



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:52 AM UTC

PDB ID : 1MUP / pdb_00001mup
Title : PHEROMONE BINDING TO TWO RODENT URINARY PROTEINS REVEALED BY X-RAY CRYSTALLOGRAPHY
Authors : Bocskei, Z.; Flower, D.R.; Groom, C.R.; Phillips, S.E.V.; North, A.C.T.
Deposited on : 1992-09-21
Resolution : 2.40 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

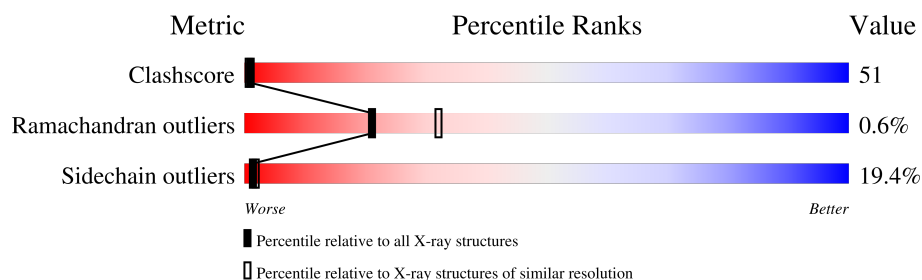
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	166	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1332 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.

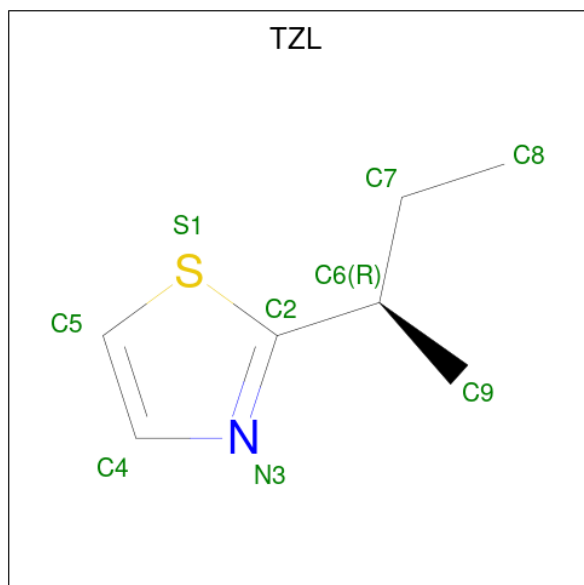
- Molecule 1 is a protein called MAJOR URINARY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1242	777	210	249	6			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cd	0	0
			4	4		

- Molecule 3 is 2-(SEC-BUTYL)THIAZOLE (CCD ID: TZL) (formula: C₇H₁₁NS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			9	7	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		

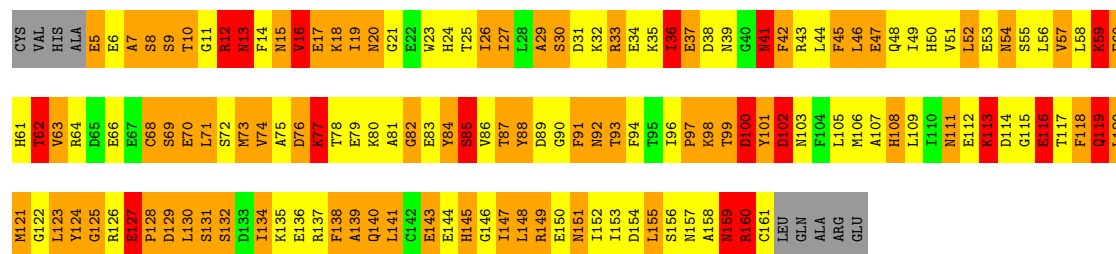
3 Residue-property plots

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: MAJOR URINARY PROTEIN

Chain A:  6% 37% 41% 10% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.30Å 57.30Å 110.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (14.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1332	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: CD, TZL

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	1.76	14/1263 (1.1%)	3.95	275/1703 (16.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	THR	C-N	-9.01	1.23	1.33
1	A	125	GLY	N-CA	8.40	1.53	1.44
1	A	34	GLU	C-O	6.51	1.32	1.24
1	A	98	LYS	CA-C	-6.25	1.45	1.52
1	A	127	GLU	C-N	-6.21	1.27	1.34
1	A	105	LEU	C-N	-6.21	1.25	1.33
1	A	83	GLU	C-N	-6.15	1.25	1.33
1	A	116	GLU	CD-OE2	5.99	1.36	1.25
1	A	130	LEU	CA-CB	5.98	1.63	1.53
1	A	120	LEU	C-O	-5.89	1.17	1.23
1	A	50	HIS	ND1-CE1	-5.61	1.26	1.32
1	A	149	ARG	NE-CZ	-5.33	1.27	1.33
1	A	117	THR	CB-OG1	5.24	1.52	1.43
1	A	50	HIS	CG-ND1	5.17	1.44	1.38

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASP	CA-CB-CG	31.41	144.01	112.60
1	A	149	ARG	NE-CZ-NH2	22.78	139.70	119.20
1	A	26	ILE	CB-CG1-CD1	16.67	148.81	113.80
1	A	129	ASP	CA-CB-CG	16.34	128.94	112.60
1	A	20	ASN	CA-CB-CG	16.09	128.69	112.60
1	A	48	GLN	CA-CB-CG	16.02	146.14	114.10
1	A	91	PHE	CA-C-O	15.22	136.64	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASN	OD1-CG-ND2	-14.64	107.96	122.60
1	A	149	ARG	NE-CZ-NH1	-14.28	107.22	121.50
1	A	10	THR	CA-C-N	14.08	133.47	120.10
1	A	10	THR	C-N-CA	14.08	133.47	120.10
1	A	50	HIS	CA-CB-CG	13.99	127.79	113.80
1	A	84	TYR	CA-C-O	-13.45	107.05	121.45
1	A	118	PHE	CA-C-N	13.33	142.52	122.65
1	A	118	PHE	C-N-CA	13.33	142.52	122.65
1	A	108	HIS	CA-CB-CG	-12.90	100.90	113.80
1	A	148	LEU	O-C-N	12.63	137.08	122.94
1	A	20	ASN	CB-CG-ND2	12.28	134.82	116.40
1	A	124	TYR	CA-C-N	-12.26	111.56	122.47
1	A	124	TYR	C-N-CA	-12.26	111.56	122.47
1	A	124	TYR	CA-C-O	-12.12	107.41	121.11
1	A	99	THR	CA-CB-OG1	-12.11	91.43	109.60
1	A	74	VAL	CA-C-O	-11.86	107.44	120.48
1	A	112	GLU	CB-CG-CD	11.48	132.11	112.60
1	A	7	ALA	CA-C-N	11.11	141.53	122.64
1	A	7	ALA	C-N-CA	11.11	141.53	122.64
1	A	130	LEU	N-CA-CB	-10.95	94.63	111.05
1	A	129	ASP	CB-CA-C	10.51	132.32	109.94
1	A	20	ASN	OD1-CG-ND2	-10.48	112.12	122.60
1	A	119	GLN	CA-CB-CG	10.35	134.81	114.10
1	A	51	VAL	CA-C-O	-10.34	109.25	121.04
1	A	42	PHE	CA-CB-CG	-10.31	103.49	113.80
1	A	74	VAL	O-C-N	10.27	133.97	122.99
1	A	119	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	132	SER	CA-C-N	9.63	134.95	120.31
1	A	132	SER	C-N-CA	9.63	134.95	120.31
1	A	83	GLU	CA-C-O	-9.58	110.34	121.16
1	A	92	ASN	O-C-N	9.57	134.50	123.31
1	A	49	ILE	CA-C-O	-9.51	110.40	120.48
1	A	9	SER	CA-C-N	9.47	136.78	120.68
1	A	9	SER	C-N-CA	9.47	136.78	120.68
1	A	81	ALA	O-C-N	9.38	134.58	122.95
1	A	111	ASN	CB-CG-ND2	9.32	130.38	116.40
1	A	10	THR	CA-C-O	9.30	130.76	119.79
1	A	31	ASP	OD1-CG-OD2	9.21	145.02	122.90
1	A	25	THR	N-CA-CB	9.13	124.72	110.21
1	A	158	ALA	CA-C-N	9.12	140.17	121.94
1	A	158	ALA	C-N-CA	9.12	140.17	121.94
1	A	31	ASP	CA-CB-CG	-9.05	103.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	GLY	N-CA-C	8.94	126.31	112.45
1	A	118	PHE	CA-CB-CG	8.88	122.68	113.80
1	A	58	LEU	CA-C-N	-8.87	110.75	123.00
1	A	58	LEU	C-N-CA	-8.87	110.75	123.00
1	A	141	LEU	CA-C-O	8.86	130.07	120.24
1	A	134	ILE	O-C-N	8.81	133.36	121.90
1	A	36	ILE	CA-CB-CG2	8.76	125.39	110.50
1	A	63	VAL	CA-C-N	8.71	135.66	122.77
1	A	63	VAL	C-N-CA	8.71	135.66	122.77
1	A	138	PHE	N-CA-C	-8.69	101.77	111.07
1	A	12	ARG	CA-C-O	8.67	130.21	119.11
1	A	19	ILE	N-CA-C	-8.65	101.31	113.07
1	A	17	GLU	CB-CG-CD	8.63	127.27	112.60
1	A	70	GLU	CB-CG-CD	8.62	127.25	112.60
1	A	60	PHE	CA-CB-CG	8.57	122.37	113.80
1	A	136	GLU	O-C-N	8.55	131.32	122.09
1	A	84	TYR	O-C-N	8.53	132.91	123.10
1	A	78	THR	N-CA-CB	8.46	122.06	110.38
1	A	140	GLN	O-C-N	-8.46	111.39	122.39
1	A	107	ALA	CA-C-O	8.45	131.34	121.46
1	A	136	GLU	N-CA-CB	8.45	122.32	110.07
1	A	128	PRO	CA-C-O	-8.40	106.21	118.89
1	A	147	ILE	CB-CA-C	-8.18	99.02	110.96
1	A	123	LEU	N-CA-CB	8.15	123.34	110.55
1	A	7	ALA	O-C-N	-8.11	114.40	123.48
1	A	31	ASP	CA-C-N	8.08	135.41	123.12
1	A	31	ASP	C-N-CA	8.08	135.41	123.12
1	A	123	LEU	CA-C-O	-8.07	111.44	120.32
1	A	124	TYR	O-C-N	7.97	133.55	123.19
1	A	47	GLU	N-CA-C	-7.94	102.38	112.93
1	A	128	PRO	O-C-N	7.91	133.68	122.37
1	A	74	VAL	N-CA-CB	7.88	121.82	111.90
1	A	66	GLU	N-CA-CB	7.85	123.76	110.49
1	A	9	SER	CA-CB-OG	7.80	126.71	111.10
1	A	98	LYS	CA-C-O	7.79	130.72	120.21
1	A	12	ARG	CA-CB-CG	-7.78	98.54	114.10
1	A	140	GLN	CA-C-N	7.76	133.84	120.58
1	A	140	GLN	C-N-CA	7.76	133.84	120.58
1	A	84	TYR	N-CA-CB	-7.72	99.36	111.56
1	A	99	THR	N-CA-C	7.70	121.08	108.99
1	A	35	LYS	CB-CA-C	7.69	123.92	110.85
1	A	122	GLY	O-C-N	7.67	130.19	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	HIS	CA-C-O	-7.66	112.26	120.46
1	A	59	LYS	CA-C-O	-7.66	112.03	120.38
1	A	143	GLU	CB-CG-CD	7.62	125.55	112.60
1	A	23	TRP	O-C-N	-7.53	112.35	122.74
1	A	6	GLU	O-C-N	7.53	131.75	123.10
1	A	93	THR	CA-CB-OG1	-7.53	98.31	109.60
1	A	70	GLU	CA-C-N	7.52	135.18	121.94
1	A	70	GLU	C-N-CA	7.52	135.18	121.94
1	A	34	GLU	CB-CG-CD	7.46	125.28	112.60
1	A	8	SER	CA-C-O	-7.45	112.49	121.28
1	A	118	PHE	O-C-N	-7.42	115.17	123.48
1	A	62	THR	N-CA-CB	-7.39	99.22	111.20
1	A	73	MET	CA-C-O	-7.39	113.05	121.40
1	A	42	PHE	CA-C-O	7.39	128.00	119.35
1	A	113	LYS	CA-C-O	7.38	129.15	120.66
1	A	132	SER	CA-CB-OG	7.38	125.86	111.10
1	A	58	LEU	CA-C-O	-7.34	112.69	120.40
1	A	62	THR	CA-CB-OG1	-7.33	98.60	109.60
1	A	159	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	A	57	VAL	CB-CA-C	7.28	121.68	110.83
1	A	78	THR	CA-CB-CG2	7.28	122.88	110.50
1	A	27	ILE	CA-C-N	7.24	134.46	122.73
1	A	27	ILE	C-N-CA	7.24	134.46	122.73
1	A	128	PRO	CA-C-N	-7.22	109.06	121.85
1	A	128	PRO	C-N-CA	-7.22	109.06	121.85
1	A	30	SER	CA-CB-OG	-7.19	96.72	111.10
1	A	159	ASN	CA-CB-CG	7.19	119.79	112.60
1	A	73	MET	O-C-N	7.15	131.82	123.17
1	A	52	LEU	N-CA-CB	7.14	121.65	110.87
1	A	160	ARG	CA-C-O	7.14	128.07	120.36
1	A	144	GLU	O-C-N	-7.11	111.86	122.39
1	A	46	LEU	CB-CA-C	7.08	121.48	109.72
1	A	50	HIS	ND1-CE1-NE2	7.01	115.41	108.40
1	A	91	PHE	O-C-N	-6.98	115.26	123.22
1	A	139	ALA	O-C-N	-6.96	114.90	122.07
1	A	85	SER	O-C-N	6.95	132.47	122.94
1	A	105	LEU	CB-CA-C	6.94	123.46	109.38
1	A	39	ASN	CB-CA-C	6.90	122.24	111.13
1	A	115	GLY	CA-C-O	-6.90	111.73	119.04
1	A	83	GLU	CB-CA-C	-6.86	96.81	109.37
1	A	37	GLU	N-CA-C	6.86	118.84	110.41
1	A	9	SER	N-CA-CB	6.84	120.84	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	CYS	O-C-N	6.80	130.92	123.10
1	A	129	ASP	CA-C-O	6.78	128.58	120.99
1	A	52	LEU	O-C-N	6.77	132.43	122.81
1	A	100	ASP	CA-C-N	6.77	134.47	121.54
1	A	100	ASP	C-N-CA	6.77	134.47	121.54
1	A	60	PHE	CB-CA-C	-6.76	96.96	110.42
1	A	145	HIS	CA-CB-CG	-6.72	107.08	113.80
1	A	100	ASP	CA-C-O	6.70	127.55	119.78
1	A	146	GLY	CA-C-N	6.69	131.82	123.12
1	A	146	GLY	C-N-CA	6.69	131.82	123.12
1	A	50	HIS	N-CA-CB	6.63	121.48	110.47
1	A	141	LEU	O-C-N	-6.63	113.61	122.23
1	A	19	ILE	CA-CB-CG1	6.61	121.63	110.40
1	A	116	GLU	CA-CB-CG	6.59	127.29	114.10
1	A	126	ARG	CB-CG-CD	-6.58	96.16	111.30
1	A	132	SER	O-C-N	-6.57	113.63	122.43
1	A	92	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	147	ILE	N-CA-CB	6.55	119.71	111.46
1	A	111	ASN	O-C-N	-6.53	115.62	123.13
1	A	56	LEU	N-CA-CB	-6.51	99.91	110.71
1	A	97	PRO	CB-CA-C	-6.50	102.07	112.21
1	A	79	GLU	N-CA-C	6.48	120.28	112.38
1	A	112	GLU	CG-CD-OE1	6.46	133.26	118.40
1	A	56	LEU	CA-C-N	-6.44	115.20	123.19
1	A	56	LEU	C-N-CA	-6.44	115.20	123.19
1	A	155	LEU	CD1-CG-CD2	-6.43	96.66	110.80
1	A	5	GLU	CA-C-O	6.38	131.64	120.80
1	A	83	GLU	N-CA-C	6.33	120.02	109.95
1	A	34	GLU	O-C-N	6.29	130.56	122.39
1	A	112	GLU	CB-CA-C	-6.26	101.52	111.17
1	A	112	GLU	N-CA-CB	6.25	121.06	110.87
1	A	152	ILE	CA-C-N	6.22	131.29	123.14
1	A	152	ILE	C-N-CA	6.22	131.29	123.14
1	A	73	MET	CA-C-N	-6.19	114.84	123.13
1	A	73	MET	C-N-CA	-6.19	114.84	123.13
1	A	100	ASP	CB-CA-C	6.18	120.99	110.85
1	A	16	VAL	O-C-N	6.18	130.30	122.57
1	A	31	ASP	CB-CG-OD2	-6.17	104.20	118.40
1	A	114	ASP	CA-C-O	-6.17	114.68	121.84
1	A	134	ILE	CA-C-N	-6.17	111.93	120.38
1	A	134	ILE	C-N-CA	-6.17	111.93	120.38
1	A	43	ARG	CA-C-O	-6.15	114.20	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	GLU	CB-CA-C	-6.10	101.26	110.90
1	A	29	ALA	O-C-N	-6.09	116.28	123.41
1	A	81	ALA	CA-C-O	-6.09	113.97	120.92
1	A	128	PRO	N-CA-CB	6.09	109.31	103.52
1	A	66	GLU	CB-CG-CD	6.09	122.95	112.60
1	A	150	GLU	CA-C-N	6.03	132.69	122.26
1	A	150	GLU	C-N-CA	6.03	132.69	122.26
1	A	74	VAL	CG1-CB-CG2	-6.03	97.54	110.80
1	A	15	ASN	CA-CB-CG	-6.02	106.58	112.60
1	A	49	ILE	CA-CB-CG2	5.96	120.64	110.50
1	A	121	MET	CA-C-N	5.96	127.13	121.46
1	A	121	MET	C-N-CA	5.96	127.13	121.46
1	A	69	SER	CA-C-N	5.94	129.91	121.42
1	A	69	SER	C-N-CA	5.94	129.91	121.42
1	A	147	ILE	CA-CB-CG1	-5.93	100.33	110.40
1	A	77	LYS	CA-C-O	-5.92	112.04	120.51
1	A	129	ASP	O-C-N	-5.91	116.65	123.33
1	A	112	GLU	CA-CB-CG	5.89	125.88	114.10
1	A	16	VAL	CG1-CB-CG2	5.85	123.68	110.80
1	A	136	GLU	CB-CG-CD	5.85	122.54	112.60
1	A	15	ASN	CA-C-O	-5.82	114.71	122.51
1	A	96	ILE	CA-C-O	-5.79	112.19	119.95
1	A	31	ASP	N-CA-CB	-5.78	101.67	110.33
1	A	13	ASN	N-CA-CB	-5.77	101.79	110.91
1	A	108	HIS	N-CA-CB	-5.74	101.94	110.90
1	A	45	PHE	CD1-CE1-CZ	-5.74	109.67	120.00
1	A	100	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	111	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	148	LEU	CD1-CG-CD2	-5.68	98.31	110.80
1	A	73	MET	CB-CG-SD	-5.66	95.72	112.70
1	A	120	LEU	CA-C-O	-5.64	113.34	120.28
1	A	131	SER	O-C-N	5.64	129.22	122.79
1	A	37	GLU	CB-CG-CD	5.64	122.18	112.60
1	A	145	HIS	N-CA-C	-5.64	105.15	113.61
1	A	78	THR	CA-CB-OG1	-5.63	101.15	109.60
1	A	107	ALA	O-C-N	-5.63	115.56	123.11
1	A	38	ASP	CA-C-N	-5.63	114.25	122.86
1	A	38	ASP	C-N-CA	-5.63	114.25	122.86
1	A	82	GLY	O-C-N	5.63	129.54	122.39
1	A	76	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	35	LYS	CA-CB-CG	-5.62	102.86	114.10
1	A	6	GLU	CB-CG-CD	5.61	122.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	THR	O-C-N	5.61	130.11	123.27
1	A	66	GLU	CA-C-N	-5.59	115.01	122.72
1	A	66	GLU	C-N-CA	-5.59	115.01	122.72
1	A	43	ARG	N-CA-CB	5.58	119.31	110.49
1	A	10	THR	OG1-CB-CG2	5.57	120.44	109.30
1	A	54	ASN	CB-CG-ND2	5.57	124.75	116.40
1	A	80	LYS	CA-C-O	-5.52	114.08	120.49
1	A	18	LYS	CA-C-N	-5.52	111.98	121.09
1	A	18	LYS	C-N-CA	-5.52	111.98	121.09
1	A	118	PHE	CA-C-O	5.52	126.96	120.89
1	A	49	ILE	CA-C-N	5.51	130.94	123.11
1	A	49	ILE	C-N-CA	5.51	130.94	123.11
1	A	119	GLN	CB-CA-C	5.51	118.73	109.48
1	A	37	GLU	N-CA-CB	5.50	117.91	110.38
1	A	145	HIS	N-CA-CB	5.49	118.98	110.80
1	A	36	ILE	N-CA-CB	-5.49	99.31	111.50
1	A	94	PHE	N-CA-C	5.48	117.40	109.07
1	A	16	VAL	CB-CA-C	-5.48	102.31	111.29
1	A	116	GLU	N-CA-CB	-5.46	101.39	110.23
1	A	98	LYS	N-CA-C	5.43	118.26	108.48
1	A	13	ASN	CA-C-O	-5.42	113.16	120.15
1	A	88	TYR	N-CA-CB	-5.42	101.38	110.32
1	A	151	ASN	CA-C-N	5.42	129.76	122.93
1	A	151	ASN	C-N-CA	5.42	129.76	122.93
1	A	64	ARG	O-C-N	5.41	129.23	122.63
1	A	41	ASN	CB-CA-C	5.41	119.70	110.56
1	A	119	GLN	N-CA-CB	-5.40	101.61	110.52
1	A	27	ILE	O-C-N	-5.38	117.08	123.05
1	A	138	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	79	GLU	CA-C-N	5.35	129.48	121.72
1	A	79	GLU	C-N-CA	5.35	129.48	121.72
1	A	11	GLY	O-C-N	5.30	129.43	122.91
1	A	42	PHE	N-CA-C	-5.30	106.49	113.17
1	A	71	LEU	CA-CB-CG	5.29	134.83	116.30
1	A	112	GLU	OE1-CD-OE2	-5.29	110.19	122.90
1	A	132	SER	CA-C-O	5.29	125.88	119.38
1	A	47	GLU	N-CA-CB	5.26	119.50	110.34
1	A	130	LEU	CB-CG-CD1	-5.22	95.05	110.70
1	A	26	ILE	CA-CB-CG2	-5.21	101.64	110.50
1	A	137	ARG	CD-NE-CZ	-5.18	117.15	124.40
1	A	79	GLU	CA-CB-CG	-5.17	103.75	114.10
1	A	115	GLY	O-C-N	5.17	128.96	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLU	CB-CG-CD	5.16	121.36	112.60
1	A	45	PHE	CB-CA-C	5.15	119.19	110.79
1	A	105	LEU	CA-C-O	-5.14	114.43	120.60
1	A	35	LYS	CA-C-N	5.14	129.06	120.64
1	A	35	LYS	C-N-CA	5.14	129.06	120.64
1	A	78	THR	N-CA-C	-5.11	103.31	110.35
1	A	44	LEU	N-CA-CB	-5.09	102.33	110.63
1	A	12	ARG	CB-CA-C	5.08	120.06	109.95
1	A	116	GLU	CB-CA-C	5.05	117.86	109.53
1	A	33	ARG	CD-NE-CZ	5.04	131.46	124.40
1	A	88	TYR	CA-CB-CG	-5.04	104.83	113.90
1	A	80	LYS	CA-C-N	5.02	127.90	120.82
1	A	80	LYS	C-N-CA	5.02	127.90	120.82
1	A	88	TYR	CB-CA-C	5.02	117.36	110.34
1	A	151	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	82	GLY	CA-C-O	-5.01	113.46	119.02

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	1242	0	1168	122	1
2	A	4	0	0	0	0
3	A	9	0	11	4	0
4	A	77	0	0	16	1
All	All	1332	0	1179	125	1

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 51.

All (125) 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:54:ASN:O	1:A:77:LYS:HG3	1.51	1.08
1:A:124:TYR:OH	4:A:377:HOH:O	1.73	1.07
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.19	1.05
1:A:12:ARG:HD3	4:A:347:HOH:O	1.60	1.00
1:A:30:SER:HB2	1:A:36:ILE:HG12	1.42	1.00
1:A:106:MET:HE2	1:A:138:PHE:HB2	1.44	0.97
1:A:91:PHE:HZ	4:A:300:HOH:O	1.48	0.95
1:A:36:ILE:HD11	1:A:120:LEU:CD1	1.96	0.94
3:A:167:TZL:C9	4:A:349:HOH:O	2.14	0.94
1:A:36:ILE:HD11	1:A:120:LEU:HD11	1.46	0.94
1:A:125:GLY:HA3	1:A:130:LEU:HD21	1.49	0.92
1:A:24:HIS:CE1	4:A:353:HOH:O	2.23	0.91
3:A:167:TZL:H91	4:A:349:HOH:O	1.69	0.90
1:A:99:THR:OG1	1:A:100:ASP:N	2.07	0.84
1:A:149:ARG:HD3	4:A:326:HOH:O	1.76	0.83
1:A:131:SER:O	1:A:135:LYS:HG3	1.78	0.83
1:A:12:ARG:HG2	1:A:12:ARG:NH1	1.79	0.83
1:A:33:ARG:HG3	1:A:151:ASN:HD22	1.42	0.81
1:A:123:LEU:HD21	1:A:134:ILE:HG22	1.64	0.79
1:A:102:ASP:OD1	4:A:312:HOH:O	2.01	0.78
1:A:153:ILE:HG22	1:A:155:LEU:HD22	1.66	0.78
1:A:13:ASN:H	1:A:13:ASN:HD22	1.31	0.77
1:A:108:HIS:NE2	1:A:119:GLN:NE2	2.32	0.77
1:A:141:LEU:O	1:A:145:HIS:HD2	1.66	0.77
1:A:30:SER:CB	1:A:36:ILE:HG12	2.17	0.75
1:A:159:ASN:ND2	1:A:160:ARG:NH1	2.35	0.75
1:A:33:ARG:HG3	1:A:151:ASN:ND2	2.02	0.74
1:A:154:ASP:OD1	1:A:156:SER:HB3	1.85	0.74
1:A:36:ILE:HG22	1:A:153:ILE:CD1	2.19	0.73
1:A:70:GLU:HG3	4:A:330:HOH:O	1.90	0.69
1:A:90:GLY:HA3	1:A:113:LYS:HB3	1.73	0.69
1:A:45:PHE:HZ	1:A:155:LEU:HD12	1.56	0.69
1:A:36:ILE:HG22	1:A:153:ILE:HD12	1.74	0.68
1:A:125:GLY:CA	1:A:130:LEU:HD21	2.23	0.68
1:A:5:GLU:O	1:A:100:ASP:HA	1.94	0.67
1:A:41:ASN:H	1:A:41:ASN:HD22	1.43	0.65
1:A:159:ASN:HD21	1:A:160:ARG:NH1	1.95	0.64
1:A:46:LEU:HD22	3:A:167:TZL:H4	1.81	0.63
1:A:36:ILE:CG2	1:A:153:ILE:HD12	2.29	0.63
1:A:85:SER:HA	1:A:92:ASN:O	1.99	0.62
1:A:12:ARG:HH11	1:A:12:ARG:CG	2.05	0.61
1:A:36:ILE:HD11	1:A:120:LEU:HD12	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:CD1	1:A:120:LEU:HD11	2.26	0.60
1:A:157:ASN:HA	1:A:160:ARG:HH12	1.67	0.60
1:A:111:ASN:CG	1:A:118:PHE:CE2	2.80	0.60
1:A:61:HIS:HA	1:A:69:SER:O	2.02	0.60
1:A:45:PHE:CD2	1:A:159:ASN:HA	2.37	0.59
1:A:9:SER:OG	1:A:82:GLY:O	2.18	0.59
1:A:73:MET:CE	1:A:88:TYR:CD1	2.85	0.59
1:A:60:PHE:HE1	1:A:73:MET:HG3	1.67	0.59
1:A:32:LYS:HG3	1:A:118:PHE:HB2	1.85	0.59
3:A:167:TZL:H92	4:A:377:HOH:O	2.02	0.58
1:A:59:LYS:HD3	1:A:72:SER:OG	2.02	0.58
1:A:100:ASP:O	1:A:102:ASP:N	2.26	0.58
1:A:45:PHE:CZ	1:A:155:LEU:HD12	2.37	0.58
1:A:86:VAL:N	1:A:92:ASN:O	2.31	0.58
1:A:106:MET:HE2	1:A:138:PHE:CB	2.27	0.58
1:A:33:ARG:O	1:A:36:ILE:HB	2.03	0.57
1:A:29:ALA:HA	1:A:151:ASN:O	2.03	0.57
1:A:73:MET:HE2	1:A:88:TYR:CD1	2.39	0.57
1:A:149:ARG:NE	4:A:344:HOH:O	2.24	0.57
1:A:85:SER:HB3	1:A:93:THR:HG22	1.87	0.57
1:A:24:HIS:O	1:A:124:TYR:HA	2.05	0.56
1:A:88:TYR:O	1:A:89:ASP:C	2.45	0.56
1:A:45:PHE:CE2	1:A:159:ASN:HA	2.41	0.56
1:A:26:ILE:HG13	1:A:130:LEU:HG	1.88	0.55
1:A:111:ASN:CB	1:A:118:PHE:CE2	2.91	0.54
1:A:63:VAL:HG22	1:A:68:CYS:SG	2.48	0.54
1:A:36:ILE:CD1	1:A:120:LEU:CD1	2.79	0.53
1:A:111:ASN:HB3	1:A:118:PHE:CE2	2.44	0.53
1:A:154:ASP:OD1	1:A:156:SER:CB	2.57	0.53
1:A:116:GLU:HG3	4:A:375:HOH:O	2.08	0.53
1:A:140:GLN:HB3	4:A:343:HOH:O	2.09	0.52
1:A:42:PHE:HB3	1:A:120:LEU:HD13	1.92	0.52
1:A:41:ASN:HD22	1:A:41:ASN:N	2.05	0.52
1:A:88:TYR:HB3	1:A:92:ASN:ND2	2.25	0.52
1:A:13:ASN:H	1:A:13:ASN:ND2	2.03	0.52
1:A:27:ILE:CG2	1:A:138:PHE:HE2	2.23	0.51
1:A:61:HIS:HB3	1:A:70:GLU:OE1	2.11	0.51
1:A:15:ASN:C	1:A:15:ASN:HD22	2.19	0.50
1:A:160:ARG:HH11	1:A:160:ARG:HB2	1.75	0.49
1:A:73:MET:HE1	1:A:88:TYR:CD1	2.46	0.49
1:A:100:ASP:C	1:A:102:ASP:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ALA:O	1:A:99:THR:HG22	2.13	0.49
1:A:76:ASP:O	1:A:84:TYR:HA	2.13	0.49
1:A:91:PHE:CZ	4:A:300:HOH:O	2.35	0.49
1:A:15:ASN:O	1:A:16:VAL:C	2.56	0.49
1:A:159:ASN:HD21	1:A:160:ARG:CZ	2.25	0.48
1:A:61:HIS:CA	1:A:69:SER:O	2.62	0.48
1:A:18:LYS:HB2	1:A:101:TYR:CD1	2.49	0.47
1:A:57:VAL:HG22	1:A:74:VAL:HG22	1.95	0.47
1:A:17:GLU:O	1:A:20:ASN:HB2	2.15	0.47
1:A:147:ILE:HG23	1:A:151:ASN:HB3	1.97	0.47
1:A:85:SER:CA	1:A:92:ASN:O	2.63	0.47
1:A:27:ILE:CG2	1:A:138:PHE:CE2	2.98	0.46
1:A:45:PHE:O	1:A:60:PHE:HB3	2.14	0.46
1:A:147:ILE:HG23	1:A:151:ASN:CB	2.45	0.46
1:A:149:ARG:HD3	1:A:149:ARG:HH11	1.30	0.46
1:A:8:SER:O	1:A:14:PHE:HB2	2.15	0.46
1:A:16:VAL:HG12	1:A:19:ILE:HG12	1.98	0.46
1:A:97:PRO:HD2	1:A:106:MET:O	2.15	0.46
1:A:123:LEU:HG	1:A:130:LEU:HD12	1.98	0.46
1:A:148:LEU:O	1:A:151:ASN:HB2	2.16	0.46
1:A:128:PRO:HB2	1:A:160:ARG:NH2	2.31	0.46
1:A:27:ILE:HG21	1:A:138:PHE:HE2	1.81	0.46
1:A:84:TYR:O	1:A:93:THR:HA	2.17	0.45
1:A:71:LEU:HD21	1:A:73:MET:HE3	1.99	0.44
1:A:36:ILE:CD1	1:A:120:LEU:HD12	2.48	0.43
1:A:54:ASN:C	1:A:77:LYS:HG3	2.35	0.43
1:A:63:VAL:HG21	4:A:351:HOH:O	2.18	0.43
1:A:111:ASN:HB3	1:A:118:PHE:CD2	2.53	0.43
1:A:149:ARG:NH2	4:A:371:HOH:O	2.52	0.43
1:A:62:THR:N	1:A:69:SER:O	2.44	0.43
1:A:123:LEU:HG	1:A:130:LEU:CD1	2.49	0.43
1:A:9:SER:HB2	1:A:82:GLY:HA2	2.02	0.42
1:A:13:ASN:HD22	1:A:13:ASN:N	2.00	0.42
1:A:47:GLU:OE2	1:A:61:HIS:ND1	2.46	0.42
1:A:26:ILE:CD1	1:A:127:GLU:O	2.68	0.42
1:A:52:LEU:O	1:A:53:GLU:C	2.61	0.42
1:A:75:ALA:HA	1:A:85:SER:O	2.19	0.42
1:A:15:ASN:C	1:A:15:ASN:ND2	2.76	0.42
1:A:128:PRO:O	1:A:129:ASP:HB2	2.19	0.41
1:A:135:LYS:O	1:A:139:ALA:N	2.40	0.41
1:A:86:VAL:HG22	1:A:87:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:NE	1:A:37:GLU:OE2	2.55	0.40

All (1) 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)
1:A:143:GLU:OE2	4:A:355:HOH:O[5_545]	2.04	0.16

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	155/166 (93%)	142 (92%)	12 (8%)	1 (1%)	21	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	TYR

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	134/148 (90%)	108 (81%)	26 (19%)	1	2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	12	ARG
1	A	13	ASN
1	A	16	VAL
1	A	36	ILE
1	A	41	ASN
1	A	55	SER
1	A	59	LYS
1	A	62	THR
1	A	77	LYS
1	A	85	SER
1	A	87	THR
1	A	98	LYS
1	A	100	ASP
1	A	102	ASP
1	A	103	ASN
1	A	109	LEU
1	A	113	LYS
1	A	116	GLU
1	A	119	GLN
1	A	121	MET
1	A	127	GLU
1	A	132	SER
1	A	159	ASN
1	A	160	ARG
1	A	161	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	15	ASN
1	A	41	ASN
1	A	54	ASN
1	A	140	GLN
1	A	151	ASN
1	A	159	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 5 ligands modelled in this entry, 4 are 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	TZL	A	167	-	9,9,9	4.46	3 (33%)	8,11,11	8.63	5 (62%)

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	TZL	A	167	-	-	2/6/6/6	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	167	TZL	C4-N3	9.88	1.56	1.38
3	A	167	TZL	C4-C5	7.82	1.52	1.34
3	A	167	TZL	C5-S1	4.24	1.89	1.70

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	167	TZL	C5-S1-C2	16.53	100.09	89.70
3	A	167	TZL	S1-C2-N3	-12.40	102.11	114.22
3	A	167	TZL	C5-C4-N3	-8.04	104.53	116.12
3	A	167	TZL	C4-N3-C2	7.69	124.48	109.86
3	A	167	TZL	C4-C5-S1	-6.65	101.79	110.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	167	TZL	C9-C6-C7-C8
3	A	167	TZL	S1-C2-C6-C9

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	167	TZL	4	0

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.