Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:21 AM EDT

PDB ID	:	1LXD
Title	:	CRYSTAL STRUCTURE OF THE RAS INTERACTING DOMAIN OF RALGDS, A GUANINE NUCLEOTIDE DISSOCIATION STIMULATOR OF RAL PROTEIN
Authors	:	Huang, L.; Weng, X.W.; Hofer, F.; Martin, G.S.; Kim, S.H.
Deposited on	:	1997-03-05
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 (i) 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 (1)) were used in the production of this report:

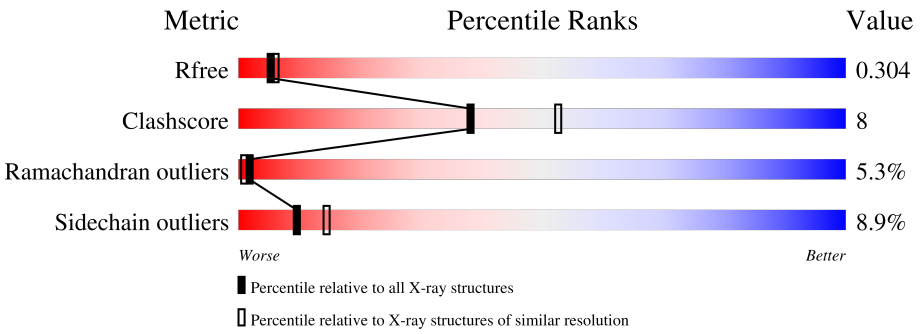
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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))
R_{free}	130704	3907 (2.40-2.40)
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 <=5%

Mol	Chain	Length	Quality of chain
1	A	100	55% 23% 7% • 13%
1	B	100	58% 24% • • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1878 atoms, of which 426 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 RALGDSB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	87	852	436	155	117	139	5	0	0	0
1	B	87	852	436	155	117	139	5	0	0	0

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	ASP	DELETION	UNP Q03386
A	?	-	VAL	DELETION	UNP Q03386
A	?	-	GLU	DELETION	UNP Q03386
A	?	-	GLU	DELETION	UNP Q03386
A	?	-	ILE	DELETION	UNP Q03386
A	?	-	ASN	DELETION	UNP Q03386
A	?	-	MET	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	PHE	DELETION	UNP Q03386
A	?	-	VAL	DELETION	UNP Q03386
A	?	-	PRO	DELETION	UNP Q03386
A	?	-	GLU	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	PRO	DELETION	UNP Q03386
A	?	-	ASP	DELETION	UNP Q03386
A	?	-	GLY	DELETION	UNP Q03386
A	?	-	GLN	DELETION	UNP Q03386
A	?	-	GLU	DELETION	UNP Q03386
A	?	-	LYS	DELETION	UNP Q03386
A	?	-	LYS	DELETION	UNP Q03386
A	?	-	PHE	DELETION	UNP Q03386
A	?	-	TRP	DELETION	UNP Q03386

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	ALA	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	GLN	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	PRO	DELETION	UNP Q03386
A	?	-	GLU	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	GLY	DELETION	UNP Q03386
A	?	-	ILE	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	ALA	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	ALA	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	PRO	DELETION	UNP Q03386
A	?	-	VAL	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	ARG	DELETION	UNP Q03386
A	?	-	THR	DELETION	UNP Q03386
A	?	-	HIS	DELETION	UNP Q03386
A	?	-	LYS	DELETION	UNP Q03386
A	?	-	ARG	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	VAL	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	GLY	DELETION	UNP Q03386

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP Q03386
A	?	-	CYS	DELETION	UNP Q03386
A	?	-	SER	DELETION	UNP Q03386
A	?	-	TYR	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	ASP	DELETION	UNP Q03386
B	?	-	VAL	DELETION	UNP Q03386
B	?	-	GLU	DELETION	UNP Q03386
B	?	-	GLU	DELETION	UNP Q03386
B	?	-	ILE	DELETION	UNP Q03386
B	?	-	ASN	DELETION	UNP Q03386
B	?	-	MET	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	PHE	DELETION	UNP Q03386
B	?	-	VAL	DELETION	UNP Q03386
B	?	-	PRO	DELETION	UNP Q03386
B	?	-	GLU	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	PRO	DELETION	UNP Q03386
B	?	-	ASP	DELETION	UNP Q03386
B	?	-	GLY	DELETION	UNP Q03386
B	?	-	GLN	DELETION	UNP Q03386
B	?	-	GLU	DELETION	UNP Q03386
B	?	-	LYS	DELETION	UNP Q03386
B	?	-	LYS	DELETION	UNP Q03386
B	?	-	PHE	DELETION	UNP Q03386
B	?	-	TRP	DELETION	UNP Q03386
B	?	-	GLU	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	ALA	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	GLN	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	PRO	DELETION	UNP Q03386
B	?	-	GLU	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	GLY	DELETION	UNP Q03386
B	?	-	ILE	DELETION	UNP Q03386

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	ALA	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	ALA	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	PRO	DELETION	UNP Q03386
B	?	-	VAL	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	ARG	DELETION	UNP Q03386
B	?	-	THR	DELETION	UNP Q03386
B	?	-	HIS	DELETION	UNP Q03386
B	?	-	LYS	DELETION	UNP Q03386
B	?	-	ARG	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	VAL	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	GLY	DELETION	UNP Q03386
B	?	-	VAL	DELETION	UNP Q03386
B	?	-	CYS	DELETION	UNP Q03386
B	?	-	SER	DELETION	UNP Q03386
B	?	-	TYR	DELETION	UNP Q03386

- Molecule 2 is water.

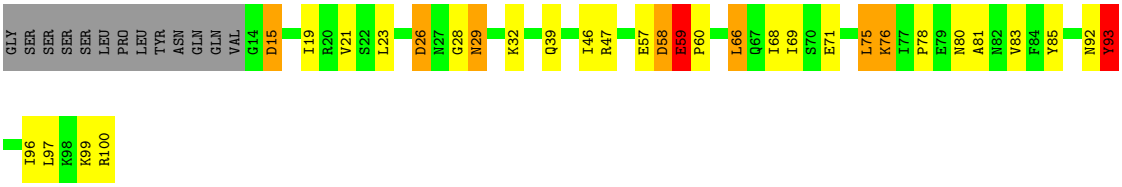
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
2	A	28	84	56	28	0	0
			Total	H	O		
2	B	30	90	60	30	0	0

3 Residue-property plots (i)

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.

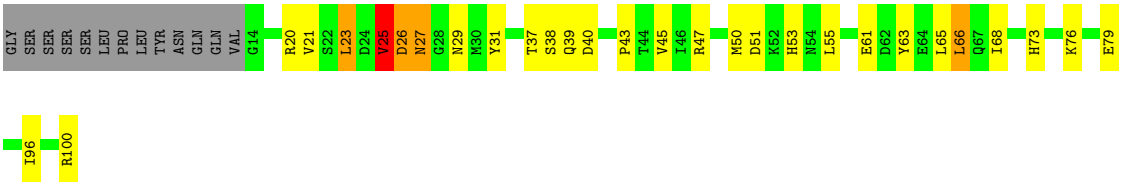
- Molecule 1: RALGDSB

Chain A:



- Molecule 1: RALGDSB

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.28Å 30.71Å 51.33Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40 9.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.0 (6.00-2.40) 91.9 (9.99-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.212 , 0.298 0.222 , 0.304	Depositor DCC
R_{free} test set	942 reflections (10.52%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.50 , 87.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	1878	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.97	2/707 (0.3%)	1.85	15/953 (1.6%)
1	B	0.92	0/707	1.77	14/953 (1.5%)
All	All	0.95	2/1414 (0.1%)	1.81	29/1906 (1.5%)

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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLU	CD-OE2	-6.14	1.19	1.25
1	A	59	GLU	CG-CD	-5.81	1.43	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	ARG	NE-CZ-NH1	13.28	126.94	120.30
1	B	65	LEU	O-C-N	-11.99	103.51	122.70
1	B	65	LEU	CA-C-N	10.38	140.03	117.20
1	A	47	ARG	NE-CZ-NH1	10.33	125.46	120.30
1	A	47	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	29	ASN	N-CA-C	7.48	131.19	111.00
1	A	58	ASP	N-CA-C	7.42	131.03	111.00
1	B	29	ASN	OD1-CG-ND2	-7.19	105.35	121.90
1	A	58	ASP	CA-C-N	-7.19	101.38	117.20
1	B	27	ASN	N-CA-C	7.01	129.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	47	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	29	ASN	CB-CG-ND2	6.13	131.41	116.70
1	B	26	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	83	VAL	CG1-CB-CG2	-6.00	101.31	110.90
1	A	57	GLU	CA-C-N	-5.61	104.86	117.20
1	A	29	ASN	CA-C-N	5.57	129.46	117.20
1	A	100	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	A	21	VAL	CG1-CB-CG2	-5.38	102.30	110.90
1	A	59	GLU	N-CA-C	5.38	125.52	111.00
1	A	99	LYS	CA-CB-CG	-5.35	101.63	113.40
1	B	51	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	40	ASP	N-CA-C	5.20	125.03	111.00
1	B	39	GLN	OE1-CD-NE2	-5.19	109.97	121.90
1	B	39	GLN	CG-CD-NE2	5.17	129.11	116.70
1	A	15	ASP	N-CA-CB	-5.13	101.36	110.60
1	B	66	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	85	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	B	25	VAL	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ASN	Peptide
1	A	93	TYR	Sidechain
1	B	31	TYR	Sidechain
1	B	63	TYR	Sidechain

5.2 Too-close contacts (i)

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	697	155	686	11	0
1	B	697	155	686	10	0
2	A	28	56	0	4	0
2	B	30	60	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1452	426	1372	21	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 8.

All (21) 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:68:ILE:HD11	1:A:96:ILE:HG12	1.61	0.83
1:A:78:PRO:HG2	1:A:81:ALA:HB2	1.70	0.72
1:B:25:VAL:HG13	1:B:26:ASP:H	1.59	0.65
1:A:69:ILE:HD11	1:A:75:LEU:HD12	1.84	0.60
1:A:46:ILE:HD12	2:A:335:HOH:O	2.02	0.59
1:A:76:LYS:HD3	2:A:312:HOH:O	2.05	0.56
1:A:46:ILE:HG23	1:A:97:LEU:HD11	1.88	0.56
1:B:76:LYS:HD2	2:B:329:HOH:O	2.06	0.55
1:A:66:LEU:HD12	1:A:76:LYS:HG3	1.92	0.51
1:A:32:LYS:HE3	2:A:313:HOH:O	2.12	0.49
1:B:55:LEU:HG	2:B:348:HOH:O	2.14	0.48
1:B:50:MET:HB2	1:B:55:LEU:HB2	1.97	0.47
1:A:15:ASP:HB3	2:A:325:HOH:O	2.15	0.46
1:B:68:ILE:HD11	1:B:96:ILE:HG12	1.98	0.45
1:B:23:LEU:HB2	1:B:25:VAL:HG12	2.00	0.44
1:B:43:PRO:HD3	1:B:79:GLU:O	2.18	0.44
1:B:73:HIS:CG	2:B:321:HOH:O	2.72	0.43
1:A:59:GLU:HA	1:A:60:PRO:HD3	1.84	0.42
1:B:21:VAL:O	1:B:53:HIS:HE1	2.02	0.42
1:B:96:ILE:HD13	1:B:96:ILE:HG21	1.77	0.42
1:A:19:ILE:HG22	1:A:93:TYR:HD1	1.84	0.41

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	85/100 (85%)	75 (88%)	5 (6%)	5 (6%)	1 0
1	B	85/100 (85%)	76 (89%)	5 (6%)	4 (5%)	2 1
All	All	170/200 (85%)	151 (89%)	10 (6%)	9 (5%)	2 1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	B	27	ASN
1	B	66	LEU
1	A	58	ASP
1	B	38	SER
1	A	28	GLY
1	A	93	TYR
1	A	26	ASP
1	B	25	VAL

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	79/91 (87%)	70 (89%)	9 (11%)	5 7
1	B	79/91 (87%)	74 (94%)	5 (6%)	18 28
All	All	158/182 (87%)	144 (91%)	14 (9%)	9 14

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	26	ASP
1	A	39	GLN
1	A	66	LEU

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Mol	Chain	Res	Type
1	A	71	GLU
1	A	75	LEU
1	A	76	LYS
1	A	80	ASN
1	A	92	ASN
1	B	20	ARG
1	B	23	LEU
1	B	37	THR
1	B	45	VAL
1	B	61	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	GLN

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)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.