



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:30 PM UTC

PDB ID : 1BHW / pdb_00001bhw
Title : LOW TEMPERATURE MIDDLE RESOLUTION STRUCTURE OF XY-LOSE ISOMERASE FROM MASC DATA
Authors : Ramin, M.; Shepard, W.; Fourme, R.; Kahn, R.
Deposited on : 1998-06-10
Resolution : 4.10 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
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

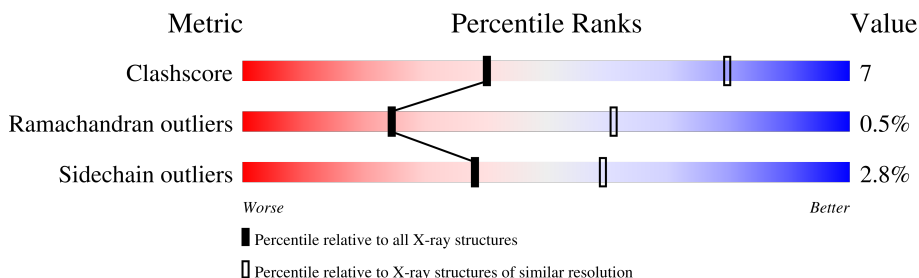
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)

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	393	67% 27% 5% .
1	B	393	69% 25% 5% .
1	C	393	70% 26% .
1	D	393	66% 29% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12248 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			
1	B	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			
1	C	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			
1	D	392	Total	C	N	O	S	0	0	0
			3062	1942	533	583	4			

There are 4 discrepancies between the modelled and reference sequences:

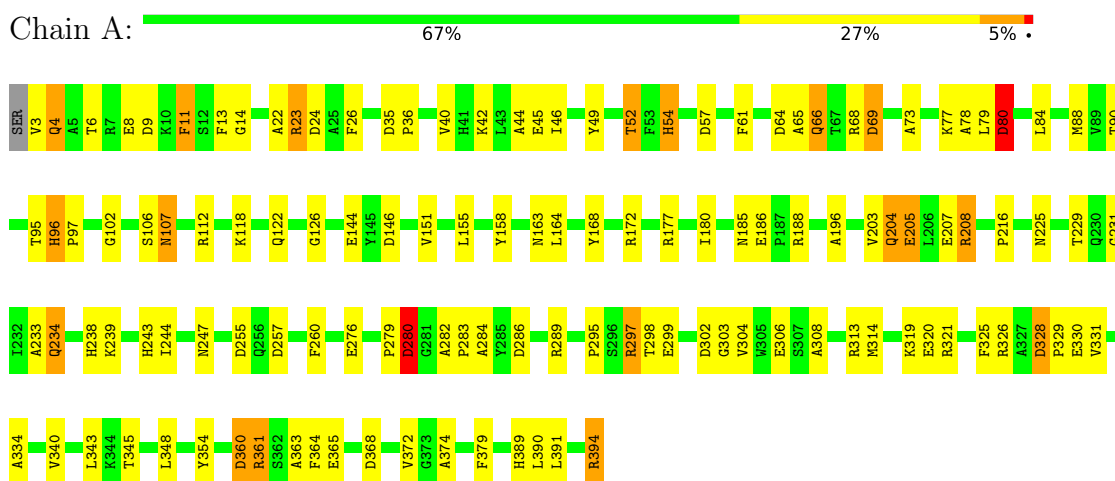
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	ASN	HIS	conflict	UNP P12851
B	220	ASN	HIS	conflict	UNP P12851
C	220	ASN	HIS	conflict	UNP P12851
D	220	ASN	HIS	conflict	UNP P12851

3 Residue-property plots

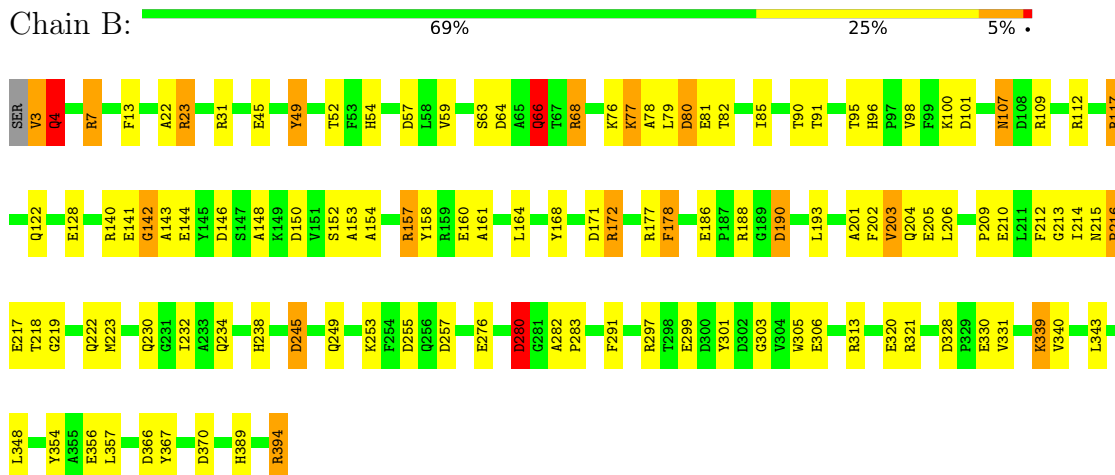
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

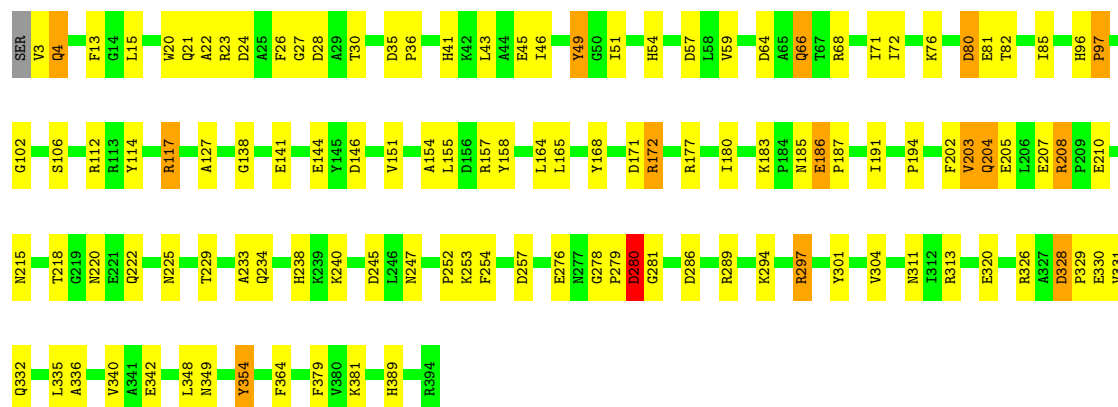


• Molecule 1: XYLOSE ISOMERASE



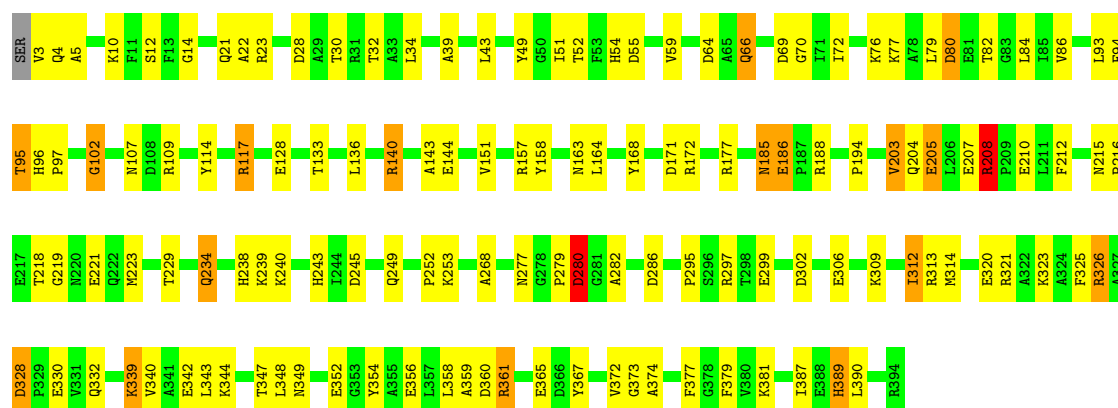
• Molecule 1: XYLOSE ISOMERASE





• Molecule 1: XYLOSE ISOMERASE

Chain D: 66% 29% . .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.91Å 141.91Å 227.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 4.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-4.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.315 , 0.321	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12248	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	2.17	11/3133 (0.4%)	4.11	125/4243 (2.9%)
1	B	2.05	12/3133 (0.4%)	3.72	116/4243 (2.7%)
1	C	2.16	12/3133 (0.4%)	3.94	118/4243 (2.8%)
1	D	1.99	12/3133 (0.4%)	3.63	135/4243 (3.2%)
All	All	2.09	47/12532 (0.4%)	3.86	494/16972 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4	GLN	CG-CD	-44.38	0.41	1.52
1	C	4	GLN	CG-CD	-43.32	0.43	1.52
1	A	66	GLN	CG-CD	-43.30	0.43	1.52
1	C	66	GLN	CG-CD	-43.30	0.43	1.52
1	A	4	GLN	CG-CD	-42.11	0.46	1.52
1	A	66	GLN	CD-OE1	-42.03	0.43	1.23
1	B	4	GLN	CD-OE1	-42.00	0.43	1.23
1	C	4	GLN	CD-OE1	-42.00	0.43	1.23
1	C	66	GLN	CD-OE1	-42.00	0.43	1.23
1	A	4	GLN	CD-OE1	-41.97	0.43	1.23
1	B	66	GLN	CD-NE2	37.76	2.12	1.33
1	B	4	GLN	CG-CD	-36.13	0.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GLN	CG-CD	-36.13	0.61	1.52
1	D	66	GLN	CG-CD	-36.13	0.61	1.52
1	C	66	GLN	CB-CG	-36.11	0.44	1.52
1	D	280	ASP	CB-CG	-35.66	0.62	1.52
1	A	66	GLN	CB-CG	-35.47	0.46	1.52
1	B	66	GLN	CB-CG	-34.77	0.48	1.52
1	D	4	GLN	CB-CG	-34.43	0.49	1.52
1	A	4	GLN	CB-CG	-32.47	0.55	1.52
1	B	4	GLN	CB-CG	-32.38	0.55	1.52
1	A	280	ASP	CB-CG	-32.01	0.72	1.52
1	D	66	GLN	CB-CG	-30.50	0.60	1.52
1	D	280	ASP	CG-OD2	-28.12	0.71	1.25
1	C	4	GLN	CB-CG	-26.64	0.72	1.52
1	B	280	ASP	CG-OD2	-26.26	0.75	1.25
1	B	280	ASP	CB-CG	-25.70	0.87	1.52
1	C	280	ASP	CB-CG	-24.89	0.89	1.52
1	C	280	ASP	CG-OD2	-22.11	0.83	1.25
1	D	66	GLN	CD-NE2	-22.08	0.86	1.33
1	A	66	GLN	CD-NE2	-22.03	0.86	1.33
1	B	4	GLN	CD-NE2	-22.00	0.87	1.33
1	C	4	GLN	CD-NE2	-21.97	0.87	1.33
1	A	4	GLN	CD-NE2	-21.94	0.87	1.33
1	D	66	GLN	CD-OE1	-21.16	0.83	1.23
1	C	280	ASP	CG-OD1	18.45	1.60	1.25
1	D	328	ASP	C-N	-16.97	1.13	1.34
1	D	280	ASP	CG-OD1	15.99	1.55	1.25
1	C	66	GLN	CD-NE2	-14.18	1.03	1.33
1	D	4	GLN	CD-NE2	-11.69	1.08	1.33
1	B	328	ASP	C-N	-9.60	1.21	1.34
1	A	328	ASP	C-N	-9.12	1.20	1.33
1	B	66	GLN	CD-OE1	-8.98	1.06	1.23
1	D	4	GLN	CD-OE1	-8.93	1.06	1.23
1	C	328	ASP	C-N	-7.99	1.15	1.33
1	A	280	ASP	CG-OD2	7.56	1.39	1.25
1	B	280	ASP	CG-OD1	-5.43	1.15	1.25

All (494) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GLN	OE1-CD-NE2	-122.60	0.00	122.60
1	A	66	GLN	OE1-CD-NE2	-122.55	0.05	122.60
1	C	4	GLN	OE1-CD-NE2	-122.55	0.05	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	GLN	OE1-CD-NE2	-122.51	0.09	122.60
1	B	4	GLN	OE1-CD-NE2	-122.51	0.09	122.60
1	C	66	GLN	OE1-CD-NE2	-111.15	11.45	122.60
1	A	280	ASP	CA-CB-CG	-106.59	6.01	112.60
1	C	280	ASP	CA-CB-CG	-97.07	15.53	112.60
1	D	4	GLN	OE1-CD-NE2	-95.82	26.78	122.60
1	D	280	ASP	CA-CB-CG	-93.88	18.72	112.60
1	D	66	GLN	OE1-CD-NE2	-93.06	29.54	122.60
1	B	280	ASP	CA-CB-CG	-53.17	59.43	112.60
1	C	4	GLN	CA-CB-CG	-49.69	14.71	114.10
1	A	66	GLN	CA-CB-CG	-48.07	17.97	114.10
1	D	280	ASP	OD1-CG-OD2	-46.20	12.02	122.90
1	A	66	GLN	CG-CD-NE2	42.34	179.91	116.40
1	C	4	GLN	CG-CD-NE2	42.30	179.86	116.40
1	B	66	GLN	CG-CD-NE2	-41.10	54.75	116.40
1	C	280	ASP	OD1-CG-OD2	-40.15	26.55	122.90
1	A	4	GLN	CA-CB-CG	-39.92	34.27	114.10
1	A	4	GLN	CG-CD-NE2	39.02	174.93	116.40
1	B	280	ASP	OD1-CG-OD2	-39.02	29.26	122.90
1	D	66	GLN	CA-CB-CG	-37.06	39.97	114.10
1	D	4	GLN	CB-CG-CD	36.59	174.81	112.60
1	D	4	GLN	CG-CD-NE2	35.37	169.45	116.40
1	A	280	ASP	OD1-CG-OD2	-34.93	39.07	122.90
1	C	66	GLN	CG-CD-NE2	34.73	168.50	116.40
1	D	4	GLN	CA-CB-CG	-34.51	45.09	114.10
1	B	66	GLN	CG-CD-OE1	-33.02	54.75	120.80
1	A	66	GLN	CB-CG-CD	32.50	167.86	112.60
1	A	4	GLN	CB-CG-CD	30.42	164.31	112.60
1	D	66	GLN	CB-CG-CD	30.26	164.04	112.60
1	A	66	GLN	CG-CD-OE1	29.55	179.89	120.80
1	C	66	GLN	CA-CB-CG	-29.55	55.01	114.10
1	C	66	GLN	CG-CD-OE1	29.55	179.89	120.80
1	C	4	GLN	CG-CD-OE1	29.51	179.81	120.80
1	B	4	GLN	CG-CD-NE2	29.40	160.50	116.40
1	C	66	GLN	CB-CG-CD	28.55	161.14	112.60
1	B	66	GLN	CA-CB-CG	-28.00	58.11	114.10
1	B	4	GLN	CA-CB-CG	-27.86	58.38	114.10
1	A	4	GLN	CG-CD-OE1	27.11	175.01	120.80
1	D	328	ASP	O-C-N	25.10	144.44	121.35
1	B	280	ASP	CB-CG-OD2	22.98	171.25	118.40
1	C	280	ASP	CB-CG-OD2	22.29	169.67	118.40
1	D	280	ASP	CB-CG-OD1	20.13	164.69	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	GLN	CG-CD-OE1	19.89	160.58	120.80
1	B	66	GLN	CB-CG-CD	19.71	146.11	112.60
1	A	80	ASP	CA-CB-CG	-18.36	94.24	112.60
1	C	328	ASP	O-C-N	17.28	136.00	121.31
1	D	328	ASP	CA-C-N	-16.67	101.52	119.19
1	D	328	ASP	C-N-CA	-16.67	101.52	119.19
1	D	204	GLN	OE1-CD-NE2	-15.80	106.80	122.60
1	D	66	GLN	CG-CD-OE1	-15.36	90.08	120.80
1	D	280	ASP	CB-CG-OD2	15.21	153.39	118.40
1	B	328	ASP	O-C-N	14.63	135.91	121.28
1	B	204	GLN	OE1-CD-NE2	-14.21	108.39	122.60
1	A	328	ASP	O-C-N	14.11	133.90	121.20
1	A	280	ASP	CB-CG-OD2	-13.83	86.59	118.40
1	D	4	GLN	CG-CD-OE1	13.24	147.28	120.80
1	C	280	ASP	CB-CG-OD1	10.77	143.17	118.40
1	A	204	GLN	OE1-CD-NE2	-10.58	112.02	122.60
1	B	280	ASP	CB-CG-OD1	10.49	142.53	118.40
1	D	172	ARG	CD-NE-CZ	10.35	138.89	124.40
1	C	204	GLN	OE1-CD-NE2	-10.01	112.59	122.60
1	A	286	ASP	CA-CB-CG	-9.75	102.85	112.60
1	D	80	ASP	CA-CB-CG	-9.26	103.34	112.60
1	B	328	ASP	CA-C-N	-9.23	108.81	119.05
1	B	328	ASP	C-N-CA	-9.23	108.81	119.05
1	C	80	ASP	CA-CB-CG	-9.18	103.42	112.60
1	B	117	ARG	NE-CZ-NH1	8.86	130.36	121.50
1	B	394	ARG	NE-CZ-NH2	-8.52	111.53	119.20
1	D	328	ASP	CA-CB-CG	8.38	120.98	112.60
1	A	172	ARG	CD-NE-CZ	8.38	136.13	124.40
1	A	244	ILE	CA-C-O	-8.38	111.94	120.90
1	A	320	GLU	CB-CG-CD	8.29	126.68	112.60
1	B	245	ASP	CA-CB-CG	8.25	120.85	112.60
1	A	188	ARG	CD-NE-CZ	8.24	135.94	124.40
1	D	54	HIS	N-CA-C	-8.17	97.32	110.32
1	C	4	GLN	CB-CG-CD	-8.14	98.75	112.60
1	A	107	ASN	CA-CB-CG	8.12	120.72	112.60
1	C	64	ASP	CA-CB-CG	-8.05	104.55	112.60
1	A	26	PHE	CA-C-O	-8.03	110.01	119.48
1	C	185	ASN	OD1-CG-ND2	-8.02	114.58	122.60
1	C	229	THR	CA-CB-OG1	-8.02	97.58	109.60
1	B	142	GLY	CA-C-O	-7.99	115.39	120.91
1	B	95	THR	N-CA-C	7.93	119.83	111.03
1	B	172	ARG	NE-CZ-NH1	7.89	129.40	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	THR	N-CA-C	7.67	119.42	111.14
1	C	54	HIS	N-CA-C	-7.66	99.18	110.52
1	C	24	ASP	CA-CB-CG	7.60	120.20	112.60
1	B	13	PHE	CA-CB-CG	7.54	121.34	113.80
1	D	286	ASP	CA-C-O	-7.50	110.63	119.48
1	C	28	ASP	CA-CB-CG	7.47	120.07	112.60
1	D	313	ARG	NE-CZ-NH2	7.45	125.91	119.20
1	B	394	ARG	N-CA-CB	7.45	123.16	110.50
1	B	150	ASP	CA-CB-CG	-7.40	105.20	112.60
1	D	171	ASP	CA-C-O	-7.36	112.62	120.42
1	D	188	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	A	95	THR	N-CA-C	7.25	118.97	111.14
1	A	319	LYS	CA-C-O	7.22	128.63	120.90
1	D	349	ASN	CA-CB-CG	-7.21	105.39	112.60
1	D	377	PHE	CA-C-O	-7.21	110.93	119.15
1	B	117	ARG	NE-CZ-NH2	-7.18	112.73	119.20
1	C	328	ASP	CA-C-N	-7.16	110.89	119.84
1	C	328	ASP	C-N-CA	-7.16	110.89	119.84
1	C	57	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	79	LEU	CA-C-O	7.13	128.11	120.55
1	C	146	ASP	CA-C-O	-7.09	113.03	120.55
1	B	141	GLU	CB-CG-CD	7.08	124.63	112.60
1	C	15	LEU	CA-C-O	7.04	128.01	120.55
1	B	4	GLN	CB-CG-CD	-7.03	100.64	112.60
1	A	394	ARG	NH1-CZ-NH2	7.03	128.44	119.30
1	C	222	GLN	OE1-CD-NE2	-7.00	115.61	122.60
1	D	54	HIS	N-CA-CB	6.99	121.80	110.41
1	B	82	THR	CA-C-O	-6.98	111.10	119.27
1	D	389	HIS	CA-CB-CG	-6.95	106.85	113.80
1	D	342	GLU	CB-CG-CD	6.95	124.42	112.60
1	D	10	LYS	CB-CA-C	-6.95	102.03	111.89
1	D	144	GLU	N-CA-C	-6.93	105.10	113.97
1	D	204	GLN	CB-CG-CD	6.93	124.38	112.60
1	B	161	ALA	CA-C-O	-6.92	113.09	120.42
1	A	379	PHE	CA-CB-CG	6.90	120.70	113.80
1	C	354	TYR	CA-C-O	-6.88	113.26	120.55
1	B	80	ASP	CA-CB-CG	-6.84	105.76	112.60
1	C	304	VAL	CA-C-O	-6.84	113.92	121.17
1	A	13	PHE	CA-C-O	-6.76	113.22	121.06
1	D	286	ASP	CA-CB-CG	-6.76	105.84	112.60
1	D	52	THR	CA-C-O	-6.75	113.75	121.58
1	A	26	PHE	O-C-N	6.72	130.32	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	278	GLY	CA-C-N	6.68	128.19	119.84
1	C	278	GLY	C-N-CA	6.68	128.19	119.84
1	C	191	ILE	CA-CB-CG2	6.67	121.83	110.50
1	D	55	ASP	O-C-N	6.66	129.02	122.09
1	C	340	VAL	CB-CA-C	6.65	120.39	111.88
1	B	172	ARG	NE-CZ-NH2	-6.65	113.22	119.20
1	B	257	ASP	CA-C-O	-6.64	113.88	121.65
1	B	157	ARG	NE-CZ-NH1	6.63	128.13	121.50
1	B	85	ILE	CA-C-O	-6.63	115.36	121.72
1	D	239	LYS	CB-CA-C	-6.63	103.34	111.82
1	C	389	HIS	CA-CB-CG	-6.62	107.18	113.80
1	C	208	ARG	CD-NE-CZ	-6.61	115.14	124.40
1	D	28	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	297	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	C	71	ILE	O-C-N	6.59	128.37	121.91
1	B	77	LYS	O-C-N	6.57	129.19	122.09
1	B	68	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	D	95	THR	O-C-N	6.56	129.18	122.09
1	D	151	VAL	CA-C-O	6.54	127.75	120.95
1	C	247	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	D	151	VAL	N-CA-C	6.53	117.28	110.62
1	C	194	PRO	N-CA-C	6.52	122.01	113.86
1	C	81	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	118	LYS	CA-C-N	6.48	128.86	120.56
1	A	118	LYS	C-N-CA	6.48	128.86	120.56
1	D	14	GLY	N-CA-C	-6.48	103.29	112.37
1	A	180	ILE	N-CA-CB	6.47	117.59	110.53
1	C	177	ARG	N-CA-CB	6.46	121.08	110.69
1	D	64	ASP	CA-CB-CG	-6.45	106.15	112.60
1	A	61	PHE	CA-C-O	-6.43	114.52	120.95
1	B	320	GLU	CB-CG-CD	6.43	123.52	112.60
1	B	389	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	231	GLY	CA-C-N	6.42	129.54	120.42
1	A	231	GLY	C-N-CA	6.42	129.54	120.42
1	C	180	ILE	N-CA-CB	6.42	117.53	110.53
1	B	313	ARG	CA-C-N	6.42	128.79	120.44
1	B	313	ARG	C-N-CA	6.42	128.79	120.44
1	D	79	LEU	CA-C-O	6.42	127.35	120.55
1	A	229	THR	CA-CB-OG1	-6.41	99.98	109.60
1	A	14	GLY	N-CA-C	-6.41	103.40	112.37
1	D	313	ARG	N-CA-CB	6.41	119.30	110.01
1	C	185	ASN	O-C-N	6.41	129.70	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	LEU	CA-C-O	-6.40	113.78	121.34
1	A	11	PHE	CA-C-O	-6.40	113.40	120.69
1	D	64	ASP	N-CA-C	-6.39	102.56	110.41
1	B	45	GLU	CB-CG-CD	6.38	123.45	112.60
1	A	394	ARG	CA-CB-CG	6.38	126.86	114.10
1	C	313	ARG	CD-NE-CZ	6.37	133.32	124.40
1	D	218	THR	CA-C-O	-6.36	114.08	121.07
1	D	109	ARG	CD-NE-CZ	6.35	133.29	124.40
1	A	57	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	68	ARG	CD-NE-CZ	6.33	133.26	124.40
1	D	253	LYS	CA-C-O	-6.32	114.36	121.25
1	A	243	HIS	CA-CB-CG	6.32	120.12	113.80
1	C	165	LEU	O-C-N	6.31	128.81	122.12
1	A	328	ASP	CA-C-N	-6.30	112.16	119.47
1	A	328	ASP	C-N-CA	-6.30	112.16	119.47
1	C	331	VAL	N-CA-C	-6.28	104.62	110.53
1	A	204	GLN	CB-CG-CD	6.28	123.27	112.60
1	D	299	GLU	N-CA-C	6.27	120.14	110.42
1	B	90	THR	CA-CB-OG1	-6.27	100.20	109.60
1	A	244	ILE	O-C-N	6.26	130.35	123.09
1	C	328	ASP	CA-CB-CG	6.25	118.85	112.60
1	D	302	ASP	CA-C-O	-6.23	114.28	120.70
1	C	202	PHE	CA-C-N	6.23	128.99	120.46
1	C	202	PHE	C-N-CA	6.23	128.99	120.46
1	A	295	PRO	N-CA-C	-6.22	101.40	110.80
1	B	213	GLY	O-C-N	6.22	130.79	122.70
1	B	91	THR	CA-C-O	-6.22	113.98	120.70
1	C	172	ARG	CD-NE-CZ	-6.21	115.70	124.40
1	D	143	ALA	N-CA-CB	-6.21	102.13	111.56
1	D	326	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	C	13	PHE	CA-C-O	-6.18	113.89	121.06
1	A	313	ARG	N-CA-CB	-6.16	101.07	110.01
1	B	54	HIS	N-CA-C	-6.16	100.52	110.32
1	B	178	PHE	O-C-N	6.15	130.62	123.30
1	A	126	GLY	CA-C-N	6.14	128.51	120.28
1	A	126	GLY	C-N-CA	6.14	128.51	120.28
1	B	140	ARG	NE-CZ-NH2	-6.14	113.67	119.20
1	C	257	ASP	CA-C-O	-6.14	114.46	121.65
1	D	207	GLU	CA-CB-CG	6.14	126.38	114.10
1	A	257	ASP	CA-C-O	-6.12	114.49	121.65
1	D	243	HIS	CA-C-O	-6.11	114.90	121.38
1	D	136	LEU	CA-C-O	-6.10	114.00	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	GLN	CB-CG-CD	-6.10	102.24	112.60
1	C	281	GLY	N-CA-C	-6.08	98.77	113.18
1	B	144	GLU	N-CA-C	-6.08	106.41	113.88
1	D	216	PRO	CA-C-O	-6.08	114.26	121.67
1	C	117	ARG	NE-CZ-NH1	6.07	127.57	121.50
1	A	69	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	44	ALA	CA-C-O	6.05	126.96	120.55
1	C	304	VAL	O-C-N	6.05	127.84	121.91
1	A	276	GLU	N-CA-C	6.05	120.85	112.45
1	A	180	ILE	CB-CA-C	-6.04	103.30	111.15
1	B	146	ASP	CA-C-O	-6.03	114.16	120.55
1	C	379	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	394	ARG	CD-NE-CZ	-6.02	115.97	124.40
1	D	374	ALA	CA-C-O	-6.01	112.03	119.18
1	B	52	THR	CA-C-O	-6.00	114.62	121.58
1	A	80	ASP	OD1-CG-OD2	5.99	137.26	122.90
1	A	122	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	C	138	GLY	CA-C-N	5.98	127.61	120.14
1	C	138	GLY	C-N-CA	5.98	127.61	120.14
1	A	326	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	D	239	LYS	O-C-N	5.97	129.41	122.67
1	A	334	ALA	CA-C-O	-5.95	114.11	120.42
1	A	8	GLU	CA-CB-CG	-5.95	102.20	114.10
1	B	77	LYS	CB-CA-C	-5.95	101.50	110.90
1	B	57	ASP	N-CA-C	-5.94	104.38	111.69
1	D	133	THR	CA-CB-OG1	-5.94	100.70	109.60
1	B	96	HIS	CA-C-O	-5.93	114.00	120.17
1	D	349	ASN	O-C-N	5.93	127.88	121.60
1	D	245	ASP	CA-CB-CG	5.92	118.52	112.60
1	C	207	GLU	CA-C-O	-5.92	114.61	120.70
1	B	276	GLU	N-CA-C	5.91	120.62	113.41
1	C	311	ASN	O-C-N	5.88	128.13	122.07
1	D	342	GLU	CG-CD-OE2	5.88	131.91	118.40
1	C	157	ARG	CA-C-O	-5.87	113.22	119.97
1	B	31	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	C	172	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	D	212	PHE	N-CA-C	5.87	118.97	109.40
1	B	107	ASN	N-CA-C	-5.85	104.90	111.28
1	A	78	ALA	CA-C-O	-5.85	114.35	120.55
1	A	394	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	B	23	ARG	N-CA-C	-5.85	99.00	108.41
1	D	55	ASP	CA-CB-CG	5.85	118.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	LEU	O-C-N	5.84	128.31	122.12
1	B	57	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	364	PHE	CA-C-N	5.83	128.41	120.54
1	A	364	PHE	C-N-CA	5.83	128.41	120.54
1	C	45	GLU	CA-CB-CG	5.82	125.73	114.10
1	B	331	VAL	N-CA-C	-5.81	104.85	110.72
1	D	312	ILE	CA-C-O	-5.78	114.72	120.85
1	B	190	ASP	N-CA-CB	5.78	120.52	110.81
1	A	158	TYR	CA-C-N	5.77	127.94	120.44
1	A	158	TYR	C-N-CA	5.77	127.94	120.44
1	A	216	PRO	CA-C-O	-5.76	114.64	121.67
1	C	23	ARG	N-CA-C	-5.76	99.13	108.41
1	A	205	GLU	CG-CD-OE2	5.75	131.63	118.40
1	A	389	HIS	CA-CB-CG	-5.75	108.05	113.80
1	B	291	PHE	CA-C-O	-5.75	114.43	120.58
1	D	203	VAL	CA-CB-CG1	5.74	120.16	110.40
1	B	79	LEU	CA-C-O	5.74	126.63	120.55
1	D	240	LYS	CA-C-O	-5.73	112.72	119.48
1	B	313	ARG	CB-CA-C	5.73	120.30	110.79
1	D	314	MET	N-CA-CB	5.73	118.47	109.94
1	A	54	HIS	CA-C-O	-5.72	114.53	121.28
1	C	41	HIS	CA-CB-CG	-5.72	108.08	113.80
1	D	32	THR	CA-CB-OG1	-5.72	101.02	109.60
1	A	374	ALA	CA-C-O	-5.72	112.38	119.18
1	C	276	GLU	CG-CD-OE2	5.71	131.53	118.40
1	D	203	VAL	CB-CA-C	5.70	119.51	112.04
1	D	140	ARG	NH1-CZ-NH2	5.70	126.71	119.30
1	A	284	ALA	N-CA-C	-5.68	106.18	113.23
1	D	234	GLN	CA-C-O	-5.68	114.40	120.42
1	D	358	LEU	CA-C-O	5.68	126.52	120.10
1	D	328	ASP	C-N-CD	5.67	148.27	125.00
1	C	286	ASP	CA-CB-CG	-5.67	106.93	112.60
1	D	86	VAL	O-C-N	5.67	127.56	121.10
1	C	141	GLU	CB-CG-CD	5.66	122.23	112.60
1	D	194	PRO	N-CA-C	5.64	120.96	113.57
1	C	328	ASP	CB-CA-C	5.63	118.51	109.51
1	B	177	ARG	CA-C-O	-5.62	114.81	121.16
1	D	30	THR	O-C-N	5.61	128.82	122.20
1	B	356	GLU	CA-C-O	-5.61	114.47	120.42
1	C	349	ASN	N-CA-C	-5.60	102.06	110.24
1	B	122	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	D	306	GLU	N-CA-C	-5.59	105.10	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLU	CA-CB-CG	5.59	125.28	114.10
1	A	57	ASP	CA-C-O	-5.59	114.04	120.24
1	A	304	VAL	CA-C-O	-5.59	115.25	121.17
1	A	308	ALA	N-CA-C	-5.59	105.11	111.14
1	A	80	ASP	O-C-N	5.58	127.83	122.03
1	C	172	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	D	140	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	A	172	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	A	57	ASP	N-CA-CB	5.57	118.50	110.20
1	D	320	GLU	CA-CB-CG	5.57	125.24	114.10
1	B	202	PHE	CA-C-N	5.57	129.26	120.47
1	B	202	PHE	C-N-CA	5.57	129.26	120.47
1	C	15	LEU	O-C-N	-5.57	116.22	122.12
1	B	305	TRP	CA-CB-CG	-5.56	103.04	113.60
1	D	117	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	B	158	TYR	N-CA-C	-5.56	105.14	111.14
1	D	210	GLU	CB-CG-CD	5.55	122.04	112.60
1	C	245	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	10	LYS	O-C-N	5.55	129.43	122.55
1	C	158	TYR	N-CA-C	-5.54	105.32	111.36
1	B	63	SER	O-C-N	5.54	129.67	123.19
1	A	158	TYR	CA-C-O	5.54	126.40	120.70
1	D	325	PHE	CA-C-O	5.54	126.82	120.90
1	B	215	ASN	CA-CB-CG	-5.53	107.07	112.60
1	A	255	ASP	CB-CA-C	5.53	119.07	110.67
1	B	299	GLU	N-CA-C	5.52	119.06	110.17
1	B	216	PRO	CA-C-O	-5.51	114.94	121.67
1	C	21	GLN	CA-C-N	5.51	130.40	122.35
1	C	21	GLN	C-N-CA	5.51	130.40	122.35
1	B	201	ALA	CA-C-N	5.50	127.60	120.44
1	B	201	ALA	C-N-CA	5.50	127.60	120.44
1	A	96	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	107	ASN	N-CA-CB	5.49	118.19	110.12
1	D	69	ASP	CA-C-N	5.49	125.92	119.94
1	D	69	ASP	C-N-CA	5.49	125.92	119.94
1	B	96	HIS	CA-CB-CG	-5.48	108.32	113.80
1	D	177	ARG	N-CA-C	-5.48	100.47	109.40
1	C	240	LYS	CA-C-O	-5.47	113.02	119.48
1	B	370	ASP	CA-C-O	-5.47	114.75	120.55
1	A	177	ARG	N-CA-C	-5.46	100.50	109.40
1	D	171	ASP	O-C-N	5.46	128.38	122.15
1	A	73	ALA	CA-C-N	5.46	126.00	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ALA	C-N-CA	5.46	126.00	120.00
1	A	394	ARG	NE-CZ-NH2	-5.45	114.30	119.20
1	B	54	HIS	N-CA-CB	5.45	119.29	110.41
1	C	127	ALA	CA-C-N	5.45	127.58	120.28
1	C	127	ALA	C-N-CA	5.45	127.58	120.28
1	D	367	TYR	CA-C-O	-5.45	114.48	120.69
1	C	210	GLU	CB-CG-CD	5.44	121.85	112.60
1	C	320	GLU	CB-CG-CD	5.43	121.84	112.60
1	C	26	PHE	CA-C-O	-5.42	113.49	119.78
1	A	102	GLY	O-C-N	5.42	128.90	123.48
1	A	188	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	A	340	VAL	O-C-N	5.40	127.11	121.87
1	B	204	GLN	CG-CD-OE1	5.40	131.59	120.80
1	A	260	PHE	CA-CB-CG	-5.38	108.42	113.80
1	D	163	ASN	O-C-N	5.38	127.82	122.12
1	A	297	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	D	133	THR	O-C-N	5.37	129.82	123.27
1	D	277	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	A	340	VAL	CA-C-O	-5.36	115.37	120.95
1	C	215	ASN	CA-CB-CG	-5.36	107.24	112.60
1	D	185	ASN	CA-C-O	-5.36	115.54	121.28
1	D	328	ASP	CB-CA-C	5.36	117.10	109.38
1	B	218	THR	CA-CB-OG1	-5.36	101.57	109.60
1	D	204	GLN	CG-CD-NE2	5.36	124.43	116.40
1	B	340	VAL	CB-CA-C	5.35	118.73	111.88
1	B	202	PHE	O-C-N	-5.35	116.56	122.07
1	D	328	ASP	CA-C-O	5.35	123.28	119.32
1	C	66	GLN	N-CA-CB	5.35	117.76	110.01
1	C	207	GLU	CG-CD-OE1	5.34	130.69	118.40
1	B	253	LYS	CA-C-O	-5.34	115.39	120.94
1	D	215	ASN	CA-CB-CG	-5.33	107.27	112.60
1	B	366	ASP	CA-C-O	-5.33	113.66	119.95
1	B	366	ASP	O-C-N	5.33	128.82	122.26
1	A	45	GLU	CA-C-O	-5.33	114.90	120.55
1	C	289	ARG	CD-NE-CZ	5.33	131.86	124.40
1	D	306	GLU	CB-CA-C	-5.33	102.48	110.90
1	C	301	TYR	CA-C-O	-5.32	114.09	120.10
1	B	109	ARG	N-CA-C	5.32	117.08	111.28
1	D	70	GLY	O-C-N	5.31	127.29	122.19
1	D	205	GLU	CG-CD-OE2	5.31	130.62	118.40
1	B	177	ARG	N-CA-C	-5.31	101.51	109.95
1	A	42	LYS	CB-CG-CD	-5.31	99.09	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	THR	CA-CB-OG1	-5.31	101.64	109.60
1	C	203	VAL	N-CA-CB	-5.29	103.34	110.54
1	A	155	LEU	CB-CA-C	5.29	119.57	110.79
1	D	128	GLU	CA-CB-CG	5.28	124.66	114.10
1	A	196	ALA	CA-C-N	5.27	125.79	119.94
1	A	196	ALA	C-N-CA	5.27	125.79	119.94
1	C	311	ASN	CA-C-O	-5.27	115.28	120.82
1	A	163	ASN	O-C-N	5.26	127.70	122.12
1	C	180	ILE	CB-CA-C	-5.25	104.32	111.15
1	B	339	LYS	CB-CA-C	-5.25	103.22	111.51
1	D	221	GLU	CG-CD-OE1	5.25	130.46	118.40
1	D	309	LYS	CA-C-O	-5.24	114.99	120.55
1	B	13	PHE	CA-C-O	-5.24	114.98	121.06
1	C	15	LEU	CA-C-N	5.24	131.56	121.18
1	C	15	LEU	C-N-CA	5.24	131.56	121.18
1	C	294	LYS	CB-CA-C	-5.24	102.16	110.02
1	D	158	TYR	CA-C-O	5.24	126.32	120.82
1	B	218	THR	CA-C-N	5.23	125.78	119.98
1	B	218	THR	C-N-CA	5.23	125.78	119.98
1	C	354	TYR	O-C-N	5.23	127.66	122.12
1	A	225	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	C	225	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	D	93	LEU	O-C-N	5.22	129.00	121.95
1	D	340	VAL	CB-CA-C	5.22	118.66	111.97
1	A	24	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	303	GLY	N-CA-C	-5.22	106.09	112.77
1	C	155	LEU	CB-CA-C	5.22	119.46	110.79
1	A	234	GLN	CA-C-O	-5.22	115.32	120.70
1	B	188	ARG	CA-C-O	-5.22	115.47	121.47
1	C	28	ASP	O-C-N	5.22	129.06	122.65
1	D	239	LYS	CA-C-O	-5.22	115.19	121.40
1	A	46	ILE	CA-C-O	-5.21	112.77	119.39
1	A	280	ASP	CB-CG-OD1	-5.21	106.42	118.40
1	C	85	ILE	CA-C-O	5.21	126.72	121.72
1	D	55	ASP	CA-C-O	-5.21	115.33	120.90
1	A	52	THR	CA-CB-OG1	-5.21	101.79	109.60
1	B	210	GLU	CB-CG-CD	5.21	121.45	112.60
1	C	158	TYR	CA-CB-CG	5.21	123.27	113.90
1	C	253	LYS	CA-C-O	-5.21	115.57	121.25
1	A	64	ASP	N-CA-C	-5.20	104.01	110.41
1	C	222	GLN	CG-CD-NE2	5.20	124.20	116.40
1	A	243	HIS	CA-C-N	-5.20	114.09	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	HIS	C-N-CA	-5.20	114.09	122.25
1	D	295	PRO	CB-CA-C	5.20	118.19	111.64
1	C	144	GLU	N-CA-CB	5.20	117.89	110.67
1	D	144	GLU	N-CA-CB	5.19	117.89	110.67
1	B	230	GLN	CA-C-O	-5.19	115.05	120.55
1	D	339	LYS	CB-CA-C	-5.18	103.32	111.51
1	A	54	HIS	N-CA-C	-5.18	101.84	110.17
1	A	247	ASN	OD1-CG-ND2	-5.17	117.42	122.60
1	B	7	ARG	CA-CB-CG	-5.17	103.75	114.10
1	C	177	ARG	N-CA-C	-5.17	101.27	109.59
1	A	345	THR	O-C-N	5.16	126.89	121.42
1	A	361	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	C	218	THR	CA-C-N	5.15	125.70	119.98
1	C	218	THR	C-N-CA	5.15	125.70	119.98
1	C	102	GLY	CA-C-O	-5.15	118.61	122.37
1	C	336	ALA	CA-C-O	-5.15	115.40	120.70
1	A	144	GLU	N-CA-CB	5.14	117.81	110.67
1	B	78	ALA	CA-C-O	-5.13	115.11	120.55
1	C	97	PRO	O-C-N	5.13	128.38	122.17
1	A	208	ARG	CA-CB-CG	5.13	124.36	114.10
1	B	112	ARG	CG-CD-NE	5.12	123.27	112.00
1	D	23	ARG	N-CA-C	-5.12	100.17	108.41
1	D	309	LYS	CA-C-N	5.12	127.14	120.28
1	D	309	LYS	C-N-CA	5.12	127.14	120.28
1	D	82	THR	CA-CB-OG1	-5.11	101.93	109.60
1	A	42	LYS	CB-CA-C	-5.11	102.31	110.79
1	D	268	ALA	N-CA-C	-5.10	105.80	111.36
1	B	45	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	286	ASP	CA-C-O	-5.09	113.45	119.05
1	B	255	ASP	N-CA-CB	-5.09	101.89	110.49
1	A	298	THR	CA-CB-CG2	5.09	119.15	110.50
1	B	370	ASP	O-C-N	5.08	127.51	122.12
1	D	361	ARG	CA-CB-CG	5.08	124.27	114.10
1	D	59	VAL	O-C-N	5.08	125.59	120.92
1	B	112	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	B	301	TYR	CA-CB-CG	-5.07	104.77	113.90
1	B	59	VAL	O-C-N	5.07	125.83	121.12
1	B	193	LEU	O-C-N	5.07	127.15	121.32
1	A	107	ASN	N-CA-C	-5.06	105.95	111.82
1	B	321	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	C	80	ASP	OD1-CG-OD2	5.05	135.03	122.90
1	A	146	ASP	CA-C-O	-5.05	115.20	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	N-CA-C	-5.05	99.10	108.24
1	A	302	ASP	O-C-N	5.05	127.27	122.07
1	D	94	PHE	O-C-N	5.05	128.23	121.67
1	B	330	GLU	OE1-CD-OE2	5.04	135.00	122.90
1	C	49	TYR	N-CA-C	-5.04	107.30	113.50
1	C	64	ASP	N-CA-C	-5.04	103.88	110.53
1	C	294	LYS	O-C-N	5.04	126.22	121.38
1	D	102	GLY	CA-C-O	5.04	127.25	122.26
1	A	289	ARG	CA-C-N	5.04	129.29	122.19
1	A	289	ARG	C-N-CA	5.04	129.29	122.19
1	D	77	LYS	CA-C-N	5.04	126.99	120.44
1	D	77	LYS	C-N-CA	5.04	126.99	120.44
1	D	279	PRO	CA-C-O	5.04	126.77	121.03
1	D	313	ARG	CA-CB-CG	5.04	124.17	114.10
1	A	360	ASP	CA-C-N	5.03	127.53	120.28
1	A	360	ASP	C-N-CA	5.03	127.53	120.28
1	C	144	GLU	N-CA-C	-5.03	107.53	113.97
1	B	204	GLN	CB-CG-CD	5.03	121.16	112.60
1	B	232	ILE	N-CA-C	-5.02	105.65	110.72
1	C	97	PRO	CA-C-O	-5.01	111.72	119.64
1	D	249	GLN	CA-CB-CG	5.01	124.13	114.10
1	D	94	PHE	CA-C-O	-5.01	112.22	118.54
1	D	12	SER	CA-C-O	-5.01	115.58	121.44
1	D	80	ASP	N-CA-CB	-5.01	102.75	110.01
1	D	117	ARG	CA-C-O	-5.01	115.24	120.55
1	B	143	ALA	N-CA-CB	-5.01	103.16	111.57
1	D	229	THR	CA-CB-OG1	-5.01	102.09	109.60
1	B	152	SER	O-C-N	-5.01	116.91	122.07
1	D	215	ASN	CB-CG-ND2	5.00	123.91	116.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	A	280	ASP	Sidechain
1	B	172	ARG	Sidechain
1	C	172	ARG	Sidechain
1	D	208	ARG	Sidechain

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	3062	0	2967	62	0
1	B	3062	0	2967	59	0
1	C	3062	0	2964	42	0
1	D	3062	0	2967	62	0
All	All	12248	0	11865	160	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 7.

All (160) 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:66:GLN:CD	1:A:66:GLN:C	1.97	1.31
1:A:66:GLN:CD	1:A:66:GLN:N	1.99	1.20
1:A:66:GLN:CD	1:A:66:GLN:HB2	1.61	1.17
1:A:66:GLN:CD	1:A:66:GLN:HB3	1.69	1.11
1:D:208:ARG:HG2	1:D:208:ARG:HH11	1.27	1.00
1:A:66:GLN:CD	1:A:66:GLN:CB	0.88	0.93
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.18	0.92
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.51	0.91
1:A:66:GLN:CD	1:A:66:GLN:HE22	1.49	0.88
1:A:279:PRO:O	1:A:280:ASP:OD2	1.92	0.87
1:A:66:GLN:CD	1:A:66:GLN:HE21	1.49	0.86
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.19	0.86
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.21	0.84
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.83
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.62	0.79
1:A:66:GLN:CD	1:A:66:GLN:CA	0.72	0.77
1:A:66:GLN:CD	1:A:66:GLN:NE2	0.87	0.77
1:B:354:TYR:CD1	1:D:168:TYR:HD1	2.07	0.73
1:D:326:ARG:O	1:D:332:GLN:NE2	2.24	0.70
1:A:66:GLN:CD	1:A:66:GLN:HA	1.11	0.68
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.76	0.67
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.78	0.66
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLN:CD	1:A:66:GLN:HG2	1.09	0.65
1:A:66:GLN:CD	1:A:66:GLN:HG3	1.09	0.65
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.80	0.65
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.78	0.64
1:A:36:PRO:O	1:A:40:VAL:HG23	1.97	0.63
1:B:164:LEU:HD12	1:D:348:LEU:CD1	2.24	0.63
1:B:354:TYR:CD1	1:D:168:TYR:CD1	2.86	0.62
1:B:154:ALA:CB	1:D:343:LEU:HD21	2.29	0.62
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.82	0.61
1:D:208:ARG:HG2	1:D:208:ARG:NH1	2.04	0.59
1:B:339:LYS:HB2	1:D:107:ASN:HB3	1.85	0.58
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.86	0.58
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.85	0.57
1:B:171:ASP:CB	1:D:354:TYR:OH	2.52	0.57
1:C:59:VAL:HG11	1:C:68:ARG:HG3	1.87	0.56
1:A:168:TYR:HD1	1:C:354:TYR:CD1	2.23	0.56
1:A:354:TYR:CD1	1:C:168:TYR:HD1	2.23	0.56
1:B:107:ASN:HB3	1:D:339:LYS:HB2	1.88	0.55
1:B:164:LEU:CD1	1:D:348:LEU:HD21	2.37	0.55
1:C:72:ILE:O	1:C:76:LYS:HG3	2.06	0.55
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.87	0.55
1:A:391:LEU:HD22	1:D:390:LEU:HD12	1.88	0.54
1:B:153:ALA:HB2	1:D:344:LYS:HG2	1.88	0.54
1:B:77:LYS:O	1:B:80:ASP:HB2	2.08	0.53
1:A:233:ALA:HB1	1:C:151:VAL:HB	1.91	0.53
1:D:328:ASP:OD1	1:D:330:GLU:N	2.33	0.53
1:B:98:VAL:HA	1:D:373:GLY:HA2	1.90	0.53
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.10	0.52
1:A:348:LEU:HD11	1:C:164:LEU:CD1	2.40	0.52
1:B:160:GLU:CD	1:D:347:THR:H	2.18	0.52
1:B:354:TYR:CE1	1:D:168:TYR:HD1	2.28	0.51
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.92	0.51
1:B:3:VAL:HG12	1:B:4:GLN:H	1.77	0.50
1:B:164:LEU:C	1:B:164:LEU:HD23	2.37	0.49
1:C:254:PHE:CD1	1:D:186:GLU:HB2	2.47	0.49
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.94	0.49
1:A:6:THR:O	1:A:9:ASP:HB2	2.13	0.49
1:A:360:ASP:O	1:C:117:ARG:NH1	2.46	0.49
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.95	0.49
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.78	0.49
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:O	1:A:69:ASP:HB2	2.13	0.48
1:C:326:ARG:O	1:C:332:GLN:NE2	2.45	0.48
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.95	0.48
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.95	0.48
1:C:27:GLY:HA2	1:D:95:THR:HA	1.94	0.48
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.49	0.48
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.94	0.48
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.50	0.47
1:B:171:ASP:HB2	1:D:354:TYR:OH	2.14	0.47
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.74	0.47
1:C:106:SER:O	1:C:112:ARG:HD3	2.15	0.47
1:D:321:ARG:HG2	1:D:389:HIS:O	2.15	0.47
1:A:204:GLN:HB2	1:C:204:GLN:OE1	2.15	0.46
1:B:168:TYR:HD1	1:D:354:TYR:CD1	2.34	0.46
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.95	0.46
1:B:64:ASP:OD2	1:B:66:GLN:CD	2.59	0.46
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.50	0.46
1:A:343:LEU:HD21	1:C:154:ALA:HB2	1.98	0.46
1:A:238:HIS:O	1:A:239:LYS:HB2	2.15	0.46
1:A:348:LEU:HD11	1:C:164:LEU:HD12	1.97	0.46
1:C:252:PRO:HB2	1:D:252:PRO:HB2	1.97	0.46
1:A:164:LEU:C	1:A:164:LEU:HD23	2.41	0.45
1:B:348:LEU:HD11	1:D:164:LEU:HD12	1.98	0.45
1:A:368:ASP:O	1:A:372:VAL:HG23	2.17	0.45
1:B:154:ALA:HB2	1:D:343:LEU:CD2	2.41	0.45
1:B:171:ASP:OD2	1:D:354:TYR:OH	2.25	0.45
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.97	0.45
1:B:107:ASN:HB3	1:D:339:LYS:CB	2.46	0.45
1:B:154:ALA:CA	1:D:343:LEU:HD21	2.47	0.45
1:B:101:ASP:CG	1:B:101:ASP:O	2.58	0.45
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.92	0.45
1:A:77:LYS:O	1:A:80:ASP:CB	2.65	0.44
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.13	0.44
1:A:363:ALA:O	1:C:114:TYR:HA	2.17	0.44
1:C:30:THR:HG22	1:D:97:PRO:HB3	1.99	0.44
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.90	0.44
1:A:325:PHE:O	1:A:331:VAL:HG11	2.17	0.44
1:A:354:TYR:OH	1:C:171:ASP:CB	2.66	0.44
1:A:151:VAL:HB	1:C:233:ALA:CB	2.48	0.44
1:A:164:LEU:HD12	1:C:348:LEU:CD1	2.47	0.44
1:A:314:MET:HE1	1:D:387:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:HE2	1:D:373:GLY:O	2.17	0.44
1:B:219:GLY:O	1:B:223:MET:HG3	2.17	0.44
1:B:148:ALA:HB1	1:D:379:PHE:CE1	2.53	0.43
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.84	0.43
1:A:391:LEU:HD22	1:D:390:LEU:O	2.17	0.43
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.99	0.43
1:A:321:ARG:HD3	1:A:390:LEU:HA	2.01	0.43
1:B:357:LEU:O	1:D:117:ARG:HD3	2.19	0.43
1:A:348:LEU:CD1	1:C:164:LEU:HD12	2.49	0.43
1:A:52:THR:HG21	1:A:88:MET:HE3	2.00	0.43
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.54	0.43
1:B:280:ASP:C	1:B:282:ALA:H	2.26	0.42
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.54	0.42
1:B:282:ALA:HB1	1:B:283:PRO:HD2	2.01	0.42
1:B:343:LEU:O	1:D:157:ARG:HD2	2.19	0.42
1:A:233:ALA:CB	1:C:151:VAL:HB	2.49	0.42
1:D:356:GLU:O	1:D:359:ALA:HB3	2.19	0.42
1:B:142:GLY:HA3	1:B:190:ASP:O	2.19	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.42
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.01	0.42
1:C:328:ASP:O	1:C:329:PRO:C	2.61	0.42
1:A:330:GLU:OE1	1:A:394:ARG:NH1	2.52	0.42
1:B:348:LEU:HD11	1:D:164:LEU:CD1	2.50	0.42
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.35	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.89	0.42
1:A:354:TYR:CG	1:C:168:TYR:HD1	2.37	0.42
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.46	0.42
1:D:22:ALA:HB1	1:D:297:ARG:HG3	2.02	0.42
1:C:186:GLU:HA	1:C:187:PRO:HA	1.91	0.41
1:B:206:LEU:O	1:B:209:PRO:HD3	2.19	0.41
1:B:148:ALA:HB1	1:D:379:PHE:CD1	2.55	0.41
1:C:59:VAL:HG21	1:C:68:ARG:HG3	2.02	0.41
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.86	0.41
1:B:367:TYR:CD2	1:D:114:TYR:CD1	3.09	0.41
1:D:72:ILE:O	1:D:76:LYS:HG3	2.21	0.41
1:D:280:ASP:C	1:D:282:ALA:H	2.28	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:D:219:GLY:O	1:D:223:MET:HG3	2.20	0.41
1:A:107:ASN:O	1:C:342:GLU:HB3	2.21	0.41
1:B:117:ARG:NH1	1:D:360:ASP:O	2.54	0.41
1:A:151:VAL:HB	1:C:233:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG23	1:D:372:VAL:HB	2.02	0.41
1:B:157:ARG:HG3	1:D:343:LEU:HD12	2.01	0.41
1:B:164:LEU:CD1	1:D:348:LEU:HD11	2.37	0.41
1:C:183:LYS:HG3	1:C:220:ASN:CG	2.45	0.41
1:C:328:ASP:C	1:C:330:GLU:N	2.78	0.41
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.51	0.41
1:A:65:ALA:C	1:A:66:GLN:HE22	1.63	0.41
1:A:106:SER:O	1:A:112:ARG:HD3	2.21	0.40
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.36	0.40
1:B:214:ILE:HG13	1:B:216:PRO:HD3	2.04	0.40
1:B:217:GLU:HA	1:B:245:ASP:O	2.22	0.40
1:B:339:LYS:CB	1:D:107:ASN:HB3	2.50	0.40
1:A:328:ASP:C	1:A:330:GLU:N	2.76	0.40
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.54	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	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	70
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	70
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	12	46
1	D	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	24	61
All	All	1560/1572 (99%)	1504 (96%)	48 (3%)	8 (0%)	24	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP

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Mol	Chain	Res	Type
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO
1	D	186	GLU
1	D	280	ASP
1	C	364	PHE

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	309/310 (100%)	301 (97%)	8 (3%)	40	61
1	B	309/310 (100%)	301 (97%)	8 (3%)	40	61
1	C	309/310 (100%)	301 (97%)	8 (3%)	40	61
1	D	309/310 (100%)	299 (97%)	10 (3%)	34	56
All	All	1236/1240 (100%)	1202 (97%)	34 (3%)	38	59

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	4	GLN
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	185	ASN
1	A	203	VAL
1	A	208	ARG
1	B	3	VAL
1	B	4	GLN
1	B	49	TYR
1	B	66	GLN
1	B	81	GLU
1	B	203	VAL

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Mol	Chain	Res	Type
1	B	280	ASP
1	B	394	ARG
1	C	3	VAL
1	C	4	GLN
1	C	46	ILE
1	C	49	TYR
1	C	66	GLN
1	C	80	ASP
1	C	203	VAL
1	C	280	ASP
1	D	3	VAL
1	D	49	TYR
1	D	66	GLN
1	D	80	ASP
1	D	84	LEU
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG
1	D	280	ASP
1	D	323	LYS

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	238	HIS
1	B	222	GLN
1	B	238	HIS
1	C	4	GLN
1	C	54	HIS
1	C	185	ASN
1	C	222	GLN
1	C	238	HIS
1	C	250	HIS
1	D	4	GLN
1	D	41	HIS
1	D	54	HIS
1	D	185	ASN
1	D	222	GLN
1	D	238	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	328:ASP	C	329:PRO	N	1.15
1	D	328:ASP	C	329:PRO	N	1.13

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.