wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:16 PM GMT

PDB ID	:	1JH5
Title	:	Crystal Structure of sTALL-1 of TNF family ligand
Authors	:	Liu, Y.; Xu, L.; Opalka, N.; Shu, H.-B.; Zhang, G.
Deposited on	:	2001-06-27
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

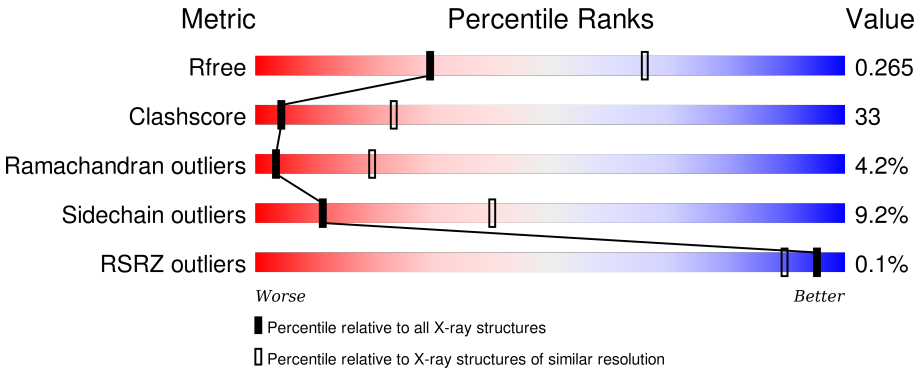
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=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	144	46% 46% 8%
1	B	144	% 49% 42% 8%
1	C	144	48% 42% 9%
1	D	144	44% 48% 8%
1	E	144	47% 44% 8%

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Mol	Chain	Length	Quality of chain
1	F	144	
1	G	144	
1	H	144	
1	I	144	
1	J	144	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11430 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 TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B.

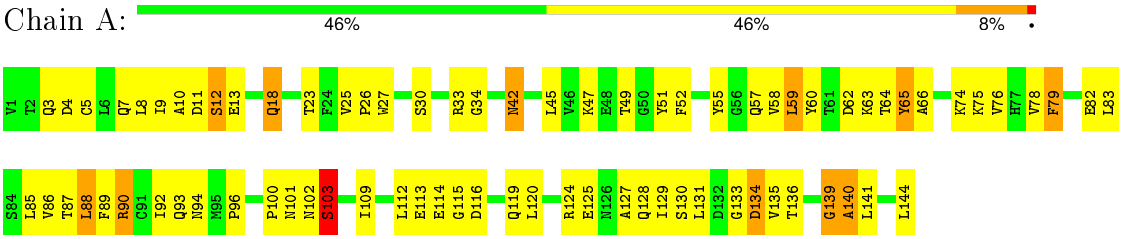
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	B	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	C	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	D	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	E	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	F	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	G	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	H	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	I	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	J	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			

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 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.

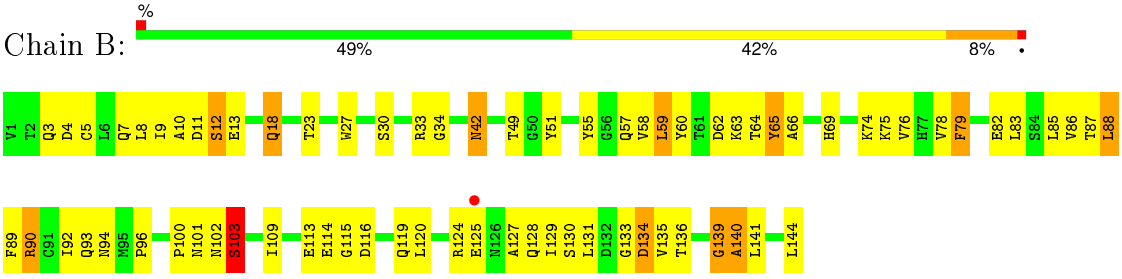
- Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain A:



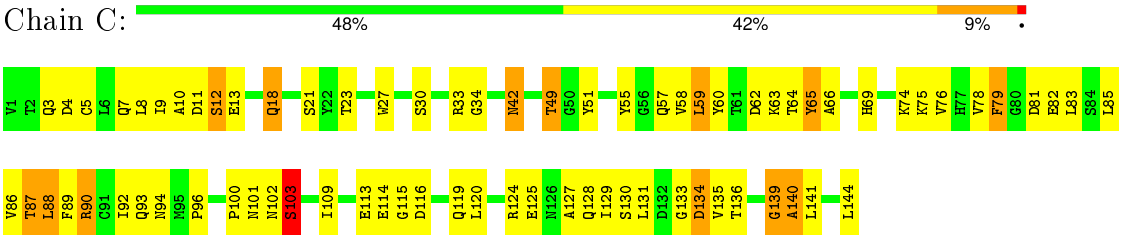
- Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain B:



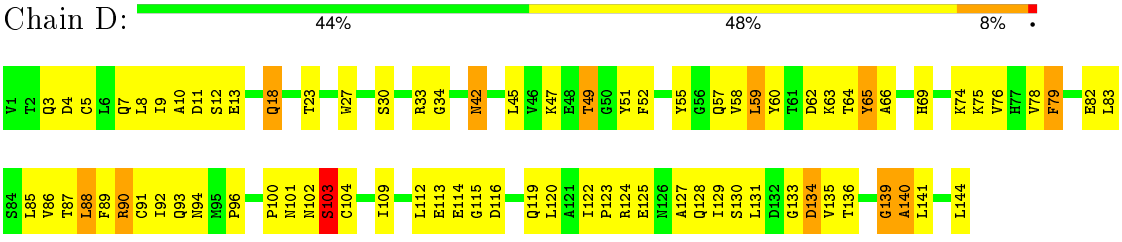
- Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain C:



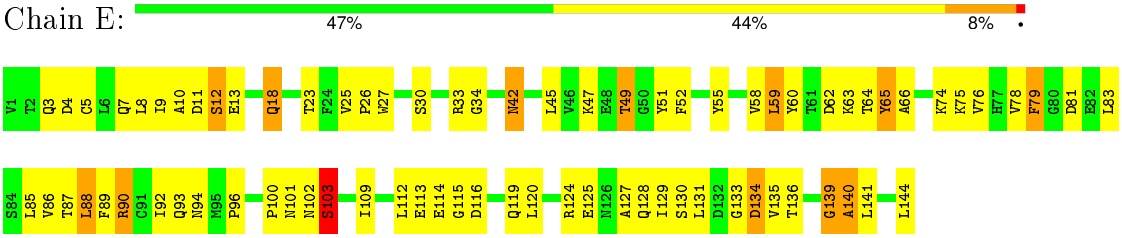
- Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain D:



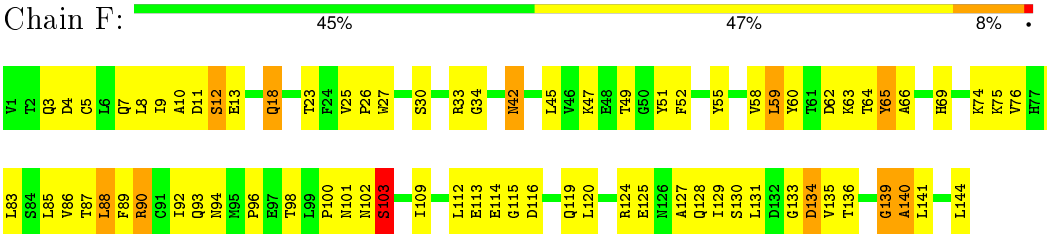
• Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain E:



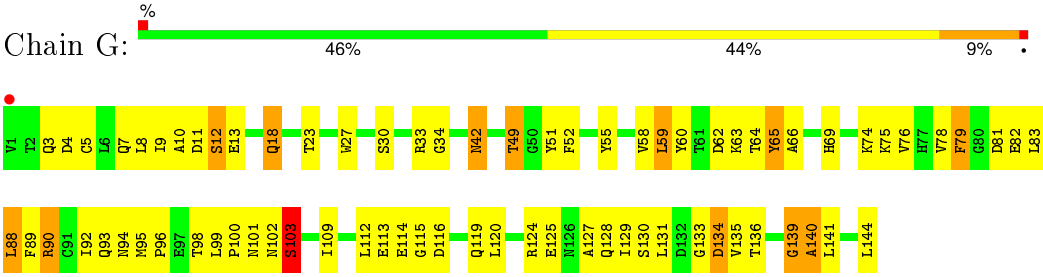
• Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain F:



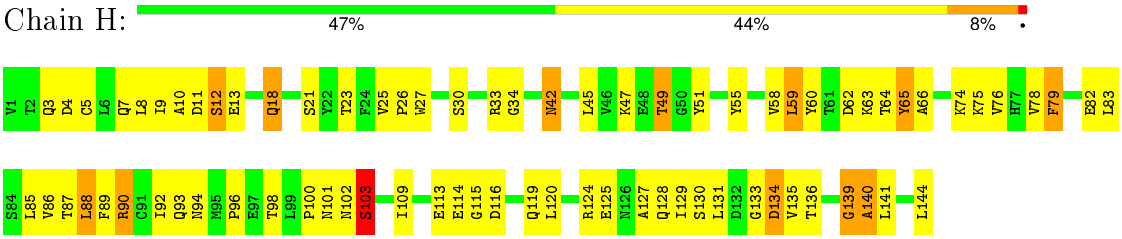
• Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain G:



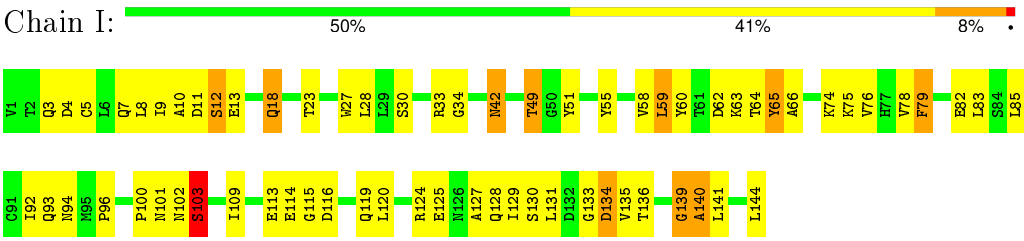
• Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain H:



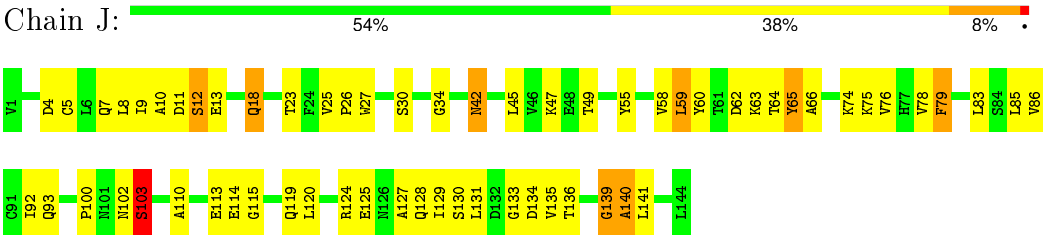
• Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain I:



• Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

Chain J:


54%
38%
8%
V1
D4
C5
L6
Q7
I8
I9
A10
D11
S12
E13
Q18
T23
F24
V25
P26
W27
S30
G34
N42
L45
V46
K47
E48
T49
Y55
V58
L59
Y60
T61
D62
K63
T64
Y65
A66
K74
K75
V76
H77
V78
F79
L83
S84
L85
V86
T87
L88
F89
R90
C91
I92
Q93
P100
N101
N102
S103
A110
E113
E114
G115
Q119
L120
R124
E125
N126
A127
Q128
I129
S130
L131
D132
G133
D134
V135
T136
G139
A140
L141
L144

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	234.24Å 234.24Å 212.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.00 37.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	79.3 (19.99-3.00) 88.3 (37.90-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.236 , 0.252 0.251 , 0.265	Depositor DCC
R_{free} test set	3064 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 22.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 60885 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	11430	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.46	0/1165	0.75	1/1574 (0.1%)
1	B	0.46	0/1165	0.75	1/1574 (0.1%)
1	C	0.46	0/1165	0.75	1/1574 (0.1%)
1	D	0.47	0/1165	0.75	1/1574 (0.1%)
1	E	0.46	0/1165	0.75	1/1574 (0.1%)
1	F	0.47	0/1165	0.75	1/1574 (0.1%)
1	G	0.48	0/1165	0.75	1/1574 (0.1%)
1	H	0.47	0/1165	0.75	1/1574 (0.1%)
1	I	0.47	0/1165	0.75	1/1574 (0.1%)
1	J	0.46	0/1165	0.76	1/1574 (0.1%)
All	All	0.47	0/11650	0.75	10/15740 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	139	GLY	N-CA-C	6.15	128.48	113.10
1	J	139	GLY	N-CA-C	6.13	128.42	113.10
1	E	139	GLY	N-CA-C	6.11	128.38	113.10
1	H	139	GLY	N-CA-C	6.09	128.32	113.10
1	C	139	GLY	N-CA-C	5.97	128.04	113.10

There are no chirality outliers.

There are no planarity outliers.

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	1143	0	1150	92	0
1	B	1143	0	1150	92	0
1	C	1143	0	1150	91	0
1	D	1143	0	1150	91	0
1	E	1143	0	1150	92	0
1	F	1143	0	1150	91	0
1	G	1143	0	1150	94	0
1	H	1143	0	1150	91	0
1	I	1143	0	1150	90	0
1	J	1143	0	1150	61	0
All	All	11430	0	11500	753	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 33.

The worst 5 of 753 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:C:49:THR:HG22	1:C:114:GLU:H	1.16	1.11
1:B:49:THR:HG22	1:B:114:GLU:H	1.17	1.10
1:J:49:THR:HG22	1:J:114:GLU:H	1.16	1.06
1:F:49:THR:HG22	1:F:114:GLU:H	1.16	1.05
1:D:49:THR:HG22	1:D:114:GLU:H	1.17	1.05

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	142/144 (99%)	125 (88%)	11 (8%)	6 (4%)	3 20
1	B	142/144 (99%)	127 (89%)	9 (6%)	6 (4%)	3 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	142/144 (99%)	124 (87%)	12 (8%)	6 (4%)	3 20
1	D	142/144 (99%)	126 (89%)	10 (7%)	6 (4%)	3 20
1	E	142/144 (99%)	127 (89%)	9 (6%)	6 (4%)	3 20
1	F	142/144 (99%)	125 (88%)	11 (8%)	6 (4%)	3 20
1	G	142/144 (99%)	125 (88%)	11 (8%)	6 (4%)	3 20
1	H	142/144 (99%)	126 (89%)	10 (7%)	6 (4%)	3 20
1	I	142/144 (99%)	125 (88%)	11 (8%)	6 (4%)	3 20
1	J	142/144 (99%)	125 (88%)	11 (8%)	6 (4%)	3 20
All	All	1420/1440 (99%)	1255 (88%)	105 (7%)	60 (4%)	3 20

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	TYR
1	B	65	TYR
1	C	65	TYR
1	D	65	TYR
1	E	65	TYR

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	126/126 (100%)	115 (91%)	11 (9%)	13 43
1	B	126/126 (100%)	115 (91%)	11 (9%)	13 43
1	C	126/126 (100%)	114 (90%)	12 (10%)	11 38
1	D	126/126 (100%)	114 (90%)	12 (10%)	11 38
1	E	126/126 (100%)	114 (90%)	12 (10%)	11 38
1	F	126/126 (100%)	115 (91%)	11 (9%)	13 43
1	G	126/126 (100%)	114 (90%)	12 (10%)	11 38
1	H	126/126 (100%)	114 (90%)	12 (10%)	11 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	126/126 (100%)	114 (90%)	12 (10%)	11 38
1	J	126/126 (100%)	115 (91%)	11 (9%)	13 43
All	All	1260/1260 (100%)	1144 (91%)	116 (9%)	11 40

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	65	TYR
1	F	87	THR
1	J	18	GLN
1	E	88	LEU
1	F	5	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	18	GLN
1	F	42	ASN
1	I	126	ASN
1	E	42	ASN
1	E	126	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, 95^{th} 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	144/144 (100%)	-0.29	0 100 100	26, 30, 33, 34	0
1	B	144/144 (100%)	-0.31	1 (0%) 89 70	27, 31, 33, 35	0
1	C	144/144 (100%)	-0.30	0 100 100	27, 30, 33, 34	0
1	D	144/144 (100%)	-0.39	0 100 100	27, 31, 33, 34	0
1	E	144/144 (100%)	-0.45	0 100 100	27, 30, 33, 34	0
1	F	144/144 (100%)	-0.37	0 100 100	27, 31, 32, 33	0
1	G	144/144 (100%)	-0.34	1 (0%) 89 70	26, 31, 33, 34	0
1	H	144/144 (100%)	-0.33	0 100 100	27, 31, 33, 34	0
1	I	144/144 (100%)	-0.38	0 100 100	26, 31, 33, 35	0
1	J	144/144 (100%)	-0.36	0 100 100	27, 31, 33, 35	0
All	All	1440/1440 (100%)	-0.35	2 (0%) 95 90	26, 31, 33, 35	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1	VAL	2.3
1	B	125	GLU	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.