



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:02 PM GMT

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

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

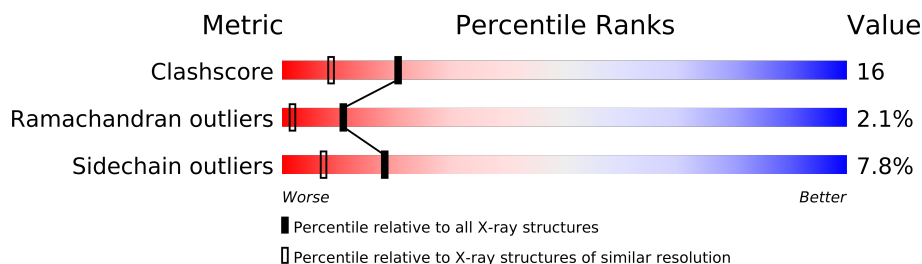
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	

2 Entry composition i

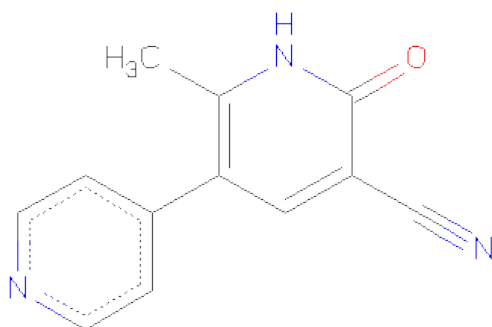
There are 3 unique types of molecules in this entry. The entry contains 2040 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (three-letter code: 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

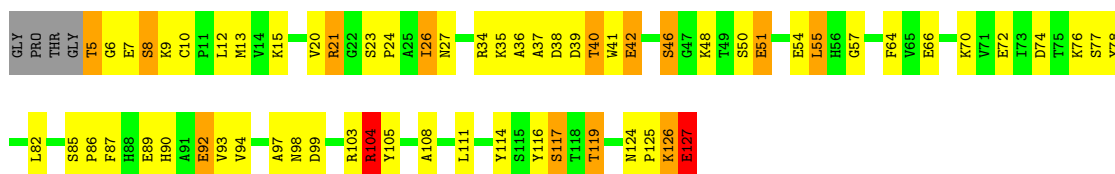
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

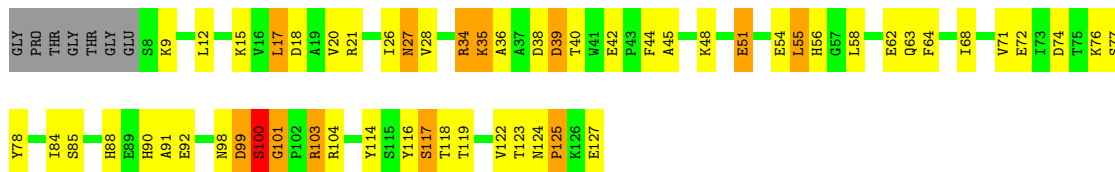
• Molecule 1: TRANSTHYRETIN

Chain A: 



• Molecule 1: TRANSTHYRETIN

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	1.36	4/973 (0.4%)	2.39	56/1325 (4.2%)
1	B	1.19	0/953	2.37	52/1298 (4.0%)
All	All	1.28	4/1926 (0.2%)	2.38	108/2623 (4.1%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	SER	CB-OG	-8.66	1.30	1.42
1	A	46	SER	CA-CB	6.69	1.62	1.52
1	A	50	SER	CB-OG	6.29	1.50	1.42
1	A	54	GLU	CD-OE1	-5.20	1.20	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	GLU	CB-CG-CD	17.97	162.72	114.20
1	A	74	ASP	CB-CG-OD1	16.18	132.86	118.30
1	A	116	TYR	CB-CG-CD2	-13.48	112.91	121.00
1	B	38	ASP	CB-CG-OD1	12.24	129.32	118.30
1	A	21	ARG	NE-CZ-NH1	11.98	126.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	GLU	OE1-CD-OE2	11.14	136.66	123.30
1	B	99	ASP	CB-CG-OD1	10.61	127.85	118.30
1	A	34	ARG	NE-CZ-NH2	10.42	125.51	120.30
1	B	104	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	99	ASP	N-CA-CB	-10.15	92.33	110.60
1	B	78	TYR	CB-CG-CD2	9.59	126.75	121.00
1	B	63	GLN	CB-CG-CD	9.52	136.35	111.60
1	B	116	TYR	CB-CG-CD1	9.40	126.64	121.00
1	A	85	SER	N-CA-CB	-9.39	96.41	110.50
1	A	27	ASN	CB-CG-OD1	8.98	139.56	121.60
1	B	114	TYR	CB-CG-CD1	-8.88	115.67	121.00
1	A	21	ARG	CD-NE-CZ	8.87	136.01	123.60
1	A	117	SER	N-CA-CB	8.86	123.79	110.50
1	B	119	THR	OG1-CB-CG2	-8.84	89.66	110.00
1	A	78	TYR	CB-CG-CD1	-8.80	115.72	121.00
1	A	46	SER	CB-CA-C	-8.78	93.42	110.10
1	A	119	THR	CA-CB-CG2	8.74	124.64	112.40
1	A	98	ASN	C-N-CA	8.63	143.26	121.70
1	B	116	TYR	CB-CG-CD2	-8.16	116.10	121.00
1	B	78	TYR	CG-CD1-CE1	8.14	127.81	121.30
1	B	38	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	B	78	TYR	CB-CG-CD1	-7.45	116.53	121.00
1	A	111	LEU	O-C-N	7.27	134.33	122.70
1	A	20	VAL	CA-CB-CG1	7.26	121.79	110.90
1	B	36	ALA	CB-CA-C	7.26	120.99	110.10
1	B	114	TYR	CB-CG-CD2	7.20	125.32	121.00
1	A	51	GLU	CB-CG-CD	7.19	133.61	114.20
1	A	99	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	87	PHE	CB-CG-CD1	-7.08	115.84	120.80
1	A	54	GLU	CG-CD-OE2	-7.03	104.24	118.30
1	A	103	ARG	CD-NE-CZ	-6.97	113.84	123.60
1	A	103	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	B	42	GLU	CA-CB-CG	6.89	128.56	113.40
1	B	34	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	40	THR	CA-CB-CG2	6.81	121.93	112.40
1	A	127	GLU	CB-CG-CD	6.76	132.45	114.20
1	A	92	GLU	CG-CD-OE2	-6.75	104.80	118.30
1	B	21	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	B	119	THR	CA-CB-CG2	6.67	121.73	112.40
1	B	103	ARG	CD-NE-CZ	6.63	132.88	123.60
1	B	78	TYR	CD1-CE1-CZ	-6.60	113.86	119.80
1	B	63	GLN	CG-CD-OE1	6.57	134.73	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	72	GLU	OE1-CD-OE2	6.47	131.07	123.30
1	B	77	SER	CB-CA-C	-6.41	97.93	110.10
1	A	92	GLU	OE1-CD-OE2	6.38	130.96	123.30
1	A	105	TYR	CZ-CE2-CD2	-6.35	114.08	119.80
1	B	28	VAL	CG1-CB-CG2	-6.35	100.75	110.90
1	A	114	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	74	ASP	OD1-CG-OD2	-6.27	111.39	123.30
1	A	103	ARG	CA-CB-CG	6.22	127.07	113.40
1	A	54	GLU	CG-CD-OE1	6.21	130.71	118.30
1	A	37	ALA	CB-CA-C	6.15	119.32	110.10
1	A	99	ASP	OD1-CG-OD2	6.12	134.93	123.30
1	A	15	LYS	CD-CE-NZ	-6.07	97.75	111.70
1	A	78	TYR	CB-CG-CD2	6.06	124.64	121.00
1	A	119	THR	OG1-CB-CG2	-6.05	96.08	110.00
1	A	76	LYS	CD-CE-NZ	-6.03	97.84	111.70
1	B	103	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	A	41	TRP	O-C-N	-6.01	113.09	122.70
1	B	117	SER	N-CA-CB	5.98	119.46	110.50
1	A	34	ARG	NH1-CZ-NH2	-5.92	112.89	119.40
1	A	13	MET	CA-CB-CG	-5.91	103.25	113.30
1	B	116	TYR	CG-CD1-CE1	5.90	126.02	121.30
1	A	97	ALA	C-N-CA	5.90	136.45	121.70
1	A	99	ASP	CB-CG-OD1	-5.85	113.04	118.30
1	A	46	SER	N-CA-CB	-5.84	101.73	110.50
1	B	39	ASP	N-CA-CB	-5.83	100.10	110.60
1	A	57	GLY	CA-C-O	-5.81	110.15	120.60
1	A	26	ILE	CG1-CB-CG2	-5.81	98.63	111.40
1	A	116	TYR	CB-CG-CD1	5.80	124.48	121.00
1	A	104	ARG	CD-NE-CZ	5.77	131.68	123.60
1	B	18	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	27	ASN	CA-CB-CG	-5.68	100.90	113.40
1	B	51	GLU	CB-CG-CD	5.61	129.34	114.20
1	B	116	TYR	CD1-CE1-CZ	-5.61	114.75	119.80
1	B	39	ASP	CB-CA-C	5.58	121.57	110.40
1	B	17	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	B	84	ILE	O-C-N	-5.57	113.78	122.70
1	A	86	PRO	CA-C-N	5.52	129.34	117.20
1	B	104	ARG	N-CA-CB	5.50	120.50	110.60
1	A	7	GLU	O-C-N	5.49	131.48	122.70
1	A	66	GLU	CA-CB-CG	5.49	125.47	113.40
1	B	91	ALA	CB-CA-C	5.48	118.32	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	VAL	CG1-CB-CG2	-5.47	102.15	110.90
1	B	71	VAL	CA-CB-CG2	5.47	119.10	110.90
1	B	44	PHE	CB-CA-C	5.37	121.14	110.40
1	B	103	ARG	CA-CB-CG	5.34	125.16	113.40
1	A	111	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	85	SER	N-CA-CB	5.31	118.46	110.50
1	A	55	LEU	CB-CG-CD2	5.29	119.99	111.00
1	A	77	SER	O-C-N	-5.27	114.26	122.70
1	B	63	GLN	OE1-CD-NE2	-5.27	109.78	121.90
1	B	127	GLU	CG-CD-OE2	-5.24	107.83	118.30
1	B	48	LYS	O-C-N	5.22	131.06	122.70
1	B	35	LYS	CD-CE-NZ	-5.13	99.89	111.70
1	B	45	ALA	N-CA-CB	-5.13	102.92	110.10
1	B	15	LYS	CB-CG-CD	5.10	124.87	111.60
1	B	34	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	127	GLU	CG-CD-OE1	5.08	128.46	118.30
1	A	94	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	B	20	VAL	CG1-CB-CG2	-5.05	102.83	110.90
1	A	12	LEU	CA-CB-CG	5.03	126.86	115.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	949	0	923	31	0
1	B	929	0	908	29	0
2	A	16	0	9	0	0
2	B	16	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	73	0	0	10	0
3	B	57	0	0	10	0
All	All	2040	0	1849	59	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:9:LYS:NZ	1:A:126:LYS:HB2	2.01	0.76
1:A:125:PRO:O	1:A:126:LYS:C	2.26	0.73
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:127:GLU:HG2	1:A:127:GLU:O	1.89	0.71
1:A:48:LYS:HE2	3:A:177:HOH:O	1.90	0.71
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:5:THR:OG1	1:A:6:GLY:N	2.28	0.65
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:98:ASN:C	1:B:103:ARG:HH11	2.00	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:99:ASP:O	1:B:100:SER:C	2.40	0.59
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:A:117:SER:HB3	1:B:117:SER:HB3	1.90	0.54
1:B:99:ASP:O	1:B:101:GLY:N	2.41	0.53
1:B:88:HIS:CD2	3:B:148:HOH:O	2.61	0.53
1:A:93:VAL:HG13	3:B:148:HOH:O	2.09	0.52
1:B:122:VAL:C	1:B:123:THR:CG2	2.79	0.51
1:A:64:PHE:CE1	3:A:196:HOH:O	2.49	0.49
1:A:8:SER:O	1:A:104:ARG:NH1	2.45	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:98:ASN:C	1:B:100:SER:H	2.16	0.46
1:A:21:ARG:CZ	3:A:135:HOH:O	2.62	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:124:ASN:HA	1:B:125:PRO:HD3	1.83	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:HD23	1:B:58:LEU:HA	1.82	0.42
1:B:98:ASN:C	1:B:103:ARG:NH1	2.72	0.41
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:B:98:ASN:C	1:B:100:SER:N	2.73	0.41
1:B:117:SER:O	2:B:128:MIL:N5A	2.54	0.41
1:A:70:LYS:HD3	1:A:92:GLU:HG3	2.02	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

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	121/127 (95%)	114 (94%)	5 (4%)	2 (2%)	14	3
1	B	118/127 (93%)	113 (96%)	2 (2%)	3 (2%)	9	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	239/254 (94%)	227 (95%)	7 (3%)	5 (2%)	11	2

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 ⓘ

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	103/105 (98%)	94 (91%)	9 (9%)	15	6
1	B	101/105 (96%)	94 (93%)	7 (7%)	22	10
All	All	204/210 (97%)	188 (92%)	16 (8%)	18	7

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	10	CYS
1	A	38	ASP
1	A	40	THR
1	A	42	GLU
1	A	46	SER
1	A	55	LEU
1	A	82	LEU
1	A	127	GLU
1	B	9	LYS
1	B	39	ASP
1	B	40	THR
1	B	51	GLU
1	B	55	LEU

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Mol	Chain	Res	Type
1	B	68	ILE
1	B	100	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	B	27	ASN
1	B	56	HIS
1	B	124	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	128	-	17,17,17	0.69	0	20,23,23	2.63	8 (40%)
2	MIL	B	128	-	17,17,17	0.74	1 (5%)	20,23,23	2.01	6 (30%)

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	A	128	-	-	0/5/6/6	0/2/2/2
2	MIL	B	128	-	-	0/5/6/6	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	128	MIL	C1-C2	-2.03	1.36	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	128	MIL	C5-C5A-N5A	-8.57	154.08	176.84
2	A	128	MIL	C1-C2-N3	4.21	119.28	117.31
2	B	128	MIL	C2A-C2-C1	3.86	129.66	126.94
2	B	128	MIL	C5-C4-N3	-3.42	112.51	115.40
2	B	128	MIL	C4-N3-C2	3.29	129.94	124.95
2	B	128	MIL	C6-C5-C5A	3.10	125.96	119.75
2	B	128	MIL	C5-C5A-N5A	-3.05	168.75	176.84
2	A	128	MIL	C6-C5-C5A	2.94	125.63	119.75
2	A	128	MIL	C2A-C2-C1	2.62	128.79	126.94
2	A	128	MIL	C6'-C1'-C1	2.29	124.49	120.92
2	B	128	MIL	C6-C1-C2	2.28	119.24	118.20
2	A	128	MIL	C2'-C1'-C1	-2.28	117.37	120.92
2	A	128	MIL	C2A-C2-N3	-2.26	111.92	117.15
2	A	128	MIL	C1'-C1-C2	2.21	126.32	122.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.