



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:16 AM UTC

PDB ID : 2TRM / pdb_00002trm
Title : THE THREE-DIMENSIONAL STRUCTURE OF ASN102 MUTANT OF TRYPSIN. ROLE OF ASP102 IN SERINE PROTEASE CATALYSIS
Authors : Stroud, R.M.; Finer-Moore, J.
Deposited on : 1988-04-25
Resolution : 2.80 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

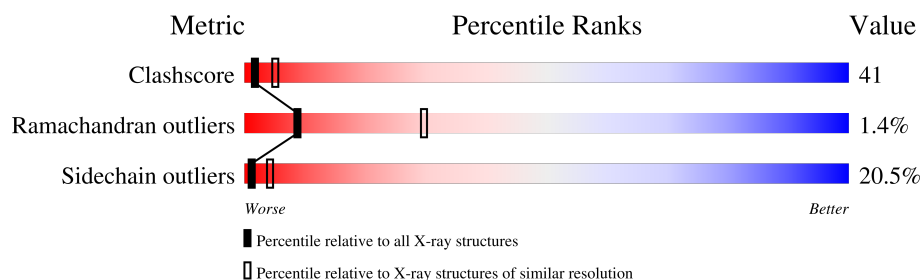
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

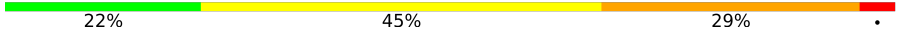
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	223	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1798 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	0	0
			1666	1041	286	325	14			

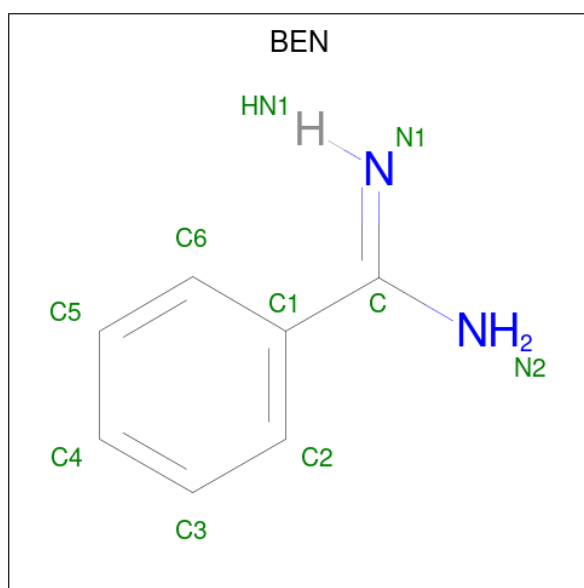
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	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		

- 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		

- Molecule 4 is water.

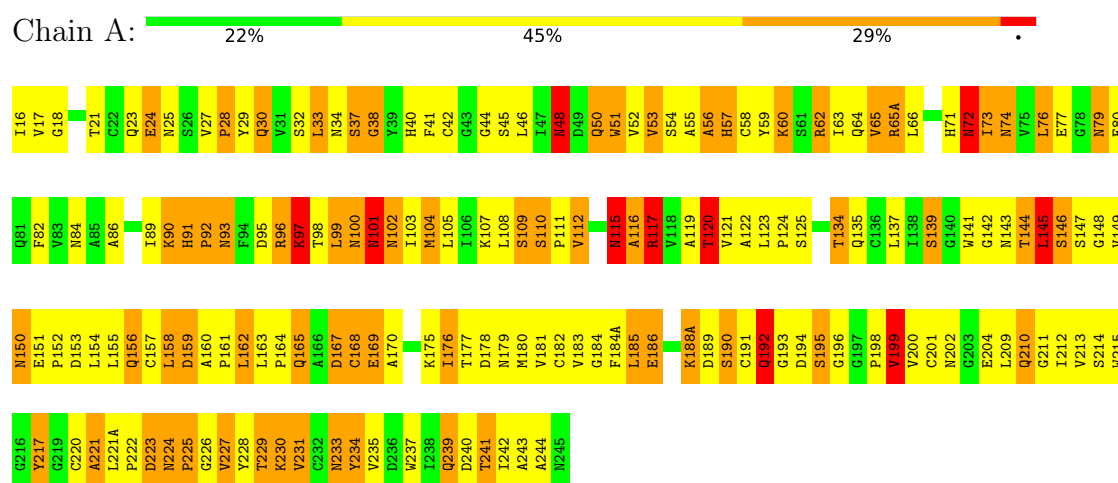
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		

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: TRYPSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	124.38Å 124.38Å 124.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1798	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: CA, BEN

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	1.01	0/1701	2.58	147/2318 (6.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	199	VAL	CB-CA-C	10.52	128.54	111.29
1	A	202	ASN	CA-CB-CG	-10.45	102.15	112.60
1	A	74	ASN	CA-CB-CG	-10.31	102.29	112.60
1	A	84	ASN	CA-CB-CG	-10.15	102.45	112.60
1	A	234	TYR	N-CA-C	10.06	125.85	113.17
1	A	117	ARG	N-CA-CB	9.72	123.52	110.59
1	A	117	ARG	N-CA-C	-9.65	102.00	113.88
1	A	96	ARG	CD-NE-CZ	9.64	137.89	124.40
1	A	122	ALA	CA-C-O	-9.11	111.06	121.81
1	A	74	ASN	N-CA-C	8.19	123.44	112.88
1	A	233	ASN	CA-CB-CG	-8.01	104.59	112.60
1	A	57	HIS	N-CA-C	-7.96	103.68	113.15
1	A	120	THR	N-CA-CB	-7.95	98.34	110.42
1	A	233	ASN	OD1-CG-ND2	7.94	130.54	122.60
1	A	30	GLN	CB-CG-CD	7.92	126.06	112.60
1	A	135	GLN	CB-CG-CD	7.89	126.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	GLN	CA-CB-CG	-7.85	98.40	114.10
1	A	89	ILE	N-CA-C	7.83	118.95	107.37
1	A	145	LEU	CA-C-O	-7.76	111.99	120.30
1	A	151	GLU	O-C-N	7.72	128.44	121.19
1	A	97	LYS	CA-C-O	-7.54	112.88	120.80
1	A	221	ALA	N-CA-C	-7.52	104.05	113.23
1	A	38	GLY	CA-C-O	7.47	127.54	119.03
1	A	135	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	A	48	ASN	CA-C-O	-7.35	113.57	121.36
1	A	185	LEU	CB-CA-C	7.23	125.42	110.31
1	A	144	THR	CA-CB-OG1	-7.20	98.80	109.60
1	A	229	THR	CA-C-O	-7.17	113.13	121.16
1	A	97	LYS	N-CA-CB	7.14	120.56	110.07
1	A	192	GLN	CB-CA-C	7.11	121.53	109.72
1	A	180	MET	CA-C-O	-7.08	111.56	120.20
1	A	217	TYR	CA-C-O	-7.03	112.25	120.62
1	A	185	LEU	N-CA-CB	-6.96	98.84	110.39
1	A	115	ASN	CB-CA-C	6.91	124.17	110.42
1	A	135	GLN	N-CA-CB	6.89	120.64	109.95
1	A	102	ASN	CA-CB-CG	-6.88	105.72	112.60
1	A	230	LYS	N-CA-CB	-6.87	100.32	110.49
1	A	42	CYS	CA-C-O	-6.83	114.00	121.31
1	A	44	GLY	CA-C-O	-6.81	114.95	121.49
1	A	148	GLY	N-CA-C	-6.79	97.10	113.18
1	A	23	GLN	CB-CA-C	6.78	119.92	110.16
1	A	125	SER	CA-C-O	6.77	127.80	120.55
1	A	198	PRO	N-CA-C	6.75	121.18	111.13
1	A	30	GLN	CA-C-O	-6.74	113.01	120.69
1	A	151	GLU	CA-C-O	-6.67	113.75	119.36
1	A	241	THR	N-CA-CB	6.65	119.66	110.01
1	A	199	VAL	CA-C-N	6.64	131.40	122.90
1	A	199	VAL	C-N-CA	6.64	131.40	122.90
1	A	157	CYS	O-C-N	6.63	131.40	123.24
1	A	199	VAL	CA-C-O	6.62	129.06	120.78
1	A	102	ASN	OD1-CG-ND2	6.59	129.19	122.60
1	A	42	CYS	O-C-N	6.59	130.04	122.99
1	A	97	LYS	O-C-N	6.54	129.70	122.11
1	A	152	PRO	CA-C-O	-6.48	113.77	121.67
1	A	237	TRP	O-C-N	6.43	128.93	122.12
1	A	178	ASP	O-C-N	6.39	130.01	122.34
1	A	100	ASN	CA-C-O	-6.36	114.20	121.19
1	A	101	ASN	OD1-CG-ND2	6.33	128.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASP	CB-CA-C	6.33	122.74	110.46
1	A	65	VAL	CA-C-O	-6.33	113.58	121.11
1	A	30	GLN	N-CA-C	6.32	119.81	109.76
1	A	202	ASN	OD1-CG-ND2	6.26	128.86	122.60
1	A	224	ASN	O-C-N	6.26	126.49	121.17
1	A	159	ASP	CB-CA-C	6.23	120.02	109.50
1	A	170	ALA	N-CA-C	-6.20	104.63	111.82
1	A	104	MET	CA-C-O	-6.18	113.89	121.06
1	A	210	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	159	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	65(A)	ARG	CA-C-O	-6.15	113.69	120.33
1	A	182	CYS	CA-CB-SG	6.12	128.47	114.40
1	A	221	ALA	CA-C-O	-6.11	113.09	120.12
1	A	157	CYS	CA-C-O	-6.11	113.96	121.11
1	A	51	TRP	CA-C-N	6.09	131.12	123.14
1	A	51	TRP	C-N-CA	6.09	131.12	123.14
1	A	182	CYS	N-CA-CB	6.06	120.31	110.43
1	A	229	THR	N-CA-C	-6.06	101.32	110.28
1	A	169	GLU	N-CA-C	6.05	118.83	111.82
1	A	90	LYS	N-CA-C	-6.04	101.54	110.48
1	A	244	ALA	CA-C-O	-6.04	111.95	119.38
1	A	30	GLN	CA-CB-CG	6.04	126.18	114.10
1	A	79	ASN	N-CA-C	6.04	120.33	113.15
1	A	33	LEU	CB-CA-C	6.02	119.68	109.75
1	A	71	HIS	N-CA-CB	6.01	120.65	110.49
1	A	103	ILE	CA-C-O	-6.00	114.48	120.90
1	A	193	GLY	N-CA-C	-5.98	107.58	114.69
1	A	226	GLY	CA-C-O	-5.97	114.84	121.94
1	A	190	SER	CB-CA-C	5.96	121.78	110.51
1	A	105	LEU	CA-C-O	-5.93	114.45	121.16
1	A	115	ASN	CA-C-O	-5.93	112.02	120.51
1	A	76	LEU	CB-CA-C	5.93	118.70	110.16
1	A	77	GLU	CA-C-O	-5.91	112.57	119.24
1	A	226	GLY	N-CA-C	-5.88	104.13	112.37
1	A	167	ASP	CA-CB-CG	-5.87	106.73	112.60
1	A	198	PRO	CB-CA-C	-5.83	102.13	110.75
1	A	123	LEU	CB-CA-C	5.81	117.50	108.61
1	A	181	VAL	CA-C-O	-5.79	113.68	121.32
1	A	91	HIS	N-CA-C	-5.78	102.50	109.83
1	A	192	GLN	CB-CG-CD	5.76	122.40	112.60
1	A	90	LYS	CA-C-O	-5.76	114.84	121.47
1	A	23	GLN	N-CA-C	-5.75	101.39	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	A	199	VAL	N-CA-C	-5.74	97.41	109.34
1	A	57	HIS	N-CA-CB	5.72	119.27	110.46
1	A	53	VAL	CA-CB-CG1	5.67	120.04	110.40
1	A	143	ASN	CB-CA-C	5.66	118.33	109.84
1	A	110	SER	O-C-N	5.62	127.78	121.32
1	A	134	THR	N-CA-C	5.61	118.67	109.76
1	A	48	ASN	N-CA-CB	5.60	120.56	111.21
1	A	229	THR	O-C-N	5.53	129.63	122.89
1	A	56	ALA	N-CA-C	-5.52	106.50	113.18
1	A	145	LEU	N-CA-C	5.49	117.36	108.41
1	A	102	ASN	CA-C-O	-5.49	115.93	122.13
1	A	93	ASN	CB-CA-C	5.44	119.80	110.01
1	A	60	LYS	N-CA-C	-5.41	100.85	109.23
1	A	156	GLN	OE1-CD-NE2	5.39	127.99	122.60
1	A	72	ASN	N-CA-C	-5.38	101.21	109.76
1	A	100	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	109	SER	CA-CB-OG	-5.37	100.36	111.10
1	A	178	ASP	CA-C-O	-5.37	113.28	119.56
1	A	96	ARG	CG-CD-NE	5.35	123.78	112.00
1	A	117	ARG	CA-CB-CG	5.33	124.75	114.10
1	A	51	TRP	CA-C-O	5.32	126.22	120.32
1	A	227	VAL	CB-CA-C	5.30	118.87	110.81
1	A	60	LYS	CA-C-O	-5.28	114.93	121.06
1	A	125	SER	N-CA-C	-5.28	104.96	111.40
1	A	192	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	71	HIS	N-CA-C	-5.26	99.59	110.80
1	A	201	CYS	CA-C-O	-5.24	114.70	120.36
1	A	90	LYS	O-C-N	5.21	128.85	122.96
1	A	168	CYS	CA-C-N	5.20	128.22	120.31
1	A	168	CYS	C-N-CA	5.20	128.22	120.31
1	A	122	ALA	O-C-N	5.20	128.78	122.85
1	A	225	PRO	N-CA-C	-5.19	103.62	111.41
1	A	79	ASN	N-CA-CB	-5.17	102.50	110.46
1	A	116	ALA	CB-CA-C	5.16	118.89	110.17
1	A	143	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	A	176	ILE	N-CA-C	5.16	115.90	107.24
1	A	24	GLU	N-CA-C	5.15	118.03	110.30
1	A	48	ASN	CB-CG-ND2	-5.13	108.71	116.40
1	A	76	LEU	O-C-N	5.12	129.81	123.01
1	A	28	PRO	O-C-N	5.10	129.24	122.30
1	A	152	PRO	CB-CA-C	-5.07	104.34	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ILE	N-CA-CB	-5.06	105.62	112.10
1	A	184	GLY	CA-C-O	5.05	125.14	120.79
1	A	76	LEU	CA-C-O	-5.05	114.90	120.70
1	A	223	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	92	PRO	O-C-N	5.02	128.70	122.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	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	1666	0	1605	134	0
2	A	1	0	0	0	0
3	A	9	0	7	3	0
4	A	122	0	0	7	0
All	All	1798	0	1612	134	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 41.

All (134) 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:79:ASN:HB3	1:A:117:ARG:HG3	1.39	1.02
1:A:214:SER:HG	1:A:215:TRP:HD1	1.11	0.98
1:A:115:ASN:HD22	1:A:116:ALA:H	1.10	0.96
1:A:72:ASN:ND2	1:A:74:ASN:H	1.82	0.77
1:A:48:ASN:ND2	1:A:51:TRP:HB2	2.01	0.74
1:A:72:ASN:HD22	1:A:74:ASN:H	1.34	0.74
1:A:115:ASN:ND2	1:A:116:ALA:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:HG2	3:A:246:BEN:H4	1.73	0.70
1:A:212:ILE:HD12	1:A:231:VAL:HG22	1.73	0.69
1:A:115:ASN:HD22	1:A:116:ALA:N	1.87	0.69
1:A:86:ALA:HB2	1:A:109:SER:HA	1.74	0.68
1:A:64:GLN:NE2	1:A:65(A):ARG:HE	1.91	0.68
1:A:212:ILE:CD1	1:A:231:VAL:HG22	2.27	0.64
1:A:214:SER:HG	1:A:215:TRP:CD1	2.03	0.63
1:A:79:ASN:ND2	1:A:117:ARG:HH11	1.96	0.63
1:A:192:GLN:HG2	3:A:246:BEN:C4	2.28	0.62
1:A:184(A):PHE:HB3	1:A:186:GLU:OE2	2.00	0.62
1:A:99:LEU:O	1:A:102:ASN:HB2	1.99	0.61
1:A:101:ASN:ND2	1:A:234:TYR:OH	2.33	0.61
1:A:46:LEU:HD13	1:A:66:LEU:HD21	1.83	0.61
1:A:79:ASN:CG	1:A:117:ARG:HH11	2.09	0.60
1:A:34:ASN:ND2	1:A:38:GLY:H	1.98	0.60
1:A:56:ALA:HB1	1:A:90:LYS:HB3	1.84	0.60
1:A:144:THR:OG1	1:A:150:ASN:ND2	2.34	0.60
1:A:46:LEU:HD22	1:A:66:LEU:CD2	2.31	0.60
1:A:134:THR:O	1:A:161:PRO:HA	2.03	0.59
1:A:27:VAL:HG12	1:A:30:GLN:HB2	1.84	0.58
1:A:72:ASN:HD22	1:A:74:ASN:N	2.01	0.58
1:A:99:LEU:HD13	1:A:102:ASN:ND2	2.19	0.58
1:A:37:SER:HB2	1:A:41:PHE:CD2	2.39	0.58
1:A:100:ASN:CG	1:A:177:THR:HG21	2.29	0.57
1:A:141:TRP:CH2	1:A:155:LEU:HD13	2.40	0.57
1:A:32:SER:OG	1:A:40:HIS:HD2	1.88	0.57
1:A:16:ILE:N	4:A:251:HOH:O	2.37	0.56
1:A:79:ASN:HB2	4:A:265:HOH:O	2.05	0.56
1:A:164:PRO:HD2	1:A:167:ASP:OD1	2.05	0.56
1:A:48:ASN:HD21	1:A:51:TRP:HB2	1.67	0.56
1:A:145:LEU:HD22	1:A:150:ASN:CB	2.36	0.56
1:A:64:GLN:NE2	4:A:336:HOH:O	2.39	0.56
1:A:79:ASN:CG	1:A:117:ARG:HD3	2.31	0.55
1:A:165:GLN:O	1:A:169:GLU:HG3	2.07	0.55
1:A:64:GLN:HE21	1:A:65(A):ARG:HE	1.54	0.55
1:A:233:ASN:ND2	4:A:286:HOH:O	2.39	0.55
1:A:50:GLN:CD	1:A:111:PRO:HG3	2.32	0.55
1:A:145:LEU:HD22	1:A:150:ASN:HB3	1.88	0.55
1:A:51:TRP:CH2	1:A:107:LYS:HB2	2.42	0.55
1:A:124:PRO:HD3	1:A:209:LEU:O	2.06	0.54
1:A:79:ASN:OD1	1:A:117:ARG:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:OG	1:A:60:LYS:HD3	2.07	0.54
1:A:210:GLN:NE2	1:A:210:GLN:HA	2.23	0.54
1:A:195:SER:HA	1:A:213:VAL:HB	1.89	0.54
1:A:115:ASN:ND2	1:A:116:ALA:N	2.50	0.54
1:A:33:LEU:HD22	1:A:65:VAL:HG22	1.90	0.54
1:A:54:SER:HB3	1:A:104:MET:HE2	1.90	0.53
1:A:65(A):ARG:NH1	4:A:308:HOH:O	2.34	0.53
1:A:46:LEU:HD21	1:A:112:VAL:HG21	1.91	0.53
1:A:93:ASN:HB2	1:A:101:ASN:OD1	2.09	0.52
1:A:98:THR:C	1:A:100:ASN:H	2.17	0.52
1:A:141:TRP:CZ2	1:A:155:LEU:HD13	2.45	0.52
1:A:52:VAL:HG23	1:A:108:LEU:HD21	1.90	0.52
1:A:243:ALA:HB3	4:A:313:HOH:O	2.08	0.52
1:A:86:ALA:HB2	1:A:109:SER:CA	2.40	0.52
1:A:220:CYS:O	1:A:221:ALA:HB3	2.10	0.51
1:A:79:ASN:ND2	1:A:117:ARG:NH1	2.58	0.51
1:A:222:PRO:O	1:A:223:ASP:HB2	2.11	0.51
1:A:191:CYS:C	3:A:246:BEN:C5	2.84	0.51
1:A:21:THR:HG21	1:A:154:LEU:HD12	1.92	0.51
1:A:189:ASP:OD2	1:A:190:SER:N	2.39	0.50
1:A:100:ASN:O	1:A:101:ASN:HB2	2.12	0.50
1:A:29:TYR:HA	1:A:119:ALA:O	2.11	0.50
1:A:72:ASN:HD22	1:A:72:ASN:C	2.19	0.49
1:A:209:LEU:HD23	1:A:231:VAL:HG11	1.95	0.49
1:A:155:LEU:C	1:A:156:GLN:HG2	2.36	0.49
1:A:56:ALA:C	1:A:58:CYS:H	2.21	0.48
1:A:210:GLN:C	1:A:231:VAL:HG23	2.38	0.48
1:A:37:SER:HB2	1:A:41:PHE:CE2	2.49	0.48
1:A:57:HIS:CD2	1:A:57:HIS:O	2.66	0.48
1:A:46:LEU:O	1:A:120:THR:HA	2.13	0.48
1:A:48:ASN:HD21	1:A:51:TRP:CB	2.26	0.48
1:A:159:ASP:O	1:A:160:ALA:HB2	2.13	0.48
1:A:65:VAL:HB	1:A:108:LEU:HD11	1.95	0.48
1:A:217:TYR:HB3	1:A:224:ASN:OD1	2.14	0.47
1:A:52:VAL:HG23	1:A:108:LEU:CD2	2.45	0.47
1:A:200:VAL:HA	1:A:204:GLU:O	2.15	0.47
1:A:162:LEU:HD12	1:A:183:VAL:HG22	1.97	0.46
1:A:101:ASN:HA	1:A:234:TYR:OH	2.15	0.46
1:A:59:TYR:CG	1:A:90:LYS:HE2	2.51	0.46
1:A:72:ASN:ND2	1:A:74:ASN:N	2.58	0.46
1:A:162:LEU:HD12	1:A:183:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:TYR:CD2	1:A:228:TYR:N	2.83	0.45
1:A:57:HIS:CE1	1:A:195:SER:HB3	2.52	0.45
1:A:96:ARG:HG3	4:A:258:HOH:O	2.16	0.45
1:A:98:THR:C	1:A:100:ASN:N	2.74	0.45
1:A:211:GLY:N	1:A:231:VAL:HG23	2.32	0.45
1:A:27:VAL:CG1	1:A:30:GLN:HB2	2.44	0.45
1:A:55:ALA:O	1:A:58:CYS:HB2	2.17	0.45
1:A:183:VAL:HB	1:A:228:TYR:CE2	2.52	0.45
1:A:220:CYS:H	1:A:221(A):LEU:HG	1.80	0.45
1:A:163:LEU:HD13	1:A:185:LEU:HD13	2.00	0.44
1:A:175:LYS:HE2	1:A:215:TRP:CZ3	2.53	0.44
1:A:95:ASP:C	1:A:97:LYS:N	2.75	0.44
1:A:199:VAL:HG13	1:A:211:GLY:C	2.43	0.44
1:A:80:GLU:HB3	1:A:82:PHE:CE2	2.52	0.44
1:A:73:ILE:HD13	1:A:141:TRP:CE2	2.52	0.44
1:A:158:LEU:CD1	1:A:188(A):LYS:HB3	2.47	0.43
1:A:210:GLN:HA	1:A:210:GLN:HE21	1.82	0.43
1:A:18:GLY:O	1:A:188(A):LYS:HD3	2.18	0.43
1:A:74:ASN:ND2	1:A:153:ASP:OD1	2.42	0.43
1:A:139:SER:HA	1:A:156:GLN:O	2.17	0.43
1:A:158:LEU:HD13	1:A:188(A):LYS:HB3	2.01	0.43
1:A:41:PHE:CE1	1:A:60:LYS:HD2	2.53	0.43
1:A:211:GLY:HA2	1:A:229:THR:O	2.18	0.43
1:A:168:CYS:SG	1:A:176:ILE:HD12	2.59	0.42
1:A:50:GLN:HG3	1:A:111:PRO:HA	2.02	0.42
1:A:29:TYR:HB2	1:A:121:VAL:HB	2.01	0.42
1:A:27:VAL:HG13	1:A:29:TYR:CE2	2.55	0.42
1:A:137:LEU:HD12	1:A:137:LEU:HA	1.85	0.42
1:A:24:GLU:O	1:A:25:ASN:HB2	2.20	0.42
1:A:185:LEU:CD1	1:A:225:PRO:HG3	2.50	0.42
1:A:210:GLN:HE21	1:A:210:GLN:CA	2.32	0.42
1:A:86:ALA:HB3	1:A:107:LYS:O	2.20	0.41
1:A:191:CYS:O	1:A:194:ASP:HB2	2.19	0.41
1:A:199:VAL:HG13	1:A:211:GLY:CA	2.49	0.41
1:A:142:GLY:HA3	1:A:194:ASP:OD2	2.20	0.41
1:A:196:GLY:O	1:A:212:ILE:HG23	2.21	0.41
1:A:66:LEU:HD13	1:A:112:VAL:HG11	2.03	0.41
1:A:28:PRO:HB2	1:A:119:ALA:HB3	2.03	0.41
1:A:41:PHE:HZ	1:A:63:ILE:HG12	1.86	0.41
1:A:54:SER:HB3	1:A:104:MET:CE	2.50	0.41
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:O	1:A:188(A):LYS:HA	2.21	0.41
1:A:51:TRP:CZ3	1:A:107:LYS:HB2	2.55	0.40
1:A:160:ALA:HA	1:A:161:PRO:HD3	1.70	0.40
1:A:189:ASP:CG	1:A:190:SER:H	2.29	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	221/223 (99%)	192 (87%)	26 (12%)	3 (1%)	9	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	146	SER
1	A	110	SER

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	185/185 (100%)	147 (80%)	38 (20%)	1	4

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	45	SER
1	A	48	ASN
1	A	50	GLN
1	A	53	VAL
1	A	62	ARG
1	A	72	ASN
1	A	73	ILE
1	A	76	LEU
1	A	97	LYS
1	A	99	LEU
1	A	101	ASN
1	A	112	VAL
1	A	115	ASN
1	A	117	ARG
1	A	120	THR
1	A	139	SER
1	A	145	LEU
1	A	146	SER
1	A	147	SER
1	A	149	VAL
1	A	150	ASN
1	A	158	LEU
1	A	162	LEU
1	A	165	GLN
1	A	179	ASN
1	A	186	GLU
1	A	188(A)	LYS
1	A	192	GLN
1	A	195	SER
1	A	199	VAL
1	A	227	VAL
1	A	230	LYS
1	A	231	VAL
1	A	235	VAL
1	A	239	GLN
1	A	241	THR
1	A	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	34	ASN
1	A	40	HIS
1	A	48	ASN
1	A	64	GLN
1	A	72	ASN
1	A	93	ASN
1	A	101	ASN
1	A	115	ASN
1	A	150	ASN
1	A	165	GLN
1	A	210	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	A	246	-	9,9,9	2.19	4 (44%)	7,11,11	2.44	3 (42%)

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	A	246	-	-	2/4/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	BEN	C1-C	-3.53	1.40	1.47
3	A	246	BEN	C3-C2	3.01	1.44	1.38
3	A	246	BEN	C6-C1	2.38	1.43	1.39
3	A	246	BEN	C2-C1	-2.08	1.36	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	BEN	C3-C2-C1	-5.10	115.35	120.36
3	A	246	BEN	C5-C4-C3	-2.88	115.92	119.87
3	A	246	BEN	C4-C3-C2	-2.17	117.56	120.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	246	BEN	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.