



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:27 PM UTC

PDB ID : 1DPO / pdb_00001dpo
Title : STRUCTURE OF RAT TRYPSIN
Authors : Stroud, R.M.
Deposited on : 1997-03-31
Resolution : 1.59 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

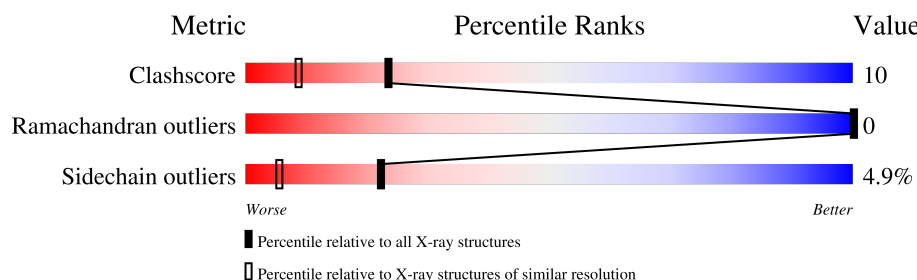
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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
4	BEN	A	247	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1926 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
			Total	C	N	O	S			
1	A	223	1671	1045	285	326	15	0	2	0

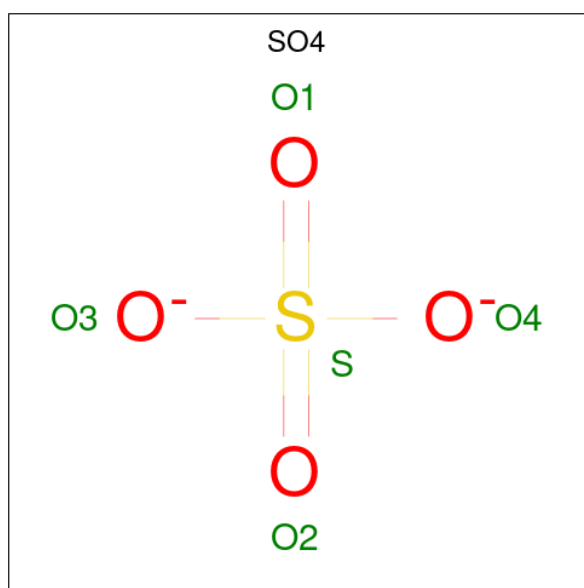
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	CYS	SER	engineered mutation	UNP P00763

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

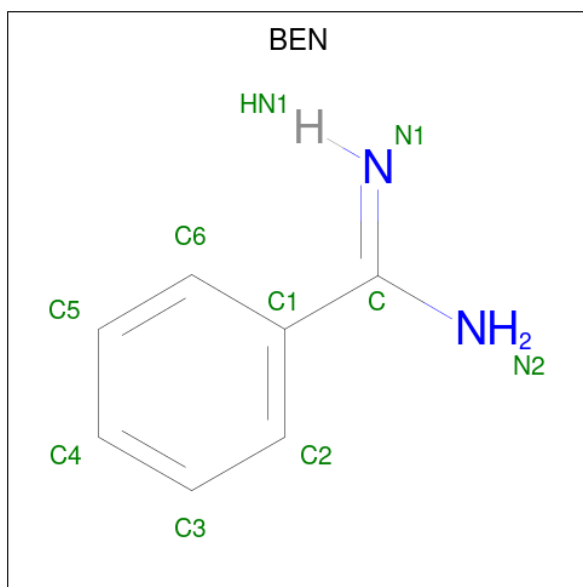
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	217	Total O 217 217	0	0

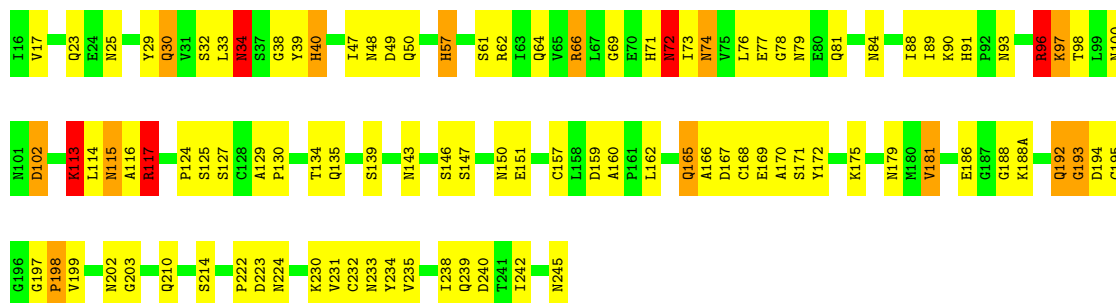
3 Residue-property plots

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

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	123.12Å 123.12Å 123.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.59	Depositor
% Data completeness (in resolution range)	97.0 (12.00-1.59)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1926	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: BEN, SO4, 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	1.73	11/1715 (0.6%)	2.79	152/2337 (6.5%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LYS	N-CA	6.90	1.54	1.45
1	A	169	GLU	C-O	6.80	1.32	1.24
1	A	40	HIS	ND1-CE1	6.28	1.38	1.32
1	A	113	LYS	CA-CB	-6.03	1.45	1.53
1	A	134	THR	N-CA	5.88	1.53	1.46
1	A	181	VAL	C-O	5.81	1.29	1.24
1	A	23	GLN	N-CA	5.37	1.52	1.45
1	A	69	GLY	N-CA	5.32	1.52	1.45
1	A	102	ASP	C-N	-5.08	1.27	1.33
1	A	230	LYS	N-CA	5.08	1.53	1.46
1	A	147	SER	N-CA	5.02	1.52	1.46

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	CD-NE-CZ	34.38	172.53	124.40
1	A	202	ASN	OD1-CG-ND2	-15.69	106.91	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	LYS	CG-CD-CE	15.50	146.95	111.30
1	A	113	LYS	CA-CB-CG	15.33	144.75	114.10
1	A	179	ASN	OD1-CG-ND2	12.31	134.91	122.60
1	A	96	ARG	CB-CG-CD	11.65	138.09	111.30
1	A	117	ARG	NE-CZ-NH1	11.62	133.12	121.50
1	A	242	ILE	O-C-N	11.25	132.78	121.87
1	A	62	ARG	CG-CD-NE	-10.94	87.93	112.00
1	A	245	ASN	CA-CB-CG	-10.54	102.06	112.60
1	A	166	ALA	CA-C-O	-10.41	109.52	120.55
1	A	62	ARG	NE-CZ-NH2	-10.25	109.97	119.20
1	A	23	GLN	OE1-CD-NE2	-10.14	112.46	122.60
1	A	62	ARG	CD-NE-CZ	-9.94	110.49	124.40
1	A	197	GLY	O-C-N	9.25	131.43	122.18
1	A	175	LYS	CD-CE-NZ	9.02	140.77	111.90
1	A	49	ASP	CA-CB-CG	-8.93	103.67	112.60
1	A	84	ASN	CB-CG-ND2	8.75	129.53	116.40
1	A	84	ASN	CA-CB-CG	-8.60	104.00	112.60
1	A	160	ALA	CA-C-O	8.44	127.95	119.76
1	A	89	ILE	O-C-N	8.22	132.69	122.66
1	A	40	HIS	CA-CB-CG	-8.18	105.62	113.80
1	A	159	ASP	O-C-N	-8.18	113.89	123.22
1	A	240	ASP	O-C-N	7.97	130.28	122.07
1	A	127	SER	CA-C-O	-7.95	112.72	121.23
1	A	239	GLN	OE1-CD-NE2	7.78	130.38	122.60
1	A	73	ILE	CA-C-O	-7.69	109.45	119.53
1	A	79	ASN	CB-CG-ND2	7.54	127.71	116.40
1	A	175	LYS	CA-CB-CG	7.54	129.18	114.10
1	A	202	ASN	CA-CB-CG	-7.39	105.21	112.60
1	A	235	VAL	O-C-N	7.30	128.95	121.87
1	A	116	ALA	CA-C-O	-7.29	111.59	119.97
1	A	125	SER	CB-CA-C	7.24	122.24	109.65
1	A	231	VAL	O-C-N	7.20	129.14	121.87
1	A	30	GLN	OE1-CD-NE2	-7.18	115.42	122.60
1	A	239	GLN	O-C-N	7.13	129.67	122.12
1	A	224	ASN	CB-CG-ND2	7.10	127.05	116.40
1	A	97	LYS	CA-C-O	-7.04	111.36	119.60
1	A	91	HIS	CA-CB-CG	-7.03	106.77	113.80
1	A	96	ARG	CD-NE-CZ	-7.01	114.58	124.40
1	A	239	GLN	CG-CD-NE2	-7.00	105.90	116.40
1	A	100	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	171	SER	CA-C-O	-6.81	112.14	119.97
1	A	96	ARG	CA-C-O	-6.77	111.30	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASN	OD1-CG-ND2	6.73	129.33	122.60
1	A	202	ASN	CB-CG-OD1	6.69	134.17	120.80
1	A	47	ILE	CA-C-O	-6.66	112.63	118.96
1	A	165	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	A	49	ASP	CA-C-O	-6.62	110.44	119.05
1	A	198	PRO	N-CA-C	6.62	122.73	111.68
1	A	224	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	89	ILE	N-CA-C	6.60	117.21	106.72
1	A	76	LEU	CA-C-O	-6.58	113.17	120.60
1	A	167	ASP	O-C-N	6.52	129.59	122.15
1	A	240	ASP	CA-C-O	-6.52	113.98	120.82
1	A	88	ILE	CA-C-O	-6.50	113.94	120.31
1	A	193	GLY	N-CA-C	-6.49	106.96	114.69
1	A	96	ARG	CA-CB-CG	6.46	127.01	114.10
1	A	114	LEU	CA-C-O	-6.45	113.69	121.05
1	A	235	VAL	CA-C-O	-6.44	114.25	120.95
1	A	93	ASN	CA-CB-CG	-6.37	106.23	112.60
1	A	231	VAL	CA-C-O	-6.33	113.80	120.57
1	A	48	ASN	CA-C-O	-6.27	114.73	121.38
1	A	71	HIS	CA-CB-CG	-6.26	107.54	113.80
1	A	233	ASN	CA-C-O	-6.24	111.75	119.18
1	A	61	SER	CA-C-O	-6.17	112.87	119.97
1	A	117	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	186	GLU	CG-CD-OE2	-6.16	104.23	118.40
1	A	127	SER	O-C-N	6.13	129.98	123.42
1	A	188	GLY	CA-C-O	-6.09	111.55	120.25
1	A	114	LEU	CD1-CG-CD2	-6.08	97.42	110.80
1	A	72	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	81	GLN	N-CA-CB	6.07	121.30	110.80
1	A	96	ARG	NE-CZ-NH1	6.05	127.55	121.50
1	A	79	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	A	98	THR	CA-C-O	-5.97	112.34	119.15
1	A	202	ASN	CA-C-O	-5.96	114.62	121.54
1	A	125	SER	CA-C-O	-5.96	112.35	119.15
1	A	89	ILE	N-CA-CB	-5.95	104.95	112.15
1	A	98	THR	N-CA-C	-5.94	106.07	113.38
1	A	181	VAL	CA-C-O	-5.93	114.23	120.76
1	A	72	ASN	CA-C-O	-5.90	113.93	120.60
1	A	167	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	73	ILE	CA-C-N	-5.88	113.43	122.60
1	A	73	ILE	C-N-CA	-5.88	113.43	122.60
1	A	222	PRO	CA-C-O	5.87	128.03	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ILE	CA-C-N	-5.84	111.99	120.29
1	A	242	ILE	C-N-CA	-5.84	111.99	120.29
1	A	34	ASN	O-C-N	5.81	130.35	123.27
1	A	157	CYS	N-CA-CB	-5.78	101.49	111.55
1	A	29	TYR	N-CA-C	-5.77	106.24	113.28
1	A	73	ILE	O-C-N	5.74	130.12	122.31
1	A	203	GLY	CA-C-N	-5.73	113.68	122.62
1	A	203	GLY	C-N-CA	-5.73	113.68	122.62
1	A	238	ILE	O-C-N	5.72	127.85	121.90
1	A	116	ALA	O-C-N	5.65	129.22	122.27
1	A	210	GLN	CA-C-N	-5.63	115.55	121.35
1	A	210	GLN	C-N-CA	-5.63	115.55	121.35
1	A	39	TYR	N-CA-C	-5.63	99.75	108.42
1	A	91	HIS	ND1-CE1-NE2	5.61	114.01	108.40
1	A	23	GLN	CG-CD-NE2	5.61	124.82	116.40
1	A	146[A]	SER	CA-C-O	-5.61	112.50	119.18
1	A	146[B]	SER	CA-C-O	-5.61	112.50	119.18
1	A	88	ILE	CB-CA-C	5.61	117.40	110.73
1	A	97	LYS	N-CA-CB	5.61	118.74	110.33
1	A	125	SER	N-CA-C	-5.61	106.48	113.38
1	A	139	SER	O-C-N	5.54	129.56	123.25
1	A	151	GLU	CA-CB-CG	-5.50	103.10	114.10
1	A	130	PRO	N-CA-CB	-5.48	97.83	103.15
1	A	50	GLN	CA-C-N	-5.42	113.34	122.29
1	A	50	GLN	C-N-CA	-5.42	113.34	122.29
1	A	39	TYR	O-C-N	5.39	128.80	123.46
1	A	66	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	193	GLY	CA-C-O	-5.37	113.53	119.27
1	A	84	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	245	ASN	OD1-CG-ND2	5.33	127.93	122.60
1	A	114	LEU	O-C-N	5.32	129.29	123.01
1	A	139	SER	CA-C-N	-5.31	112.93	121.32
1	A	139	SER	C-N-CA	-5.31	112.93	121.32
1	A	125	SER	CA-CB-OG	-5.30	100.50	111.10
1	A	74	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	79	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	77	GLU	CA-CB-CG	-5.23	103.64	114.10
1	A	78	GLY	CA-C-O	-5.21	113.08	119.03
1	A	168	CYS	O-C-N	5.21	127.72	122.09
1	A	224	ASN	O-C-N	5.21	125.45	121.23
1	A	245	ASN	CA-C-O	-5.20	105.41	121.00
1	A	165	GLN	N-CA-CB	5.20	117.85	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASN	O-C-N	5.18	129.91	123.28
1	A	71	HIS	N-CA-C	-5.17	99.79	110.80
1	A	223	ASP	CA-C-O	-5.16	114.18	120.12
1	A	203	GLY	O-C-N	5.16	128.86	122.41
1	A	203	GLY	CA-C-O	-5.16	112.84	119.13
1	A	48	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	A	150	ASN	CA-C-O	-5.15	113.92	120.20
1	A	194	ASP	N-CA-C	-5.15	107.00	113.28
1	A	48	ASN	N-CA-CB	5.13	119.36	111.46
1	A	172	TYR	N-CA-CB	-5.12	104.74	111.09
1	A	233	ASN	N-CA-C	-5.12	107.03	113.28
1	A	50	GLN	CA-CB-CG	-5.11	103.88	114.10
1	A	62	ARG	NH1-CZ-NH2	5.08	125.90	119.30
1	A	234	TYR	N-CA-CB	-5.06	102.84	111.20
1	A	97	LYS	CA-CB-CG	5.04	124.18	114.10
1	A	33	LEU	N-CA-C	-5.04	101.03	109.24
1	A	40	HIS	CB-CG-CD2	-5.04	124.66	131.20
1	A	197	GLY	CA-C-O	-5.02	117.21	122.38
1	A	199	VAL	CA-C-O	-5.02	115.39	120.31
1	A	170	ALA	CB-CA-C	-5.02	101.04	110.67
1	A	57	HIS	N-CA-CB	5.01	119.43	110.32
1	A	72	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	170	ALA	CA-C-N	-5.00	112.71	120.31
1	A	170	ALA	C-N-CA	-5.00	112.71	120.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	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	1671	0	1611	34	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	0	0
4	A	27	0	21	0	0
5	A	217	0	0	4	3
All	All	1926	0	1632	34	3

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 10.

All (34) 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:162[B]:LEU:HD21	1:A:181:VAL:CG2	1.36	1.51
1:A:162[B]:LEU:CD2	1:A:181:VAL:CG2	2.15	1.24
1:A:162[B]:LEU:CD2	1:A:181:VAL:HG21	1.79	1.02
1:A:57:HIS:NE2	1:A:195:CYS:HB3	1.80	0.97
1:A:162[B]:LEU:CD2	1:A:181:VAL:HG22	1.90	0.96
1:A:72:ASN:HD22	1:A:74:ASN:H	1.26	0.83
1:A:162[B]:LEU:HD21	1:A:181:VAL:HG21	0.82	0.82
1:A:25:ASN:HD22	1:A:117:ARG:NH1	1.79	0.80
1:A:135:GLN:NE2	5:A:459:HOH:O	2.15	0.80
1:A:34:ASN:ND2	1:A:38:GLY:H	1.82	0.77
1:A:25:ASN:HD22	1:A:117:ARG:HH11	1.29	0.76
1:A:72:ASN:ND2	1:A:74:ASN:H	1.85	0.75
1:A:64:GLN:HE21	1:A:66:ARG:HE	1.38	0.71
1:A:64:GLN:NE2	1:A:66:ARG:HE	1.92	0.68
1:A:115:ASN:HD22	1:A:117:ARG:H	1.45	0.64
1:A:64:GLN:HE22	1:A:66:ARG:HH21	1.45	0.63
1:A:32:SER:OG	1:A:40:HIS:HD2	1.82	0.62
1:A:115:ASN:HD22	1:A:115:ASN:C	2.10	0.60
1:A:57:HIS:NE2	1:A:195:CYS:CB	2.64	0.56
1:A:115:ASN:ND2	1:A:117:ARG:H	2.02	0.56
1:A:72:ASN:HD22	1:A:72:ASN:C	2.14	0.55
1:A:162[B]:LEU:HD13	5:A:359:HOH:O	2.06	0.55
1:A:162[B]:LEU:HD23	1:A:181:VAL:HG22	1.88	0.52
1:A:40:HIS:HE1	1:A:193:GLY:O	1.98	0.47
1:A:57:HIS:HE1	1:A:214:SER:HA	1.79	0.47
1:A:195:CYS:SG	5:A:354:HOH:O	2.23	0.46
1:A:192:GLN:NE2	1:A:192:GLN:H	2.13	0.46
1:A:57:HIS:ND1	1:A:102:ASP:OD2	2.42	0.45
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.82	0.44
1:A:57:HIS:CD2	5:A:354:HOH:O	2.71	0.43

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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	2.20	0.42
1:A:124:PRO:HG2	1:A:232:CYS:HA	2.03	0.41
1:A:129:ALA:HB3	1:A:162[A]:LEU:HD11	2.03	0.41
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.69	0.40

All (3) 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)
5:A:404:HOH:O	5:A:404:HOH:O[4_566]	1.98	0.22
5:A:399:HOH:O	5:A:402:HOH:O[3_556]	2.04	0.16
5:A:323:HOH:O	5:A:323:HOH:O[2_565]	2.17	0.03

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	223/223 (100%)	219 (98%)	4 (2%)	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	187/185 (101%)	178 (95%)	9 (5%)	23 6

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	72	ASN
1	A	96	ARG
1	A	97	LYS
1	A	113	LYS
1	A	115	ASN
1	A	117	ARG
1	A	165	GLN
1	A	192	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
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	72	ASN
1	A	93	ASN
1	A	101	ASN
1	A	115	ASN
1	A	135	GLN
1	A	192	GLN
1	A	210	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
4	BEN	A	248	-	9,9,9	2.08	4 (44%)	7,11,11	1.97	3 (42%)
3	SO4	A	251	-	4,4,4	0.75	0	6,6,6	0.57	0
4	BEN	A	249	-	9,9,9	2.23	3 (33%)	7,11,11	2.55	4 (57%)
3	SO4	A	250	-	4,4,4	0.62	0	6,6,6	0.86	0
4	BEN	A	247	-	9,9,9	2.08	6 (66%)	7,11,11	3.48	5 (71%)

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
4	BEN	A	248	-	-	2/4/4/4	0/1/1/1
4	BEN	A	247	-	-	0/4/4/4	0/1/1/1
4	BEN	A	249	-	-	0/4/4/4	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	249	BEN	C1-C	-4.28	1.39	1.47
4	A	248	BEN	C1-C	-3.29	1.41	1.47
4	A	249	BEN	C4-C3	3.25	1.45	1.38
4	A	248	BEN	C3-C2	3.03	1.44	1.38
4	A	247	BEN	C5-C6	2.88	1.43	1.38
4	A	247	BEN	C1-C	-2.84	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	248	BEN	C4-C3	2.47	1.43	1.38
4	A	247	BEN	C5-C4	2.34	1.43	1.38
4	A	247	BEN	C2-C1	-2.33	1.35	1.39
4	A	249	BEN	C3-C2	2.24	1.42	1.38
4	A	248	BEN	C5-C6	2.22	1.42	1.38
4	A	247	BEN	C4-C3	2.19	1.43	1.38
4	A	247	BEN	C3-C2	2.06	1.42	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	247	BEN	C4-C3-C2	5.09	126.52	120.24
4	A	247	BEN	C3-C2-C1	-4.48	115.96	120.36
4	A	249	BEN	C6-C1-C2	4.10	123.79	118.57
4	A	247	BEN	C5-C4-C3	-4.04	114.34	119.87
4	A	249	BEN	C4-C3-C2	-3.64	115.75	120.24
4	A	249	BEN	C5-C6-C1	-3.32	117.10	120.36
4	A	248	BEN	C5-C6-C1	3.27	123.58	120.36
4	A	247	BEN	C1-C-N2	3.20	122.87	118.01
4	A	247	BEN	C6-C1-C2	2.63	121.92	118.57
4	A	248	BEN	C5-C4-C3	-2.49	116.45	119.87
4	A	248	BEN	C6-C1-C2	-2.36	115.57	118.57
4	A	249	BEN	C5-C4-C3	2.04	122.66	119.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	248	BEN	N2-C-C1-C2
4	A	248	BEN	N2-C-C1-C6

There are no ring outliers.

No monomer is involved in short contacts.

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.