



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 01:03 PM EDT

PDB ID : 1MUP
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

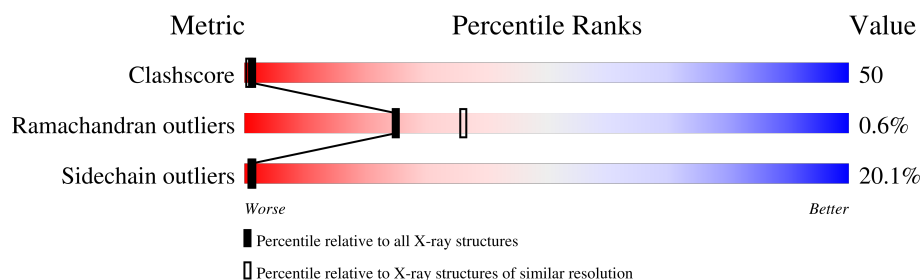
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

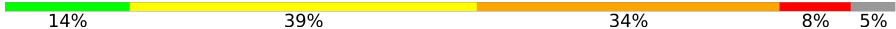
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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.

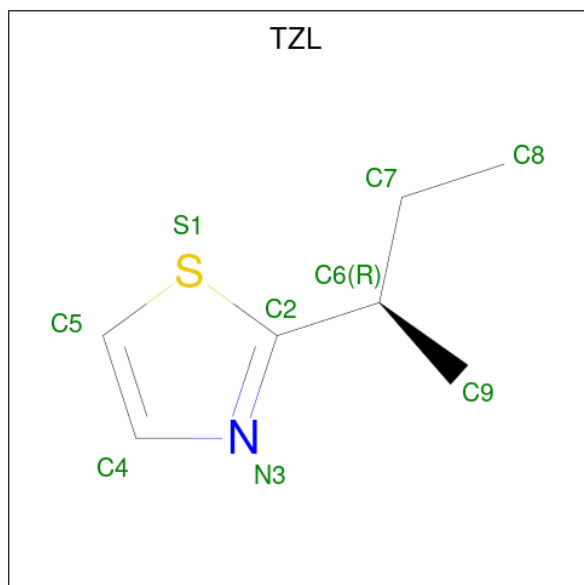
- Molecule 1 is a protein called MAJOR URINARY PROTEIN.

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 (three-letter code: 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 (three-letter code: 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.

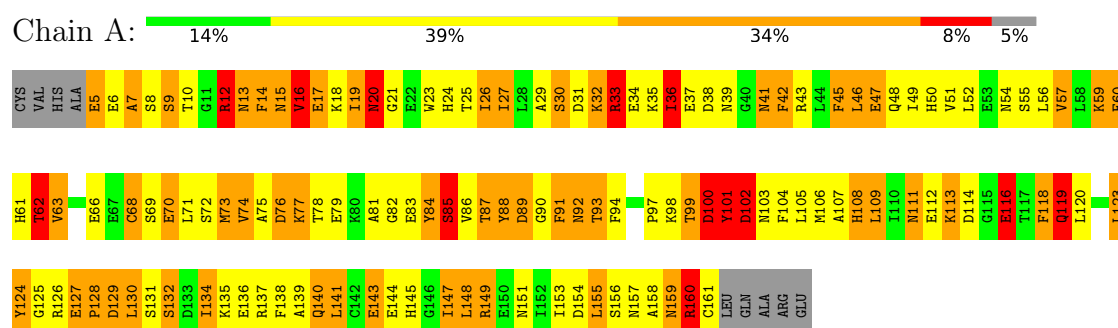
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total 77	O 77	0	0

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: MAJOR URINARY PROTEIN



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	1.42	7/1263 (0.6%)	3.26	166/1703 (9.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	GLU	CD-OE2	10.07	1.36	1.25
1	A	17	GLU	CD-OE1	7.82	1.34	1.25
1	A	79	GLU	CD-OE1	6.40	1.32	1.25
1	A	79	GLU	CD-OE2	6.10	1.32	1.25
1	A	116	GLU	CG-CD	5.81	1.60	1.51
1	A	47	GLU	CD-OE2	5.48	1.31	1.25
1	A	79	GLU	CB-CG	5.25	1.62	1.52

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	NE-CZ-NH2	38.80	139.70	120.30
1	A	149	ARG	NE-CZ-NH1	-26.16	107.22	120.30
1	A	31	ASP	CB-CG-OD2	-15.66	104.20	118.30
1	A	48	GLN	CA-CB-CG	14.88	146.14	113.40
1	A	102	ASP	CA-CB-CG	13.91	144.01	113.40
1	A	26	ILE	CB-CG1-CD1	12.47	148.81	113.90
1	A	124	TYR	CB-CG-CD2	12.02	128.21	121.00
1	A	101	TYR	CB-CG-CD2	-12.01	113.79	121.00
1	A	129	ASP	CB-CG-OD1	-11.66	107.81	118.30
1	A	31	ASP	OD1-CG-OD2	11.43	145.02	123.30
1	A	129	ASP	CB-CA-C	10.96	132.32	110.40
1	A	112	GLU	OE1-CD-OE2	-10.92	110.19	123.30
1	A	114	ASP	CB-CG-OD2	-10.66	108.70	118.30
1	A	114	ASP	CB-CG-OD1	9.95	127.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLN	CA-CB-CG	9.73	134.81	113.40
1	A	126	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	A	130	LEU	CB-CG-CD1	-9.38	95.05	111.00
1	A	129	ASP	CB-CG-OD2	9.30	126.67	118.30
1	A	148	LEU	O-C-N	8.99	137.08	122.70
1	A	160	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	A	12	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	45	PHE	CD1-CE1-CZ	-8.69	109.67	120.10
1	A	109	LEU	CB-CG-CD1	-8.67	96.26	111.00
1	A	71	LEU	CA-CB-CG	8.49	134.83	115.30
1	A	79	GLU	OE1-CD-OE2	8.41	133.40	123.30
1	A	99	THR	CA-CB-OG1	-8.37	91.43	109.00
1	A	102	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	31	ASP	CB-CG-OD1	-8.36	110.78	118.30
1	A	74	VAL	CG1-CB-CG2	-8.35	97.54	110.90
1	A	50	HIS	CA-CB-CG	8.35	127.79	113.60
1	A	118	PHE	C-N-CA	8.33	142.52	121.70
1	A	101	TYR	CB-CG-CD1	8.08	125.85	121.00
1	A	16	VAL	CG1-CB-CG2	7.99	123.68	110.90
1	A	7	ALA	C-N-CA	7.93	141.53	121.70
1	A	130	LEU	N-CA-CB	-7.88	94.63	110.40
1	A	91	PHE	CA-C-O	7.88	136.64	120.10
1	A	76	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	25	THR	N-CA-CB	7.59	124.72	110.30
1	A	137	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	20	ASN	CB-CG-ND2	7.55	134.82	116.70
1	A	78	THR	CA-CB-CG2	7.48	122.88	112.40
1	A	112	GLU	CG-CD-OE1	7.48	133.26	118.30
1	A	108	HIS	CA-CB-CG	-7.47	100.90	113.60
1	A	158	ALA	C-N-CA	7.39	140.17	121.70
1	A	92	ASN	O-C-N	7.38	134.50	122.70
1	A	100	ASP	CB-CG-OD1	-7.38	111.66	118.30
1	A	33	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	A	124	TYR	CB-CG-CD1	-7.34	116.59	121.00
1	A	66	GLU	N-CA-CB	7.31	123.76	110.60
1	A	45	PHE	CG-CD1-CE1	7.28	128.81	120.80
1	A	36	ILE	CA-CB-CG2	7.25	125.39	110.90
1	A	126	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	144	GLU	OE1-CD-OE2	7.12	131.84	123.30
1	A	143	GLU	OE1-CD-OE2	-7.11	114.77	123.30
1	A	140	GLN	O-C-N	-7.07	111.39	122.70
1	A	129	ASP	CA-CB-CG	7.06	128.94	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	GLU	OE1-CD-OE2	7.05	131.75	123.30
1	A	74	VAL	O-C-N	7.05	133.97	122.70
1	A	105	LEU	CB-CA-C	6.98	123.46	110.20
1	A	20	ASN	CA-CB-CG	6.95	128.69	113.40
1	A	9	SER	N-CA-CB	6.89	120.84	110.50
1	A	128	PRO	O-C-N	6.86	133.68	122.70
1	A	83	GLU	CB-CA-C	-6.79	96.81	110.40
1	A	144	GLU	O-C-N	-6.77	111.86	122.70
1	A	35	LYS	CB-CA-C	6.76	123.92	110.40
1	A	12	ARG	CA-CB-CG	-6.75	98.54	113.40
1	A	47	GLU	OE1-CD-OE2	-6.72	115.24	123.30
1	A	60	PHE	CB-CA-C	-6.72	96.96	110.40
1	A	81	ALA	O-C-N	6.69	134.58	123.20
1	A	134	ILE	O-C-N	6.66	133.36	122.70
1	A	45	PHE	CB-CG-CD1	6.66	125.46	120.80
1	A	89	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	A	112	GLU	CB-CG-CD	6.63	132.11	114.20
1	A	136	GLU	N-CA-CB	6.51	122.32	110.60
1	A	123	LEU	N-CA-CB	6.47	123.34	110.40
1	A	23	TRP	O-C-N	-6.47	112.35	122.70
1	A	38	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	84	TYR	O-C-N	6.38	132.91	122.70
1	A	92	ASN	CA-C-N	-6.35	103.23	117.20
1	A	116	GLU	CA-CB-CG	6.31	127.29	113.40
1	A	147	ILE	CB-CA-C	-6.29	99.02	111.60
1	A	84	TYR	N-CA-CB	-6.25	99.36	110.60
1	A	84	TYR	CA-C-O	-6.21	107.05	120.10
1	A	32	LYS	CD-CE-NZ	-6.20	97.43	111.70
1	A	78	THR	N-CA-CB	6.19	122.06	110.30
1	A	123	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	85	SER	O-C-N	6.10	132.47	122.70
1	A	124	TYR	O-C-N	6.09	133.55	123.20
1	A	52	LEU	O-C-N	6.08	132.43	122.70
1	A	111	ASN	OD1-CG-ND2	-6.06	107.96	121.90
1	A	50	HIS	N-CA-CB	6.04	121.48	110.60
1	A	124	TYR	CA-C-O	-6.04	107.41	120.10
1	A	9	SER	C-N-CA	6.03	136.78	121.70
1	A	74	VAL	CA-C-O	-6.03	107.44	120.10
1	A	130	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	126	ARG	CB-CG-CD	-5.94	96.16	111.60
1	A	46	LEU	CB-CA-C	5.93	121.48	110.20
1	A	39	ASN	CB-CA-C	5.92	122.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	THR	N-CA-CB	-5.83	99.22	110.30
1	A	128	PRO	CA-C-O	-5.83	106.21	120.20
1	A	112	GLU	N-CA-CB	5.81	121.06	110.60
1	A	14	PHE	CZ-CE2-CD2	-5.80	113.14	120.10
1	A	42	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	A	149	ARG	NH1-CZ-NH2	-5.78	113.05	119.40
1	A	9	SER	CA-CB-OG	5.74	126.71	111.20
1	A	73	MET	O-C-N	5.70	131.82	122.70
1	A	111	ASN	CB-CG-ND2	5.70	130.38	116.70
1	A	141	LEU	O-C-N	-5.68	113.61	122.70
1	A	112	GLU	CA-CB-CG	5.67	125.88	113.40
1	A	51	VAL	CA-C-N	5.67	129.67	117.20
1	A	132	SER	O-C-N	-5.67	113.63	122.70
1	A	6	GLU	O-C-N	5.66	131.75	122.70
1	A	49	ILE	CA-C-N	5.65	129.62	117.20
1	A	52	LEU	N-CA-CB	5.63	121.65	110.40
1	A	147	ILE	CA-CB-CG1	-5.62	100.33	111.00
1	A	33	ARG	CD-NE-CZ	5.61	131.46	123.60
1	A	19	ILE	CA-CB-CG1	5.60	121.63	111.00
1	A	63	VAL	C-N-CA	5.59	135.66	121.70
1	A	19	ILE	CB-CA-C	5.56	122.73	111.60
1	A	73	MET	CB-CG-SD	-5.56	95.72	112.40
1	A	34	GLU	CA-C-N	-5.55	104.99	117.20
1	A	12	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	A	5	GLU	CA-C-O	5.50	131.64	120.10
1	A	31	ASP	C-N-CA	5.48	135.41	121.70
1	A	132	SER	CA-CB-OG	5.43	125.86	111.20
1	A	42	PHE	CG-CD1-CE1	-5.42	114.83	120.80
1	A	57	VAL	CB-CA-C	5.41	121.68	111.40
1	A	136	GLU	O-C-N	5.39	131.32	122.70
1	A	70	GLU	C-N-CA	5.39	135.18	121.70
1	A	30	SER	CA-CB-OG	-5.36	96.72	111.20
1	A	85	SER	CA-C-N	-5.36	105.41	117.20
1	A	107	ALA	CA-C-O	5.35	131.34	120.10
1	A	144	GLU	CG-CD-OE1	-5.35	107.60	118.30
1	A	104	PHE	CD1-CE1-CZ	-5.34	113.69	120.10
1	A	10	THR	C-N-CA	5.32	133.47	122.30
1	A	132	SER	C-N-CA	5.30	134.95	121.70
1	A	100	ASP	CB-CA-C	5.30	120.99	110.40
1	A	21	GLY	N-CA-C	5.28	126.31	113.10
1	A	109	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	7	ALA	N-CA-CB	-5.26	102.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ARG	CD-NE-CZ	5.26	130.96	123.60
1	A	148	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	147	ILE	CG1-CB-CG2	5.25	122.95	111.40
1	A	56	LEU	N-CA-CB	-5.25	99.91	110.40
1	A	62	THR	CA-CB-CG2	-5.23	105.07	112.40
1	A	148	LEU	CA-C-N	-5.22	105.72	117.20
1	A	94	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	A	23	TRP	CA-C-N	5.19	128.62	117.20
1	A	141	LEU	CA-CB-CG	-5.19	103.36	115.30
1	A	7	ALA	O-C-N	-5.19	114.40	122.70
1	A	116	GLU	CG-CD-OE1	5.17	128.65	118.30
1	A	51	VAL	CA-C-O	-5.17	109.25	120.10
1	A	118	PHE	CB-CG-CD1	5.16	124.42	120.80
1	A	68	CYS	O-C-N	5.14	130.92	122.70
1	A	88	TYR	N-CA-CB	-5.12	101.38	110.60
1	A	116	GLU	N-CA-CB	-5.12	101.39	110.60
1	A	124	TYR	C-N-CA	-5.11	111.56	122.30
1	A	100	ASP	C-N-CA	5.11	134.47	121.70
1	A	27	ILE	C-N-CA	5.11	134.46	121.70
1	A	93	THR	CA-CB-OG1	-5.09	98.31	109.00
1	A	10	THR	CA-C-O	5.08	130.76	120.10
1	A	98	LYS	CA-C-O	5.06	130.72	120.10
1	A	128	PRO	C-N-CA	-5.05	109.06	121.70
1	A	35	LYS	CD-CE-NZ	5.04	123.28	111.70
1	A	155	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	128	PRO	N-CA-CB	5.01	109.31	103.30

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	1166	119	1
2	A	4	0	0	0	0
3	A	9	0	11	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	77	0	0	16	1
All	All	1332	0	1177	122	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 50.

All (122) 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: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:106:MET:HE2	1:A:138:PHE:HB2	1.61	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:106:MET:HE2	1:A:123:LEU:HD13	1.83	0.59
1:A:32:LYS:HG3	1:A:118:PHE:HB2	1.85	0.59
1:A:73:MET:HE1	1:A:88:TYR:CD1	2.37	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: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: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: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:CG	1:A:118:PHE:CE2	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TYR:O	1:A:89:ASP:C	2.45	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:160:ARG:HH11	1:A:160:ARG:HB2	1.75	0.49
1:A:106:MET:CE	1:A:138:PHE:HB2	2.40	0.49
1:A:7:ALA:O	1:A:99:THR:HG22	2.13	0.49
1:A:73:MET:HE2	1:A:88:TYR:CD1	2.48	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: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:77:LYS:HZ2	1:A:77:LYS:HB3	1.78	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:15:ASN:C	1:A:15:ASN:HD22	2.19	0.45
1:A:84:TYR:O	1:A:93:THR:HA	2.17	0.45
1:A:15:ASN:O	1:A:16:VAL:C	2.56	0.44
1:A:36:ILE:CD1	1:A:120:LEU:HD12	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:75:ALA:HA	1:A:85:SER:O	2.19	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
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

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	155/166 (93%)	142 (92%)	12 (8%)	1 (1%)	25	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	TYR

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	134/148 (90%)	107 (80%)	27 (20%)	1 1

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	ASN
1	A	15	ASN
1	A	16	VAL
1	A	20	ASN
1	A	33	ARG
1	A	36	ILE
1	A	41	ASN
1	A	43	ARG
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	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	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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	15	ASN
1	A	41	ASN

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Mol	Chain	Res	Type
1	A	151	ASN
1	A	159	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	8,9,9	2.14	3 (37%)	5,11,11	1.97	1 (20%)

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	-	-	1/3/6/6	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	4.09	1.56	1.37
3	A	167	TZL	C5-S1	3.75	1.89	1.71
3	A	167	TZL	C5-C4	2.07	1.52	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	167	TZL	C6-C2-N3	4.30	133.27	125.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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.