



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 AM UTC

PDB ID : 1TRM / pdb_00001trm
Title : THE THREE-DIMENSIONAL STRUCTURE OF ASN102 MUTANT OF TRYPSIN. ROLE OF ASP102 IN SERINE PROTEASE CATALYSIS
Authors : Sprang, S.; Standing, T.; Fletterick, R.J.
Deposited on : 1987-10-21
Resolution : 2.30 Å(reported)

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

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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

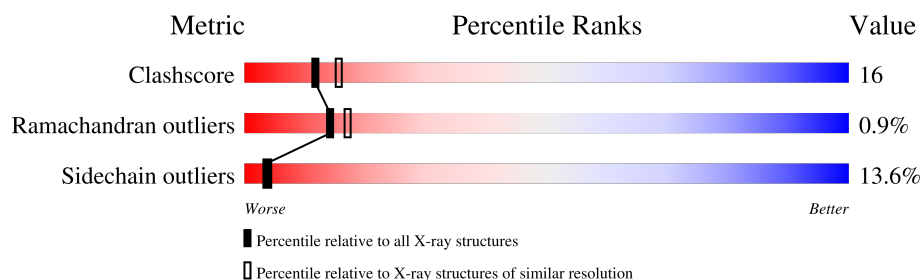
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	223	
1	B	223	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BEN	B	246	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3594 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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1672	1045	288	325	14			
1	B	223	Total	C	N	O	S	0	1	0
			1672	1045	288	325	14			

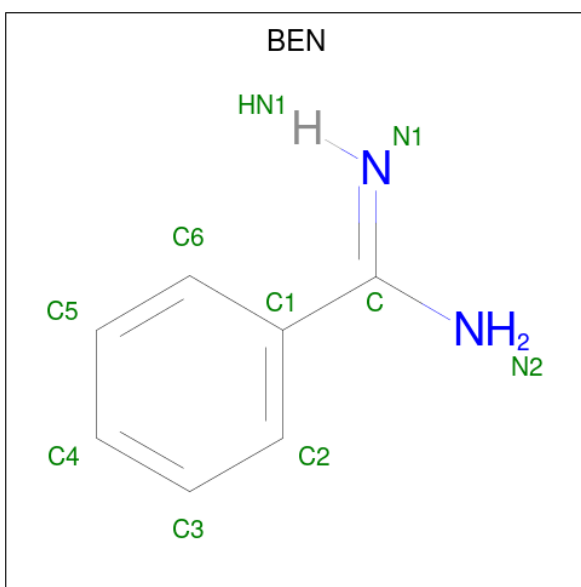
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ASN	ASP	conflict	UNP P00763
B	102	ASN	ASP	conflict	UNP P00763

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is water.

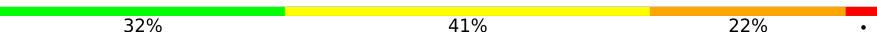
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		
4	B	115	Total	O	0	0
			115	115		

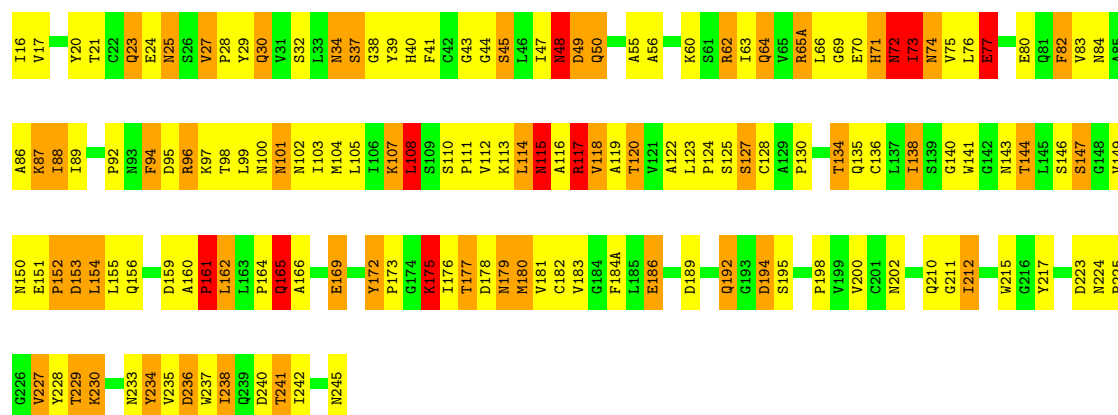
3 Residue-property plots [i](#)

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.

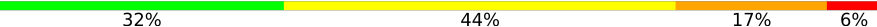
Note EDS was not executed.

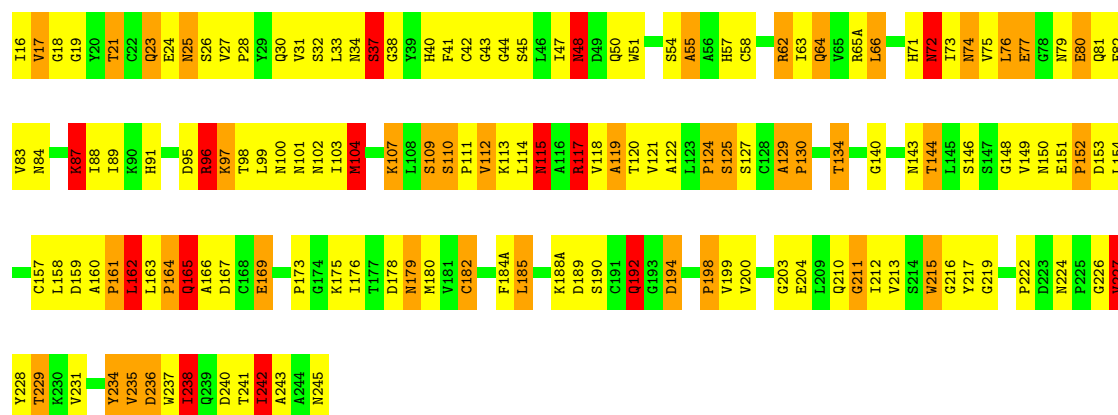
• Molecule 1: TRYPSIN

Chain A: 



• Molecule 1: TRYPSIN

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.40 Å 92.00 Å 127.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3594	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: BEN, CA

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	1.97	31/1708 (1.8%)	2.93	202/2328 (8.7%)
1	B	1.99	38/1708 (2.2%)	2.99	212/2328 (9.1%)
All	All	1.98	69/3416 (2.0%)	2.96	414/4656 (8.9%)

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	2	2
1	B	1	7
All	All	3	9

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	LYS	N-CA	7.53	1.55	1.46
1	B	115	ASN	C-O	7.46	1.31	1.23
1	B	100	ASN	C-O	7.37	1.32	1.23
1	B	89	ILE	C-O	7.34	1.32	1.24
1	A	161	PRO	N-CD	7.15	1.57	1.47
1	A	237	TRP	N-CA	-6.90	1.37	1.46
1	A	123	LEU	C-N	6.78	1.42	1.33
1	B	161	PRO	N-CD	6.75	1.57	1.47
1	B	37	SER	CA-CB	6.61	1.62	1.53
1	A	115	ASN	C-O	6.60	1.31	1.23
1	A	104	MET	N-CA	6.39	1.54	1.45
1	B	83	VAL	CA-CB	6.39	1.64	1.54
1	B	24	GLU	CA-CB	-6.38	1.43	1.53
1	A	111	PRO	N-CD	6.33	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	ILE	N-CA	6.20	1.53	1.46
1	B	245	ASN	C-OXT	6.16	1.35	1.23
1	B	43	GLY	N-CA	6.16	1.49	1.44
1	A	37	SER	C-N	-6.14	1.27	1.34
1	A	235	VAL	C-N	-5.98	1.25	1.33
1	A	43	GLY	N-CA	5.97	1.50	1.44
1	B	104	MET	CA-C	5.94	1.60	1.52
1	B	227	VAL	CA-CB	-5.93	1.47	1.54
1	A	169	GLU	C-O	5.89	1.31	1.24
1	A	24	GLU	CA-CB	-5.85	1.44	1.53
1	A	135	GLN	N-CA	-5.84	1.39	1.46
1	B	121	VAL	CA-C	5.77	1.59	1.52
1	A	63	ILE	N-CA	5.67	1.52	1.46
1	B	87	LYS	N-CA	5.67	1.53	1.46
1	A	140	GLY	N-CA	5.65	1.52	1.45
1	B	194	ASP	CA-CB	-5.64	1.44	1.53
1	A	180	MET	N-CA	5.63	1.52	1.45
1	B	245	ASN	C-O	5.62	1.34	1.23
1	B	140	GLY	N-CA	5.61	1.52	1.45
1	B	104	MET	N-CA	5.57	1.53	1.45
1	B	112	VAL	CA-CB	5.56	1.62	1.54
1	A	40	HIS	ND1-CE1	-5.56	1.26	1.32
1	B	111	PRO	N-CD	5.52	1.55	1.47
1	B	203	GLY	C-N	-5.51	1.26	1.33
1	A	194	ASP	CA-CB	-5.49	1.45	1.53
1	B	182	CYS	N-CA	5.46	1.52	1.46
1	B	110	SER	N-CA	-5.42	1.41	1.45
1	B	130	PRO	N-CD	5.42	1.55	1.47
1	A	107	LYS	N-CA	5.40	1.52	1.46
1	A	147	SER	N-CA	5.35	1.52	1.46
1	A	175	LYS	CA-C	-5.35	1.45	1.52
1	B	122	ALA	C-O	5.33	1.30	1.23
1	A	166	ALA	C-N	-5.32	1.26	1.33
1	B	199	VAL	C-N	-5.32	1.25	1.33
1	A	184(A)	PHE	N-CA	5.30	1.52	1.46
1	A	55	ALA	N-CA	5.29	1.52	1.46
1	A	227	VAL	N-CA	5.26	1.52	1.46
1	B	213	VAL	C-O	5.25	1.29	1.24
1	A	30	GLN	N-CA	5.24	1.52	1.46
1	A	83	VAL	CA-CB	5.22	1.62	1.54
1	A	241	THR	CB-OG1	5.22	1.52	1.43
1	B	245	ASN	CA-CB	5.21	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184(A)	PHE	N-CA	5.21	1.52	1.46
1	B	71	HIS	CA-CB	-5.15	1.44	1.53
1	A	233	ASN	C-N	-5.15	1.26	1.34
1	B	178	ASP	CG-OD2	5.12	1.35	1.25
1	B	18	GLY	C-O	5.10	1.30	1.24
1	A	223	ASP	CG-OD2	5.09	1.35	1.25
1	A	212	ILE	CA-CB	5.08	1.61	1.54
1	B	63	ILE	N-CA	5.08	1.52	1.46
1	B	159	ASP	CA-CB	-5.07	1.46	1.53
1	B	64	GLN	CA-C	5.06	1.58	1.52
1	B	245	ASN	CA-C	5.05	1.63	1.52
1	B	40	HIS	ND1-CE1	-5.03	1.27	1.32
1	B	234	TYR	C-N	-5.00	1.26	1.33

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	PRO	CB-CA-C	15.32	131.23	111.46
1	B	115	ASN	OD1-CG-ND2	-14.70	107.90	122.60
1	B	235	VAL	CA-C-O	14.40	138.78	120.78
1	A	236	ASP	CA-CB-CG	13.91	126.51	112.60
1	B	235	VAL	O-C-N	-12.32	107.17	122.57
1	A	124	PRO	N-CA-CB	-12.26	92.69	103.35
1	B	175	LYS	CA-C-N	12.12	137.51	122.37
1	B	175	LYS	C-N-CA	12.12	137.51	122.37
1	B	241	THR	CA-CB-OG1	-12.11	91.43	109.60
1	B	234	TYR	CA-C-O	-12.06	105.61	119.24
1	B	227	VAL	CB-CA-C	11.62	128.15	110.83
1	B	118	VAL	CA-C-O	11.57	132.66	120.51
1	A	241	THR	CA-CB-OG1	-11.53	92.30	109.60
1	A	82	PHE	CA-CB-CG	11.41	125.21	113.80
1	B	235	VAL	N-CA-CB	-10.79	93.43	111.23
1	B	236	ASP	CA-CB-CG	10.66	123.26	112.60
1	B	96	ARG	NE-CZ-NH1	10.64	132.14	121.50
1	A	127	SER	CA-C-O	-10.50	109.80	121.25
1	A	210	GLN	OE1-CD-NE2	-10.49	112.11	122.60
1	B	115	ASN	CB-CG-OD1	10.48	141.76	120.80
1	A	194	ASP	CA-CB-CG	10.45	123.05	112.60
1	B	210	GLN	OE1-CD-NE2	-10.29	112.31	122.60
1	B	37	SER	N-CA-CB	-10.19	96.77	111.54
1	A	24	GLU	N-CA-CB	10.13	125.19	109.48
1	A	37	SER	CA-C-N	10.03	133.94	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	SER	C-N-CA	10.03	133.94	123.30
1	B	118	VAL	O-C-N	-9.97	113.04	122.71
1	A	27	VAL	CA-CB-CG2	9.96	127.33	110.40
1	B	242	ILE	CA-CB-CG1	9.88	127.20	110.40
1	B	169	GLU	CB-CG-CD	9.81	129.28	112.60
1	A	100	ASN	OD1-CG-ND2	9.79	132.38	122.60
1	B	37	SER	CA-C-N	9.76	134.01	123.08
1	B	37	SER	C-N-CA	9.76	134.01	123.08
1	A	224	ASN	CA-C-O	-9.72	110.58	121.28
1	A	175	LYS	CB-CA-C	9.68	126.25	110.09
1	B	82	PHE	CA-CB-CG	9.65	123.45	113.80
1	B	189	ASP	CA-CB-CG	9.60	122.20	112.60
1	B	100	ASN	OD1-CG-ND2	9.48	132.08	122.60
1	A	236	ASP	CB-CA-C	9.46	128.02	110.70
1	A	96	ARG	CD-NE-CZ	9.36	137.50	124.40
1	A	186	GLU	CB-CG-CD	9.32	128.45	112.60
1	B	152	PRO	CB-CA-C	-9.18	98.93	110.95
1	A	127	SER	CA-C-N	-9.15	107.09	122.64
1	A	127	SER	C-N-CA	-9.15	107.09	122.64
1	A	143	ASN	CA-C-O	9.06	131.16	121.19
1	B	144	THR	CA-CB-CG2	9.03	125.86	110.50
1	B	109	SER	CA-CB-OG	-9.03	93.04	111.10
1	A	245	ASN	OD1-CG-ND2	-9.01	113.59	122.60
1	A	23	GLN	CB-CG-CD	8.92	127.76	112.60
1	B	24	GLU	N-CA-CB	8.90	123.28	109.48
1	A	104	MET	CA-CB-CG	8.87	131.84	114.10
1	B	227	VAL	CA-CB-CG2	8.79	125.35	110.40
1	A	147	SER	O-C-N	-8.79	112.64	123.36
1	A	241	THR	O-C-N	8.67	131.31	122.12
1	A	144	THR	CA-CB-CG2	8.54	125.01	110.50
1	B	240	ASP	N-CA-CB	8.51	122.33	109.91
1	A	124	PRO	CA-N-CD	8.50	123.91	112.00
1	A	241	THR	OG1-CB-CG2	-8.31	92.67	109.30
1	A	176	ILE	CB-CG1-CD1	8.29	131.21	113.80
1	A	236	ASP	CA-C-N	8.27	137.33	121.54
1	A	236	ASP	C-N-CA	8.27	137.33	121.54
1	B	129	ALA	CA-C-N	8.25	129.65	120.66
1	B	129	ALA	C-N-CA	8.25	129.65	120.66
1	B	245	ASN	CA-C-O	-8.25	96.25	121.00
1	A	235	VAL	CA-C-N	8.25	134.68	120.58
1	A	235	VAL	C-N-CA	8.25	134.68	120.58
1	B	95	ASP	CA-C-O	8.23	129.17	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	GLU	CA-C-N	8.16	128.10	120.03
1	B	151	GLU	C-N-CA	8.16	128.10	120.03
1	B	216	GLY	CA-C-O	-8.09	113.73	121.49
1	B	231	VAL	CB-CA-C	8.06	122.59	112.04
1	A	186	GLU	CA-CB-CG	8.03	130.17	114.10
1	A	101	ASN	CA-C-O	-8.03	111.73	121.28
1	A	143	ASN	OD1-CG-ND2	-8.03	114.57	122.60
1	A	224	ASN	O-C-N	8.02	127.73	121.23
1	A	110	SER	CA-C-N	7.95	127.71	119.76
1	A	110	SER	C-N-CA	7.95	127.71	119.76
1	A	73	ILE	CA-CB-CG2	7.95	124.01	110.50
1	B	40	HIS	CA-CB-CG	-7.95	105.86	113.80
1	A	189	ASP	CA-CB-CG	7.91	120.51	112.60
1	B	243	ALA	CA-C-O	-7.91	110.87	119.97
1	B	173	PRO	CB-CA-C	7.91	124.61	111.56
1	B	235	VAL	CA-CB-CG1	-7.87	97.02	110.40
1	A	153	ASP	CA-C-O	-7.82	110.57	119.41
1	A	96	ARG	N-CA-CB	7.78	121.55	110.12
1	B	37	SER	CA-CB-OG	-7.75	95.60	111.10
1	A	161	PRO	O-C-N	7.74	133.09	122.64
1	B	149	VAL	CA-C-O	7.71	128.65	120.48
1	A	123	LEU	CA-C-O	-7.68	112.72	120.63
1	B	237	TRP	CB-CA-C	7.66	123.66	110.79
1	B	125	SER	CA-CB-OG	-7.66	95.78	111.10
1	B	149	VAL	CB-CA-C	7.65	122.23	110.83
1	B	37	SER	CB-CA-C	-7.65	99.25	111.18
1	B	227	VAL	N-CA-CB	7.62	121.61	111.25
1	B	200	VAL	CB-CA-C	7.58	121.15	110.84
1	A	202	ASN	CA-CB-CG	7.54	120.14	112.60
1	A	55	ALA	CA-C-O	-7.54	112.56	120.70
1	B	245	ASN	CB-CA-C	-7.44	95.96	110.10
1	A	48	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	B	104	MET	N-CA-C	-7.35	98.19	109.14
1	A	77	GLU	CG-CD-OE2	-7.34	101.52	118.40
1	A	202	ASN	CA-C-N	7.32	135.76	121.41
1	A	202	ASN	C-N-CA	7.32	135.76	121.41
1	A	27	VAL	CA-C-N	7.31	127.95	119.47
1	A	27	VAL	C-N-CA	7.31	127.95	119.47
1	A	125	SER	N-CA-C	-7.29	104.39	113.28
1	A	227	VAL	CA-CB-CG2	7.24	122.71	110.40
1	A	84	ASN	OD1-CG-ND2	7.22	129.82	122.60
1	B	159	ASP	O-C-N	-7.21	115.01	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ASP	N-CA-CB	-7.17	99.27	110.30
1	A	192	GLN	CG-CD-NE2	7.13	127.10	116.40
1	B	27	VAL	CA-CB-CG2	7.13	122.52	110.40
1	A	117	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	B	194	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	167	ASP	CA-C-O	7.05	127.90	120.42
1	B	103	ILE	O-C-N	7.05	130.76	123.00
1	A	242	ILE	CA-CB-CG1	7.04	122.36	110.40
1	B	104	MET	N-CA-CB	-7.00	100.28	111.62
1	B	117	ARG	N-CA-CB	7.00	120.82	110.53
1	A	102	ASN	CB-CA-C	6.97	122.99	111.83
1	B	120	THR	N-CA-CB	-6.97	100.48	110.44
1	B	99	LEU	CA-C-O	6.96	128.13	120.12
1	A	153	ASP	N-CA-C	-6.95	104.94	113.41
1	A	39	TYR	CA-C-N	6.87	130.46	120.71
1	A	39	TYR	C-N-CA	6.87	130.46	120.71
1	A	34	ASN	CB-CA-C	6.85	121.06	109.75
1	B	190	SER	CB-CA-C	6.83	121.78	109.83
1	A	127	SER	CB-CA-C	-6.82	98.28	111.78
1	A	120	THR	OG1-CB-CG2	6.81	122.92	109.30
1	A	48	ASN	O-C-N	-6.78	114.92	122.72
1	A	230	LYS	CA-C-N	6.76	130.07	120.53
1	A	230	LYS	C-N-CA	6.76	130.07	120.53
1	B	151	GLU	CB-CG-CD	6.75	124.08	112.60
1	B	30	GLN	O-C-N	-6.73	114.67	122.89
1	B	143	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	B	76	LEU	CB-CA-C	6.67	120.26	110.26
1	A	245	ASN	CB-CG-OD1	6.66	134.12	120.80
1	A	30	GLN	CA-CB-CG	6.65	127.40	114.10
1	A	159	ASP	O-C-N	-6.62	115.52	123.13
1	A	24	GLU	CA-CB-CG	6.60	127.30	114.10
1	B	21	THR	N-CA-CB	6.60	119.87	109.71
1	B	30	GLN	CA-C-O	6.56	128.51	121.16
1	B	192	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	A	149	VAL	CA-C-N	6.55	130.50	121.33
1	A	149	VAL	C-N-CA	6.55	130.50	121.33
1	A	210	GLN	CA-C-O	6.54	126.33	119.14
1	B	222	PRO	CB-CA-C	6.53	119.87	111.64
1	B	23	GLN	CB-CG-CD	6.52	123.68	112.60
1	A	69	GLY	N-CA-C	-6.50	104.89	114.90
1	B	80	GLU	CA-CB-CG	6.50	127.10	114.10
1	B	75	VAL	CA-C-N	6.50	130.59	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	VAL	C-N-CA	6.50	130.59	121.24
1	B	150	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	A	88	ILE	CB-CG1-CD1	6.47	127.39	113.80
1	B	215	TRP	N-CA-C	6.46	117.10	108.38
1	B	33	LEU	N-CA-CB	6.45	120.39	109.87
1	B	134	THR	CA-CB-OG1	-6.45	99.93	109.60
1	B	27	VAL	CA-C-N	6.42	126.11	119.56
1	B	27	VAL	C-N-CA	6.42	126.11	119.56
1	B	176	ILE	N-CA-CB	6.42	118.32	111.00
1	A	117	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	94	PHE	CB-CG-CD2	-6.40	109.82	120.70
1	B	235	VAL	N-CA-C	6.39	122.63	109.34
1	A	147	SER	CA-C-N	6.38	132.85	122.00
1	A	147	SER	C-N-CA	6.38	132.85	122.00
1	B	74	ASN	N-CA-C	6.37	121.83	113.30
1	A	44	GLY	O-C-N	6.35	131.44	123.56
1	B	21	THR	O-C-N	6.34	130.94	122.96
1	B	124	PRO	CA-C-O	6.33	128.56	121.34
1	B	228	TYR	CA-C-O	6.31	127.91	120.66
1	A	146	SER	CB-CA-C	6.31	121.57	110.85
1	B	112	VAL	CG1-CB-CG2	-6.30	96.93	110.80
1	A	24	GLU	N-CA-C	6.30	119.50	110.24
1	A	60	LYS	N-CA-CB	6.30	122.53	111.13
1	A	227	VAL	N-CA-CB	6.29	119.81	111.25
1	A	179	ASN	OD1-CG-ND2	6.28	128.88	122.60
1	A	94	PHE	N-CA-CB	6.27	119.20	109.48
1	B	47	ILE	O-C-N	-6.27	116.08	122.23
1	B	237	TRP	CB-CG-CD1	6.27	136.30	126.90
1	A	195	SER	CA-C-N	6.27	134.09	121.93
1	A	195	SER	C-N-CA	6.27	134.09	121.93
1	B	148	GLY	CA-C-O	6.25	126.95	122.45
1	A	25	ASN	OD1-CG-ND2	6.24	128.84	122.60
1	A	169	GLU	CB-CG-CD	6.24	123.21	112.60
1	A	118	VAL	CB-CA-C	6.24	118.15	110.73
1	B	84	ASN	CB-CG-ND2	-6.23	107.05	116.40
1	B	117	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	B	124	PRO	N-CA-C	6.22	120.84	111.14
1	B	153	ASP	CA-C-O	-6.22	112.42	120.00
1	A	86	ALA	N-CA-C	-6.20	105.84	113.41
1	A	99	LEU	CB-CA-C	6.20	121.61	111.26
1	B	96	ARG	N-CA-CB	6.18	119.31	110.16
1	A	151	GLU	N-CA-CB	-6.15	102.17	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	PHE	CB-CA-C	6.15	117.09	109.16
1	A	116	ALA	CA-C-N	6.14	132.54	121.92
1	A	116	ALA	C-N-CA	6.14	132.54	121.92
1	A	149	VAL	CA-C-O	6.14	126.83	120.39
1	A	154	LEU	CA-C-O	-6.13	114.00	121.36
1	A	192	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	71	HIS	CG-CD2-NE2	-6.11	101.09	107.20
1	A	76	LEU	N-CA-CB	6.09	120.78	110.49
1	B	34	ASN	CB-CA-C	6.06	120.80	109.71
1	A	117	ARG	N-CA-CB	6.04	119.42	110.53
1	A	225	PRO	O-C-N	-6.04	115.60	122.91
1	B	115	ASN	O-C-N	-6.04	114.94	122.73
1	B	204	GLU	CA-CB-CG	6.03	126.16	114.10
1	A	124	PRO	CA-CB-CG	6.02	115.94	104.50
1	B	44	GLY	CA-C-O	-6.01	115.83	121.96
1	B	96	ARG	NH1-CZ-NH2	-6.01	111.49	119.30
1	A	64	GLN	N-CA-C	-5.99	99.43	109.07
1	B	40	HIS	CG-CD2-NE2	-5.99	101.21	107.20
1	B	210	GLN	N-CA-CB	-5.97	101.12	110.44
1	B	150	ASN	N-CA-CB	5.97	119.08	110.37
1	A	38	GLY	CA-C-O	5.96	124.90	119.83
1	B	180	MET	CA-C-O	-5.96	114.26	120.70
1	B	229	THR	CA-CB-OG1	-5.95	100.68	109.60
1	B	211	GLY	CA-C-N	5.95	131.37	122.75
1	B	211	GLY	C-N-CA	5.95	131.37	122.75
1	A	234	TYR	N-CA-CB	-5.94	101.62	111.49
1	B	219	GLY	O-C-N	-5.93	116.13	122.95
1	A	181	VAL	CG1-CB-CG2	-5.91	97.79	110.80
1	A	96	ARG	NE-CZ-NH1	5.91	127.41	121.50
1	A	165	GLN	OE1-CD-NE2	5.90	128.50	122.60
1	B	143	ASN	CB-CG-ND2	5.90	125.25	116.40
1	B	40	HIS	ND1-CG-CD2	5.89	112.00	106.10
1	A	74	ASN	CA-CB-CG	5.89	118.49	112.60
1	B	161	PRO	O-C-N	5.89	130.59	122.64
1	A	215	TRP	CA-C-N	5.89	132.95	121.41
1	A	215	TRP	C-N-CA	5.89	132.95	121.41
1	B	238	ILE	CA-C-O	-5.89	115.15	121.27
1	B	240	ASP	O-C-N	5.88	128.14	122.03
1	A	143	ASN	O-C-N	-5.87	115.65	122.87
1	B	84	ASN	OD1-CG-ND2	5.87	128.47	122.60
1	A	233	ASN	CA-C-N	5.86	131.93	122.14
1	A	233	ASN	C-N-CA	5.86	131.93	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASN	CA-C-O	-5.86	111.44	119.12
1	A	100	ASN	CB-CG-ND2	-5.86	107.61	116.40
1	A	45	SER	CA-C-N	5.85	130.78	121.66
1	A	45	SER	C-N-CA	5.85	130.78	121.66
1	A	176	ILE	CA-CB-CG2	5.84	120.44	110.50
1	B	87	LYS	CA-CB-CG	5.84	125.79	114.10
1	A	147	SER	CA-C-O	5.84	127.47	120.28
1	B	32	SER	CA-C-N	5.83	130.18	121.72
1	B	32	SER	C-N-CA	5.83	130.18	121.72
1	A	242	ILE	N-CA-C	-5.82	104.84	110.72
1	A	77	GLU	CG-CD-OE1	5.81	131.76	118.40
1	B	204	GLU	CA-C-N	5.80	132.62	121.54
1	B	204	GLU	C-N-CA	5.80	132.62	121.54
1	B	120	THR	OG1-CB-CG2	5.79	120.89	109.30
1	B	55	ALA	CA-C-O	-5.79	114.41	121.36
1	A	154	LEU	O-C-N	5.79	129.54	123.06
1	A	217	TYR	CB-CA-C	5.78	119.56	110.19
1	B	119	ALA	O-C-N	-5.78	116.13	123.24
1	B	117	ARG	CA-CB-CG	5.78	125.65	114.10
1	B	37	SER	O-C-N	-5.77	114.45	122.19
1	B	48	ASN	N-CA-CB	5.77	120.35	111.46
1	B	151	GLU	CG-CD-OE1	5.76	131.66	118.40
1	B	179	ASN	CB-CA-C	5.76	120.29	110.56
1	B	30	GLN	N-CA-CB	-5.73	101.54	109.97
1	A	240	ASP	CA-C-N	5.72	127.95	120.28
1	A	240	ASP	C-N-CA	5.72	127.95	120.28
1	B	224	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	54	SER	CA-C-N	5.72	131.85	122.07
1	B	54	SER	C-N-CA	5.72	131.85	122.07
1	B	124	PRO	N-CA-CB	-5.70	98.24	103.31
1	A	153	ASP	O-C-N	5.69	130.44	122.36
1	B	103	ILE	CA-C-O	-5.68	115.34	121.19
1	B	241	THR	CB-CA-C	5.68	119.71	110.96
1	A	150	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	242	ILE	CB-CG1-CD1	5.66	125.68	113.80
1	A	71	HIS	CA-CB-CG	-5.65	108.15	113.80
1	B	47	ILE	CA-C-N	5.65	131.46	121.80
1	B	47	ILE	C-N-CA	5.65	131.46	121.80
1	B	100	ASN	CB-CG-ND2	-5.63	107.95	116.40
1	A	21	THR	O-C-N	5.63	129.95	123.02
1	A	37	SER	N-CA-C	5.63	119.26	111.71
1	B	25	ASN	OD1-CG-ND2	5.63	128.23	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	GLU	CA-C-N	-5.62	115.06	122.99
1	B	80	GLU	C-N-CA	-5.62	115.06	122.99
1	B	89	ILE	N-CA-CB	-5.61	104.60	111.67
1	B	162	LEU	N-CA-CB	-5.61	101.60	110.06
1	B	17	VAL	CA-CB-CG2	5.60	119.92	110.40
1	B	72	ASN	CA-C-O	5.60	126.57	120.58
1	A	17	VAL	CB-CA-C	5.59	117.85	110.91
1	A	128	CYS	N-CA-CB	-5.59	101.52	110.63
1	B	23	GLN	N-CA-C	-5.58	102.03	110.28
1	B	88	ILE	CA-C-N	-5.58	115.52	123.11
1	B	88	ILE	C-N-CA	-5.58	115.52	123.11
1	B	21	THR	CA-C-N	-5.57	112.34	120.75
1	B	21	THR	C-N-CA	-5.57	112.34	120.75
1	A	104	MET	N-CA-C	-5.57	100.61	109.07
1	A	25	ASN	CB-CG-ND2	-5.55	108.08	116.40
1	B	120	THR	CA-C-O	-5.55	115.56	121.94
1	B	130	PRO	CB-CA-C	-5.55	102.13	110.17
1	B	231	VAL	CA-C-N	5.54	129.47	120.60
1	B	231	VAL	C-N-CA	5.54	129.47	120.60
1	B	238	ILE	N-CA-C	5.51	116.15	110.36
1	B	235	VAL	CG1-CB-CG2	-5.50	98.71	110.80
1	B	143	ASN	CB-CA-C	5.49	118.84	109.72
1	A	37	SER	CA-C-O	5.48	125.91	120.32
1	A	229	THR	OG1-CB-CG2	-5.46	98.37	109.30
1	B	245	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	143	ASN	CB-CA-C	5.45	118.77	109.72
1	B	80	GLU	N-CA-C	5.45	118.34	110.28
1	A	200	VAL	CA-C-O	5.44	126.11	120.39
1	A	115	ASN	N-CA-C	-5.44	101.59	108.45
1	A	178	ASP	O-C-N	-5.44	114.96	122.46
1	B	81	GLN	CA-C-N	5.43	130.83	123.11
1	B	81	GLN	C-N-CA	5.43	130.83	123.11
1	B	166	ALA	N-CA-CB	-5.42	101.92	110.06
1	B	76	LEU	CA-C-O	-5.42	114.29	120.58
1	B	185	LEU	CB-CG-CD1	5.42	126.95	110.70
1	B	190	SER	N-CA-C	-5.41	102.51	110.52
1	A	122	ALA	O-C-N	-5.41	116.05	122.65
1	B	55	ALA	CB-CA-C	5.41	118.76	109.51
1	B	237	TRP	CA-C-O	5.40	126.33	120.55
1	A	178	ASP	CB-CA-C	5.40	121.19	110.17
1	B	165	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	A	95	ASP	CA-C-O	5.40	126.16	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	A	236	ASP	N-CA-CB	-5.39	102.16	110.20
1	B	130	PRO	N-CD-CG	-5.39	95.11	103.20
1	B	242	ILE	CA-CB-CG2	5.39	119.67	110.50
1	B	175	LYS	N-CA-C	5.39	119.98	113.41
1	A	111	PRO	O-C-N	-5.38	116.64	123.10
1	A	87	LYS	CA-CB-CG	5.38	124.85	114.10
1	B	242	ILE	CB-CG1-CD1	5.37	125.08	113.80
1	B	42	CYS	CA-CB-SG	5.36	126.74	114.40
1	A	105	LEU	O-C-N	5.36	130.20	123.23
1	B	80	GLU	CA-C-O	-5.36	115.16	121.16
1	B	210	GLN	CA-C-O	5.36	125.54	119.27
1	A	182	CYS	CA-C-O	5.35	126.74	120.80
1	A	17	VAL	CA-CB-CG2	5.34	119.48	110.40
1	A	84	ASN	CB-CG-ND2	-5.34	108.39	116.40
1	B	166	ALA	N-CA-C	5.34	117.79	111.33
1	B	77	GLU	CG-CD-OE1	5.34	130.67	118.40
1	B	77	GLU	CG-CD-OE2	-5.34	106.13	118.40
1	A	40	HIS	CA-C-N	-5.33	112.25	121.52
1	A	40	HIS	C-N-CA	-5.33	112.25	121.52
1	A	72	ASN	OD1-CG-ND2	5.33	127.92	122.60
1	A	156	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	A	71	HIS	ND1-CG-CD2	5.32	111.42	106.10
1	A	89	ILE	CA-C-O	5.32	127.60	120.69
1	A	49	ASP	CB-CA-C	5.31	120.19	110.11
1	B	159	ASP	CA-C-O	5.30	126.04	120.36
1	A	95	ASP	CB-CG-OD2	-5.30	106.21	118.40
1	A	70	GLU	N-CA-C	5.28	117.68	110.55
1	A	34	ASN	CA-C-O	5.27	126.18	120.43
1	A	108	LEU	N-CA-CB	-5.26	102.59	110.17
1	B	38	GLY	N-CA-C	-5.25	108.23	114.48
1	A	138	ILE	CA-CB-CG2	5.25	119.43	110.50
1	B	91	HIS	CA-C-N	5.25	125.56	119.47
1	B	91	HIS	C-N-CA	5.25	125.56	119.47
1	A	47	ILE	CB-CG1-CD1	5.25	124.81	113.80
1	B	150	ASN	CB-CG-ND2	5.24	124.25	116.40
1	A	172	TYR	CA-C-N	5.23	126.38	119.84
1	A	172	TYR	C-N-CA	5.23	126.38	119.84
1	A	235	VAL	CA-CB-CG1	-5.23	101.51	110.40
1	B	153	ASP	O-C-N	5.23	129.96	122.28
1	B	97	LYS	CA-CB-CG	5.22	124.54	114.10
1	A	141	TRP	CA-C-O	5.21	127.49	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	PRO	CB-CA-C	-5.19	104.76	111.46
1	B	34	ASN	CA-C-O	5.19	125.97	120.36
1	B	120	THR	O-C-N	5.19	129.03	122.65
1	B	95	ASP	O-C-N	-5.18	117.31	123.22
1	A	134	THR	CA-C-N	5.18	129.29	122.30
1	A	134	THR	C-N-CA	5.18	129.29	122.30
1	B	192	GLN	CA-C-O	-5.17	115.46	121.15
1	A	224	ASN	CA-C-N	5.17	125.45	119.92
1	A	224	ASN	C-N-CA	5.17	125.45	119.92
1	A	172	TYR	N-CA-C	5.16	119.20	110.02
1	B	98	THR	CA-CB-CG2	5.15	119.26	110.50
1	A	227	VAL	CB-CA-C	5.14	118.50	110.83
1	A	194	ASP	CA-C-O	5.14	124.79	119.14
1	A	62	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	241	THR	O-C-N	5.13	127.36	122.03
1	A	73	ILE	CG1-CB-CG2	5.13	126.08	110.70
1	B	241	THR	CA-C-O	-5.12	115.62	121.00
1	B	149	VAL	CA-C-N	5.11	129.16	121.40
1	B	149	VAL	C-N-CA	5.11	129.16	121.40
1	B	109	SER	N-CA-C	5.10	116.84	111.28
1	B	122	ALA	O-C-N	-5.10	116.54	122.81
1	A	242	ILE	CA-C-O	-5.10	115.45	120.85
1	B	110	SER	CA-C-N	5.09	125.00	119.85
1	B	110	SER	C-N-CA	5.09	125.00	119.85
1	A	200	VAL	CB-CA-C	5.08	118.15	110.63
1	B	160	ALA	CA-C-N	5.08	126.19	119.84
1	B	160	ALA	C-N-CA	5.08	126.19	119.84
1	A	101	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	B	96	ARG	CA-C-N	5.07	127.52	120.63
1	B	96	ARG	C-N-CA	5.07	127.52	120.63
1	A	161	PRO	CA-C-N	-5.07	113.68	120.87
1	A	161	PRO	C-N-CA	-5.07	113.68	120.87
1	A	177	THR	CB-CA-C	5.06	121.15	111.48
1	B	99	LEU	CA-C-N	-5.06	114.19	121.42
1	B	99	LEU	C-N-CA	-5.06	114.19	121.42
1	A	76	LEU	CA-C-O	-5.05	113.28	120.51
1	A	71	HIS	CA-C-O	5.05	127.72	120.51
1	B	192	GLN	CG-CD-NE2	5.05	123.97	116.40
1	A	229	THR	CA-C-O	5.04	126.66	120.92
1	A	120	THR	CA-CB-CG2	5.04	119.06	110.50
1	A	155	LEU	CD1-CG-CD2	-5.04	99.72	110.80
1	A	30	GLN	CG-CD-OE1	5.03	130.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	182	CYS	CA-C-O	5.03	126.39	120.80
1	A	110	SER	CB-CA-C	5.03	117.77	109.97
1	B	217	TYR	CB-CA-C	5.03	118.33	110.19
1	A	245	ASN	CA-C-O	-5.02	105.94	121.00
1	B	66	LEU	CA-C-O	-5.01	115.50	121.56
1	B	243	ALA	N-CA-CB	5.01	118.04	110.28
1	A	30	GLN	CB-CG-CD	5.01	121.11	112.60
1	A	166	ALA	CA-C-N	5.00	127.40	120.29
1	A	166	ALA	C-N-CA	5.00	127.40	120.29
1	B	198	PRO	CA-C-N	5.00	129.84	123.13
1	B	198	PRO	C-N-CA	5.00	129.84	123.13

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	120	THR	CB
1	A	175	LYS	CA
1	B	120	THR	CB

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	LEU	Mainchain
1	A	65(A)	ARG	Sidechain
1	B	104	MET	Mainchain
1	B	112	VAL	Mainchain
1	B	117	ARG	Sidechain
1	B	234	TYR	Mainchain
1	B	238	ILE	Mainchain
1	B	62	ARG	Sidechain
1	B	96	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1672	0	1605	55	8

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1672	0	1605	50	7
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	9	0	7	0	0
3	B	9	0	7	0	0
4	A	115	0	0	5	13
4	B	115	0	0	3	14
All	All	3594	0	3224	105	25

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 16.

All (105) 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:72:ASN:HD22	1:B:74:ASN:H	1.13	0.91
1:A:92:PRO:HG2	4:A:281:HOH:O	1.71	0.90
1:B:72:ASN:ND2	1:B:74:ASN:H	1.73	0.86
1:A:64:GLN:NE2	1:A:65(A):ARG:HE	1.87	0.73
1:A:115:ASN:HD22	1:A:117:ARG:H	1.36	0.72
1:A:64:GLN:HE22	1:A:65(A):ARG:HH21	1.37	0.72
1:A:72:ASN:HD22	1:A:74:ASN:H	1.41	0.69
1:B:79:ASN:OD1	1:B:117:ARG:HD2	1.92	0.69
1:B:144:THR:HG23	1:B:152:PRO:HD3	1.75	0.68
1:B:101:ASN:H	1:B:179:ASN:HD21	1.42	0.67
1:A:165:GLN:HG3	1:A:169:GLU:OE2	1.95	0.67
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.60	0.66
1:B:72:ASN:HD22	1:B:72:ASN:C	2.04	0.66
1:A:64:GLN:HE21	1:A:65(A):ARG:HE	1.43	0.65
1:B:64:GLN:HE22	1:B:65(A):ARG:HH21	1.43	0.65
1:B:28:PRO:HB2	1:B:119:ALA:HB3	1.78	0.65
1:B:87:LYS:HB2	1:B:107:LYS:HB3	1.80	0.63
1:A:72:ASN:ND2	1:A:74:ASN:H	1.97	0.62
1:B:64:GLN:HE21	1:B:65(A):ARG:HE	1.46	0.62
1:A:212:ILE:HB	1:A:229:THR:HB	1.83	0.61
1:B:215:TRP:NE1	1:B:227:VAL:HG22	2.15	0.60
1:A:28:PRO:HB2	1:A:119:ALA:HB3	1.84	0.59
1:B:48:ASN:HD22	1:B:50:GLN:H	1.50	0.58
1:A:75:VAL:O	1:A:77:GLU:HG3	2.03	0.58
1:A:234:TYR:O	1:A:238:ILE:HG13	2.04	0.58
1:A:72:ASN:HD22	1:A:72:ASN:C	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:O	1:A:169:GLU:HG3	2.03	0.57
1:B:165:GLN:O	1:B:169:GLU:HG3	2.04	0.57
1:B:64:GLN:NE2	1:B:65(A):ARG:HE	2.01	0.57
1:B:134:THR:O	1:B:161:PRO:HA	2.04	0.57
1:B:16:ILE:O	1:B:144:THR:HA	2.05	0.56
1:B:101:ASN:H	1:B:179:ASN:ND2	2.02	0.56
1:B:115:ASN:HD22	1:B:115:ASN:C	2.13	0.56
1:A:101:ASN:H	1:A:179:ASN:HD21	1.51	0.56
1:B:64:GLN:HE22	1:B:65(A):ARG:NH2	2.04	0.56
1:A:115:ASN:ND2	1:A:118:VAL:H	2.05	0.55
1:B:31:VAL:HG12	1:B:66:LEU:HD23	1.89	0.54
1:B:130:PRO:HD2	1:B:134:THR:OG1	2.07	0.54
1:B:45:SER:OG	1:B:198:PRO:HB3	2.07	0.54
1:A:177:THR:HG23	1:A:180:MET:HE3	1.90	0.54
1:A:50:GLN:O	1:A:107:LYS:HA	2.08	0.53
1:B:23:GLN:HB3	1:B:26:SER:HB3	1.91	0.52
1:A:27:VAL:HG13	1:A:29:TYR:CZ	2.45	0.52
1:B:21:THR:HG21	1:B:154:LEU:HD13	1.90	0.52
1:A:108:LEU:HD23	1:A:112:VAL:HG13	1.92	0.52
1:A:25:ASN:CG	1:A:117:ARG:HD3	2.35	0.51
1:A:101:ASN:H	1:A:179:ASN:ND2	2.07	0.51
1:B:96:ARG:HD2	4:B:258:HOH:O	2.10	0.51
1:A:71:HIS:NE2	1:A:154:LEU:HD13	2.26	0.51
1:B:211:GLY:HA2	1:B:229:THR:O	2.12	0.50
1:B:72:ASN:HD21	1:B:74:ASN:HB2	1.78	0.49
1:A:48:ASN:HD22	1:A:48:ASN:C	2.20	0.49
1:A:73:ILE:HG12	4:A:254:HOH:O	2.13	0.49
1:A:25:ASN:ND2	1:A:117:ARG:HD3	2.28	0.49
1:B:238:ILE:O	1:B:242:ILE:HD13	2.13	0.48
1:A:62:ARG:HA	4:A:318:HOH:O	2.12	0.48
1:A:56:ALA:HB3	1:A:94:PHE:CD2	2.50	0.47
1:A:64:GLN:HE22	1:A:65(A):ARG:NH2	2.10	0.47
1:A:64:GLN:NE2	1:A:65(A):ARG:NE	2.59	0.47
1:B:37:SER:HB2	1:B:41:PHE:CD2	2.49	0.47
1:A:134:THR:O	1:A:161:PRO:HA	2.14	0.47
1:A:87:LYS:C	1:A:88:ILE:HG13	2.38	0.46
1:B:212:ILE:HB	1:B:229:THR:HB	1.97	0.46
1:A:183:VAL:HG23	1:A:228:TYR:CD2	2.51	0.46
1:B:55:ALA:O	1:B:58:CYS:HB2	2.15	0.46
1:B:64:GLN:NE2	1:B:65(A):ARG:HH21	2.12	0.46
1:B:57[A]:HIS:HD2	4:B:317:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:CYS:SG	1:A:162:LEU:HD12	2.57	0.45
1:A:101:ASN:HA	1:A:234:TYR:OH	2.16	0.45
1:A:144:THR:HG23	1:A:152:PRO:HD3	1.99	0.45
1:B:72:ASN:HD22	1:B:74:ASN:N	1.96	0.44
1:B:64:GLN:NE2	1:B:65(A):ARG:NE	2.65	0.44
1:B:17:VAL:O	1:B:188(A):LYS:HA	2.16	0.44
1:B:19:GLY:HA2	1:B:158:LEU:HD12	2.00	0.43
1:A:130:PRO:O	1:A:134:THR:OG1	2.36	0.43
1:B:48:ASN:HD22	1:B:48:ASN:C	2.26	0.43
1:B:162:LEU:HD23	4:B:334:HOH:O	2.17	0.43
1:B:129:ALA:HA	1:B:130:PRO:HD3	1.80	0.43
1:A:211:GLY:HA2	1:A:229:THR:O	2.19	0.43
1:A:241:THR:HA	4:A:359:HOH:O	2.17	0.43
1:B:19:GLY:HA3	1:B:157:CYS:O	2.19	0.43
1:A:20:TYR:N	1:A:20:TYR:CD2	2.87	0.42
1:A:101:ASN:HA	1:A:234:TYR:HH	1.84	0.42
1:B:57[B]:HIS:CE1	1:B:102:ASN:HD21	2.37	0.42
1:B:182:CYS:HA	1:B:226:GLY:O	2.19	0.42
1:B:51:TRP:CE2	1:B:107:LYS:HG3	2.55	0.42
1:B:25:ASN:CG	1:B:117:ARG:HD3	2.44	0.42
1:B:16:ILE:N	1:B:194:ASP:OD1	2.53	0.42
1:B:163:LEU:HA	1:B:164:PRO:HD3	1.94	0.42
1:A:115:ASN:HD22	1:A:117:ARG:N	2.12	0.41
1:B:25:ASN:HB3	1:B:117:ARG:HB3	2.01	0.41
1:A:32:SER:OG	1:A:73:ILE:HD11	2.20	0.41
1:A:74:ASN:ND2	1:A:153:ASP:OD1	2.53	0.41
1:A:115:ASN:ND2	1:A:117:ARG:H	2.09	0.41
1:A:32:SER:CB	1:A:73:ILE:HD11	2.51	0.41
1:B:192:GLN:H	1:B:192:GLN:NE2	2.18	0.41
1:A:66:LEU:HD22	1:A:118:VAL:HG13	2.02	0.41
1:A:120:THR:HG21	4:A:311:HOH:O	2.20	0.41
1:A:115:ASN:ND2	1:A:118:VAL:N	2.67	0.41
1:B:21:THR:HG21	1:B:154:LEU:CD1	2.50	0.41
1:A:66:LEU:O	1:A:80:GLU:HA	2.21	0.40
1:A:160:ALA:HA	1:A:161:PRO:HD3	1.83	0.40
1:A:172:TYR:HB3	1:A:175:LYS:HG2	2.02	0.40
1:A:65(A):ARG:HD3	1:A:82:PHE:CE2	2.56	0.40
1:A:16:ILE:N	1:A:194:ASP:OD1	2.54	0.40

All (25) 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)
4:A:358:HOH:O	4:B:311:HOH:O[4_466]	0.28	1.92
4:A:348:HOH:O	4:B:362:HOH:O[4_566]	0.60	1.60
4:A:361:HOH:O	4:B:349:HOH:O[4_466]	0.89	1.31
1:B:23:GLN:OE1	1:B:96:ARG:NH2[1_655]	1.07	1.13
1:B:23:GLN:CD	1:B:96:ARG:NH2[1_655]	1.34	0.86
1:A:23:GLN:OE1	1:A:96:ARG:NH2[1_655]	1.39	0.81
4:A:310:HOH:O	4:B:359:HOH:O[4_566]	1.44	0.76
4:A:327:HOH:O	4:B:329:HOH:O[3_546]	1.51	0.69
4:A:327:HOH:O	4:B:328:HOH:O[3_546]	1.58	0.62
1:A:23:GLN:OE1	1:A:96:ARG:CZ[1_655]	1.73	0.47
1:B:23:GLN:OE1	1:B:96:ARG:CZ[1_655]	1.73	0.47
1:B:23:GLN:NE2	1:B:96:ARG:NH2[1_655]	1.77	0.43
4:A:311:HOH:O	4:B:360:HOH:O[4_566]	1.78	0.42
4:A:349:HOH:O	4:B:361:HOH:O[4_566]	1.83	0.37
4:A:314:HOH:O	4:B:282:HOH:O[4_566]	1.93	0.27
1:A:236:ASP:OD2	1:B:114:LEU:O[4_466]	1.94	0.26
1:A:23:GLN:CD	1:A:96:ARG:NH2[1_655]	1.97	0.23
4:A:360:HOH:O	4:B:350:HOH:O[4_466]	1.98	0.22
1:A:49:ASP:OD1	4:B:282:HOH:O[4_566]	2.01	0.19
1:A:23:GLN:OE1	1:A:96:ARG:NE[1_655]	2.05	0.15
4:A:359:HOH:O	4:B:312:HOH:O[4_466]	2.10	0.10
4:A:326:HOH:O	4:B:329:HOH:O[3_546]	2.11	0.09
1:A:114:LEU:O	1:B:236:ASP:OD2[4_566]	2.12	0.08
1:A:147:SER:OG	1:B:146:SER:O[3_546]	2.17	0.03
4:A:281:HOH:O	4:B:315:HOH:O[4_466]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/223 (100%)	207 (93%)	12 (5%)	3 (1%)	9	9
1	B	222/223 (100%)	212 (96%)	9 (4%)	1 (0%)	24	31
All	All	444/446 (100%)	419 (94%)	21 (5%)	4 (1%)	14	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	VAL
1	A	173	PRO
1	A	238	ILE
1	A	161	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/185 (100%)	160 (86%)	25 (14%)	4	4
1	B	185/185 (100%)	160 (86%)	25 (14%)	4	4
All	All	370/370 (100%)	320 (86%)	50 (14%)	3	4

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

Mol	Chain	Res	Type
1	A	34	ASN
1	A	37	SER
1	A	45	SER
1	A	48	ASN
1	A	50	GLN
1	A	72	ASN
1	A	73	ILE
1	A	77	GLU
1	A	97	LYS
1	A	98	THR
1	A	108	LEU
1	A	113	LYS
1	A	115	ASN
1	A	117	ARG
1	A	127	SER
1	A	138	ILE
1	A	152	PRO
1	A	162	LEU
1	A	164	PRO

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Mol	Chain	Res	Type
1	A	165	GLN
1	A	175	LYS
1	A	186	GLU
1	A	192	GLN
1	A	227	VAL
1	A	230	LYS
1	B	37	SER
1	B	48	ASN
1	B	62	ARG
1	B	72	ASN
1	B	73	ILE
1	B	76	LEU
1	B	77	GLU
1	B	80	GLU
1	B	87	LYS
1	B	97	LYS
1	B	104	MET
1	B	109	SER
1	B	110	SER
1	B	113	LYS
1	B	115	ASN
1	B	117	ARG
1	B	124	PRO
1	B	125	SER
1	B	127	SER
1	B	162	LEU
1	B	165	GLN
1	B	185	LEU
1	B	192	GLN
1	B	227	VAL
1	B	242	ILE

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	34	ASN
1	A	48	ASN
1	A	50	GLN
1	A	64	GLN
1	A	72	ASN
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	115	ASN
1	A	179	ASN
1	A	210	GLN
1	A	224	ASN
1	B	25	ASN
1	B	30	GLN
1	B	34	ASN
1	B	48	ASN
1	B	50	GLN
1	B	64	GLN
1	B	72	ASN
1	B	135	GLN
1	B	150	ASN
1	B	165	GLN
1	B	179	ASN
1	B	192	GLN
1	B	224	ASN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	BEN	B	246	-	9,9,9	2.86	5 (55%)	7,11,11	2.09	2 (28%)
3	BEN	A	246	-	9,9,9	3.03	6 (66%)	7,11,11	1.75	2 (28%)

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	BEN	B	246	-	-	3/4/4/4	0/1/1/1
3	BEN	A	246	-	-	1/4/4/4	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	BEN	C6-C1	4.22	1.45	1.39
3	B	246	BEN	C4-C3	4.14	1.47	1.38
3	A	246	BEN	C4-C3	4.13	1.47	1.38
3	B	246	BEN	C1-C	-4.05	1.39	1.47
3	A	246	BEN	C1-C	-3.84	1.40	1.47
3	A	246	BEN	C3-C2	3.68	1.45	1.38
3	B	246	BEN	C3-C2	3.54	1.45	1.38
3	A	246	BEN	C5-C6	3.29	1.44	1.38
3	B	246	BEN	C6-C1	3.16	1.44	1.39
3	B	246	BEN	C5-C6	2.96	1.44	1.38
3	A	246	BEN	C5-C4	2.26	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	246	BEN	C5-C4-C3	-4.16	114.17	119.87
3	A	246	BEN	C1-C-N2	3.32	123.05	118.01
3	A	246	BEN	C5-C4-C3	-3.12	115.60	119.87
3	B	246	BEN	C1-C-N2	2.80	122.26	118.01

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	246	BEN	N2-C-C1-C6

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Mol	Chain	Res	Type	Atoms
3	B	246	BEN	N2-C-C1-C2
3	B	246	BEN	N2-C-C1-C6
3	B	246	BEN	N1-C-C1-C2

There are no ring outliers.

No monomer is involved in short contacts.

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.