



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:34 PM UTC

PDB ID : 1ANB / pdb_00001anb
Title : ANIONIC TRYPSIN MUTANT WITH SER 214 REPLACED BY GLU
Authors : Fletterick, R.J.; Mcgrath, M.E.
Deposited on : 1994-12-21
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

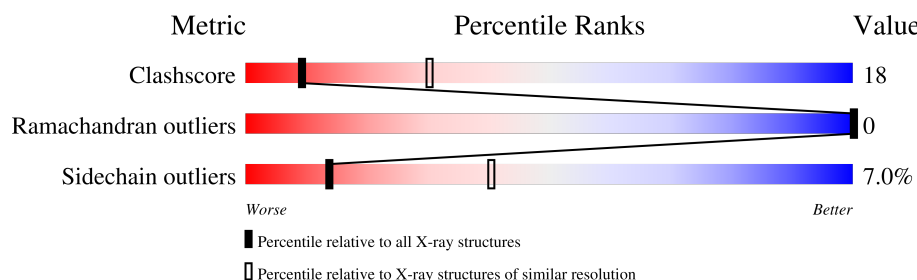
1 Overall quality at a glance

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	

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	A	370	-	X	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1837 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 ANIONIC TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1669	1043	285	327	14			

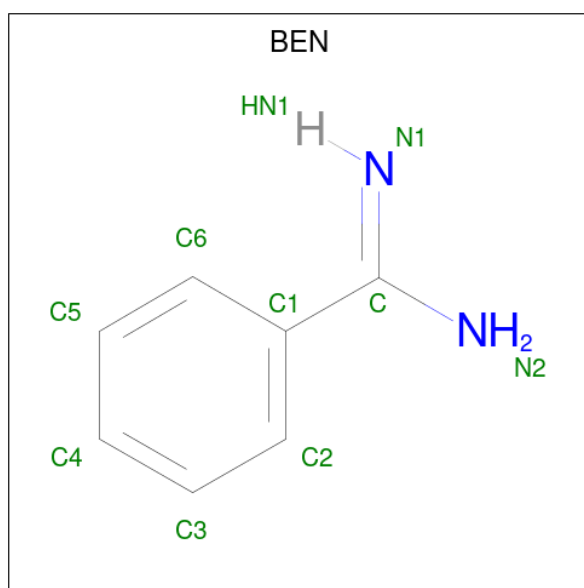
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	GLU	SER	engineered mutation	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		
3	A	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is water.

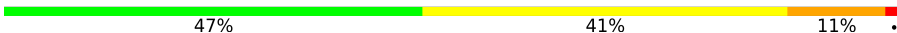
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		

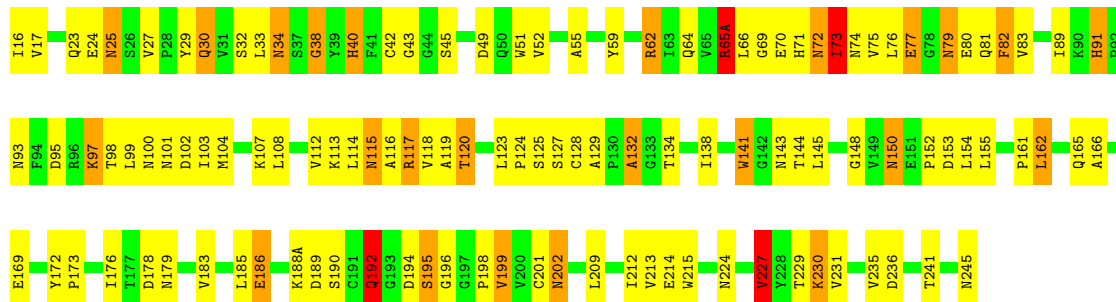
3 Residue-property plots

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: ANIONIC TRYPSIN

Chain A: 



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}	0.13	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1837	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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	1.00	1/1704 (0.1%)	2.31	89/2322 (3.8%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	GLY	N-CA	5.72	1.49	1.44

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	GLN	CB-CG-CD	12.33	133.56	112.60
1	A	120	THR	N-CA-CB	-11.44	92.16	110.46
1	A	82	PHE	CA-CB-CG	11.24	125.04	113.80
1	A	199	VAL	CB-CA-C	10.28	122.13	110.41
1	A	91	HIS	CA-CB-CG	-9.25	104.55	113.80
1	A	128	CYS	CA-C-O	-8.07	111.49	120.69
1	A	192	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	A	190	SER	N-CA-C	-7.76	99.04	110.52
1	A	24	GLU	CA-C-O	7.52	128.93	120.80
1	A	196	GLY	N-CA-C	-7.43	105.59	115.40
1	A	224	ASN	O-C-N	7.42	127.95	121.34
1	A	38	GLY	CA-C-O	7.33	127.27	119.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ILE	CA-CB-CG2	7.31	122.93	110.50
1	A	183	VAL	O-C-N	7.11	130.94	123.05
1	A	154	LEU	O-C-N	7.00	131.27	123.16
1	A	23	GLN	N-CA-C	-6.91	99.81	110.10
1	A	42	CYS	O-C-N	6.88	130.49	123.26
1	A	202	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	162	LEU	N-CA-CB	-6.85	98.86	110.16
1	A	189	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	241	THR	CA-CB-OG1	-6.69	99.56	109.60
1	A	34	ASN	CA-CB-CG	-6.69	105.91	112.60
1	A	138	ILE	O-C-N	6.68	129.96	123.14
1	A	62	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	A	123	LEU	N-CA-C	-6.58	100.64	110.24
1	A	24	GLU	CA-CB-CG	6.57	127.23	114.10
1	A	227	VAL	CB-CA-C	6.56	120.78	110.81
1	A	162	LEU	CB-CA-C	6.51	120.48	109.80
1	A	183	VAL	CA-C-O	-6.50	113.61	120.76
1	A	59	TYR	CA-C-O	6.49	128.33	121.19
1	A	199	VAL	N-CA-CB	6.47	120.75	112.34
1	A	245	ASN	CA-CB-CG	6.40	119.00	112.60
1	A	100	ASN	CB-CA-C	6.29	120.17	109.53
1	A	101	ASN	CA-CB-CG	-6.28	106.32	112.60
1	A	40	HIS	CA-CB-CG	-6.24	107.56	113.80
1	A	141	TRP	CA-C-O	6.24	127.31	119.95
1	A	119	ALA	CA-C-O	6.21	128.42	121.40
1	A	123	LEU	CB-CA-C	6.08	118.23	109.11
1	A	245	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	A	25	ASN	CB-CA-C	6.01	121.00	111.51
1	A	76	LEU	O-C-N	5.98	130.60	122.82
1	A	127	SER	CA-C-O	-5.89	115.14	121.45
1	A	100	ASN	N-CA-C	-5.88	100.90	110.20
1	A	33	LEU	CA-C-O	5.86	126.85	120.58
1	A	132	ALA	CA-C-O	-5.86	114.74	121.19
1	A	235	VAL	CB-CA-C	5.85	119.37	111.88
1	A	55	ALA	O-C-N	5.83	130.01	123.19
1	A	52	VAL	CA-C-O	5.83	126.51	120.39
1	A	79	ASN	N-CA-C	-5.71	106.18	114.12
1	A	91	HIS	N-CA-C	-5.71	101.26	109.48
1	A	93	ASN	O-C-N	5.69	129.65	122.37
1	A	107	LYS	CA-C-O	-5.61	114.20	120.54
1	A	30	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	A	51	TRP	CA-C-O	5.61	127.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	GLU	CG-CD-OE2	-5.61	105.50	118.40
1	A	155	LEU	N-CA-CB	-5.55	101.44	109.83
1	A	192	GLN	CB-CA-C	5.55	118.64	109.70
1	A	89	ILE	CB-CA-C	-5.50	103.84	110.99
1	A	65(A)	ARG	CA-C-O	-5.46	114.45	120.30
1	A	230	LYS	N-CA-CB	-5.46	102.70	110.46
1	A	93	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	178	ASP	CA-C-O	-5.43	110.23	118.91
1	A	43	GLY	N-CA-C	-5.42	103.20	112.64
1	A	143	ASN	OD1-CG-ND2	5.41	128.01	122.60
1	A	199	VAL	CA-C-O	5.40	125.03	120.22
1	A	69	GLY	O-C-N	5.39	128.45	122.31
1	A	101	ASN	OD1-CG-ND2	5.39	127.99	122.60
1	A	148	GLY	N-CA-C	-5.37	103.08	112.53
1	A	166	ALA	CA-C-O	-5.36	115.17	120.90
1	A	51	TRP	N-CA-C	5.31	118.09	108.69
1	A	71	HIS	N-CA-CB	5.30	119.44	110.49
1	A	104	MET	CA-C-O	-5.28	114.94	121.06
1	A	129	ALA	O-C-N	5.27	127.33	121.43
1	A	77	GLU	OE1-CD-OE2	5.26	135.53	122.90
1	A	81	GLN	N-CA-CB	5.24	119.00	110.77
1	A	212	ILE	CA-C-O	-5.21	114.84	120.36
1	A	29	TYR	CA-C-O	5.21	125.38	119.18
1	A	33	LEU	CB-CA-C	5.20	119.39	110.81
1	A	125	SER	N-CA-C	-5.20	106.09	112.90
1	A	59	TYR	CA-C-N	5.13	130.94	121.85
1	A	59	TYR	C-N-CA	5.13	130.94	121.85
1	A	229	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	215	TRP	CA-CB-CG	5.10	123.29	113.60
1	A	186	GLU	CG-CD-OE1	-5.09	106.68	118.40
1	A	113	LYS	O-C-N	5.08	129.03	122.93
1	A	128	CYS	N-CA-C	-5.08	101.69	109.76
1	A	150	ASN	N-CA-CB	5.06	118.94	110.59
1	A	132	ALA	N-CA-C	-5.04	102.92	110.23
1	A	179	ASN	OD1-CG-ND2	5.02	127.62	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65(A)	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	1669	0	1604	60	0
2	A	1	0	0	0	0
3	A	18	0	15	0	18
4	A	149	0	0	10	3
All	All	1837	0	1619	60	21

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 18.

All (60) 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:192:GLN:HB3	4:A:517:HOH:O	0.96	1.12
1:A:214:GLU:HG2	4:A:515:HOH:O	1.46	1.12
1:A:64:GLN:HE22	1:A:65(A):ARG:HH21	1.03	1.00
1:A:72:ASN:HD22	1:A:74:ASN:H	1.15	0.90
1:A:72:ASN:ND2	1:A:74:ASN:H	1.72	0.86
1:A:34:ASN:ND2	1:A:38:GLY:H	1.82	0.77
1:A:64:GLN:NE2	1:A:65(A):ARG:HH21	1.82	0.73
1:A:192:GLN:CB	4:A:517:HOH:O	1.75	0.71
1:A:115:ASN:HD22	1:A:116:ALA:N	1.89	0.70
1:A:115:ASN:ND2	1:A:117:ARG:H	1.91	0.68
1:A:115:ASN:HD22	1:A:117:ARG:H	1.41	0.68
1:A:64:GLN:HE21	1:A:65(A):ARG:HE	1.41	0.67
1:A:80:GLU:HB3	1:A:82:PHE:CE1	2.34	0.62
1:A:64:GLN:HE22	1:A:65(A):ARG:NH2	1.87	0.61
1:A:64:GLN:NE2	1:A:65(A):ARG:HE	1.99	0.61
1:A:70:GLU:HB2	4:A:390:HOH:O	2.00	0.60
1:A:34:ASN:HD21	1:A:38:GLY:H	1.49	0.59
1:A:72:ASN:HD22	1:A:72:ASN:C	2.11	0.59
1:A:91:HIS:HB2	1:A:103:ILE:HG23	1.85	0.59
1:A:25:ASN:HB3	1:A:117:ARG:HB3	1.85	0.59
1:A:79:ASN:HB3	1:A:117:ARG:HG3	1.85	0.58
1:A:74:ASN:ND2	1:A:153:ASP:OD1	2.34	0.58
1:A:214:GLU:CG	4:A:515:HOH:O	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:SER:OG	1:A:40:HIS:HD2	1.88	0.56
1:A:214:GLU:HB3	1:A:227:VAL:O	2.06	0.56
1:A:16:ILE:N	1:A:194:ASP:OD2	2.39	0.56
1:A:79:ASN:HB2	4:A:411:HOH:O	2.08	0.53
1:A:195:SER:HA	1:A:213:VAL:HB	1.91	0.52
1:A:27:VAL:HG12	1:A:30:GLN:HB2	1.91	0.52
1:A:124:PRO:HD3	1:A:209:LEU:O	2.09	0.51
1:A:144:THR:HG23	1:A:152:PRO:HG3	1.93	0.50
1:A:172:TYR:HB2	1:A:176:ILE:HD11	1.93	0.50
1:A:165:GLN:O	1:A:169:GLU:HG3	2.13	0.48
1:A:134:THR:O	1:A:161:PRO:HA	2.13	0.48
1:A:83:VAL:CG1	1:A:108:LEU:HB3	2.44	0.48
1:A:45:SER:OG	1:A:198:PRO:HB3	2.14	0.47
1:A:98:THR:O	1:A:99:LEU:HB2	2.13	0.47
1:A:49:ASP:O	1:A:112:VAL:HG22	2.15	0.47
1:A:209:LEU:HG	1:A:231:VAL:HG21	1.97	0.47
1:A:132:ALA:HA	1:A:162:LEU:HD22	1.97	0.46
1:A:83:VAL:HG11	1:A:108:LEU:HB3	1.97	0.46
1:A:117:ARG:N	1:A:117:ARG:HD2	2.31	0.45
1:A:102:ASP:OD2	1:A:214:GLU:OE2	2.35	0.45
1:A:214:GLU:CD	4:A:515:HOH:O	2.57	0.45
1:A:95:ASP:OD1	1:A:97:LYS:HB2	2.16	0.45
1:A:230:LYS:HE2	4:A:505:HOH:O	2.17	0.44
1:A:17:VAL:O	1:A:188(A):LYS:HA	2.16	0.44
1:A:145:LEU:HG	1:A:150:ASN:HB3	1.99	0.44
1:A:75:VAL:O	1:A:77:GLU:HG3	2.18	0.43
1:A:72:ASN:ND2	1:A:72:ASN:C	2.76	0.43
1:A:91:HIS:HB2	1:A:103:ILE:CG2	2.49	0.43
1:A:62:ARG:HG2	4:A:398:HOH:O	2.18	0.42
1:A:99:LEU:HD13	1:A:214:GLU:OE2	2.20	0.42
1:A:172:TYR:HB2	1:A:176:ILE:CD1	2.50	0.41
1:A:144:THR:CG2	1:A:152:PRO:HG3	2.49	0.41
1:A:114:LEU:HA	1:A:118:VAL:O	2.21	0.41
1:A:201:CYS:O	1:A:202:ASN:C	2.63	0.41
1:A:66:LEU:HD13	1:A:112:VAL:HG11	2.03	0.41
1:A:236:ASP:HB2	4:A:469:HOH:O	2.21	0.40
1:A:73:ILE:HD13	1:A:141:TRP:CE2	2.57	0.40

All (21) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:370:BEN:C3	3:A:370:BEN:C4[2_565]	0.92	1.28
3:A:370:BEN:C2	3:A:370:BEN:C6[2_565]	1.18	1.02
3:A:370:BEN:N1	3:A:370:BEN:N2[2_565]	1.22	0.98
3:A:370:BEN:C2	3:A:370:BEN:C5[2_565]	1.30	0.90
3:A:370:BEN:C3	3:A:370:BEN:C3[2_565]	1.33	0.87
3:A:370:BEN:C3	3:A:370:BEN:C5[2_565]	1.40	0.80
3:A:370:BEN:C1	3:A:370:BEN:C2[2_565]	1.53	0.67
3:A:370:BEN:C1	3:A:370:BEN:C1[2_565]	1.53	0.67
3:A:370:BEN:C2	3:A:370:BEN:C4[2_565]	1.69	0.51
4:A:470:HOH:O	4:A:470:HOH:O[4_566]	1.83	0.37
3:A:370:BEN:C4	3:A:370:BEN:C4[2_565]	1.87	0.33
3:A:370:BEN:C	3:A:370:BEN:C[2_565]	1.90	0.30
3:A:370:BEN:C2	3:A:370:BEN:C2[2_565]	1.91	0.29
3:A:370:BEN:C	3:A:370:BEN:N2[2_565]	1.94	0.26
3:A:370:BEN:C2	3:A:370:BEN:C3[2_565]	1.96	0.24
3:A:370:BEN:C3	3:A:370:BEN:C6[2_565]	1.96	0.24
4:A:459:HOH:O	4:A:459:HOH:O[2_565]	2.02	0.18
3:A:370:BEN:C	3:A:370:BEN:N1[2_565]	2.12	0.08
3:A:370:BEN:C1	3:A:370:BEN:C3[2_565]	2.16	0.04
4:A:432:HOH:O	4:A:473:HOH:O[4_566]	2.18	0.02
3:A:370:BEN:C1	3:A:370:BEN:C6[2_565]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/223 (99%)	210 (95%)	11 (5%)	0	100	100

There are no Ramachandran outliers to report.

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%)	172 (93%)	13 (7%)	14	40

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

Mol	Chain	Res	Type
1	A	72	ASN
1	A	73	ILE
1	A	97	LYS
1	A	115	ASN
1	A	117	ARG
1	A	120	THR
1	A	173	PRO
1	A	185	LEU
1	A	186	GLU
1	A	192	GLN
1	A	195	SER
1	A	199	VAL
1	A	227	VAL

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	23	GLN
1	A	25	ASN
1	A	30	GLN
1	A	34	ASN
1	A	40	HIS
1	A	50	GLN
1	A	64	GLN
1	A	71	HIS
1	A	72	ASN
1	A	84	ASN
1	A	101	ASN
1	A	115	ASN
1	A	150	ASN
1	A	165	GLN
1	A	210	GLN
1	A	224	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	A	370	-	9,9,9	2.63	7 (77%)	7,11,11	1.73	3 (42%)
3	BEN	A	290	-	9,9,9	1.87	1 (11%)	7,11,11	0.80	0

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	370	-	-	1/4/4/4	0/1/1/1
3	BEN	A	290	-	-	1/4/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	290	BEN	C1-C	-4.07	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	370	BEN	C3-C2	3.85	1.45	1.38
3	A	370	BEN	C4-C3	3.64	1.46	1.38
3	A	370	BEN	C5-C4	2.89	1.44	1.38
3	A	370	BEN	C-N1	2.58	1.38	1.27
3	A	370	BEN	C5-C6	2.49	1.43	1.38
3	A	370	BEN	C6-C1	2.47	1.43	1.39
3	A	370	BEN	C-N2	2.10	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	370	BEN	C6-C1-C2	3.06	122.46	118.57
3	A	370	BEN	C3-C2-C1	-2.42	117.98	120.36
3	A	370	BEN	C1-C-N2	-2.11	114.81	118.01

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	290	BEN	N1-C-C1-C2
3	A	370	BEN	N1-C-C1-C6

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	370	BEN	0	18

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.