



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:46 PM GMT

PDB ID : 1LYN
Title : CRYSTAL STRUCTURE AND SUBUNIT DYNAMICS OF THE LYSIN DIMER: EGG ENVELOPES DISSOCIATE DIMERS, THE MONOMER IS THE ACTIVE SPECIES
Authors : Shaw, A.; Vacquier, V.D.; Stout, C.D.
Deposited on : 1995-03-03
Resolution : 2.75 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

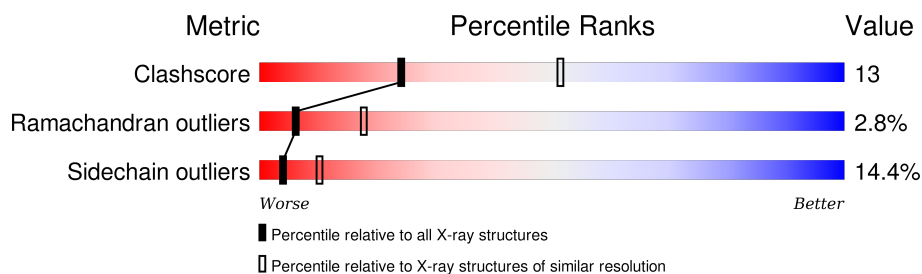
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	136	
1	B	136	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2094 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 SPERM LYSIN.

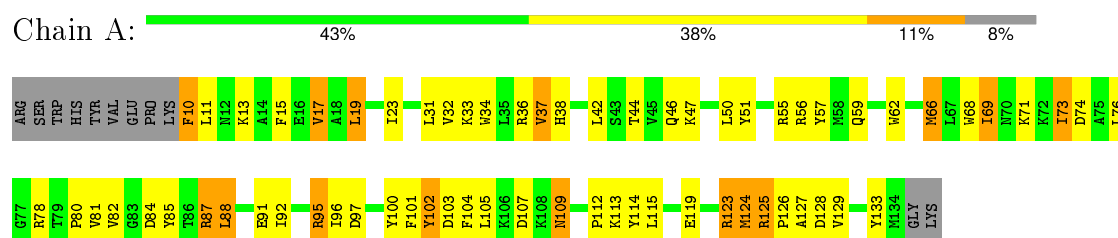
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1047	685	185	171	6			
1	B	125	Total	C	N	O	S	0	0	0
			1047	685	185	171	6			

3 Residue-property plots

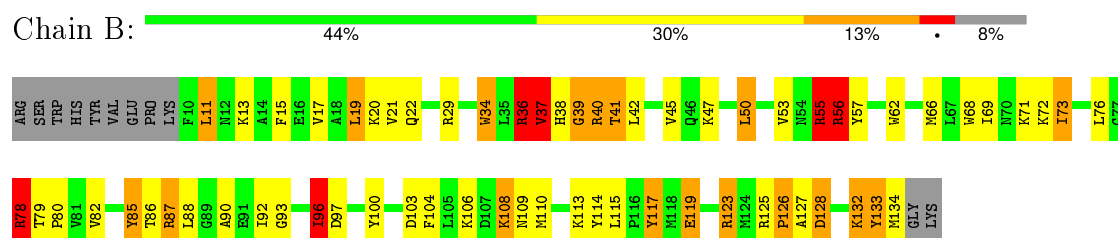
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: SPERM LYSIN



• Molecule 1: SPERM LYSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.20 Å 47.00 Å 123.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.75	Depositor
% Data completeness (in resolution range)	93.6 (8.00-2.75)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2094	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.20	1/1074 (0.1%)	2.18	56/1448 (3.9%)
1	B	1.19	1/1074 (0.1%)	2.19	56/1448 (3.9%)
All	All	1.19	2/2148 (0.1%)	2.18	112/2896 (3.9%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	GLN	CA-CB	-5.49	1.41	1.53
1	B	40	ARG	CA-CB	5.04	1.65	1.53

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	B	85	TYR	CB-CG-CD1	-10.76	114.54	121.00
1	B	68	TRP	CD1-CG-CD2	10.43	114.64	106.30
1	B	34	TRP	CD1-CG-CD2	10.36	114.59	106.30
1	B	34	TRP	CE2-CD2-CG	-9.74	99.50	107.30
1	B	78	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	A	34	TRP	CD1-CG-CD2	9.22	113.68	106.30
1	B	68	TRP	CE2-CD2-CG	-9.09	100.03	107.30
1	B	66	MET	CG-SD-CE	-9.00	85.79	100.20
1	B	62	TRP	CD1-CG-CD2	8.87	113.40	106.30
1	B	110	MET	CG-SD-CE	-8.80	86.13	100.20
1	B	21	VAL	CA-CB-CG2	-8.78	97.74	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	B	37	VAL	CG1-CB-CG2	-8.56	97.20	110.90
1	B	68	TRP	CG-CD2-CE3	8.48	141.53	133.90
1	A	125	ARG	CG-CD-NE	8.29	129.21	111.80
1	A	34	TRP	CE2-CD2-CG	-8.05	100.86	107.30
1	A	62	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	A	17	VAL	CA-CB-CG2	-7.98	98.94	110.90
1	B	62	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	A	95	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	125	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	B	34	TRP	CG-CD2-CE3	7.71	140.84	133.90
1	A	36	ARG	CA-CB-CG	7.60	130.12	113.40
1	A	62	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	B	36	ARG	CA-CB-CG	7.38	129.65	113.40
1	A	68	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	57	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	A	128	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	85	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	A	17	VAL	CA-CB-CG1	7.19	121.68	110.90
1	A	102	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	A	34	TRP	CB-CG-CD1	-7.17	117.68	127.00
1	B	123	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	133	TYR	CG-CD1-CE1	-7.04	115.67	121.30
1	B	40	ARG	CA-CB-CG	6.98	128.75	113.40
1	B	128	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	123	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	133	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	A	34	TRP	CG-CD2-CE3	6.69	139.92	133.90
1	A	133	TYR	CA-C-N	-6.65	102.58	117.20
1	B	133	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	A	34	TRP	CG-CD1-NE1	-6.58	103.52	110.10
1	B	103	ASP	O-C-N	-6.57	112.18	122.70
1	A	55	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	62	TRP	CG-CD2-CE3	6.55	139.79	133.90
1	A	56	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	68	TRP	CB-CG-CD1	-6.43	118.64	127.00
1	B	68	TRP	CG-CD1-NE1	-6.41	103.69	110.10
1	A	124	MET	CB-CA-C	-6.39	97.63	110.40
1	A	32	VAL	CG1-CB-CG2	-6.37	100.71	110.90
1	A	68	TRP	CB-CG-CD1	-6.29	118.82	127.00
1	B	17	VAL	CA-CB-CG2	-6.28	101.47	110.90
1	A	125	ARG	CD-NE-CZ	6.26	132.36	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ARG	CA-CB-CG	-6.21	99.73	113.40
1	A	10	PHE	CA-C-N	6.15	130.72	117.20
1	B	36	ARG	O-C-N	-6.14	112.87	122.70
1	A	87	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	71	LYS	O-C-N	-6.00	113.11	122.70
1	A	124	MET	CA-C-N	-5.99	104.03	117.20
1	B	133	TYR	CA-C-N	-5.97	104.06	117.20
1	A	105	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	B	62	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	62	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	B	87	ARG	CA-CB-CG	5.90	126.37	113.40
1	A	68	TRP	CG-CD2-CE3	5.84	139.15	133.90
1	A	51	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	B	41	THR	N-CA-CB	-5.77	99.33	110.30
1	B	86	THR	N-CA-CB	-5.77	99.33	110.30
1	A	74	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	55	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	103	ASP	CA-C-N	5.73	129.81	117.20
1	B	37	VAL	O-C-N	-5.72	113.55	122.70
1	B	56	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	125	ARG	CA-CB-CG	5.68	125.90	113.40
1	A	126	PRO	O-C-N	-5.67	113.64	122.70
1	B	62	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	B	57	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	B	96	ILE	CB-CA-C	-5.61	100.38	111.60
1	A	62	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	B	117	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	B	96	ILE	CB-CG1-CD1	-5.45	98.65	113.90
1	A	11	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	68	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	A	69	ILE	CA-CB-CG1	-5.36	100.81	111.00
1	A	88	LEU	CB-CG-CD2	-5.36	101.88	111.00
1	A	15	PHE	CB-CG-CD1	5.36	124.55	120.80
1	B	128	ASP	CA-CB-CG	5.36	125.19	113.40
1	A	112	PRO	CA-C-N	-5.32	105.49	117.20
1	B	134	MET	N-CA-C	-5.32	96.64	111.00
1	B	119	GLU	CA-CB-CG	-5.32	101.70	113.40
1	B	34	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	B	56	ARG	CD-NE-CZ	5.25	130.95	123.60
1	B	20	LYS	CB-CG-CD	-5.25	97.96	111.60
1	B	39	GLY	CA-C-O	-5.24	111.17	120.60
1	A	62	TRP	CB-CG-CD1	-5.23	120.20	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	LEU	N-CA-C	-5.23	96.89	111.00
1	B	114	TYR	CB-CG-CD1	-5.21	117.88	121.00
1	A	56	ARG	CA-CB-CG	-5.18	101.99	113.40
1	A	109	ASN	N-CA-CB	5.17	119.91	110.60
1	B	108	LYS	CG-CD-CE	5.16	127.38	111.90
1	A	133	TYR	CZ-CE2-CD2	-5.16	115.16	119.80
1	A	82	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	B	97	ASP	CA-C-N	-5.10	105.98	117.20
1	A	133	TYR	O-C-N	5.09	130.84	122.70
1	B	21	VAL	CA-CB-CG1	5.09	118.53	110.90
1	B	47	LYS	CA-CB-CG	5.09	124.59	113.40
1	A	46	GLN	CA-CB-CG	-5.08	102.23	113.40
1	B	29	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	85	TYR	CG-CD2-CE2	-5.04	117.27	121.30
1	A	66	MET	CA-CB-CG	5.02	121.83	113.30
1	A	57	TYR	CG-CD1-CE1	-5.01	117.29	121.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	MET	Mainchain

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	1047	0	1072	24	0
1	B	1047	0	1072	39	0
All	All	2094	0	2144	55	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 13.

All (55) 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:B:56:ARG:HG2	1:B:56:ARG:HH11	1.50	0.77
1:B:34:TRP:O	1:B:38:HIS:HD2	1.70	0.74
1:A:92:ILE:O	1:A:96:ILE:HG12	1.89	0.72
1:B:38:HIS:HB3	1:B:106:LYS:HZ3	1.55	0.71
1:B:36:ARG:HD2	1:B:36:ARG:O	1.90	0.71
1:A:17:VAL:HG22	1:A:127:ALA:HB1	1.78	0.66
1:A:113:LYS:H	1:B:56:ARG:NH2	1.96	0.64
1:A:73:ILE:HA	1:A:76:LEU:HD23	1.80	0.62
1:B:82:VAL:O	1:B:85:TYR:HB2	2.00	0.60
1:B:19:LEU:HD11	1:B:85:TYR:HD1	1.66	0.60
1:A:19:LEU:HD21	1:A:69:ILE:HD13	1.83	0.57
1:A:119:GLU:HG3	1:A:123:ARG:HE	1.70	0.56
1:A:78:ARG:NH2	1:A:81:VAL:HG22	2.20	0.56
1:A:113:LYS:HE3	1:B:117:TYR:CE2	2.42	0.54
1:B:119:GLU:O	1:B:119:GLU:HG2	2.07	0.54
1:B:132:LYS:HE3	1:B:133:TYR:O	2.08	0.53
1:B:93:GLY:O	1:B:96:ILE:HD11	2.09	0.53
1:A:113:LYS:HE3	1:B:117:TYR:CZ	2.44	0.52
1:B:76:LEU:HD22	1:B:78:ARG:NH1	2.25	0.52
1:A:73:ILE:HA	1:A:76:LEU:CD2	2.40	0.52
1:A:113:LYS:HB3	1:B:56:ARG:HH21	1.76	0.51
1:B:38:HIS:O	1:B:106:LYS:NZ	2.44	0.51
1:A:31:LEU:HD13	1:A:102:TYR:CZ	2.46	0.51
1:A:97:ASP:OD2	1:A:100:TYR:HB2	2.09	0.51
1:A:104:PHE:HE1	1:B:100:TYR:CE2	2.29	0.50
1:A:101:PHE:HA	1:B:104:PHE:HZ	1.76	0.49
1:B:56:ARG:HG2	1:B:56:ARG:NH1	2.19	0.49
1:A:59:GLN:HE21	1:A:129:VAL:HG12	1.78	0.48
1:B:88:LEU:O	1:B:92:ILE:HG13	2.12	0.48
1:B:104:PHE:O	1:B:108:LYS:HB2	2.14	0.48
1:B:39:GLY:O	1:B:41:THR:N	2.47	0.47
1:A:101:PHE:HD1	1:B:108:LYS:HD2	1.79	0.47
1:B:119:GLU:O	1:B:123:ARG:HG3	2.14	0.46
1:B:132:LYS:HB3	1:B:132:LYS:HE2	1.80	0.46
1:B:36:ARG:O	1:B:37:VAL:HG23	2.14	0.46
1:A:37:VAL:HG12	1:A:38:HIS:CD2	2.51	0.45
1:B:69:ILE:O	1:B:73:ILE:HB	2.16	0.45
1:B:73:ILE:O	1:B:76:LEU:HB2	2.17	0.44
1:B:19:LEU:CD1	1:B:85:TYR:HD1	2.31	0.43
1:A:87:ARG:HH11	1:A:87:ARG:HG3	1.82	0.43
1:B:79:THR:HA	1:B:80:PRO:HD2	1.77	0.43
1:B:69:ILE:HD11	1:B:92:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:HIS:HB3	1:B:106:LYS:NZ	2.29	0.41
1:A:42:LEU:O	1:A:47:LYS:HE2	2.20	0.41
1:B:42:LEU:HD13	1:B:106:LYS:HZ1	1.85	0.41
1:B:22:GLN:HB3	1:B:90:ALA:N	2.34	0.41
1:A:91:GLU:O	1:A:95:ARG:CG	2.68	0.41
1:B:15:PHE:O	1:B:19:LEU:HD22	2.21	0.41
1:B:50:LEU:O	1:B:53:VAL:HB	2.20	0.41
1:B:113:LYS:HG3	1:B:115:LEU:HG	2.03	0.41
1:A:115:LEU:HD13	1:B:117:TYR:HB3	2.02	0.41
1:B:36:ARG:NH1	1:B:37:VAL:HG23	2.36	0.41
1:A:103:ASP:O	1:A:107:ASP:HB2	2.21	0.41
1:A:73:ILE:HD12	1:A:80:PRO:HB3	2.03	0.40
1:B:55:ARG:HH11	1:B:55:ARG:HD2	1.73	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	123/136 (90%)	116 (94%)	5 (4%)	2 (2%)	12	34
1	B	123/136 (90%)	106 (86%)	12 (10%)	5 (4%)	3	10
All	All	246/272 (90%)	222 (90%)	17 (7%)	7 (3%)	6	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	ARG
1	A	114	TYR
1	B	37	VAL
1	B	40	ARG
1	A	23	ILE

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Mol	Chain	Res	Type
1	B	127	ALA
1	B	126	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	108/119 (91%)	94 (87%)	14 (13%)	5	14
1	B	108/119 (91%)	91 (84%)	17 (16%)	3	8
All	All	216/238 (91%)	185 (86%)	31 (14%)	4	10

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	13	LYS
1	A	19	LEU
1	A	33	LYS
1	A	37	VAL
1	A	44	THR
1	A	50	LEU
1	A	66	MET
1	A	71	LYS
1	A	73	ILE
1	A	84	ASP
1	A	88	LEU
1	A	109	ASN
1	A	125	ARG
1	B	11	LEU
1	B	13	LYS
1	B	19	LEU
1	B	36	ARG
1	B	45	VAL
1	B	50	LEU
1	B	55	ARG

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Mol	Chain	Res	Type
1	B	56	ARG
1	B	72	LYS
1	B	73	ILE
1	B	78	ARG
1	B	87	ARG
1	B	96	ILE
1	B	109	ASN
1	B	126	PRO
1	B	128	ASP
1	B	132	LYS

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

Mol	Chain	Res	Type
1	A	38	HIS
1	A	59	GLN
1	A	70	ASN
1	A	122	ASN
1	B	38	HIS
1	B	61	HIS
1	B	70	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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