ALA	CA-C-N	5.38	127.93	120.29
1	A	308	ALA	C-N-CA	5.38	127.93	120.29
1	A	331	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	B	55	LYS	O-C-N	-5.37	116.53	122.07
1	B	126	ILE	CA-CB-CG2	5.37	119.64	110.50
1	A	278	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	388	VAL	N-CA-CB	5.37	118.67	111.90
1	A	93	SER	CA-C-O	5.37	125.98	119.49
1	A	351	THR	CA-CB-OG1	-5.36	101.56	109.60
1	B	277	GLU	CA-C-O	-5.35	113.34	119.60
1	A	258	THR	N-CA-C	-5.34	106.81	113.38
1	A	344	HIS	CB-CA-C	-5.34	102.25	111.23
1	B	390	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	40	GLU	CA-C-O	-5.33	114.75	120.46
1	B	4	PHE	O-C-N	5.33	129.64	123.30
1	A	411	ALA	N-CA-CB	5.33	117.84	110.17
1	B	65	GLU	CB-CG-CD	5.32	121.65	112.60
1	A	20	GLY	N-CA-C	-5.32	105.73	112.54
1	A	179	THR	N-CA-C	5.30	117.89	109.24
1	B	115	CYS	CA-CB-SG	5.30	126.60	114.40
1	A	184	ASN	N-CA-CB	-5.29	104.15	112.46
1	A	159	ASP	CA-C-O	5.29	125.86	119.31
1	B	126	ILE	CA-C-O	5.29	126.95	121.29
1	B	195	ALA	CA-C-N	5.28	127.79	120.29
1	B	195	ALA	C-N-CA	5.28	127.79	120.29
1	A	355	HIS	O-C-N	5.28	130.09	123.12
1	B	4	PHE	N-CA-CB	5.28	119.55	110.68
1	B	323	ILE	CB-CA-C	-5.28	103.27	110.77
1	B	340	ARG	CA-C-N	5.27	131.08	122.65
1	B	340	ARG	C-N-CA	5.27	131.08	122.65
1	B	393	TYR	CA-C-O	-5.27	114.15	120.10
1	A	395	ILE	O-C-N	-5.26	116.43	121.90
1	B	306	MET	CA-C-N	5.26	127.59	120.65
1	B	306	MET	C-N-CA	5.26	127.59	120.65
1	A	250	VAL	N-CA-CB	5.25	118.97	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ASN	CA-C-N	5.25	129.50	120.72
1	B	314	ASN	C-N-CA	5.25	129.50	120.72
1	A	345	ALA	CA-C-N	-5.24	115.60	122.99
1	A	345	ALA	C-N-CA	-5.24	115.60	122.99
1	B	42	GLN	CG-CD-NE2	-5.24	108.54	116.40
1	A	197	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	19	SER	CA-C-O	-5.23	115.63	121.81
1	A	280	ILE	CA-C-N	-5.23	114.59	122.81
1	A	280	ILE	C-N-CA	-5.23	114.59	122.81
1	B	77	VAL	N-CA-C	-5.23	102.31	109.37
1	A	259	LEU	CB-CA-C	-5.22	102.28	110.85
1	A	204	LYS	CA-CB-CG	-5.22	103.66	114.10
1	A	407	ARG	CA-CB-CG	5.21	124.52	114.10
1	A	407	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	A	70	VAL	N-CA-CB	5.20	118.40	111.64
1	B	307	GLN	CG-CD-NE2	5.20	124.20	116.40
1	B	384	GLU	CA-C-N	-5.19	113.89	122.05
1	B	384	GLU	C-N-CA	-5.19	113.89	122.05
1	B	330	ASN	N-CA-CB	-5.18	104.31	112.13
1	B	93	SER	CB-CA-C	5.17	121.22	110.32
1	B	306	MET	O-C-N	-5.17	115.65	122.42
1	B	117	ILE	CA-C-O	-5.17	114.88	120.67
1	B	230	PRO	CA-C-O	-5.16	115.37	121.67
1	B	406	LEU	CA-C-O	5.16	126.24	120.82
1	A	247	GLY	N-CA-C	5.16	120.97	112.30
1	A	12	LEU	O-C-N	-5.16	117.19	123.27
1	B	391	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	143	VAL	N-CA-CB	5.15	119.04	111.52
1	B	416	VAL	N-CA-CB	-5.15	105.18	111.67
1	B	311	THR	N-CA-C	-5.14	105.58	111.14
1	A	391	ARG	CA-C-O	5.13	127.79	121.84
1	B	297	ALA	CA-C-N	5.13	125.06	119.78
1	B	297	ALA	C-N-CA	5.13	125.06	119.78
1	A	75	SER	CA-C-N	5.12	130.69	122.86
1	A	75	SER	C-N-CA	5.12	130.69	122.86
1	A	351	THR	N-CA-CB	5.12	120.60	111.69
1	B	125	HIS	CA-C-O	-5.12	115.43	120.70
1	B	187	ARG	CD-NE-CZ	5.11	131.55	124.40
1	B	237	THR	O-C-N	5.11	127.33	122.07
1	A	123	ASP	CA-CB-CG	5.11	117.70	112.60
1	B	350	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	290	LYS	CG-CD-CE	5.09	123.01	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	THR	N-CA-C	5.09	117.27	109.07
1	B	65	GLU	CG-CD-OE1	5.09	130.10	118.40
1	B	289	PRO	CA-C-O	5.09	128.59	122.08
1	B	160	LYS	CB-CG-CD	5.08	122.98	111.30
1	A	148	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	187	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	311	THR	N-CA-CB	5.06	117.41	110.07
1	B	80	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	78	ASN	CB-CG-OD1	5.06	130.91	120.80
1	B	192	VAL	N-CA-CB	5.05	116.46	110.55
1	B	370	LEU	N-CA-CB	-5.05	102.42	109.94
1	A	126	ILE	O-C-N	-5.05	116.96	121.91
1	A	110	SER	O-C-N	-5.04	116.91	122.86
1	A	220	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	B	221	LEU	CA-C-O	5.04	126.05	120.71
1	A	203	ALA	O-C-N	-5.04	117.05	122.79
1	A	210	THR	N-CA-CB	5.04	118.20	110.70
1	B	323	ILE	CA-C-N	-5.03	116.06	123.00
1	B	323	ILE	C-N-CA	-5.03	116.06	123.00
1	B	294	VAL	CB-CA-C	-5.02	102.76	110.50
1	A	50	ILE	N-CA-C	-5.02	105.81	110.53
1	B	110	SER	CA-C-O	5.02	127.24	121.47
1	A	306	MET	CA-C-N	5.01	126.96	120.44
1	A	306	MET	C-N-CA	5.01	126.96	120.44
1	A	53	THR	CA-CB-OG1	-5.01	102.08	109.60
1	B	340	ARG	O-C-N	-5.01	115.55	122.46
1	A	243	ALA	N-CA-C	5.01	117.47	111.71
1	B	108	GLN	CA-CB-CG	-5.01	104.09	114.10

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	3142	0	3220	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3142	0	3220	86	0
2	A	14	0	27	7	0
3	A	242	0	0	17	2
3	B	236	0	0	12	2
All	All	6776	0	6467	189	2

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 15.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HE3	3:A:571:HOH:O	1.50	1.09
1:A:287:LYS:CE	3:A:571:HOH:O	1.98	1.08
1:B:3:LYS:HZ1	1:B:419:GLU:HG3	1.24	1.00
1:B:335:VAL:HG22	1:B:347:ILE:HD11	1.50	0.91
1:B:137:LYS:NZ	1:B:137:LYS:HB3	1.87	0.87
1:B:248:LYS:HZ1	1:B:281:SER:HB2	1.40	0.87
1:B:83:PRO:HD2	1:B:86:LEU:HD12	1.57	0.85
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.42	0.82
1:A:139:GLU:HB2	1:A:142:TYR:CE2	2.16	0.81
2:A:479:HAI:H41	2:A:480:HAI:H41	1.63	0.81
1:A:287:LYS:HE2	3:A:571:HOH:O	1.72	0.78
1:B:248:LYS:NZ	1:B:281:SER:HB2	1.98	0.78
1:B:392:ILE:HD12	1:B:395:ILE:HD12	1.67	0.76
1:B:120:ARG:HB3	1:B:121:PRO:HD2	1.68	0.76
1:B:121:PRO:O	3:B:645:HOH:O	2.03	0.76
1:A:91:ARG:HH12	1:A:121:PRO:HG2	1.51	0.75
1:A:101:VAL:HG11	1:A:145:ALA:HB3	1.69	0.74
1:B:3:LYS:NZ	1:B:419:GLU:HG3	2.01	0.74
1:A:116:ALA:O	1:A:120:ARG:HD2	1.87	0.74
1:A:284:MET:O	1:A:287:LYS:HE2	1.88	0.74
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.69	0.73
1:B:54:MET:SD	1:B:66:ARG:HG3	2.28	0.73
1:B:278:ASP:OD1	3:B:546:HOH:O	2.07	0.72
1:B:131:LYS:NZ	1:B:131:LYS:HB3	2.06	0.71
1:A:51:ASP:O	1:A:55:LYS:HD3	1.90	0.71
1:A:347:ILE:HD13	1:A:352:VAL:HG22	1.72	0.70
1:B:34:LEU:HD22	1:B:175:LEU:HD22	1.72	0.70
1:B:299:HIS:HD2	3:B:421:HOH:O	1.75	0.70
1:A:265:LYS:HE3	1:A:268:GLU:OE1	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:N	1:B:419:GLU:HB2	2.07	0.69
1:B:98:GLY:HA3	3:B:570:HOH:O	1.91	0.69
1:B:309:GLN:HE21	1:B:309:GLN:H	1.43	0.66
1:B:139:GLU:HB2	1:B:142:TYR:CE1	2.31	0.65
1:A:299:HIS:HD2	3:A:494:HOH:O	1.78	0.65
1:A:346:GLU:OE1	1:A:355:HIS:HE1	1.81	0.64
1:B:155:HIS:HE1	1:B:183:GLU:OE2	1.81	0.64
1:B:37:GLU:HB3	1:B:38:PRO:HD2	1.78	0.63
1:A:287:LYS:NZ	3:A:705:HOH:O	2.31	0.63
1:A:394:HIS:HD2	3:A:578:HOH:O	1.82	0.63
1:A:334:HIS:H	1:A:334:HIS:CD2	2.17	0.62
1:A:89:THR:HG22	3:A:554:HOH:O	2.00	0.61
1:B:123:ASP:HB2	3:B:535:HOH:O	1.99	0.61
1:A:98:GLY:HA3	3:A:497:HOH:O	2.00	0.61
1:B:176:ALA:O	1:B:217:GLY:HA3	2.00	0.61
1:A:307:GLN:HG2	1:A:323:ILE:HG21	1.81	0.61
1:B:120:ARG:HB3	1:B:121:PRO:CD	2.31	0.61
1:A:204:LYS:HD3	1:A:216:GLU:OE1	2.01	0.60
1:B:137:LYS:HB3	1:B:137:LYS:HZ3	1.65	0.60
2:A:480:HAI:H31	1:B:279:TRP:CD1	2.37	0.60
1:B:118:GLY:O	1:B:119:ALA:C	2.45	0.59
1:B:394:HIS:HB2	3:B:554:HOH:O	2.02	0.59
1:A:97:LEU:O	1:A:101:VAL:HG13	2.05	0.57
1:B:99:PRO:HD3	3:B:570:HOH:O	2.02	0.57
1:B:177:GLU:O	1:B:177:GLU:HG3	2.04	0.57
1:A:125:HIS:HD2	1:A:168:THR:OG1	1.88	0.57
1:A:347:ILE:CD1	1:A:352:VAL:HG22	2.36	0.56
1:A:250:VAL:HG11	2:A:480:HAI:H32	1.87	0.56
1:A:297:ALA:HB3	1:A:301:ALA:CB	2.36	0.55
1:B:2:ASP:OD2	1:B:415:ARG:HD3	2.05	0.55
1:A:265:LYS:HE2	1:A:293:THR:O	2.06	0.55
1:B:131:LYS:HB3	1:B:131:LYS:HZ3	1.71	0.55
1:B:89:THR:HG22	3:B:497:HOH:O	2.06	0.55
1:A:176:ALA:O	1:A:217:GLY:HA3	2.06	0.55
2:A:480:HAI:H52	1:B:250:VAL:HG11	1.89	0.55
1:A:299:HIS:CD2	3:A:494:HOH:O	2.58	0.54
1:A:329:GLU:HB3	3:A:665:HOH:O	2.08	0.54
1:B:66:ARG:NH2	1:B:67:ASN:O	2.23	0.54
1:A:317:ALA:O	1:A:356:GLY:HA3	2.07	0.54
1:B:124:LEU:HD11	1:B:160:LYS:HG2	1.88	0.54
1:A:155:HIS:HE1	1:A:183:GLU:OE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ALA:HA	1:B:284:MET:CG	2.38	0.54
1:B:297:ALA:HB1	1:B:298:PRO:CD	2.38	0.53
1:A:59:GLN:HE21	1:A:86:LEU:HD11	1.73	0.53
1:A:297:ALA:HB1	1:A:298:PRO:HD2	1.91	0.52
1:A:188:GLU:OE1	1:A:188:GLU:N	2.41	0.52
1:B:56:LEU:HA	1:B:86:LEU:HD13	1.92	0.52
1:A:335:VAL:HG11	1:A:347:ILE:HD11	1.92	0.52
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.91	0.51
1:A:395:ILE:HG21	1:A:402:ILE:HG21	1.93	0.51
1:A:137:LYS:NZ	1:A:142:TYR:OH	2.24	0.51
1:B:40:GLU:HB3	1:B:225:VAL:HG22	1.93	0.51
1:A:304:THR:HG22	3:A:487:HOH:O	2.10	0.51
1:B:126:ILE:HG23	1:B:136:ILE:HG21	1.91	0.51
1:A:89:THR:CG2	3:A:554:HOH:O	2.56	0.50
1:B:152:LYS:N	1:B:152:LYS:HD3	2.25	0.50
1:B:263:LEU:HD12	3:B:575:HOH:O	2.10	0.50
1:A:332:PHE:CE1	1:A:352:VAL:HG23	2.47	0.50
2:A:479:HAI:H41	2:A:480:HAI:C4	2.38	0.50
1:A:64:VAL:HG13	1:A:72:ILE:HD13	1.93	0.50
1:A:31:ALA:HB1	1:A:198:LEU:HD21	1.93	0.49
1:A:334:HIS:HD2	3:A:512:HOH:O	1.95	0.49
1:B:309:GLN:H	1:B:309:GLN:NE2	2.10	0.49
1:B:299:HIS:CG	1:B:300:PRO:HA	2.48	0.49
1:A:63:LYS:CE	1:A:76:ASN:HD22	2.26	0.48
1:B:120:ARG:HB2	1:B:123:ASP:OD2	2.14	0.48
1:B:370:LEU:HD23	1:B:395:ILE:HA	1.96	0.48
1:A:299:HIS:CG	1:A:300:PRO:HA	2.49	0.47
1:B:1:MET:H3	1:B:419:GLU:HB2	1.79	0.47
1:A:66:ARG:HG3	1:A:70:VAL:HG22	1.96	0.47
1:A:335:VAL:HG21	1:A:347:ILE:HD11	1.96	0.47
1:B:125:HIS:HD2	1:B:168:THR:OG1	1.96	0.47
1:B:315:LEU:HD21	1:B:345:ALA:HB2	1.96	0.47
1:B:83:PRO:HG2	1:B:86:LEU:HG	1.94	0.47
1:A:267:ARG:HG3	1:A:273:ILE:HD12	1.95	0.47
1:A:91:ARG:HH11	1:A:91:ARG:CG	2.22	0.47
1:B:139:GLU:O	1:B:140:GLU:C	2.56	0.47
1:A:329:GLU:HA	3:A:665:HOH:O	2.14	0.47
1:A:359:LYS:HD2	1:A:384:GLU:OE2	2.14	0.47
1:B:83:PRO:HD2	1:B:86:LEU:CD1	2.38	0.46
1:B:232:ARG:O	1:B:259:LEU:HD21	2.15	0.46
2:A:480:HAI:C5	1:B:250:VAL:HG11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:HE2	3:B:463:HOH:O	2.14	0.46
1:A:157:VAL:HA	1:A:183:GLU:HB2	1.97	0.46
1:A:295:ARG:NH1	1:A:326:THR:HG21	2.31	0.46
1:A:288:ARG:CG	1:A:289:PRO:HD2	2.46	0.45
1:B:39:VAL:HG12	1:B:223:GLY:HA2	1.98	0.45
1:A:392:ILE:HD12	1:A:392:ILE:HA	1.63	0.45
1:A:264:ALA:O	1:A:268:GLU:HG3	2.17	0.45
1:A:403:GLU:O	1:A:407:ARG:HB2	2.17	0.45
1:A:13:GLN:HA	1:A:248:LYS:O	2.17	0.45
1:A:91:ARG:O	1:A:94:ILE:HG22	2.17	0.45
1:A:5:ARG:HH11	1:A:5:ARG:HG3	1.81	0.45
1:B:3:LYS:HZ1	1:B:419:GLU:CG	2.11	0.45
1:B:5:ARG:NH1	1:B:386:THR:HG21	2.32	0.45
1:B:87:VAL:HB	1:B:93:SER:OG	2.17	0.45
1:B:403:GLU:O	1:B:407:ARG:HB2	2.16	0.45
1:A:109:VAL:HG12	1:A:110:SER:O	2.18	0.44
1:A:21:ALA:HB2	1:A:231:ASP:HA	2.00	0.44
1:B:317:ALA:O	1:B:356:GLY:HA3	2.17	0.44
1:A:303:PRO:HG2	1:A:306:MET:HB2	2.00	0.44
1:B:370:LEU:CD2	1:B:395:ILE:HA	2.48	0.44
1:A:137:LYS:HB3	1:A:144:LYS:HB3	1.99	0.44
1:A:325:GLU:HG3	1:A:328:PHE:O	2.17	0.43
1:A:329:GLU:CA	3:A:665:HOH:O	2.66	0.43
1:A:128:GLY:HA3	1:A:169:ILE:HD11	2.00	0.43
1:A:120:ARG:HA	1:A:120:ARG:HE	1.82	0.43
1:A:267:ARG:HH11	1:A:267:ARG:HD2	1.44	0.43
1:A:276:GLY:HA3	1:A:279:TRP:NE1	2.33	0.43
1:B:120:ARG:O	1:B:121:PRO:C	2.60	0.43
1:B:299:HIS:CD2	1:B:300:PRO:HA	2.53	0.43
1:B:85:ASP:HA	1:B:88:LYS:HD3	1.99	0.43
1:B:313:LEU:HD23	1:B:313:LEU:C	2.44	0.43
1:A:3:LYS:HB2	1:A:416:VAL:HG22	2.00	0.43
1:A:101:VAL:HG11	1:A:145:ALA:CB	2.45	0.43
1:A:36:GLU:O	1:A:75:SER:HB3	2.19	0.43
1:A:83:PRO:O	1:A:87:VAL:HG13	2.18	0.43
1:B:124:LEU:HD11	1:B:160:LYS:CG	2.49	0.43
1:B:333:MET:HG3	3:B:531:HOH:O	2.19	0.43
1:B:116:ALA:O	1:B:120:ARG:HD3	2.19	0.42
1:A:12:LEU:O	1:A:247:GLY:HA3	2.19	0.42
1:A:265:LYS:HB3	1:A:310:PHE:CE2	2.55	0.42
1:B:359:LYS:O	3:B:611:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:VAL:CG1	1:B:392:ILE:HD11	2.49	0.42
1:A:320:THR:OG1	1:A:355:HIS:HD2	2.02	0.42
1:B:63:LYS:CE	1:B:65:GLU:HG3	2.50	0.42
1:A:41:ILE:O	1:A:69:SER:HA	2.20	0.42
1:A:348:GLU:O	1:A:349:SER:HB3	2.19	0.42
1:A:391:ARG:NH1	1:A:394:HIS:HE1	2.18	0.42
1:A:7:GLN:HG2	1:A:386:THR:OG1	2.19	0.42
1:A:153:GLY:HA2	1:A:180:THR:OG1	2.20	0.42
1:A:295:ARG:CZ	1:A:326:THR:HG21	2.50	0.42
1:A:335:VAL:CB	1:A:336:PRO:HD3	2.44	0.42
1:A:139:GLU:HB2	1:A:142:TYR:CZ	2.54	0.41
1:A:179:THR:HA	1:A:215:ILE:O	2.20	0.41
1:B:83:PRO:O	1:B:87:VAL:HG13	2.19	0.41
1:B:152:LYS:HD3	1:B:152:LYS:H	1.83	0.41
1:B:297:ALA:HB1	1:B:298:PRO:HD2	2.02	0.41
1:A:63:LYS:HE2	1:A:76:ASN:HD22	1.85	0.41
1:B:159:ASP:OD1	1:B:160:LYS:HG2	2.20	0.41
1:A:249:ILE:HD13	1:A:249:ILE:HG21	1.89	0.41
1:B:413:ILE:HG21	1:B:413:ILE:HD13	1.73	0.41
1:A:86:LEU:HB3	3:A:612:HOH:O	2.21	0.41
1:A:279:TRP:CH2	2:A:479:HAI:H22	2.56	0.41
1:A:3:LYS:HG2	1:A:390:ASP:OD1	2.20	0.41
1:A:9:PRO:HD3	1:A:384:GLU:OE1	2.20	0.41
1:A:59:GLN:HG2	1:A:86:LEU:HD12	2.03	0.41
1:A:334:HIS:CD2	3:A:512:HOH:O	2.71	0.41
1:B:3:LYS:HG2	1:B:390:ASP:HA	2.03	0.41
1:B:320:THR:HA	1:B:354:CYS:O	2.20	0.41
1:A:5:ARG:HD2	1:A:7:GLN:HE21	1.86	0.40
1:B:53:THR:O	1:B:57:LEU:HG	2.21	0.40
1:A:259:LEU:O	1:A:260:ASP:C	2.64	0.40
1:A:227:ARG:HH11	1:A:227:ARG:HD2	1.56	0.40
1:B:335:VAL:HG22	1:B:347:ILE:CD1	2.36	0.40
1:B:30:PHE:HE1	1:B:56:LEU:HD22	1.86	0.40
1:B:111:LEU:HA	1:B:112:PRO:HD3	1.84	0.40
1:A:4:PHE:CD2	1:A:392:ILE:HG13	2.57	0.40
1:A:197:PHE:O	1:A:200:ALA:HB3	2.21	0.40
1:B:3:LYS:HZ3	1:B:419:GLU:HA	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:642:HOH:O	3:B:491:HOH:O[3_455]	0.49	1.71
3:A:692:HOH:O	3:B:535:HOH:O[3_455]	2.19	0.01

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	417/419 (100%)	407 (98%)	8 (2%)	2 (0%)	24	21
1	B	417/419 (100%)	406 (97%)	8 (2%)	3 (1%)	18	14
All	All	834/838 (100%)	813 (98%)	16 (2%)	5 (1%)	21	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	B	67	ASN
1	A	68	GLY
1	B	119	ALA
1	B	121	PRO

5.3.2 Protein sidechains [i](#)

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	330/330 (100%)	313 (95%)	17 (5%)	21	18
1	B	330/330 (100%)	297 (90%)	33 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	660/660 (100%)	610 (92%)	50 (8%)	12 9

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	63	LYS
1	A	66	ARG
1	A	67	ASN
1	A	87	VAL
1	A	91	ARG
1	A	101	VAL
1	A	126	ILE
1	A	131	LYS
1	A	220	ARG
1	A	229	LEU
1	A	322	VAL
1	A	360	LEU
1	A	370	LEU
1	A	392	ILE
1	A	412	ASN
1	A	419	GLU
1	B	44	VAL
1	B	55	LYS
1	B	63	LYS
1	B	64	VAL
1	B	65	GLU
1	B	66	ARG
1	B	86	LEU
1	B	87	VAL
1	B	88	LYS
1	B	91	ARG
1	B	110	SER
1	B	117	ILE
1	B	122	VAL
1	B	126	ILE
1	B	131	LYS
1	B	137	LYS
1	B	150	ARG
1	B	152	LYS
1	B	160	LYS
1	B	163	VAL

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Mol	Chain	Res	Type
1	B	175	LEU
1	B	210	THR
1	B	229	LEU
1	B	248	LYS
1	B	292	VAL
1	B	309	GLN
1	B	335	VAL
1	B	370	LEU
1	B	375	SER
1	B	378	LEU
1	B	392	ILE
1	B	412	ASN
1	B	413	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	59	GLN
1	A	67	ASN
1	A	76	ASN
1	A	79	ASN
1	A	125	HIS
1	A	155	HIS
1	A	255	GLN
1	A	299	HIS
1	A	334	HIS
1	A	355	HIS
1	A	394	HIS
1	A	412	ASN
1	B	7	GLN
1	B	23	ASN
1	B	125	HIS
1	B	148	ASN
1	B	155	HIS
1	B	255	GLN
1	B	299	HIS
1	B	309	GLN
1	B	355	HIS

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HAI	A	479	-	7,7,7	1.93	2 (28%)	8,8,8	6.65	5 (62%)
2	HAI	A	480	-	7,7,7	1.50	1 (14%)	8,8,8	9.86	5 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HAI	A	479	-	-	-	0/1/1/1
2	HAI	A	480	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	479	HAI	C5-C6	3.97	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	HAI	C5-C6	-3.57	1.44	1.53
2	A	479	HAI	C2-C1	-2.76	1.43	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	HAI	C6-C1-C2	-23.78	86.10	110.29
2	A	479	HAI	C6-C1-C2	16.70	127.27	110.29
2	A	480	HAI	C4-C5-C6	-10.98	88.86	111.42
2	A	480	HAI	C5-C6-C1	8.06	122.69	111.77
2	A	479	HAI	C4-C5-C6	6.91	125.62	111.42
2	A	480	HAI	C3-C2-C1	-4.24	106.03	111.77
2	A	479	HAI	C5-C6-C1	-3.90	106.48	111.77
2	A	480	HAI	C5-C4-C3	2.48	118.56	111.19
2	A	479	HAI	C5-C4-C3	-2.45	103.93	111.19
2	A	479	HAI	C2-C1-N	2.02	117.19	111.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	479	HAI	3	0
2	A	480	HAI	6	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.