



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:33 pm GMT

PDB ID : 5LC4
Title : Xray structure of mouse FAM3C ILEI dimer
Authors : Johansson, P.; Jansson, A.
Deposited on : 2016-06-19
Resolution : 1.84 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

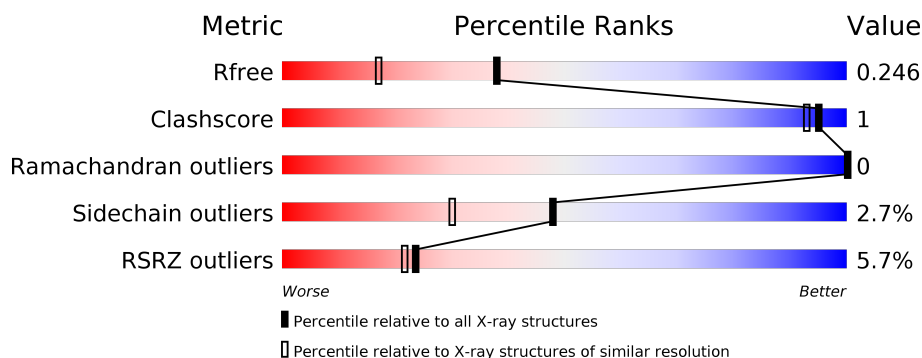
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	111664	3313 (1.86-1.82)
Clashscore	122126	3530 (1.86-1.82)
Ramachandran outliers	120053	3495 (1.86-1.82)
Sidechain outliers	120020	3496 (1.86-1.82)
RSRZ outliers	108989	3265 (1.86-1.82)

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.

Mol	Chain	Length	Quality of chain
1	A	205	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>6%</div> <div>17%</div> </div> </div>
1	B	205	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	205	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>5%</div> <div>18%</div> </div> </div>
1	D	205	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>5%</div> <div>18%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5636 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 Protein FAM3C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1311	832	221	248	10			
1	B	170	Total	C	N	O	S	0	0	0
			1302	827	219	246	10			
1	C	169	Total	C	N	O	S	0	0	0
			1293	821	217	245	10			
1	D	169	Total	C	N	O	S	0	1	0
			1307	832	219	246	10			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP Q91VU0
A	24	PRO	-	expression tag	UNP Q91VU0
A	25	LEU	-	expression tag	UNP Q91VU0
A	26	LEU	-	expression tag	UNP Q91VU0
A	27	LEU	-	expression tag	UNP Q91VU0
A	28	LEU	-	expression tag	UNP Q91VU0
A	29	LEU	-	expression tag	UNP Q91VU0
A	30	PRO	-	expression tag	UNP Q91VU0
A	31	LEU	-	expression tag	UNP Q91VU0
A	32	LEU	-	expression tag	UNP Q91VU0
A	33	TRP	-	expression tag	UNP Q91VU0
A	34	ALA	-	expression tag	UNP Q91VU0
A	35	GLY	-	expression tag	UNP Q91VU0
A	36	ALA	-	expression tag	UNP Q91VU0
A	37	LEU	-	expression tag	UNP Q91VU0
A	38	ALA	-	expression tag	UNP Q91VU0
A	39	GLU	-	expression tag	UNP Q91VU0
A	40	LEU	-	expression tag	UNP Q91VU0
A	41	HIS	-	expression tag	UNP Q91VU0
A	42	HIS	-	expression tag	UNP Q91VU0
A	43	HIS	-	expression tag	UNP Q91VU0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	44	HIS	-	expression tag	UNP Q91VU0
A	45	HIS	-	expression tag	UNP Q91VU0
A	46	HIS	-	expression tag	UNP Q91VU0
A	47	GLU	-	expression tag	UNP Q91VU0
A	48	ASN	-	expression tag	UNP Q91VU0
A	49	LEU	-	expression tag	UNP Q91VU0
A	50	TYR	-	expression tag	UNP Q91VU0
A	51	PHE	-	expression tag	UNP Q91VU0
A	52	GLN	-	expression tag	UNP Q91VU0
A	53	SER	-	expression tag	UNP Q91VU0
A	54	GLY	-	expression tag	UNP Q91VU0
B	23	MET	-	initiating methionine	UNP Q91VU0
B	24	PRO	-	expression tag	UNP Q91VU0
B	25	LEU	-	expression tag	UNP Q91VU0
B	26	LEU	-	expression tag	UNP Q91VU0
B	27	LEU	-	expression tag	UNP Q91VU0
B	28	LEU	-	expression tag	UNP Q91VU0
B	29	LEU	-	expression tag	UNP Q91VU0
B	30	PRO	-	expression tag	UNP Q91VU0
B	31	LEU	-	expression tag	UNP Q91VU0
B	32	LEU	-	expression tag	UNP Q91VU0
B	33	TRP	-	expression tag	UNP Q91VU0
B	34	ALA	-	expression tag	UNP Q91VU0
B	35	GLY	-	expression tag	UNP Q91VU0
B	36	ALA	-	expression tag	UNP Q91VU0
B	37	LEU	-	expression tag	UNP Q91VU0
B	38	ALA	-	expression tag	UNP Q91VU0
B	39	GLU	-	expression tag	UNP Q91VU0
B	40	LEU	-	expression tag	UNP Q91VU0
B	41	HIS	-	expression tag	UNP Q91VU0
B	42	HIS	-	expression tag	UNP Q91VU0
B	43	HIS	-	expression tag	UNP Q91VU0
B	44	HIS	-	expression tag	UNP Q91VU0
B	45	HIS	-	expression tag	UNP Q91VU0
B	46	HIS	-	expression tag	UNP Q91VU0
B	47	GLU	-	expression tag	UNP Q91VU0
B	48	ASN	-	expression tag	UNP Q91VU0
B	49	LEU	-	expression tag	UNP Q91VU0
B	50	TYR	-	expression tag	UNP Q91VU0
B	51	PHE	-	expression tag	UNP Q91VU0
B	52	GLN	-	expression tag	UNP Q91VU0
B	53	SER	-	expression tag	UNP Q91VU0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	54	GLY	-	expression tag	UNP Q91VU0
C	23	MET	-	initiating methionine	UNP Q91VU0
C	24	PRO	-	expression tag	UNP Q91VU0
C	25	LEU	-	expression tag	UNP Q91VU0
C	26	LEU	-	expression tag	UNP Q91VU0
C	27	LEU	-	expression tag	UNP Q91VU0
C	28	LEU	-	expression tag	UNP Q91VU0
C	29	LEU	-	expression tag	UNP Q91VU0
C	30	PRO	-	expression tag	UNP Q91VU0
C	31	LEU	-	expression tag	UNP Q91VU0
C	32	LEU	-	expression tag	UNP Q91VU0
C	33	TRP	-	expression tag	UNP Q91VU0
C	34	ALA	-	expression tag	UNP Q91VU0
C	35	GLY	-	expression tag	UNP Q91VU0
C	36	ALA	-	expression tag	UNP Q91VU0
C	37	LEU	-	expression tag	UNP Q91VU0
C	38	ALA	-	expression tag	UNP Q91VU0
C	39	GLU	-	expression tag	UNP Q91VU0
C	40	LEU	-	expression tag	UNP Q91VU0
C	41	HIS	-	expression tag	UNP Q91VU0
C	42	HIS	-	expression tag	UNP Q91VU0
C	43	HIS	-	expression tag	UNP Q91VU0
C	44	HIS	-	expression tag	UNP Q91VU0
C	45	HIS	-	expression tag	UNP Q91VU0
C	46	HIS	-	expression tag	UNP Q91VU0
C	47	GLU	-	expression tag	UNP Q91VU0
C	48	ASN	-	expression tag	UNP Q91VU0
C	49	LEU	-	expression tag	UNP Q91VU0
C	50	TYR	-	expression tag	UNP Q91VU0
C	51	PHE	-	expression tag	UNP Q91VU0
C	52	GLN	-	expression tag	UNP Q91VU0
C	53	SER	-	expression tag	UNP Q91VU0
C	54	GLY	-	expression tag	UNP Q91VU0
D	23	MET	-	initiating methionine	UNP Q91VU0
D	24	PRO	-	expression tag	UNP Q91VU0
D	25	LEU	-	expression tag	UNP Q91VU0
D	26	LEU	-	expression tag	UNP Q91VU0
D	27	LEU	-	expression tag	UNP Q91VU0
D	28	LEU	-	expression tag	UNP Q91VU0
D	29	LEU	-	expression tag	UNP Q91VU0
D	30	PRO	-	expression tag	UNP Q91VU0
D	31	LEU	-	expression tag	UNP Q91VU0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	32	LEU	-	expression tag	UNP Q91VU0
D	33	TRP	-	expression tag	UNP Q91VU0
D	34	ALA	-	expression tag	UNP Q91VU0
D	35	GLY	-	expression tag	UNP Q91VU0
D	36	ALA	-	expression tag	UNP Q91VU0
D	37	LEU	-	expression tag	UNP Q91VU0
D	38	ALA	-	expression tag	UNP Q91VU0
D	39	GLU	-	expression tag	UNP Q91VU0
D	40	LEU	-	expression tag	UNP Q91VU0
D	41	HIS	-	expression tag	UNP Q91VU0
D	42	HIS	-	expression tag	UNP Q91VU0
D	43	HIS	-	expression tag	UNP Q91VU0
D	44	HIS	-	expression tag	UNP Q91VU0
D	45	HIS	-	expression tag	UNP Q91VU0
D	46	HIS	-	expression tag	UNP Q91VU0
D	47	GLU	-	expression tag	UNP Q91VU0
D	48	ASN	-	expression tag	UNP Q91VU0
D	49	LEU	-	expression tag	UNP Q91VU0
D	50	TYR	-	expression tag	UNP Q91VU0
D	51	PHE	-	expression tag	UNP Q91VU0
D	52	GLN	-	expression tag	UNP Q91VU0
D	53	SER	-	expression tag	UNP Q91VU0
D	54	GLY	-	expression tag	UNP Q91VU0

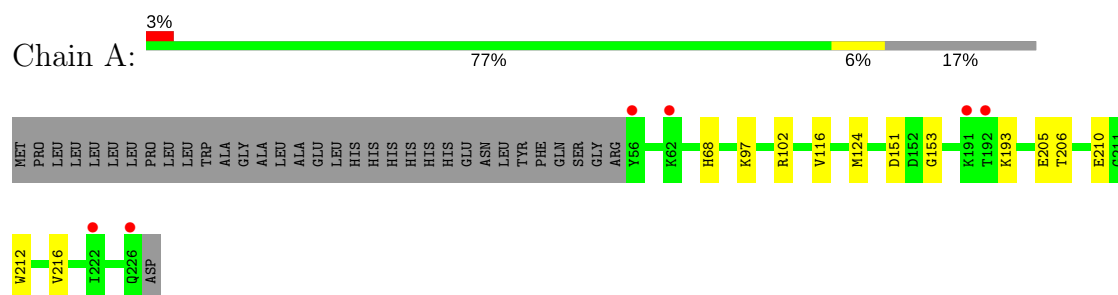
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	B	103	Total O 103 103	0	0
2	C	98	Total O 98 98	0	0
2	D	109	Total O 109 109	0	0

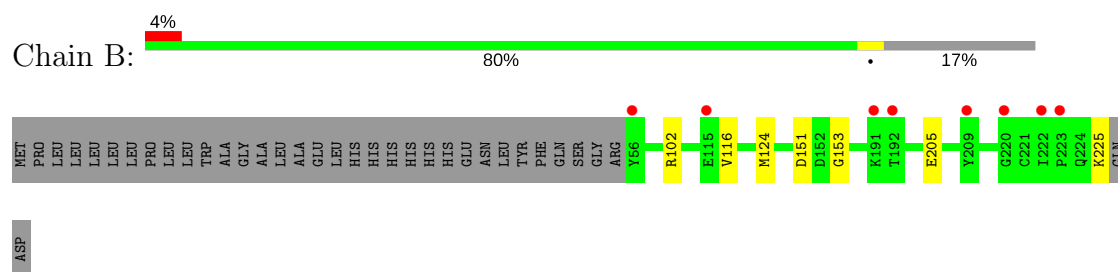
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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.

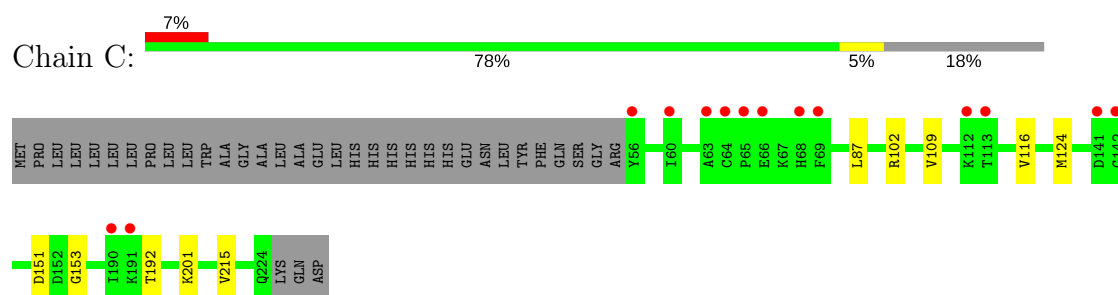
• Molecule 1: Protein FAM3C



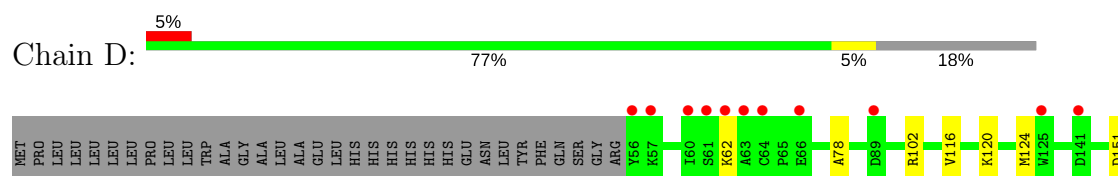
• Molecule 1: Protein FAM3C



• Molecule 1: Protein FAM3C



• Molecule 1: Protein FAM3C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.75Å 118.45Å 85.42Å 90.00° 98.78° 90.00°	Depositor
Resolution (Å)	48.48 – 1.84 42.21 – 1.84	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.48-1.84) 98.1 (42.21-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.212 , 0.230 0.227 , 0.246	Depositor DCC
R_{free} test set	3465 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5636	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.38	0/1336	0.59	0/1799
1	B	0.42	0/1327	0.60	0/1787
1	C	0.38	0/1318	0.61	0/1776
1	D	0.41	0/1334	0.58	0/1799
All	All	0.40	0/5315	0.60	0/7161

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1311	0	1306	6	0
1	B	1302	0	1298	2	0
1	C	1293	0	1285	3	0
1	D	1307	0	1294	5	0
2	A	113	0	0	0	0
2	B	103	0	0	0	0
2	C	98	0	0	0	0
2	D	109	0	0	0	0
All	All	5636	0	5183	13	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 1.

All (13) 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:102:ARG:HG3	1:B:151:ASP:HB3	1.98	0.46
1:A:124:MET:HB2	1:A:153:GLY:HA2	1.98	0.46
1:C:102:ARG:HG3	1:C:151:ASP:HB3	1.98	0.46
1:D:102:ARG:HG3	1:D:151:ASP:HB3	1.98	0.46
1:C:124:MET:HB2	1:C:153:GLY:HA2	1.98	0.45
1:A:102:ARG:HG3	1:A:151:ASP:HB3	1.98	0.45
1:D:124:MET:HB2	1:D:153:GLY:HA2	1.99	0.45
1:A:205:GLU:HG3	1:A:206:THR:HG23	1.98	0.45
1:B:124:MET:HB2	1:B:153:GLY:HA2	1.99	0.45
1:A:216:VAL:HG13	1:D:183:VAL:HG22	2.00	0.44
1:C:87:LEU:HD13	1:C:109:VAL:HG21	2.00	0.43
1:A:212:TRP:CG	1:D:78:ALA:HA	2.55	0.41
1:A:68:HIS:HB3	1:D:221:CYS:HB3	2.02	0.41

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	169/205 (82%)	164 (97%)	5 (3%)	0	100	100
1	B	168/205 (82%)	165 (98%)	3 (2%)	0	100	100
1	C	167/205 (82%)	162 (97%)	5 (3%)	0	100	100
1	D	168/205 (82%)	164 (98%)	4 (2%)	0	100	100
All	All	672/820 (82%)	655 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	141/170 (83%)	137 (97%)	4 (3%)	47	28
1	B	140/170 (82%)	137 (98%)	3 (2%)	56	41
1	C	139/170 (82%)	135 (97%)	4 (3%)	45	27
1	D	140/170 (82%)	136 (97%)	4 (3%)	45	27
All	All	560/680 (82%)	545 (97%)	15 (3%)	48	30

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	116	VAL
1	A	193	LYS
1	A	210	GLU
1	B	116	VAL
1	B	205	GLU
1	B	225	LYS
1	C	116	VAL
1	C	192	THR
1	C	201	LYS
1	C	215	VAL
1	D	62	LYS
1	D	116	VAL
1	D	120	LYS
1	D	190	ILE

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

Mol	Chain	Res	Type
1	A	203	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 [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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	171/205 (83%)	0.42	6 (3%)	44 40	22, 33, 56, 91	0
1	B	170/205 (82%)	0.49	8 (4%)	31 29	24, 36, 61, 92	0
1	C	169/205 (82%)	0.63	14 (8%)	11 10	24, 38, 63, 81	0
1	D	169/205 (82%)	0.48	11 (6%)	19 16	22, 35, 58, 79	0
All	All	679/820 (82%)	0.51	39 (5%)	24 22	22, 36, 61, 92	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	TYR	5.3
1	D	56	TYR	5.0
1	B	192	THR	4.8
1	D	64	CYS	3.9
1	C	66	GLU	3.8
1	A	56	TYR	3.6
1	D	62	LYS	3.4
1	C	65	PRO	3.3
1	B	56	TYR	3.0
1	A	191	LYS	2.8
1	B	191	LYS	2.7
1	B	223	PRO	2.7
1	C	60	ILE	2.6
1	D	60	ILE	2.6
1	C	141	ASP	2.6
1	C	64	CYS	2.6
1	D	125[A]	TRP	2.6
1	D	63	ALA	2.5
1	A	222	ILE	2.4
1	C	191	LYS	2.3
1	A	192	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	57	LYS	2.3
1	C	112	LYS	2.3
1	C	142	GLY	2.3
1	C	113	THR	2.3
1	D	141	ASP	2.3
1	B	220	GLY	2.2
1	D	66	GLU	2.2
1	C	63	ALA	2.2
1	B	222	ILE	2.2
1	A	226	GLN	2.2
1	D	89	ASP	2.1
1	D	61	SER	2.1
1	B	115	GLU	2.1
1	C	69	PHE	2.1
1	B	209	TYR	2.0
1	C	190	ILE	2.0
1	A	62	LYS	2.0
1	C	68	HIS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.