



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:09 AM UTC

PDB ID : 1TLM / pdb_00001tln
Title : STRUCTURAL ASPECTS OF INOTROPIC BIPYRIDINE BINDING:
CRYSTAL STRUCTURE DETERMINATION TO 1.9 ANGSTROMS OF
THE HUMAN SERUM TRANSTHYRETIN-MILRINONE COMPLEX
Authors : Wojtczak, A.; Luft, J.; Cody, V.
Deposited on : 1992-12-22
Resolution : 1.90 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

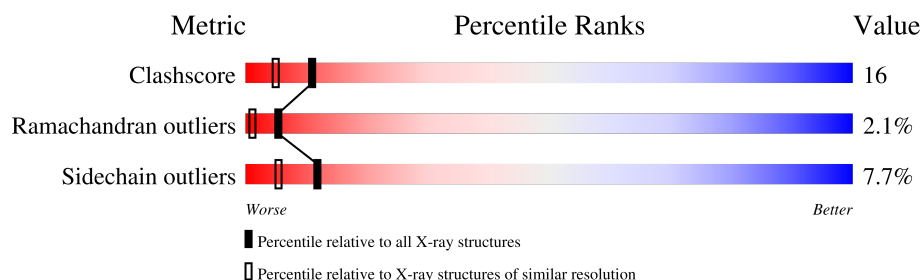
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	127	
1	B	127	

2 Entry composition [i](#)

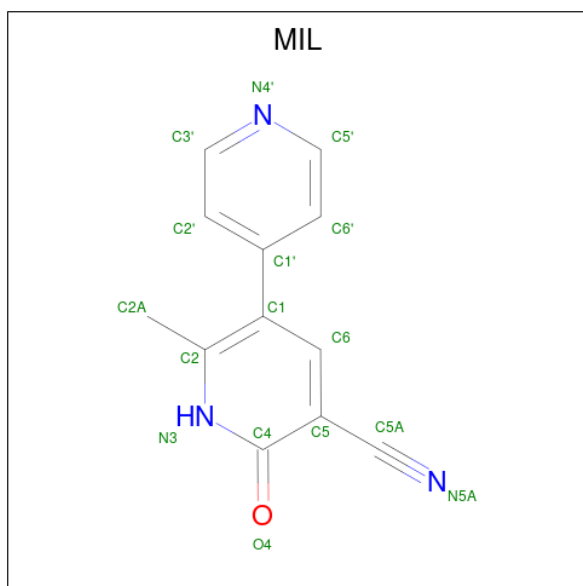
There are 3 unique types of molecules in this entry. The entry contains 2040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSTHYRETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			949	604	157	186	2			
1	B	120	Total	C	N	O	S	0	0	0
			929	593	154	180	2			

- Molecule 2 is MILRINONE (CCD ID: MIL) (formula: $C_{12}H_9N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	12	3	1		
2	B	1	Total	C	N	O	0	0
			16	12	3	1		

- Molecule 3 is water.

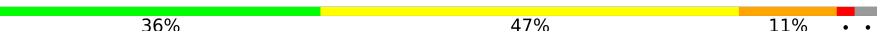
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total 73	O 73	0	0
3	B	57	Total 57	O 57	0	0

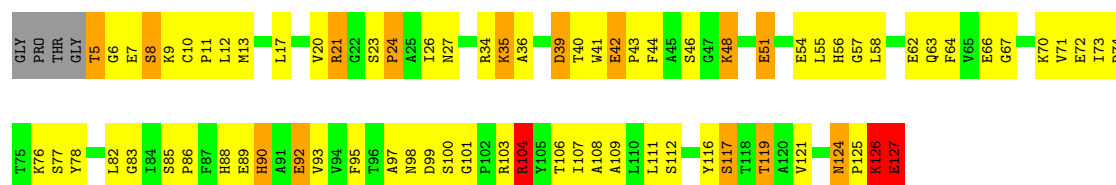
3 Residue-property plots

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.

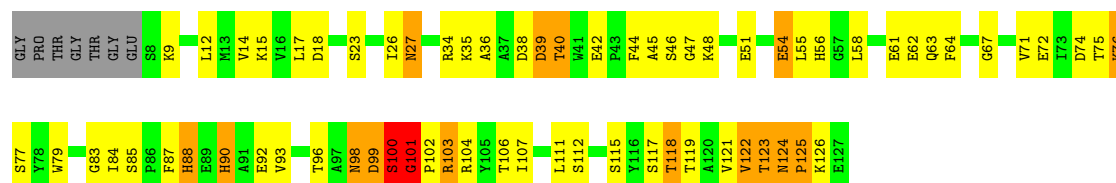
• Molecule 1: TRANSTHYRETIN

Chain A: 



• Molecule 1: TRANSTHYRETIN

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	44.18Å 86.38Å 66.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2040	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: MIL

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	1.68	10/973 (1.0%)	2.83	94/1325 (7.1%)
1	B	1.56	4/953 (0.4%)	2.83	87/1298 (6.7%)
All	All	1.62	14/1926 (0.7%)	2.83	181/2623 (6.9%)

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
1	B	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	LYS	N-CA	7.85	1.55	1.46
1	A	73	ILE	CA-CB	6.51	1.62	1.54
1	A	98	ASN	C-N	-6.21	1.25	1.33
1	B	47	GLY	CA-C	6.13	1.58	1.52
1	A	24	PRO	C-O	6.04	1.30	1.23
1	B	107	ILE	N-CA	5.74	1.53	1.46
1	A	46	SER	CB-OG	-5.58	1.30	1.42
1	A	71	VAL	C-O	5.41	1.30	1.24
1	B	75	THR	CA-CB	5.38	1.61	1.53
1	A	40	THR	CA-CB	5.24	1.61	1.53
1	A	46	SER	CA-CB	5.20	1.62	1.53
1	A	34	ARG	C-O	5.11	1.30	1.24
1	A	86	PRO	C-N	-5.09	1.27	1.33
1	A	107	ILE	C-O	5.03	1.29	1.24

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	GLU	CB-CG-CD	29.48	162.72	112.60
1	A	98	ASN	CA-C-N	16.70	143.26	120.38
1	A	98	ASN	C-N-CA	16.70	143.26	120.38
1	B	63	GLN	CB-CG-CD	13.97	136.35	112.60
1	B	63	GLN	OE1-CD-NE2	-12.82	109.78	122.60
1	A	51	GLU	CB-CG-CD	12.36	133.61	112.60
1	A	99	ASP	N-CA-CB	-11.82	92.33	110.06
1	B	27	ASN	CA-CB-CG	-11.70	100.90	112.60
1	A	127	GLU	CB-CG-CD	11.67	132.45	112.60
1	A	99	ASP	CA-CB-CG	-10.13	102.47	112.60
1	B	124	ASN	CA-CB-CG	10.02	122.62	112.60
1	B	51	GLU	CB-CG-CD	9.85	129.34	112.60
1	B	119	THR	OG1-CB-CG2	-9.82	89.66	109.30
1	A	77	SER	CA-C-N	9.80	133.19	120.44
1	A	77	SER	C-N-CA	9.80	133.19	120.44
1	A	97	ALA	CA-C-N	9.77	136.45	122.08
1	A	97	ALA	C-N-CA	9.77	136.45	122.08
1	B	107	ILE	CA-C-O	-9.62	110.11	120.59
1	A	27	ASN	CB-CG-OD1	9.38	139.56	120.80
1	A	63	GLN	OE1-CD-NE2	9.35	131.95	122.60
1	A	85	SER	N-CA-CB	-9.13	96.41	110.11
1	A	111	LEU	CA-C-O	-9.03	111.13	120.71
1	B	84	ILE	O-C-N	-8.95	113.78	123.18
1	A	85	SER	CB-CA-C	8.85	118.40	110.44
1	A	111	LEU	O-C-N	8.76	134.33	123.21
1	A	27	ASN	OD1-CG-ND2	-8.59	114.01	122.60
1	A	42	GLU	CA-C-O	-8.57	112.22	120.19
1	B	67	GLY	CA-C-O	-8.53	113.04	121.48
1	B	18	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	119	THR	CA-CB-CG2	8.31	124.64	110.50
1	A	21	ARG	CD-NE-CZ	8.29	136.01	124.40
1	A	86	PRO	CA-C-N	8.18	131.75	120.63
1	A	86	PRO	C-N-CA	8.18	131.75	120.63
1	A	124	ASN	CA-C-N	8.16	130.04	119.84
1	A	124	ASN	C-N-CA	8.16	130.04	119.84
1	A	41	TRP	O-C-N	-8.07	113.09	123.02
1	A	27	ASN	CA-CB-CG	-8.04	104.56	112.60
1	B	39	ASP	N-CA-CB	-7.97	100.10	112.13
1	A	58	LEU	CA-C-O	-7.94	112.01	120.42
1	A	46	SER	CB-CA-C	-7.92	93.42	110.45
1	B	54	GLU	CB-CG-CD	7.90	126.04	112.60
1	B	77	SER	CB-CA-C	-7.75	97.93	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ARG	CD-NE-CZ	-7.54	113.84	124.40
1	B	103	ARG	CA-C-O	-7.53	111.39	120.65
1	A	117	SER	N-CA-CB	7.43	123.79	111.08
1	A	77	SER	O-C-N	-7.41	114.26	122.12
1	A	101	GLY	CA-C-N	7.31	127.29	119.76
1	A	101	GLY	C-N-CA	7.31	127.29	119.76
1	A	17	LEU	CA-C-N	7.29	133.46	123.11
1	A	17	LEU	C-N-CA	7.29	133.46	123.11
1	A	57	GLY	CA-C-O	-7.26	110.15	119.58
1	B	42	GLU	CA-CB-CG	7.23	128.56	114.10
1	A	62	GLU	CB-CG-CD	7.15	124.76	112.60
1	B	112	SER	CA-C-N	7.11	126.94	119.05
1	B	112	SER	C-N-CA	7.11	126.94	119.05
1	B	101	GLY	O-C-N	7.09	128.86	121.77
1	B	74	ASP	CA-CB-CG	-7.08	105.52	112.60
1	A	34	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	B	63	GLN	CG-CD-OE1	6.96	134.73	120.80
1	B	39	ASP	CB-CA-C	6.93	121.57	111.73
1	A	100	SER	CA-C-N	6.88	132.67	121.87
1	A	100	SER	C-N-CA	6.88	132.67	121.87
1	A	27	ASN	CB-CG-ND2	-6.84	106.14	116.40
1	B	39	ASP	CA-C-O	6.83	129.41	121.28
1	B	36	ALA	CA-C-N	6.82	129.72	120.38
1	B	36	ALA	C-N-CA	6.82	129.72	120.38
1	A	7	GLU	O-C-N	6.80	131.48	122.30
1	B	36	ALA	CB-CA-C	6.78	120.99	109.80
1	A	40	THR	CA-CB-CG2	6.72	121.93	110.50
1	A	11	PRO	CA-C-O	-6.72	109.34	119.55
1	A	20	VAL	CA-CB-CG1	6.70	121.79	110.40
1	A	95	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	111	LEU	N-CA-C	6.63	120.27	109.59
1	A	88	HIS	CB-CG-ND1	6.63	132.64	122.70
1	B	40	THR	CA-C-O	-6.61	113.56	121.56
1	A	119	THR	OG1-CB-CG2	-6.61	96.08	109.30
1	B	119	THR	CA-CB-CG2	6.61	121.73	110.50
1	B	40	THR	CA-CB-OG1	-6.59	99.72	109.60
1	A	39	ASP	CA-CB-CG	-6.57	106.03	112.60
1	B	23	SER	CA-C-O	6.57	126.43	120.71
1	B	122	VAL	CB-CA-C	6.56	120.54	110.96
1	B	118	THR	CA-CB-OG1	-6.52	99.82	109.60
1	B	61	GLU	CA-C-O	-6.51	112.75	120.10
1	A	103	ARG	CA-CB-CG	6.49	127.07	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	VAL	CA-C-N	6.40	131.52	123.14
1	B	93	VAL	C-N-CA	6.40	131.52	123.14
1	B	40	THR	N-CA-CB	-6.39	101.00	110.85
1	B	48	LYS	O-C-N	6.39	131.06	123.27
1	B	27	ASN	N-CA-C	6.38	120.41	112.24
1	B	14	VAL	O-C-N	-6.32	116.35	123.18
1	B	111	LEU	N-CA-C	6.31	119.74	109.59
1	B	77	SER	O-C-N	6.30	128.80	122.12
1	A	112	SER	CA-C-O	-6.30	114.70	120.50
1	B	61	GLU	O-C-N	6.29	129.59	122.22
1	A	74	ASP	CB-CG-OD1	6.29	132.86	118.40
1	B	99	ASP	CA-C-O	6.27	127.21	119.05
1	A	86	PRO	CA-C-O	-6.23	114.30	121.96
1	A	86	PRO	O-C-N	-6.21	116.34	123.23
1	B	104	ARG	N-CA-CB	6.19	120.50	110.42
1	A	54	GLU	CG-CD-OE2	-6.16	104.24	118.40
1	A	78	TYR	CA-C-O	-6.15	114.36	120.82
1	B	106	THR	CA-C-N	-6.10	115.09	122.90
1	B	106	THR	C-N-CA	-6.10	115.09	122.90
1	B	90	HIS	CA-C-O	-6.09	114.43	121.26
1	A	121	VAL	N-CA-CB	6.08	119.55	111.64
1	B	103	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	63	GLN	CB-CG-CD	-6.03	102.34	112.60
1	B	87	PHE	CA-C-N	6.02	130.02	121.42
1	B	87	PHE	C-N-CA	6.02	130.02	121.42
1	B	23	SER	N-CA-CB	-6.00	103.73	111.35
1	B	102	PRO	CA-C-N	-5.99	113.03	122.79
1	B	102	PRO	C-N-CA	-5.99	113.03	122.79
1	B	98	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	B	46	SER	CA-C-O	-5.96	115.06	121.38
1	B	96	THR	CA-C-O	-5.96	113.93	120.43
1	B	44	PHE	CB-CA-C	5.95	121.14	111.26
1	A	46	SER	N-CA-CB	-5.95	101.73	111.66
1	A	66	GLU	N-CA-CB	5.92	118.75	110.04
1	A	92	GLU	CG-CD-OE2	-5.92	104.80	118.40
1	B	99	ASP	N-CA-C	-5.91	105.91	113.01
1	B	98	ASN	CA-CB-CG	5.90	118.50	112.60
1	B	15	LYS	CB-CG-CD	5.90	124.87	111.30
1	A	126	LYS	O-C-N	5.86	130.38	122.59
1	A	39	ASP	N-CA-C	5.78	120.14	113.38
1	B	62	GLU	CA-CB-CG	-5.76	102.58	114.10
1	B	15	LYS	CB-CA-C	5.75	120.10	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	GLU	OE1-CD-OE2	5.74	136.66	122.90
1	A	109	ALA	O-C-N	-5.72	116.29	123.27
1	B	79	TRP	N-CA-CB	5.71	118.62	110.16
1	B	48	LYS	CA-C-O	-5.71	114.09	120.66
1	A	66	GLU	CA-CB-CG	5.69	125.47	114.10
1	B	123	THR	CA-CB-OG1	-5.68	101.08	109.60
1	B	76	LYS	CA-C-N	5.68	127.89	120.28
1	B	76	LYS	C-N-CA	5.68	127.89	120.28
1	A	48	LYS	CG-CD-CE	-5.55	98.53	111.30
1	B	103	ARG	CA-CB-CG	5.53	125.16	114.10
1	A	41	TRP	N-CA-C	5.48	117.63	109.25
1	A	39	ASP	N-CA-CB	-5.47	104.41	112.78
1	A	107	ILE	O-C-N	-5.43	115.81	122.97
1	A	13	MET	CA-CB-CG	-5.42	103.25	114.10
1	B	83	GLY	CA-C-O	-5.41	112.91	119.68
1	B	18	ASP	CA-C-N	5.40	130.59	121.14
1	B	18	ASP	C-N-CA	5.40	130.59	121.14
1	A	99	ASP	CA-C-O	5.40	126.46	120.63
1	A	90	HIS	O-C-N	-5.39	117.43	123.04
1	B	85	SER	O-C-N	5.39	127.14	121.42
1	B	103	ARG	N-CA-C	5.37	119.44	111.87
1	A	76	LYS	CA-C-O	-5.36	114.87	120.55
1	B	51	GLU	CA-C-O	5.35	125.97	119.49
1	A	54	GLU	CG-CD-OE1	5.35	130.71	118.40
1	A	11	PRO	N-CA-CB	5.35	109.16	103.39
1	B	112	SER	CA-C-O	-5.34	115.36	120.64
1	A	56	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	35	LYS	CA-C-O	-5.32	114.41	120.58
1	A	43	PRO	N-CA-CB	5.29	107.95	103.19
1	B	9	LYS	O-C-N	5.26	129.88	123.14
1	A	72	GLU	CA-CB-CG	-5.26	103.58	114.10
1	A	116	TYR	CB-CG-CD2	-5.26	112.91	120.80
1	B	45	ALA	N-CA-CB	-5.23	102.92	111.66
1	A	73	ILE	CA-C-O	-5.22	114.95	120.48
1	A	100	SER	CA-CB-OG	5.21	121.51	111.10
1	B	88	HIS	O-C-N	5.21	129.16	123.01
1	A	104	ARG	CD-NE-CZ	5.20	131.68	124.40
1	B	85	SER	N-CA-CB	5.18	118.46	110.01
1	B	72	GLU	CA-C-O	5.18	125.95	120.36
1	B	102	PRO	O-C-N	5.16	129.61	122.64
1	B	121	VAL	N-CA-C	-5.16	100.22	107.75
1	A	83	GLY	CA-C-O	5.12	124.95	119.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	VAL	CA-CB-CG2	5.12	119.10	110.40
1	A	106	THR	CA-C-O	-5.12	114.69	120.32
1	B	38	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	27	ASN	CB-CA-C	-5.11	103.44	111.51
1	A	40	THR	CA-C-O	-5.10	115.14	120.80
1	B	126	LYS	CA-C-O	-5.07	115.99	121.36
1	B	115	SER	CA-C-O	-5.06	115.82	121.23
1	A	12	LEU	CB-CA-C	5.05	117.62	110.24
1	A	44	PHE	CB-CA-C	5.05	118.66	110.37
1	A	67	GLY	CA-C-N	5.04	129.35	122.90
1	A	67	GLY	C-N-CA	5.04	129.35	122.90
1	A	117	SER	CA-C-O	5.03	126.79	121.11
1	A	99	ASP	OD1-CG-OD2	5.01	134.93	122.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	B	34	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	949	0	923	33	0
1	B	929	0	908	30	0
2	A	16	0	9	0	0
2	B	16	0	9	3	0
3	A	73	0	0	10	0
3	B	57	0	0	10	0
All	All	2040	0	1849	62	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 16.

All (62) 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:64:PHE:CZ	3:A:196:HOH:O	2.04	1.08
1:B:35:LYS:O	3:B:140:HOH:O	1.97	0.83
1:A:64:PHE:HZ	3:A:196:HOH:O	1.46	0.81
1:A:125:PRO:O	1:A:126:LYS:C	2.26	0.78
1:A:9:LYS:NZ	1:A:126:LYS:HB2	2.01	0.76
1:A:89:GLU:OE2	3:A:157:HOH:O	2.05	0.72
1:A:35:LYS:HE3	1:A:39:ASP:OD1	1.91	0.71
1:A:48:LYS:HE2	3:A:177:HOH:O	1.90	0.71
1:A:127:GLU:HG2	1:A:127:GLU:O	1.89	0.70
1:B:98:ASN:C	1:B:103:ARG:HH11	2.00	0.69
1:B:27:ASN:ND2	3:B:143:HOH:O	2.27	0.68
1:A:21:ARG:NH2	3:A:135:HOH:O	2.25	0.68
1:B:64:PHE:CZ	3:B:153:HOH:O	2.47	0.67
1:A:36:ALA:HB2	1:A:42:GLU:HG3	1.78	0.65
1:A:9:LYS:HZ1	1:A:126:LYS:HB2	1.62	0.64
1:B:99:ASP:O	1:B:100:SER:C	2.40	0.64
1:A:5:THR:OG1	1:A:6:GLY:N	2.28	0.64
1:B:26:ILE:O	1:B:27:ASN:HB2	1.97	0.63
1:A:26:ILE:HG22	3:A:133:HOH:O	2.02	0.60
1:A:93:VAL:CG1	3:B:148:HOH:O	2.50	0.60
1:B:12:LEU:HD13	3:B:153:HOH:O	2.02	0.59
1:B:12:LEU:HB2	3:B:153:HOH:O	2.01	0.59
1:B:118:THR:HA	2:B:128:MIL:N5A	2.21	0.55
1:B:122:VAL:C	1:B:123:THR:CG2	2.79	0.55
1:A:117:SER:HB3	1:B:117:SER:HB3	1.90	0.54
1:B:88:HIS:CD2	3:B:148:HOH:O	2.61	0.53
1:B:99:ASP:O	1:B:101:GLY:N	2.41	0.53
1:A:93:VAL:HG13	3:B:148:HOH:O	2.09	0.52
1:B:98:ASN:C	1:B:100:SER:H	2.16	0.51
1:A:8:SER:O	1:A:104:ARG:NH1	2.45	0.49
1:A:64:PHE:CE1	3:A:196:HOH:O	2.49	0.49
1:A:23:SER:HB2	1:A:24:PRO:HD2	1.94	0.49
1:A:108:ALA:HB3	1:A:119:THR:HG22	1.95	0.49
1:B:54:GLU:CB	1:B:56:HIS:CE1	2.95	0.49
1:A:36:ALA:HB2	1:A:42:GLU:CG	2.43	0.48
1:B:54:GLU:HB3	1:B:56:HIS:CE1	2.48	0.48
1:A:9:LYS:HZ2	1:A:126:LYS:HB2	1.77	0.48
1:A:90:HIS:HE1	3:A:201:HOH:O	1.97	0.48
1:B:98:ASN:CB	1:B:100:SER:OG	2.62	0.47
1:B:90:HIS:CD2	1:B:92:GLU:HG3	2.49	0.47
1:A:125:PRO:O	1:A:127:GLU:N	2.47	0.46
1:A:21:ARG:CZ	3:A:135:HOH:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ASN:C	1:B:100:SER:N	2.73	0.46
1:B:98:ASN:HB3	1:B:100:SER:OG	2.15	0.46
1:A:124:ASN:HA	1:A:125:PRO:HD2	1.53	0.45
1:B:55:LEU:HD13	1:B:58:LEU:HD11	1.98	0.45
1:A:26:ILE:HD11	1:A:51:GLU:OE2	2.16	0.45
1:B:98:ASN:C	1:B:103:ARG:NH1	2.72	0.45
1:B:124:ASN:HA	1:B:125:PRO:HD3	1.83	0.44
1:A:125:PRO:C	1:A:127:GLU:N	2.74	0.44
1:B:99:ASP:N	1:B:103:ARG:HH11	2.14	0.43
1:A:26:ILE:HD12	1:A:51:GLU:HA	2.00	0.42
1:A:93:VAL:HG12	3:B:148:HOH:O	2.14	0.42
1:B:17:LEU:HD11	2:B:128:MIL:C3'	2.49	0.42
1:B:58:LEU:HA	1:B:58:LEU:HD23	1.82	0.42
1:B:76:LYS:NZ	3:B:145:HOH:O	2.54	0.41
1:B:55:LEU:CD1	1:B:58:LEU:HD21	2.51	0.41
1:A:26:ILE:HD11	1:A:51:GLU:CD	2.46	0.41
1:A:70:LYS:HD3	1:A:92:GLU:HG3	2.02	0.41
1:B:117:SER:O	2:B:128:MIL:N5A	2.54	0.41
1:B:99:ASP:C	1:B:101:GLY:N	2.78	0.41
1:A:48:LYS:CE	3:A:177:HOH:O	2.60	0.40

There are no symmetry-related clashes.

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	121/127 (95%)	114 (94%)	5 (4%)	2 (2%)	7	2
1	B	118/127 (93%)	113 (96%)	2 (2%)	3 (2%)	4	1
All	All	239/254 (94%)	227 (95%)	7 (3%)	5 (2%)	5	1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	B	100	SER
1	B	101	GLY
1	A	126	LYS
1	B	125	PRO

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	41/105 (39%)	36 (88%)	5 (12%)	5	2
1	B	63/105 (60%)	60 (95%)	3 (5%)	23	15
All	All	104/210 (50%)	96 (92%)	8 (8%)	12	5

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	10	CYS
1	A	55	LEU
1	A	82	LEU
1	A	127	GLU
1	B	39	ASP
1	B	40	THR
1	B	100	SER

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	90	HIS
1	B	27	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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	MIL	B	128	-	17,17,17	1.10	1 (5%)	23,23,23	2.16	6 (26%)
2	MIL	A	128	-	17,17,17	0.88	1 (5%)	23,23,23	3.13	6 (26%)

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
2	MIL	B	128	-	-	0/4/6/6	0/2/2/2
2	MIL	A	128	-	-	0/4/6/6	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	128	MIL	C2-N3	-3.37	1.34	1.38
2	A	128	MIL	C2-N3	-2.43	1.35	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	128	MIL	C5-C5A-N5A	-12.95	154.08	177.68
2	B	128	MIL	C4-N3-C2	5.07	129.94	126.25
2	B	128	MIL	C5-C5A-N5A	-4.90	168.75	177.68
2	B	128	MIL	C2A-C2-C1	3.53	129.66	126.25
2	A	128	MIL	C5A-C5-C4	-3.30	114.15	117.61
2	B	128	MIL	C5A-C5-C4	-3.29	114.16	117.61
2	A	128	MIL	C1'-C1-C2	2.80	126.32	122.86
2	B	128	MIL	C1-C2-N3	-2.63	116.53	118.80
2	A	128	MIL	C2A-C2-C1	2.62	128.79	126.25
2	A	128	MIL	C2'-C1'-C1	-2.52	117.37	120.98
2	A	128	MIL	C6'-C1'-C1	2.45	124.49	120.98
2	B	128	MIL	C1'-C1-C2	2.30	125.70	122.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	128	MIL	3	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.