



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:11 AM UTC

PDB ID : 1BRA / pdb_00001bra
Title : RELOCATING A NEGATIVE CHARGE IN THE BINDING POCKET OF TRYPSIN
Authors : Perona, J.J.; Mcgrath, M.E.; Fletterick, R.J.
Deposited on : 1992-12-17
Resolution : 2.20 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

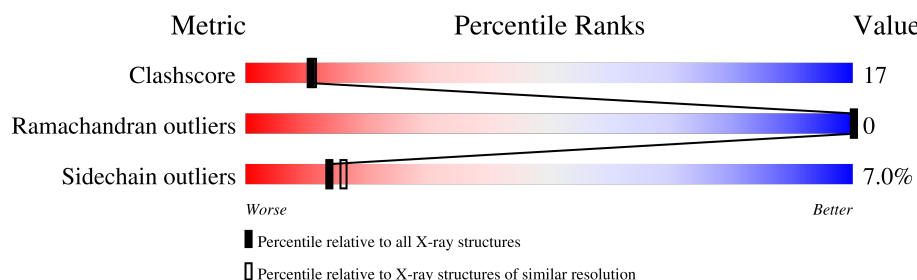
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	45% 42% 10% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1813 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	285	326	14			

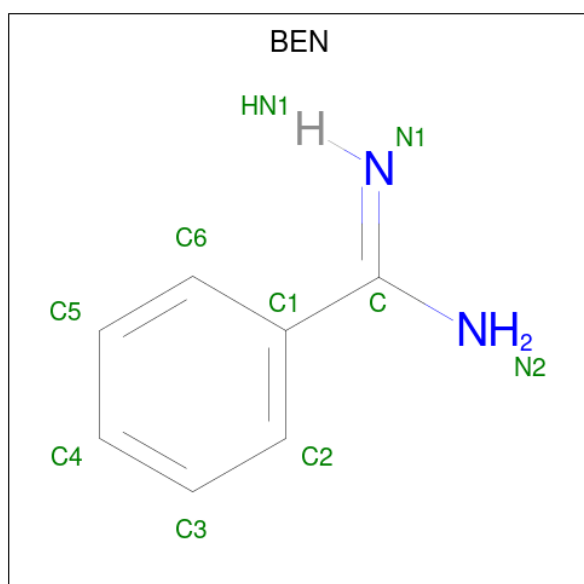
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	GLY	ASP	conflict	UNP P00763
A	226	ASP	GLY	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.

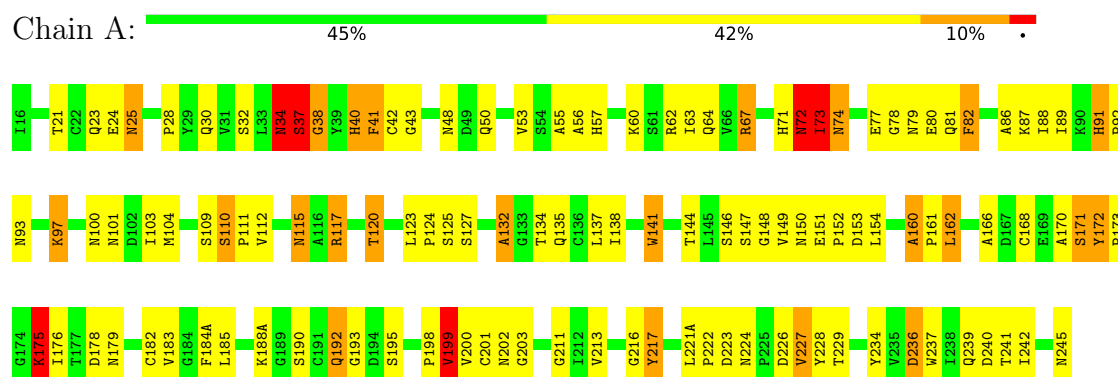
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		

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	124.40 Å 124.40 Å 124.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1813	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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	1.26	2/1701 (0.1%)	2.60	142/2318 (6.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	GLY	N-CA	6.62	1.51	1.44
1	A	211	GLY	N-CA	5.01	1.50	1.45

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASP	CA-CB-CG	-16.60	96.00	112.60
1	A	42	CYS	CA-C-O	-12.86	107.47	121.23
1	A	42	CYS	CA-C-N	-12.17	111.60	122.43
1	A	42	CYS	C-N-CA	-12.17	111.60	122.43
1	A	190	SER	CB-CA-C	11.86	129.80	109.51
1	A	192	GLN	OE1-CD-NE2	-11.19	111.41	122.60
1	A	199	VAL	N-CA-CB	10.84	125.97	112.10
1	A	199	VAL	CB-CA-C	10.17	122.83	110.73
1	A	146	SER	CA-CB-OG	-9.76	91.58	111.10
1	A	229	THR	CA-CB-OG1	-9.33	95.61	109.60
1	A	93	ASN	CA-CB-CG	-9.02	103.58	112.60
1	A	179	ASN	OD1-CG-ND2	8.76	131.36	122.60
1	A	77	GLU	CG-CD-OE2	-8.62	98.57	118.40
1	A	62	ARG	NE-CZ-NH2	-8.59	111.47	119.20
1	A	171	SER	CA-C-O	-8.55	111.36	120.42
1	A	42	CYS	O-C-N	8.38	132.38	123.42
1	A	193	GLY	CA-C-O	-8.37	110.32	119.27
1	A	154	LEU	O-C-N	8.16	132.48	123.10
1	A	202	ASN	CA-CB-CG	-8.13	104.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188(A)	LYS	CA-C-O	-8.08	111.37	120.66
1	A	91	HIS	CA-CB-CG	-8.04	105.77	113.80
1	A	21	THR	CA-C-O	-8.01	111.29	120.58
1	A	227	VAL	CB-CA-C	7.94	122.88	110.81
1	A	178	ASP	CA-C-O	-7.75	108.97	119.12
1	A	73	ILE	CA-CB-CG2	7.74	123.65	110.50
1	A	184(A)	PHE	CA-C-O	-7.62	112.40	120.40
1	A	78	GLY	CA-C-O	-7.42	110.73	118.97
1	A	23	GLN	N-CA-C	-7.33	99.44	110.28
1	A	229	THR	O-C-N	7.31	131.93	122.93
1	A	74	ASN	CA-CB-CG	-7.31	105.29	112.60
1	A	224	ASN	O-C-N	7.29	127.94	121.37
1	A	120	THR	N-CA-CB	-7.19	98.96	110.46
1	A	38	GLY	N-CA-C	-7.19	105.57	114.92
1	A	48	ASN	N-CA-CB	7.13	123.55	111.57
1	A	73	ILE	CA-C-O	-7.03	111.52	120.03
1	A	151	GLU	CA-CB-CG	-7.01	100.08	114.10
1	A	62	ARG	NE-CZ-NH1	6.99	128.49	121.50
1	A	48	ASN	O-C-N	6.96	130.25	123.29
1	A	199	VAL	O-C-N	6.96	129.78	123.03
1	A	176	ILE	N-CA-CB	-6.96	103.14	110.72
1	A	147	SER	CA-C-O	-6.95	110.82	120.21
1	A	178	ASP	N-CA-C	-6.94	104.81	113.20
1	A	245	ASN	CA-CB-CG	-6.91	105.69	112.60
1	A	192	GLN	CB-CG-CD	6.90	124.32	112.60
1	A	171	SER	O-C-N	6.86	129.97	122.15
1	A	175	LYS	CA-CB-CG	-6.84	100.42	114.10
1	A	203	GLY	CA-C-O	-6.81	110.73	119.58
1	A	100	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	A	166	ALA	CA-C-O	-6.72	112.51	120.10
1	A	82	PHE	CA-C-O	-6.69	112.97	120.32
1	A	43	GLY	N-CA-C	-6.67	103.44	112.57
1	A	162	LEU	CB-CA-C	6.65	120.67	109.84
1	A	192	GLN	CB-CA-C	6.61	119.75	109.84
1	A	171	SER	CA-C-N	-6.59	115.18	123.15
1	A	171	SER	C-N-CA	-6.59	115.18	123.15
1	A	132	ALA	N-CA-C	-6.57	101.41	110.35
1	A	160	ALA	CA-C-O	6.53	126.09	119.76
1	A	93	ASN	CA-C-O	-6.50	112.05	119.78
1	A	40	HIS	CA-CB-CG	-6.49	107.31	113.80
1	A	239	GLN	CA-CB-CG	-6.49	101.13	114.10
1	A	37	SER	N-CA-CB	-6.45	101.96	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	SER	CA-C-O	6.40	127.35	120.95
1	A	201	CYS	CA-C-O	-6.40	113.46	120.24
1	A	234	TYR	O-C-N	6.39	129.92	122.19
1	A	154	LEU	CA-C-O	-6.32	113.82	121.28
1	A	162	LEU	N-CA-CB	-6.30	100.18	109.95
1	A	53	VAL	CB-CA-C	6.30	120.39	110.81
1	A	101	ASN	CA-CB-CG	-6.26	106.34	112.60
1	A	172	TYR	O-C-N	6.24	126.89	121.34
1	A	71	HIS	N-CA-CB	6.22	121.01	110.49
1	A	30	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	A	241	THR	O-C-N	6.19	128.44	122.07
1	A	53	VAL	O-C-N	-6.18	116.83	123.14
1	A	193	GLY	N-CA-C	-6.16	107.36	114.69
1	A	81	GLN	N-CA-CB	6.11	120.18	110.65
1	A	216	GLY	CA-C-O	-6.07	115.72	121.60
1	A	81	GLN	CA-C-O	-5.97	113.92	120.30
1	A	168	CYS	CB-CA-C	5.95	120.12	110.96
1	A	125	SER	N-CA-C	-5.95	105.86	113.23
1	A	71	HIS	CA-CB-CG	-5.93	107.87	113.80
1	A	48	ASN	CA-C-O	-5.92	114.94	121.28
1	A	37	SER	CA-CB-OG	-5.92	99.26	111.10
1	A	88	ILE	CA-C-O	-5.91	113.97	120.48
1	A	50	GLN	OE1-CD-NE2	5.89	128.49	122.60
1	A	234	TYR	CA-C-O	-5.89	112.53	119.48
1	A	72	ASN	CB-CG-ND2	5.88	125.22	116.40
1	A	21	THR	O-C-N	5.86	130.35	122.96
1	A	62	ARG	CD-NE-CZ	-5.86	116.20	124.40
1	A	198	PRO	O-C-N	5.85	130.50	123.13
1	A	120	THR	OG1-CB-CG2	-5.81	97.69	109.30
1	A	93	ASN	O-C-N	5.78	129.45	122.35
1	A	134	THR	CA-C-N	5.77	130.08	122.30
1	A	134	THR	C-N-CA	5.77	130.08	122.30
1	A	175	LYS	O-C-N	5.73	128.92	122.27
1	A	176	ILE	CA-C-O	-5.66	114.31	120.71
1	A	144	THR	CA-CB-OG1	-5.66	101.11	109.60
1	A	77	GLU	O-C-N	5.62	129.79	122.42
1	A	25	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	110	SER	O-C-N	5.62	126.82	121.71
1	A	150	ASN	N-CA-CB	5.61	119.29	110.71
1	A	203	GLY	CA-C-N	-5.59	113.89	122.62
1	A	203	GLY	C-N-CA	-5.59	113.89	122.62
1	A	37	SER	CA-C-O	-5.58	114.85	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ALA	CA-C-O	5.57	126.40	120.10
1	A	89	ILE	N-CA-C	5.52	116.06	107.28
1	A	149	VAL	CA-C-O	-5.51	114.50	120.67
1	A	223	ASP	CA-C-O	-5.51	112.38	119.59
1	A	112	VAL	O-C-N	5.49	128.95	122.36
1	A	89	ILE	O-C-N	5.46	128.83	122.99
1	A	55	ALA	O-C-N	5.46	129.57	123.19
1	A	148	GLY	N-CA-C	-5.45	103.56	112.83
1	A	71	HIS	N-CA-C	-5.45	99.19	110.80
1	A	237	TRP	O-C-N	5.42	127.66	122.07
1	A	30	GLN	O-C-N	5.42	129.38	123.04
1	A	138	ILE	O-C-N	5.38	128.99	123.18
1	A	127	SER	CA-C-O	-5.38	115.68	121.38
1	A	60	LYS	N-CA-CB	5.34	121.46	111.52
1	A	199	VAL	CG1-CB-CG2	5.34	122.55	110.80
1	A	21	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	224	ASN	CB-CG-ND2	5.33	124.39	116.40
1	A	242	ILE	O-C-N	5.32	127.03	121.87
1	A	67	ARG	CG-CD-NE	-5.28	100.38	112.00
1	A	28	PRO	N-CA-C	5.24	120.64	113.84
1	A	34	ASN	CA-C-O	5.23	126.01	120.36
1	A	217	TYR	CB-CA-C	5.19	118.71	110.19
1	A	229	THR	CA-C-O	-5.17	114.86	120.81
1	A	200	VAL	O-C-N	5.17	128.61	123.18
1	A	152	PRO	N-CA-CB	-5.17	97.39	103.23
1	A	41	PHE	CB-CA-C	5.15	117.16	109.13
1	A	48	ASN	OD1-CG-ND2	5.11	127.71	122.60
1	A	141	TRP	N-CA-C	-5.11	106.36	112.59
1	A	57	HIS	N-CA-CB	5.10	119.31	110.39
1	A	137	LEU	O-C-N	5.09	129.30	123.29
1	A	190	SER	N-CA-C	-5.08	102.25	110.32
1	A	25	ASN	CB-CA-C	5.06	119.50	111.51
1	A	240	ASP	O-C-N	5.03	127.25	122.07
1	A	150	ASN	CB-CG-ND2	5.02	123.93	116.40
1	A	63	ILE	CA-C-N	-5.02	116.08	123.00
1	A	63	ILE	C-N-CA	-5.02	116.08	123.00
1	A	93	ASN	N-CA-CB	5.01	118.16	110.70
1	A	236	ASP	O-C-N	5.00	127.22	122.07
1	A	77	GLU	CA-C-O	-5.00	113.44	119.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1666	0	1603	55	0
2	A	1	0	0	0	0
3	A	9	0	7	2	0
4	A	137	0	0	5	0
All	All	1813	0	1610	55	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 17.

All (55) 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:64:GLN:HE22	1:A:67:ARG:HH21	1.02	0.94
1:A:72:ASN:HD22	1:A:74:ASN:H	1.12	0.90
1:A:64:GLN:NE2	1:A:67:ARG:HH21	1.70	0.89
1:A:72:ASN:ND2	1:A:74:ASN:H	1.72	0.86
1:A:32:SER:OG	1:A:40:HIS:HD2	1.69	0.76
1:A:172:TYR:HB3	1:A:175:LYS:NZ	2.01	0.74
1:A:115:ASN:HD22	1:A:117:ARG:H	1.38	0.72
1:A:79:ASN:HB3	1:A:117:ARG:HG3	1.76	0.68
1:A:72:ASN:HD22	1:A:74:ASN:N	1.91	0.66
1:A:213:VAL:HA	1:A:228:TYR:CD1	2.30	0.66
1:A:172:TYR:HB3	1:A:175:LYS:HZ3	1.62	0.62
1:A:213:VAL:HG22	1:A:228:TYR:HE1	1.63	0.62
1:A:73:ILE:HD13	1:A:141:TRP:CE2	2.39	0.57
1:A:64:GLN:HE21	1:A:67:ARG:HE	1.53	0.57
1:A:64:GLN:NE2	1:A:67:ARG:NH2	2.48	0.56
1:A:34:ASN:ND2	1:A:38:GLY:H	2.02	0.56
1:A:183:VAL:HB	1:A:228:TYR:CE2	2.40	0.56
1:A:74:ASN:ND2	1:A:153:ASP:OD1	2.35	0.53
1:A:117:ARG:N	1:A:117:ARG:HD2	2.23	0.53
1:A:25:ASN:HB3	1:A:117:ARG:HB3	1.91	0.53
1:A:91:HIS:HB2	1:A:103:ILE:HG23	1.89	0.52
1:A:64:GLN:NE2	1:A:67:ARG:HE	2.07	0.52
1:A:115:ASN:ND2	1:A:117:ARG:H	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:HD22	1:A:72:ASN:C	2.18	0.52
1:A:72:ASN:ND2	1:A:74:ASN:N	2.51	0.51
1:A:24:GLU:HG2	1:A:25:ASN:ND2	2.27	0.50
1:A:120:THR:HG22	4:A:272:HOH:O	2.12	0.49
1:A:64:GLN:HE22	1:A:67:ARG:NH2	1.87	0.49
1:A:213:VAL:CG1	3:A:246:BEN:H5	2.42	0.49
1:A:171:SER:C	1:A:173:PRO:HD3	2.39	0.48
1:A:115:ASN:HD22	1:A:117:ARG:N	2.09	0.47
1:A:117:ARG:HD3	4:A:381:HOH:O	2.15	0.47
1:A:213:VAL:HA	1:A:228:TYR:HD1	1.78	0.47
1:A:236:ASP:HB2	4:A:384:HOH:O	2.14	0.47
1:A:132:ALA:HA	1:A:162:LEU:HD22	1.96	0.47
1:A:115:ASN:HD21	1:A:117:ARG:HG2	1.81	0.46
1:A:213:VAL:HG13	3:A:246:BEN:H5	1.97	0.46
1:A:135:GLN:NE2	4:A:315:HOH:O	2.50	0.45
1:A:160:ALA:HA	1:A:161:PRO:HD3	1.83	0.44
1:A:110:SER:HB2	1:A:111:PRO:HD2	1.99	0.44
1:A:80:GLU:HB3	1:A:82:PHE:CE1	2.52	0.44
1:A:97:LYS:O	1:A:97:LYS:HE2	2.18	0.44
1:A:37:SER:HB2	1:A:41:PHE:CE1	2.53	0.44
1:A:117:ARG:H	1:A:117:ARG:HD2	1.84	0.42
1:A:56:ALA:HA	1:A:104:MET:HB2	2.01	0.42
1:A:86:ALA:HB2	1:A:109:SER:HA	2.00	0.42
1:A:123:LEU:HB3	1:A:124:PRO:HD2	2.01	0.42
1:A:37:SER:HB2	1:A:41:PHE:CD1	2.55	0.41
1:A:73:ILE:HD13	1:A:141:TRP:CZ2	2.55	0.41
1:A:199:VAL:HG11	1:A:228:TYR:CD1	2.56	0.41
1:A:192:GLN:HB3	4:A:383:HOH:O	2.21	0.41
1:A:221(A):LEU:HA	1:A:222:PRO:HD3	1.88	0.41
1:A:32:SER:OG	1:A:40:HIS:CD2	2.60	0.41
1:A:182:CYS:HA	1:A:226:ASP:O	2.21	0.40
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

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	221/223 (99%)	217 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	172 (93%)	13 (7%)	14	16

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	37	SER
1	A	72	ASN
1	A	73	ILE
1	A	87	LYS
1	A	97	LYS
1	A	115	ASN
1	A	117	ARG
1	A	175	LYS
1	A	185	LEU
1	A	199	VAL
1	A	217	TYR
1	A	227	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN

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Mol	Chain	Res	Type
1	A	30	GLN
1	A	34	ASN
1	A	40	HIS
1	A	50	GLN
1	A	64	GLN
1	A	72	ASN
1	A	79	ASN
1	A	93	ASN
1	A	101	ASN
1	A	115	ASN
1	A	135	GLN
1	A	150	ASN
1	A	165	GLN
1	A	192	GLN
1	A	210	GLN
1	A	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 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	1.76	1 (11%)	7,11,11	1.32	1 (14%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	BEN	C1-C	-4.10	1.39	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	BEN	C1-C-N2	2.44	121.72	118.01

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-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	246	BEN	2	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.