



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:57 PM UTC

PDB ID : 1PPN / pdb_00001ppn
Title : STRUCTURE OF MONOCLINIC PAPAIN AT 1.60 ANGSTROMS RESOLUTION
Authors : Pickersgill, R.W.; Harris, G.W.; Garman, E.
Deposited on : 1991-10-25
Resolution : 1.60 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

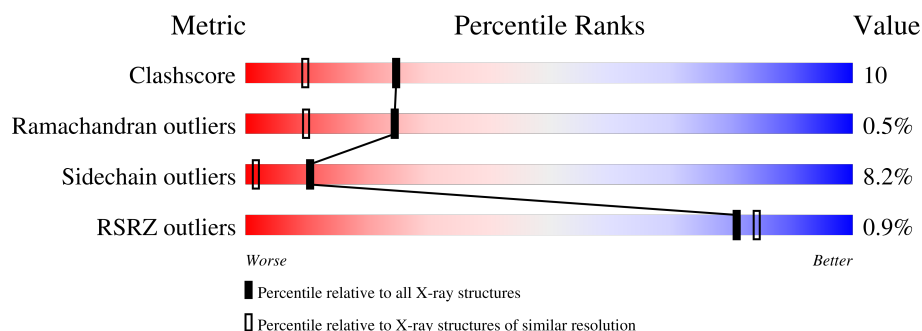
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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)
RSRZ outliers	180081	4672 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	212	43% 45% 8% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1888 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.

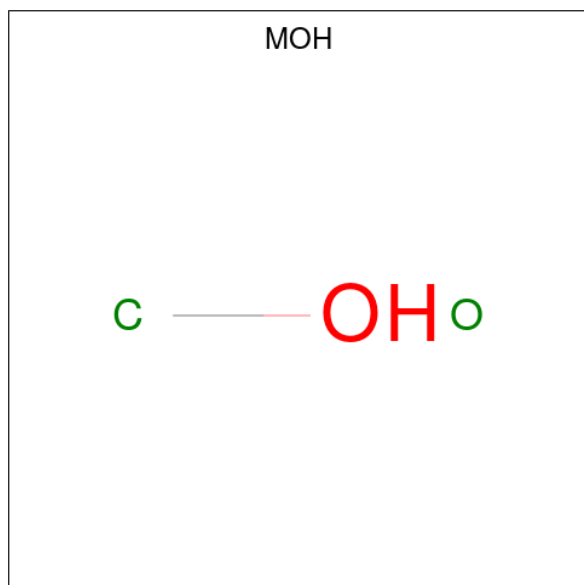
- Molecule 1 is a protein called PAPAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	1	0
			1659	1052	291	309	7			

- Molecule 2 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

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

- Molecule 3 is METHANOL (CCD ID: MOH) (formula: CH₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			2	1	1		

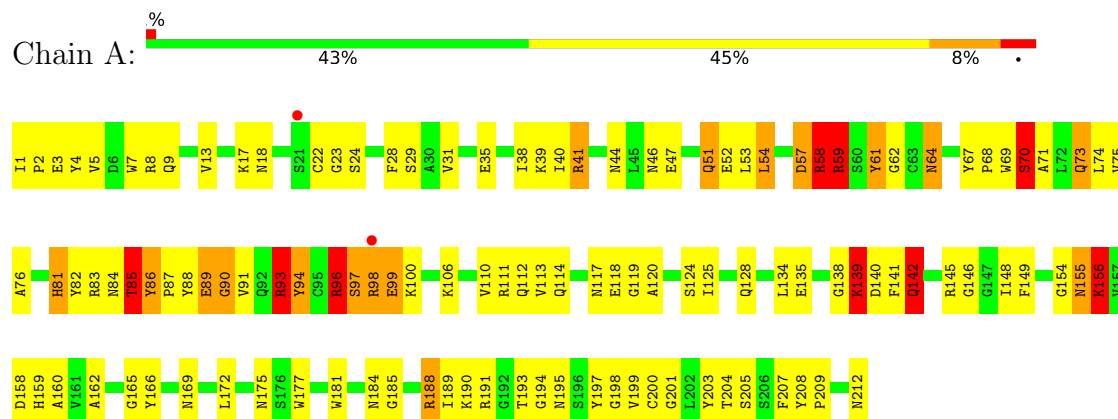
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	226	Total 226	O 226	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: PAPAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.70Å 50.70Å 31.50Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60 10.00 – 1.63	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.60) 61.7 (10.00-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 1.62Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.160 , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 92.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1888	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MOH, UNL

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	1.70	26/1707 (1.5%)	2.69	154/2317 (6.6%)

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	9

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLU	N-CA	8.07	1.56	1.46
1	A	159	HIS	ND1-CE1	8.06	1.40	1.32
1	A	199	VAL	C-O	7.71	1.31	1.24
1	A	81	HIS	ND1-CE1	6.97	1.39	1.32
1	A	159	HIS	CE1-NE2	6.96	1.39	1.32
1	A	189	ILE	N-CA	6.62	1.54	1.46
1	A	141	PHE	N-CA	5.89	1.53	1.46
1	A	142	GLN	N-CA	5.79	1.53	1.46
1	A	113	VAL	C-O	-5.65	1.17	1.24
1	A	7	TRP	NE1-CE2	-5.57	1.31	1.37
1	A	44	ASN	CG-OD1	5.48	1.33	1.23
1	A	117	ASN	CA-C	5.46	1.59	1.53
1	A	145	ARG	NE-CZ	5.37	1.39	1.33
1	A	172	LEU	N-CA	5.35	1.52	1.46
1	A	31	VAL	C-O	5.34	1.30	1.24
1	A	165	GLY	N-CA	5.26	1.51	1.45
1	A	81	HIS	CE1-NE2	5.25	1.37	1.32
1	A	212	ASN	CG-OD1	5.24	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	ALA	N-CA	5.22	1.52	1.46
1	A	177	TRP	NE1-CE2	-5.20	1.31	1.37
1	A	114	GLN	CD-OE1	5.20	1.33	1.23
1	A	73	GLN	CD-OE1	5.16	1.33	1.23
1	A	128	GLN	CD-OE1	5.13	1.33	1.23
1	A	181	TRP	NE1-CE2	-5.13	1.31	1.37
1	A	212	ASN	C-OXT	5.07	1.33	1.23
1	A	46	ASN	CG-OD1	5.04	1.33	1.23

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	CA-C-N	11.90	136.23	120.28
1	A	58	ARG	C-N-CA	11.90	136.23	120.28
1	A	28	PHE	CA-CB-CG	-11.40	102.40	113.80
1	A	184	ASN	CA-CB-CG	-9.80	102.80	112.60
1	A	139	LYS	N-CA-CB	9.58	124.21	110.12
1	A	155	ASN	OD1-CG-ND2	9.42	132.02	122.60
1	A	8	ARG	NE-CZ-NH2	-9.29	110.84	119.20
1	A	23	GLY	O-C-N	8.98	134.37	122.70
1	A	64	ASN	CB-CA-C	-8.96	94.42	110.37
1	A	59	ARG	CD-NE-CZ	8.85	136.79	124.40
1	A	59	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	A	9	GLN	CG-CD-NE2	8.37	128.95	116.40
1	A	96	ARG	CB-CA-C	8.36	124.74	110.94
1	A	96	ARG	CA-C-O	8.35	129.71	119.78
1	A	81	HIS	CA-CB-CG	-8.19	105.61	113.80
1	A	149	PHE	CA-C-O	8.19	130.03	120.69
1	A	9	GLN	OE1-CD-NE2	-8.13	114.47	122.60
1	A	9	GLN	CB-CG-CD	-8.05	98.91	112.60
1	A	124	SER	CA-CB-OG	-8.03	95.03	111.10
1	A	191	ARG	NE-CZ-NH1	-8.01	113.49	121.50
1	A	71	ALA	O-C-N	-7.92	113.86	122.09
1	A	155	ASN	CA-CB-CG	-7.88	104.72	112.60
1	A	155	ASN	CA-C-O	-7.83	111.02	120.65
1	A	195	ASN	OD1-CG-ND2	-7.80	114.80	122.60
1	A	70	SER	N-CA-CB	7.65	121.17	110.07
1	A	31	VAL	CA-C-O	-7.60	113.04	120.95
1	A	54	LEU	CB-CA-C	7.54	123.36	110.84
1	A	184	ASN	OD1-CG-ND2	-7.42	115.17	122.60
1	A	64	ASN	OD1-CG-ND2	7.34	129.94	122.60
1	A	96	ARG	N-CA-C	7.34	121.08	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	LYS	CA-C-O	7.33	128.52	120.82
1	A	193	THR	CA-C-N	7.22	135.10	120.80
1	A	193	THR	C-N-CA	7.22	135.10	120.80
1	A	24	SER	CA-C-N	7.22	129.96	120.28
1	A	24	SER	C-N-CA	7.22	129.96	120.28
1	A	194	GLY	CA-C-N	7.18	132.68	121.99
1	A	194	GLY	C-N-CA	7.18	132.68	121.99
1	A	193	THR	N-CA-C	-7.15	104.37	113.23
1	A	24	SER	O-C-N	-7.10	113.62	122.35
1	A	197	TYR	O-C-N	7.08	130.98	122.27
1	A	166	TYR	CA-C-N	7.04	132.93	121.87
1	A	166	TYR	C-N-CA	7.04	132.93	121.87
1	A	76	ALA	CA-C-O	-7.01	112.99	120.42
1	A	124	SER	CA-C-O	-6.99	113.50	120.70
1	A	114	GLN	CA-C-O	-6.93	112.72	119.51
1	A	185	GLY	O-C-N	6.93	130.85	122.60
1	A	208	TYR	O-C-N	6.91	129.19	121.94
1	A	84	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	A	89	GLU	CA-C-N	6.84	133.11	120.87
1	A	89	GLU	C-N-CA	6.84	133.11	120.87
1	A	93	ARG	CA-C-N	-6.83	110.86	122.67
1	A	93	ARG	C-N-CA	-6.83	110.86	122.67
1	A	114	GLN	CA-CB-CG	-6.82	100.45	114.10
1	A	64	ASN	CA-C-O	-6.80	111.20	119.43
1	A	13	VAL	CA-CB-CG1	6.79	121.94	110.40
1	A	120	ALA	N-CA-C	-6.76	104.00	111.36
1	A	146	GLY	N-CA-C	-6.76	102.92	110.96
1	A	29	SER	CA-C-O	6.73	127.89	120.82
1	A	3	GLU	CA-CB-CG	-6.72	100.66	114.10
1	A	191	ARG	NE-CZ-NH2	6.70	125.23	119.20
1	A	198	GLY	N-CA-C	-6.64	104.02	112.65
1	A	57	ASP	CA-C-N	6.63	134.21	121.54
1	A	57	ASP	C-N-CA	6.63	134.21	121.54
1	A	93	ARG	O-C-N	-6.58	115.60	122.84
1	A	5	VAL	CA-C-N	-6.54	111.89	121.76
1	A	5	VAL	C-N-CA	-6.54	111.89	121.76
1	A	140	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	135	GLU	CB-CG-CD	-6.47	101.61	112.60
1	A	204	THR	CA-C-N	-6.46	111.58	121.40
1	A	204	THR	C-N-CA	-6.46	111.58	121.40
1	A	112	GLN	CA-CB-CG	-6.46	101.19	114.10
1	A	85	THR	O-C-N	-6.42	113.83	122.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASN	CA-C-O	-6.41	113.75	121.89
1	A	160	ALA	CA-C-O	-6.37	113.96	120.71
1	A	156	LYS	O-C-N	6.36	130.02	122.46
1	A	94	TYR	N-CA-C	-6.33	101.08	110.46
1	A	203	TYR	N-CA-CB	6.27	119.56	110.47
1	A	155	ASN	N-CA-CB	6.26	121.16	111.39
1	A	118	GLU	CA-C-O	-6.25	114.26	120.82
1	A	51	GLN	O-C-N	-6.22	114.94	122.22
1	A	106	LYS	O-C-N	-6.21	116.07	123.27
1	A	76	ALA	N-CA-CB	6.18	119.31	110.16
1	A	112	GLN	CA-C-N	6.08	129.36	120.91
1	A	112	GLN	C-N-CA	6.08	129.36	120.91
1	A	38	ILE	O-C-N	-6.05	116.00	121.87
1	A	112	GLN	O-C-N	-6.02	116.36	123.22
1	A	51	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	A	59	ARG	N-CA-CB	6.00	118.94	110.12
1	A	197	TYR	CA-C-O	-5.98	113.09	119.97
1	A	140	ASP	N-CA-C	-5.95	104.87	111.36
1	A	81	HIS	O-C-N	-5.91	115.76	122.68
1	A	139	LYS	CA-C-O	-5.91	114.29	120.55
1	A	81	HIS	ND1-CG-CD2	5.85	111.95	106.10
1	A	18	ASN	O-C-N	-5.79	116.49	123.27
1	A	54	LEU	CA-C-N	5.79	129.12	120.31
1	A	54	LEU	C-N-CA	5.79	129.12	120.31
1	A	207	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	53	LEU	CA-C-O	-5.76	114.77	120.82
1	A	47	GLU	CA-CB-CG	-5.76	102.57	114.10
1	A	195	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	13	VAL	O-C-N	-5.76	116.94	123.10
1	A	4	TYR	CA-C-N	5.74	131.07	122.75
1	A	4	TYR	C-N-CA	5.74	131.07	122.75
1	A	145	ARG	CA-CB-CG	-5.71	102.68	114.10
1	A	9	GLN	CA-CB-CG	-5.70	102.69	114.10
1	A	119	GLY	CA-C-N	5.69	128.38	120.29
1	A	119	GLY	C-N-CA	5.69	128.38	120.29
1	A	22	CYS	N-CA-C	-5.67	100.44	109.96
1	A	9	GLN	N-CA-C	-5.62	106.38	113.18
1	A	91	VAL	CA-CB-CG1	5.59	119.90	110.40
1	A	212	ASN	CA-CB-CG	-5.56	107.04	112.60
1	A	61	TYR	O-C-N	-5.56	114.45	121.95
1	A	205	SER	N-CA-CB	-5.53	102.30	110.37
1	A	90	GLY	CA-C-N	5.52	130.66	122.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	GLY	C-N-CA	5.52	130.66	122.71
1	A	40	ILE	O-C-N	-5.52	116.52	121.87
1	A	140	ASP	CB-CG-OD2	5.51	131.08	118.40
1	A	39	LYS	O-C-N	-5.48	116.43	122.07
1	A	135	GLU	O-C-N	5.46	129.92	122.82
1	A	199	VAL	CA-C-O	-5.46	114.11	120.99
1	A	190	LYS	N-CA-CB	-5.46	101.58	109.83
1	A	125	ILE	CA-C-O	-5.42	115.31	120.95
1	A	86	TYR	CA-C-N	5.40	125.38	120.03
1	A	86	TYR	C-N-CA	5.40	125.38	120.03
1	A	162	ALA	CA-C-O	-5.40	114.33	120.32
1	A	58	ARG	NE-CZ-NH2	5.39	124.06	119.20
1	A	112	GLN	OE1-CD-NE2	5.39	127.99	122.60
1	A	185	GLY	CA-C-O	-5.33	113.10	119.07
1	A	31	VAL	O-C-N	-5.33	116.70	121.87
1	A	83	ARG	O-C-N	5.31	128.21	122.15
1	A	96	ARG	O-C-N	-5.30	115.84	122.35
1	A	114	GLN	CG-CD-OE1	-5.30	110.21	120.80
1	A	99	GLU	N-CA-C	5.28	118.98	112.54
1	A	159	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	A	188	ARG	CA-CB-CG	-5.27	103.56	114.10
1	A	141	PHE	CA-CB-CG	-5.25	108.56	113.80
1	A	209	PRO	CA-C-N	5.24	129.93	123.12
1	A	209	PRO	C-N-CA	5.24	129.93	123.12
1	A	158	ASP	O-C-N	5.23	127.23	121.85
1	A	114	GLN	CG-CD-NE2	5.21	124.21	116.40
1	A	124	SER	N-CA-C	-5.21	105.52	111.14
1	A	3	GLU	CA-C-O	-5.20	114.00	119.97
1	A	64	ASN	CA-CB-CG	-5.16	107.44	112.60
1	A	23	GLY	CA-C-O	-5.16	111.60	120.57
1	A	201	GLY	N-CA-C	-5.15	108.17	115.43
1	A	96	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	159	HIS	CG-CD2-NE2	5.12	112.32	107.20
1	A	68	PRO	O-C-N	-5.11	115.63	122.22
1	A	73	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	59	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
1	A	46	ASN	N-CA-CB	5.04	119.70	111.08
1	A	97	SER	CA-C-N	5.04	127.98	120.31
1	A	97	SER	C-N-CA	5.04	127.98	120.31
1	A	75	VAL	CA-CB-CG1	5.01	118.92	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	58	ARG	CA
1	A	96	ARG	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	17	LYS	Mainchain
1	A	188	ARG	Mainchain
1	A	41	ARG	Sidechain
1	A	57	ASP	Peptide
1	A	58	ARG	Sidechain
1	A	59	ARG	Sidechain
1	A	81	HIS	Mainchain
1	A	98	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	1659	0	1591	32	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	226	0	0	7	0
All	All	1888	0	1591	32	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 10.

All (32) 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:61:TYR:CE2	4:A:600:HOH:O	1.82	1.28
1:A:85:THR:HG22	4:A:561:HOH:O	1.01	1.16
1:A:69:TRP:O	1:A:73:GLN:HG3	1.64	0.98
1:A:148:ILE:HD13	1:A:169[A]:ASN:ND2	1.78	0.97
1:A:148:ILE:HD13	1:A:169[A]:ASN:HD22	1.29	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:CD1	1:A:169[A]:ASN:ND2	2.43	0.80
1:A:169[A]:ASN:OD1	4:A:572:HOH:O	2.03	0.75
1:A:52:GLU:HG3	1:A:86:TYR:CE2	2.29	0.68
1:A:73:GLN:HG2	1:A:110:VAL:HG21	1.79	0.64
1:A:134:LEU:HD21	4:A:566:HOH:O	1.98	0.63
1:A:94:TYR:CD1	1:A:94:TYR:N	2.69	0.61
1:A:139:LYS:HD2	4:A:567:HOH:O	2.00	0.59
1:A:96:ARG:HB2	1:A:99:GLU:CG	2.33	0.58
1:A:96:ARG:HB2	1:A:99:GLU:CD	2.32	0.55
1:A:82:TYR:HB2	1:A:85:THR:HG23	1.89	0.55
1:A:154:GLY:O	1:A:200:CYS:HA	2.08	0.54
1:A:148:ILE:CD1	1:A:169[A]:ASN:HD21	2.21	0.53
1:A:138:GLY:O	1:A:142:GLN:HG2	2.09	0.51
1:A:52:GLU:OE2	1:A:97:SER:OG	2.19	0.49
1:A:67:TYR:HB2	1:A:70:SER:OG	2.12	0.48
1:A:134:LEU:C	1:A:134:LEU:HD12	2.38	0.48
1:A:59:ARG:NH1	1:A:61:TYR:OH	2.47	0.48
1:A:88:TYR:CZ	1:A:90:GLY:HA2	2.51	0.46
1:A:86:TYR:N	1:A:87:PRO:CD	2.79	0.46
1:A:156:LYS:NZ	1:A:156:LYS:HB3	2.30	0.46
1:A:89:GLU:OE1	1:A:93:ARG:HD3	2.17	0.45
1:A:51:GLN:HB2	1:A:88:TYR:HA	1.98	0.44
1:A:85:THR:CG2	4:A:561:HOH:O	1.91	0.43
1:A:96:ARG:HB2	1:A:99:GLU:HG3	2.00	0.42
1:A:61:TYR:CD2	4:A:600:HOH:O	2.41	0.41
1:A:1:ILE:HA	1:A:2:PRO:HD3	1.92	0.41
1:A:54:LEU:HD12	1:A:62:GLY:HA2	2.03	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	211/212 (100%)	202 (96%)	8 (4%)	1 (0%)	24 10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ARG

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	171/170 (101%)	157 (92%)	14 (8%)	10 2

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	58	ARG
1	A	64	ASN
1	A	70	SER
1	A	74	LEU
1	A	85	THR
1	A	93	ARG
1	A	96	ARG
1	A	98	ARG
1	A	100	LYS
1	A	139	LYS
1	A	142	GLN
1	A	155	ASN
1	A	156	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	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 unknown - 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	MOH	A	302	-	1,1,1	0.86	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	212/212 (100%)	-0.48	2 (0%) 81 84	4, 12, 32, 47	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	SER	2.2
1	A	98	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UNL	A	301	1/-	0.81	0.29	9,9,9,9	0
3	MOH	A	302	2/2	0.88	0.08	19,19,19,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.