Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 04:34 PM EST

PDB ID	:	4P4H
Title	:	Caught-in-action signaling complex of RIG-I 2CARD domain and MAVS CARD domain
Authors	:	Wu, B.; Hur, S.
Deposited on	:	2014-03-12
Resolution	:	3.40 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:

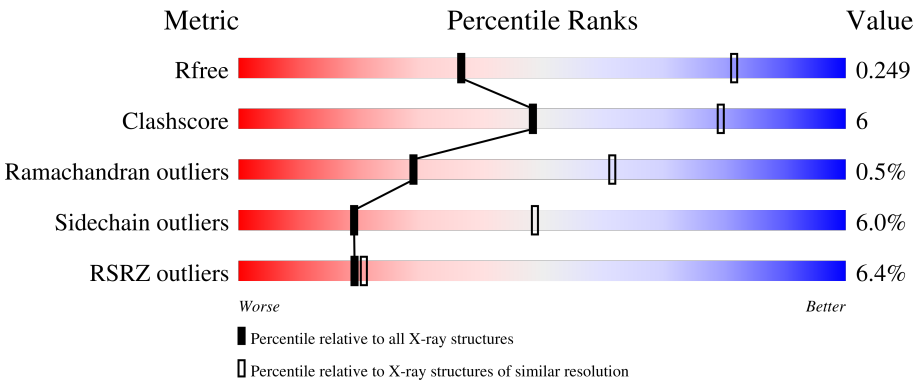
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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% 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	2% 76% 14% • 8%
1	B	205	2% 74% 16% • 8%
1	C	205	2% 69% 20% • 8%
1	D	205	3% 67% 22% • 8%
1	E	205	2% 75% 13% • 8%

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Mol	Chain	Length	Quality of chain
1	F	205	72% 18% • 8%
1	G	205	3% 74% 15% • 8%
1	H	205	4% 70% 19% • 8%
2	I	108	% 81% 8% • 10%
2	J	108	% 82% 7% 10%
2	K	108	% 72% 15% • 10%
2	L	108	2% 80% 8% • 10%
2	M	108	9% 74% 13% • • 10%
2	N	108	7% 82% 7% 10%
2	O	108	13% 78% 10% • 10%
2	P	108	11% 77% 11% • 10%
3	S	79	15% 77% 13% 10%
3	T	79	19% 81% 10% • 8%
3	U	79	24% 81% 10% 9%
3	W	79	28% 82% 8% 10%
3	X	79	15% 80% 11% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 43332 atoms, of which 21621 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	188	3112	1007	1550	255	291	9	0	0	0
1	B	189	3127	1012	1556	256	294	9	0	0	0
1	C	189	3127	1012	1556	256	294	9	0	0	0
1	D	188	3112	1007	1550	255	291	9	0	0	0
1	E	188	3073	1000	1524	250	290	9	0	0	0
1	F	189	3085	1004	1530	250	292	9	0	0	0
1	G	189	3111	1008	1548	256	290	9	0	0	0
1	H	188	3112	1007	1550	255	291	9	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O95786
A	-2	PRO	-	expression tag	UNP O95786
A	-1	GLY	-	expression tag	UNP O95786
A	0	ALA	-	expression tag	UNP O95786
A	52	ALA	GLU	engineered mutation	UNP O95786
B	-3	GLY	-	expression tag	UNP O95786
B	-2	PRO	-	expression tag	UNP O95786
B	-1	GLY	-	expression tag	UNP O95786
B	0	ALA	-	expression tag	UNP O95786
B	52	ALA	GLU	engineered mutation	UNP O95786
C	-3	GLY	-	expression tag	UNP O95786
C	-2	PRO	-	expression tag	UNP O95786
C	-1	GLY	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP O95786
C	52	ALA	GLU	engineered mutation	UNP O95786
D	-3	GLY	-	expression tag	UNP O95786
D	-2	PRO	-	expression tag	UNP O95786
D	-1	GLY	-	expression tag	UNP O95786
D	0	ALA	-	expression tag	UNP O95786
D	52	ALA	GLU	engineered mutation	UNP O95786
E	-3	GLY	-	expression tag	UNP O95786
E	-2	PRO	-	expression tag	UNP O95786
E	-1	GLY	-	expression tag	UNP O95786
E	0	ALA	-	expression tag	UNP O95786
E	52	ALA	GLU	engineered mutation	UNP O95786
F	-3	GLY	-	expression tag	UNP O95786
F	-2	PRO	-	expression tag	UNP O95786
F	-1	GLY	-	expression tag	UNP O95786
F	0	ALA	-	expression tag	UNP O95786
F	52	ALA	GLU	engineered mutation	UNP O95786
G	-3	GLY	-	expression tag	UNP O95786
G	-2	PRO	-	expression tag	UNP O95786
G	-1	GLY	-	expression tag	UNP O95786
G	0	ALA	-	expression tag	UNP O95786
G	52	ALA	GLU	engineered mutation	UNP O95786
H	-3	GLY	-	expression tag	UNP O95786
H	-2	PRO	-	expression tag	UNP O95786
H	-1	GLY	-	expression tag	UNP O95786
H	0	ALA	-	expression tag	UNP O95786
H	52	ALA	GLU	engineered mutation	UNP O95786

- Molecule 2 is a protein called Mitochondrial antiviral-signaling protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	I	97	1586	511	790	139	140	6	0	0	0
2	J	97	1586	511	790	139	140	6	0	0	0
2	K	97	1586	511	790	139	140	6	0	0	0
2	L	97	1586	511	790	139	140	6	0	0	0
2	N	97	1586	511	790	139	140	6	0	0	0
2	O	97	1586	511	790	139	140	6	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	P	97	1586	511	790	139	140	6	0	0	0
2	M	97	1581	511	785	139	140	6	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLY	-	expression tag	UNP Q7Z434
I	-7	SER	-	expression tag	UNP Q7Z434
I	-6	GLY	-	expression tag	UNP Q7Z434
I	-5	THR	-	expression tag	UNP Q7Z434
I	-4	GLY	-	expression tag	UNP Q7Z434
I	-3	SER	-	expression tag	UNP Q7Z434
I	-2	THR	-	expression tag	UNP Q7Z434
I	-1	GLY	-	expression tag	UNP Q7Z434
I	0	SER	-	expression tag	UNP Q7Z434
I	23	LYS	ASP	engineered mutation	UNP Q7Z434
I	26	LYS	GLU	engineered mutation	UNP Q7Z434
I	80	LYS	GLU	engineered mutation	UNP Q7Z434
J	-8	GLY	-	expression tag	UNP Q7Z434
J	-7	SER	-	expression tag	UNP Q7Z434
J	-6	GLY	-	expression tag	UNP Q7Z434
J	-5	THR	-	expression tag	UNP Q7Z434
J	-4	GLY	-	expression tag	UNP Q7Z434
J	-3	SER	-	expression tag	UNP Q7Z434
J	-2	THR	-	expression tag	UNP Q7Z434
J	-1	GLY	-	expression tag	UNP Q7Z434
J	0	SER	-	expression tag	UNP Q7Z434
J	23	LYS	ASP	engineered mutation	UNP Q7Z434
J	26	LYS	GLU	engineered mutation	UNP Q7Z434
J	80	LYS	GLU	engineered mutation	UNP Q7Z434
K	-8	GLY	-	expression tag	UNP Q7Z434
K	-7	SER	-	expression tag	UNP Q7Z434
K	-6	GLY	-	expression tag	UNP Q7Z434
K	-5	THR	-	expression tag	UNP Q7Z434
K	-4	GLY	-	expression tag	UNP Q7Z434
K	-3	SER	-	expression tag	UNP Q7Z434
K	-2	THR	-	expression tag	UNP Q7Z434
K	-1	GLY	-	expression tag	UNP Q7Z434
K	0	SER	-	expression tag	UNP Q7Z434
K	23	LYS	ASP	engineered mutation	UNP Q7Z434

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Chain	Residue	Modelled	Actual	Comment	Reference
K	26	LYS	GLU	engineered mutation	UNP Q7Z434
K	80	LYS	GLU	engineered mutation	UNP Q7Z434
L	-8	GLY	-	expression tag	UNP Q7Z434
L	-7	SER	-	expression tag	UNP Q7Z434
L	-6	GLY	-	expression tag	UNP Q7Z434
L	-5	THR	-	expression tag	UNP Q7Z434
L	-4	GLY	-	expression tag	UNP Q7Z434
L	-3	SER	-	expression tag	UNP Q7Z434
L	-2	THR	-	expression tag	UNP Q7Z434
L	-1	GLY	-	expression tag	UNP Q7Z434
L	0	SER	-	expression tag	UNP Q7Z434
L	23	LYS	ASP	engineered mutation	UNP Q7Z434
L	26	LYS	GLU	engineered mutation	UNP Q7Z434
L	80	LYS	GLU	engineered mutation	UNP Q7Z434
N	-8	GLY	-	expression tag	UNP Q7Z434
N	-7	SER	-	expression tag	UNP Q7Z434
N	-6	GLY	-	expression tag	UNP Q7Z434
N	-5	THR	-	expression tag	UNP Q7Z434
N	-4	GLY	-	expression tag	UNP Q7Z434
N	-3	SER	-	expression tag	UNP Q7Z434
N	-2	THR	-	expression tag	UNP Q7Z434
N	-1	GLY	-	expression tag	UNP Q7Z434
N	0	SER	-	expression tag	UNP Q7Z434
N	23	LYS	ASP	engineered mutation	UNP Q7Z434
N	26	LYS	GLU	engineered mutation	UNP Q7Z434
N	80	LYS	GLU	engineered mutation	UNP Q7Z434
O	-8	GLY	-	expression tag	UNP Q7Z434
O	-7	SER	-	expression tag	UNP Q7Z434
O	-6	GLY	-	expression tag	UNP Q7Z434
O	-5	THR	-	expression tag	UNP Q7Z434
O	-4	GLY	-	expression tag	UNP Q7Z434
O	-3	SER	-	expression tag	UNP Q7Z434
O	-2	THR	-	expression tag	UNP Q7Z434
O	-1	GLY	-	expression tag	UNP Q7Z434
O	0	SER	-	expression tag	UNP Q7Z434
O	23	LYS	ASP	engineered mutation	UNP Q7Z434
O	26	LYS	GLU	engineered mutation	UNP Q7Z434
O	80	LYS	GLU	engineered mutation	UNP Q7Z434
P	-8	GLY	-	expression tag	UNP Q7Z434
P	-7	SER	-	expression tag	UNP Q7Z434
P	-6	GLY	-	expression tag	UNP Q7Z434
P	-5	THR	-	expression tag	UNP Q7Z434

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	GLY	-	expression tag	UNP Q7Z434
P	-3	SER	-	expression tag	UNP Q7Z434
P	-2	THR	-	expression tag	UNP Q7Z434
P	-1	GLY	-	expression tag	UNP Q7Z434
P	0	SER	-	expression tag	UNP Q7Z434
P	23	LYS	ASP	engineered mutation	UNP Q7Z434
P	26	LYS	GLU	engineered mutation	UNP Q7Z434
P	80	LYS	GLU	engineered mutation	UNP Q7Z434
M	-8	GLY	-	expression tag	UNP Q7Z434
M	-7	SER	-	expression tag	UNP Q7Z434
M	-6	GLY	-	expression tag	UNP Q7Z434
M	-5	THR	-	expression tag	UNP Q7Z434
M	-4	GLY	-	expression tag	UNP Q7Z434
M	-3	SER	-	expression tag	UNP Q7Z434
M	-2	THR	-	expression tag	UNP Q7Z434
M	-1	GLY	-	expression tag	UNP Q7Z434
M	0	SER	-	expression tag	UNP Q7Z434
M	23	LYS	ASP	engineered mutation	UNP Q7Z434
M	26	LYS	GLU	engineered mutation	UNP Q7Z434
M	80	LYS	GLU	engineered mutation	UNP Q7Z434

- Molecule 3 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	S	71	1146	356	583	94	112	1	0	0	0
3	T	73	1189	368	607	99	114	1	0	0	0
3	U	72	1140	356	574	96	113	1	0	0	0
3	W	71	1126	352	571	92	110	1	0	0	0
3	X	73	1189	368	607	99	114	1	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	GLY	-	expression tag	UNP P62987
S	-1	PRO	-	expression tag	UNP P62987
S	0	GLY	-	expression tag	UNP P62987
T	-2	GLY	-	expression tag	UNP P62987

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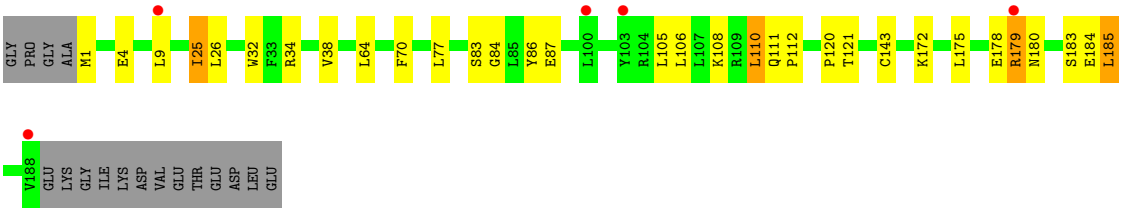
Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	PRO	-	expression tag	UNP P62987
T	0	GLY	-	expression tag	UNP P62987
U	-2	GLY	-	expression tag	UNP P62987
U	-1	PRO	-	expression tag	UNP P62987
U	0	GLY	-	expression tag	UNP P62987
W	-2	GLY	-	expression tag	UNP P62987
W	-1	PRO	-	expression tag	UNP P62987
W	0	GLY	-	expression tag	UNP P62987
X	-2	GLY	-	expression tag	UNP P62987
X	-1	PRO	-	expression tag	UNP P62987
X	0	GLY	-	expression tag	UNP P62987

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 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.

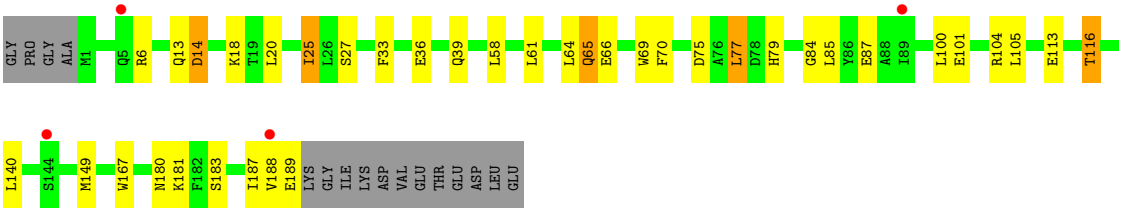
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain A:



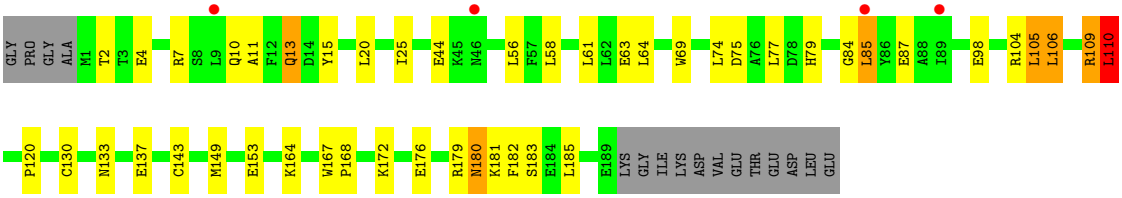
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain B:



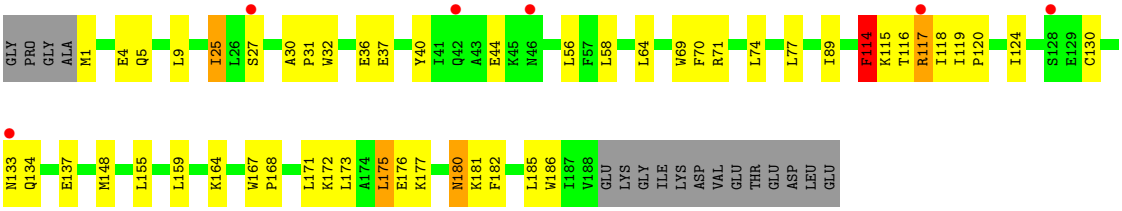
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain C:



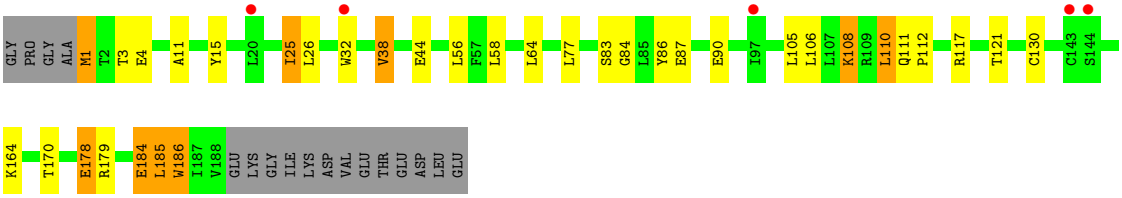
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain D:



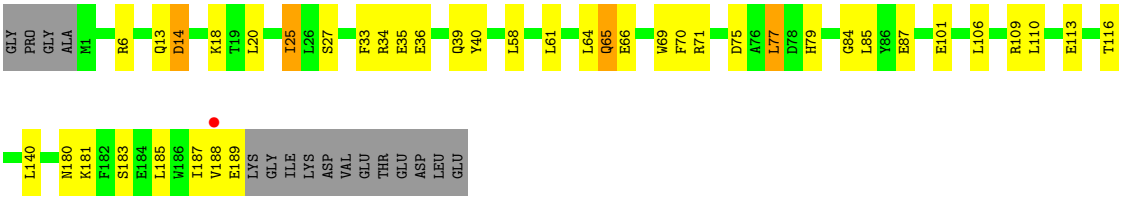
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain E:



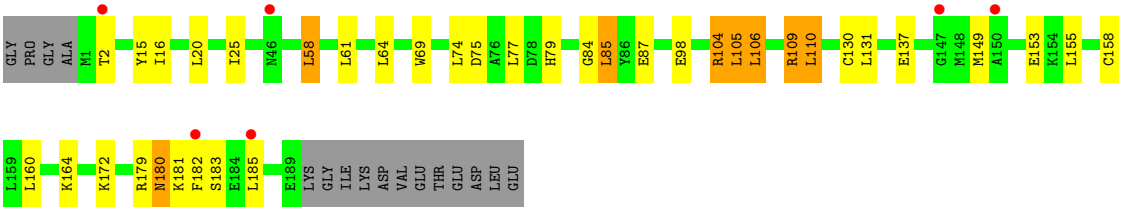
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain F:



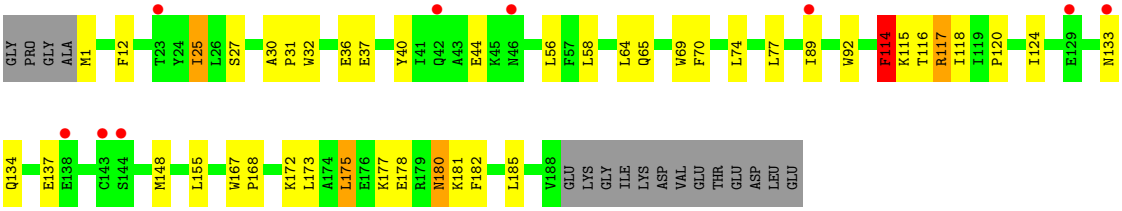
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain G:



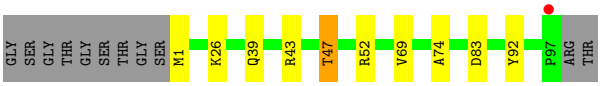
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain H:



• Molecule 2: Mitochondrial antiviral-signaling protein

Chain I:

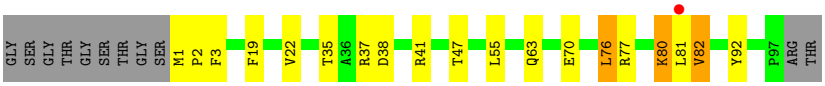


• Molecule 2: Mitochondrial antiviral-signaling protein

Chain J:

• Molecule 2: Mitochondrial antiviral-signaling protein

Chain K:



• Molecule 2: Mitochondrial antiviral-signaling protein

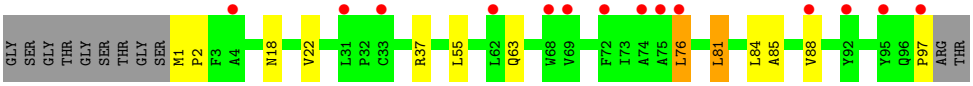
Chain L:

• Molecule 2: Mitochondrial antiviral-signaling protein

Chain N:

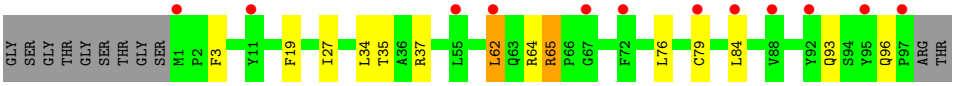
• Molecule 2: Mitochondrial antiviral-signaling protein

Chain O:



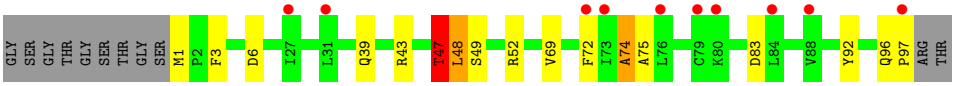
• Molecule 2: Mitochondrial antiviral-signaling protein

Chain P:



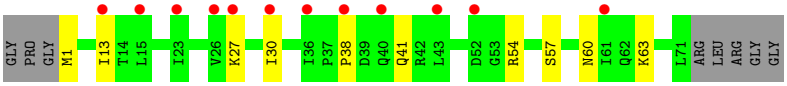
• Molecule 2: Mitochondrial antiviral-signaling protein

Chain M:



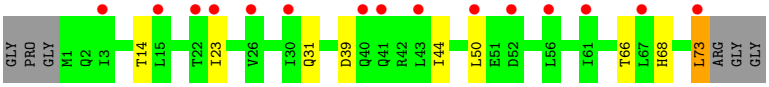
• Molecule 3: Ubiquitin-60S ribosomal protein L40

Chain S:



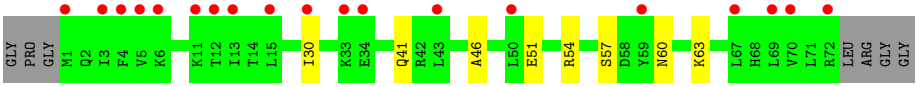
• Molecule 3: Ubiquitin-60S ribosomal protein L40

Chain T:



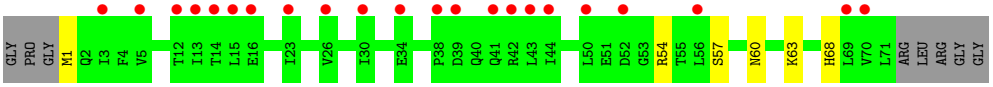
• Molecule 3: Ubiquitin-60S ribosomal protein L40

Chain U:



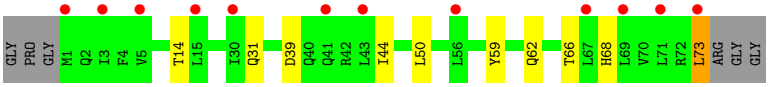
• Molecule 3: Ubiquitin-60S ribosomal protein L40

Chain W:



• Molecule 3: Ubiquitin-60S ribosomal protein L40

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.81Å 117.33Å 257.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 3.40 48.18 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.80-3.40) 99.2 (48.18-3.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.191 , 0.240 0.202 , 0.249	Depositor DCC
R_{free} test set	2361 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	104.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	43332	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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	0.59	0/1594	0.68	1/2146 (0.0%)
1	B	0.54	0/1603	0.64	0/2158
1	C	0.59	0/1603	0.70	1/2158 (0.0%)
1	D	0.69	0/1594	0.71	0/2146
1	E	0.52	0/1581	0.73	4/2131 (0.2%)
1	F	0.49	0/1587	0.60	0/2139
1	G	0.62	0/1595	0.68	0/2148
1	H	0.59	0/1594	0.67	0/2146
2	I	0.57	0/816	0.66	0/1108
2	J	0.60	1/816 (0.1%)	0.61	0/1108
2	K	0.62	0/816	0.66	0/1108
2	L	0.43	0/816	0.53	0/1108
2	M	0.42	0/816	0.71	3/1108 (0.3%)
2	N	0.41	0/816	0.57	0/1108
2	O	0.40	0/816	0.55	0/1108
2	P	0.36	0/816	0.53	0/1108
3	S	0.47	0/569	0.54	0/767
3	T	0.41	0/588	0.56	0/792
3	U	0.36	0/572	0.51	0/773
3	W	0.36	0/561	0.51	0/757
3	X	0.44	0/588	0.54	0/792
All	All	0.54	1/22157 (0.0%)	0.64	9/29917 (0.0%)

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	C	0	1
1	D	0	1
1	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	H	0	1
2	I	0	2
2	M	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	46	CYS	CB-SG	-5.95	1.72	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	184	GLU	C-N-CA	8.81	143.74	121.70
2	M	74	ALA	C-N-CA	7.34	140.06	121.70
1	A	172	LYS	CD-CE-NZ	6.93	127.64	111.70
1	E	184	GLU	CA-C-N	6.76	132.08	117.20
1	E	184	GLU	O-C-N	-6.55	112.21	122.70
2	M	74	ALA	CA-C-N	6.19	130.82	117.20
2	M	74	ALA	O-C-N	-5.84	113.36	122.70
1	C	110	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	E	185	LEU	CA-CB-CG	-5.15	103.47	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	GLU	Mainchain,Peptide
1	C	180	ASN	Mainchain
1	D	114	PHE	Mainchain
1	E	178	GLU	Mainchain
1	E	184	GLU	Mainchain
1	G	180	ASN	Mainchain
1	H	114	PHE	Mainchain
2	I	47	THR	Mainchain
2	I	74	ALA	Peptide
2	M	47	THR	Mainchain
2	M	74	ALA	Mainchain

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	1562	1550	1571	20	0
1	B	1571	1556	1577	26	0
1	C	1571	1556	1577	30	0
1	D	1562	1550	1571	27	0
1	E	1549	1524	1545	28	0
1	F	1555	1530	1551	26	0
1	G	1563	1548	1569	24	0
1	H	1562	1550	1571	23	0
2	I	796	790	793	4	0
2	J	796	790	793	5	0
2	K	796	790	793	13	0
2	L	796	790	793	5	0
2	M	796	785	793	12	0
2	N	796	790	793	5	0
2	O	796	790	793	7	0
2	P	796	790	793	7	0
3	S	563	583	586	10	0
3	T	582	607	610	5	0
3	U	566	574	577	9	0
3	W	555	571	574	4	0
3	X	582	607	610	6	0
All	All	21711	21621	21833	260	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 6.

All (260) 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:G:106:LEU:HD12	1:G:110:LEU:HD11	1.40	1.03
1:C:106:LEU:HD12	1:C:110:LEU:HD11	1.42	1.02
1:C:180:ASN:O	1:C:182:PHE:N	2.02	0.91
1:A:175:LEU:O	1:A:180:ASN:ND2	2.12	0.81
1:F:18:LYS:NZ	1:F:101:GLU:OE1	2.15	0.78
1:G:180:ASN:O	1:G:182:PHE:N	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:PHE:O	1:D:116:THR:N	2.17	0.77
1:B:18:LYS:NZ	1:B:101:GLU:OE1	2.19	0.76
1:D:117:ARG:O	1:D:117:ARG:NH1	2.20	0.75
3:S:30:ILE:HG21	3:S:41:GLN:NE2	2.05	0.72
1:F:25:ILE:HD11	1:F:77:LEU:HD12	1.72	0.72
1:H:117:ARG:O	1:H:117:ARG:NH1	2.23	0.71
1:A:180:ASN:OD1	1:A:183:SER:N	2.23	0.71
3:S:30:ILE:HG21	3:S:41:GLN:HE22	1.56	0.70
1:A:106:LEU:O	1:A:110:LEU:HD12	1.91	0.70
1:B:75:ASP:O	1:B:79:HIS:ND1	2.24	0.70
1:F:14:ASP:OD1	1:F:14:ASP:N	2.24	0.70
1:G:15:TYR:OH	1:G:98:GLU:OE1	2.09	0.69
1:F:20:LEU:HD11	1:F:25:ILE:HD12	1.74	0.69
1:F:25:ILE:HD11	1:F:77:LEU:CD1	2.23	0.69
1:B:25:ILE:HD11	1:B:77:LEU:CD1	2.21	0.69
3:U:30:ILE:HG21	3:U:41:GLN:NE2	2.08	0.68
1:A:26:LEU:HD13	1:A:38:VAL:HG13	1.75	0.68
2:M:47:THR:O	2:M:49:SER:N	2.25	0.68
2:J:53:ASP:OD1	2:K:41:ARG:NH1	2.26	0.68
2:I:39:GLN:OE1	2:I:43:ARG:NH1	2.25	0.68
1:F:75:ASP:O	1:F:79:HIS:ND1	2.25	0.66
2:M:39:GLN:OE1	2:M:43:ARG:NH1	2.29	0.65
1:G:106:LEU:CD1	1:G:110:LEU:HD11	2.24	0.64
1:E:117:ARG:NH2	2:M:6:ASP:OD1	2.31	0.64
1:B:14:ASP:N	1:B:14:ASP:OD1	2.28	0.63
1:E:106:LEU:O	1:E:110:LEU:HD12	1.99	0.62
1:G:61:LEU:HD12	1:G:64:LEU:HD12	1.80	0.62
1:D:133:ASN:OD1	1:D:134:GLN:N	2.33	0.62
3:U:30:ILE:CG2	3:U:41:GLN:HE22	2.14	0.61
1:C:61:LEU:HD12	1:C:64:LEU:HD12	1.82	0.60
1:F:61:LEU:HD12	1:F:64:LEU:HD12	1.82	0.60
1:A:110:LEU:HD23	1:A:185:LEU:HD12	1.84	0.59
2:O:84:LEU:O	2:O:88:VAL:HG13	2.03	0.59
1:B:116:THR:O	2:J:64:ARG:NH1	2.35	0.59
1:B:61:LEU:HD12	1:B:64:LEU:HD12	1.84	0.59
1:A:32:TRP:HZ2	3:T:66:THR:HG1	1.51	0.59
1:C:110:LEU:H	1:C:110:LEU:HD12	1.67	0.58
2:O:1:MET:HB3	2:O:2:PRO:HD3	1.84	0.58
1:C:7:ARG:NH2	1:E:15:TYR:OH	2.35	0.58
1:C:15:TYR:OH	1:C:98:GLU:OE1	2.12	0.58
3:U:30:ILE:HG21	3:U:41:GLN:HE22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LEU:HD23	1:E:185:LEU:HD23	1.86	0.57
3:U:51:GLU:OE1	2:M:3:PHE:HB2	2.05	0.57
2:L:21:ASN:OD1	2:L:81:LEU:HD21	2.05	0.56
2:P:19:PHE:HA	2:P:84:LEU:HD11	1.86	0.56
2:K:77:ARG:HH11	2:K:82:VAL:HG13	1.71	0.55
3:S:38:PRO:HA	3:S:41:GLN:HG2	1.89	0.55
1:B:20:LEU:HD11	1:B:25:ILE:HD12	1.89	0.54
1:A:25:ILE:HD11	1:A:77:LEU:HD12	1.89	0.54
3:U:54:ARG:HH21	2:M:3:PHE:HB3	1.73	0.54
1:G:84:GLY:HA2	1:G:87:GLU:HB3	1.91	0.53
1:H:114:PHE:O	1:H:116:THR:N	2.41	0.53
1:H:133:ASN:OD1	1:H:134:GLN:N	2.42	0.53
1:G:110:LEU:HD12	1:G:110:LEU:H	1.73	0.53
2:I:69:VAL:HG11	2:I:92:TYR:CG	2.45	0.52
1:G:137:GLU:OE2	2:N:64:ARG:NH2	2.43	0.52
1:C:11:ALA:HB2	1:E:11:ALA:HB2	1.92	0.52
1:H:25:ILE:HD11	1:H:77:LEU:HA	1.93	0.52
1:C:106:LEU:HD12	1:C:110:LEU:CD1	2.28	0.51
1:C:77:LEU:HD21	1:C:85:LEU:HD13	1.93	0.51
1:A:83:SER:HA	1:A:86:TYR:HB3	1.93	0.51
1:B:13:GLN:HG2	1:B:58:LEU:HD23	1.93	0.51
1:E:106:LEU:HG	1:E:110:LEU:CD1	2.41	0.51
1:A:106:LEU:HG	1:A:110:LEU:CD1	2.41	0.51
1:C:84:GLY:HA2	1:C:87:GLU:HB3	1.92	0.51
2:P:34:LEU:HD21	2:P:62:LEU:HD12	1.93	0.50
2:L:34:LEU:HD21	2:L:62:LEU:HD12	1.93	0.50
1:E:106:LEU:HD11	1:E:110:LEU:HD11	1.93	0.50
3:S:30:ILE:CG2	3:S:41:GLN:HE22	2.25	0.50
1:E:106:LEU:CD1	1:E:110:LEU:HD11	2.42	0.50
1:H:44:GLU:HG3	1:H:56:LEU:HD22	1.93	0.50
2:K:1:MET:HB3	2:K:2:PRO:HD3	1.93	0.49
1:G:2:THR:CG2	1:G:69:TRP:HE1	2.25	0.49
1:D:172:LYS:HA	1:D:175:LEU:HD11	1.95	0.49
2:O:22:VAL:HG12	2:O:81:LEU:HD11	1.95	0.49
1:C:106:LEU:HD11	1:C:110:LEU:HD21	1.94	0.49
1:B:149:MET:HB2	1:C:137:GLU:OE1	2.12	0.49
1:G:106:LEU:HD11	1:G:110:LEU:HD21	1.94	0.49
1:B:18:LYS:HE3	1:B:104:ARG:CD	2.43	0.48
1:H:120:PRO:HD2	1:H:148:MET:HG3	1.95	0.48
1:H:12:PHE:CE1	3:X:44:ILE:HD11	2.48	0.48
1:H:117:ARG:NH1	2:P:64:ARG:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:HG	1:E:110:LEU:HD13	1.96	0.48
1:B:36:GLU:O	1:B:39:GLN:N	2.46	0.48
1:B:149:MET:SD	1:C:133:ASN:ND2	2.87	0.47
2:M:47:THR:HG22	2:M:48:LEU:H	1.79	0.47
2:M:69:VAL:HG11	2:M:92:TYR:CG	2.49	0.47
1:A:84:GLY:HA2	1:A:87:GLU:HB2	1.96	0.47
1:D:74:LEU:HD21	1:D:89:ILE:HG13	1.96	0.47
1:F:188:VAL:HG13	1:F:189:GLU:HG3	1.95	0.47
1:G:20:LEU:HD11	1:G:25:ILE:HD12	1.96	0.47
1:G:131:LEU:HD22	1:G:158:CYS:HB3	1.97	0.47
1:H:92:TRP:HE1	3:X:73:LEU:HD22	1.79	0.47
1:A:106:LEU:CD1	1:A:110:LEU:HD11	2.45	0.47
1:C:25:ILE:HD11	1:C:77:LEU:CD1	2.45	0.47
1:E:83:SER:HA	1:E:86:TYR:HB3	1.96	0.47
1:H:74:LEU:HD21	1:H:89:ILE:HG13	1.95	0.47
2:N:5:GLU:HB2	2:N:69:VAL:HG23	1.97	0.47
1:G:25:ILE:HD11	1:G:77:LEU:CD1	2.45	0.47
3:W:1:MET:HB2	3:W:63:LYS:CG	2.45	0.47
1:D:44:GLU:HG3	1:D:56:LEU:HD22	1.95	0.46
1:E:25:ILE:HD11	1:E:77:LEU:HD12	1.97	0.46
1:G:130:CYS:HA	1:G:164:LYS:HG3	1.96	0.46
1:D:180:ASN:O	1:D:181:LYS:CB	2.64	0.46
1:C:130:CYS:HA	1:C:164:LYS:HG3	1.98	0.46
1:E:178:GLU:O	1:E:179:ARG:C	2.53	0.46
1:F:79:HIS:CD2	3:U:46:ALA:CB	2.98	0.46
1:A:178:GLU:O	1:A:179:ARG:C	2.53	0.46
1:C:120:PRO:HG2	1:C:143:CYS:SG	2.55	0.46
1:E:186:TRP:HA	1:E:186:TRP:CE3	2.49	0.46
1:B:18:LYS:HE3	1:B:104:ARG:HD2	1.96	0.46
1:C:149:MET:HB2	1:D:137:GLU:OE1	2.15	0.46
1:D:4:GLU:HG3	3:T:73:LEU:HD21	1.97	0.46
1:H:172:LYS:HA	1:H:175:LEU:HD11	1.98	0.46
2:N:5:GLU:HB2	2:N:69:VAL:CG2	2.46	0.46
1:A:120:PRO:HG2	1:A:143:CYS:SG	2.56	0.46
1:B:84:GLY:HA2	1:B:87:GLU:HB3	1.97	0.46
2:J:2:PRO:HA	2:J:5:GLU:HG2	1.98	0.46
1:F:36:GLU:O	1:F:39:GLN:N	2.49	0.45
1:D:117:ARG:NH1	2:L:64:ARG:HD2	2.31	0.45
1:E:44:GLU:HG3	1:E:56:LEU:HD22	1.97	0.45
1:E:117:ARG:NH2	2:M:6:ASP:OD2	2.50	0.45
3:W:1:MET:HB2	3:W:63:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD12	1:B:64:LEU:CD1	2.46	0.45
1:E:110:LEU:CD2	1:E:185:LEU:HD23	2.46	0.45
1:G:75:ASP:O	1:G:79:HIS:ND1	2.41	0.45
1:D:120:PRO:HD2	1:D:148:MET:HG3	1.99	0.45
3:U:54:ARG:HH12	2:M:97:PRO:HD3	1.80	0.45
1:B:180:ASN:OD1	1:B:183:SER:HB2	2.17	0.45
1:E:106:LEU:CD1	1:E:110:LEU:CD1	2.95	0.45
1:G:16:ILE:HG21	1:G:58:LEU:HD21	1.98	0.45
1:G:105:LEU:HD12	1:G:109:ARG:NH2	2.31	0.45
1:E:117:ARG:NH2	2:M:6:ASP:CG	2.70	0.45
1:F:187:ILE:O	1:F:187:ILE:HD12	2.17	0.45
2:K:35:THR:HB	2:K:38:ASP:H	1.81	0.45
1:C:25:ILE:HD11	1:C:77:LEU:HD13	1.99	0.45
3:S:1:MET:HB2	3:S:63:LYS:CG	2.46	0.45
2:K:22:VAL:HG23	2:K:55:LEU:CD2	2.46	0.45
1:F:71:ARG:HD3	3:U:63:LYS:O	2.17	0.44
1:H:180:ASN:O	1:H:181:LYS:CB	2.65	0.44
1:H:182:PHE:HA	1:H:185:LEU:HD23	2.00	0.44
3:S:1:MET:HB2	3:S:63:LYS:HG2	1.98	0.44
1:C:2:THR:CG2	1:C:69:TRP:HE1	2.30	0.44
1:C:77:LEU:HD11	1:C:85:LEU:HD12	1.98	0.44
1:D:182:PHE:HA	1:D:185:LEU:HD23	2.00	0.44
1:E:32:TRP:HZ2	3:X:66:THR:HG1	1.66	0.44
1:E:90:GLU:OE2	3:X:62:GLN:NE2	2.46	0.44
2:P:76:LEU:HD21	2:P:84:LEU:HB3	2.00	0.44
1:A:110:LEU:CD2	1:A:185:LEU:HD12	2.47	0.44
1:B:6:ARG:NH2	1:B:64:LEU:O	2.50	0.44
1:D:4:GLU:HB2	3:T:73:LEU:HD11	2.00	0.44
1:D:71:ARG:HD3	3:S:63:LYS:O	2.18	0.44
2:I:52:ARG:HG2	2:I:52:ARG:HH11	1.83	0.44
1:B:188:VAL:HG13	1:B:189:GLU:HG3	2.00	0.44
1:C:105:LEU:HD12	1:C:109:ARG:NH2	2.33	0.44
1:D:25:ILE:HD11	1:D:77:LEU:HA	2.00	0.44
1:F:69:TRP:CG	1:F:70:PHE:N	2.86	0.44
1:G:149:MET:HB2	1:H:137:GLU:OE1	2.17	0.44
3:X:44:ILE:HB	3:X:68:HIS:HB3	1.99	0.44
1:F:84:GLY:HA2	1:F:87:GLU:HB3	1.99	0.44
2:O:22:VAL:HG23	2:O:55:LEU:CD2	2.47	0.44
1:A:34:ARG:O	1:A:38:VAL:HG23	2.18	0.44
1:B:69:TRP:CG	1:B:70:PHE:N	2.86	0.44
1:B:180:ASN:O	1:B:181:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:LYS:NZ	1:G:183:SER:O	2.50	0.44
2:O:97:PRO:HD3	3:W:54:ARG:HH12	1.82	0.44
1:D:69:TRP:CG	1:D:70:PHE:N	2.86	0.44
2:K:80:LYS:HG2	2:K:81:LEU:H	1.82	0.44
1:G:77:LEU:HD21	1:G:85:LEU:HD13	1.99	0.43
3:S:41:GLN:O	3:S:41:GLN:HG3	2.17	0.43
1:A:106:LEU:HD11	1:A:110:LEU:HD11	1.99	0.43
1:D:171:LEU:HD23	1:D:186:TRP:CE2	2.53	0.43
2:K:76:LEU:O	2:K:80:LYS:HB3	2.18	0.43
1:E:110:LEU:HD23	1:E:185:LEU:CD2	2.48	0.43
1:D:114:PHE:CE1	1:D:118:ILE:HG21	2.53	0.43
1:D:130:CYS:HA	1:D:164:LYS:HG3	1.98	0.43
1:G:109:ARG:HG2	3:W:68:HIS:CG	2.53	0.43
1:H:69:TRP:CG	1:H:70:PHE:N	2.86	0.43
1:E:130:CYS:SG	1:E:170:THR:OG1	2.75	0.43
1:A:110:LEU:CD2	1:A:185:LEU:HB3	2.48	0.43
1:B:25:ILE:HD11	1:B:77:LEU:HD12	1.98	0.43
1:C:172:LYS:HE3	1:C:176:GLU:HG2	2.00	0.43
1:F:6:ARG:NH2	1:F:64:LEU:O	2.52	0.43
2:P:27:ILE:HA	2:P:79:CYS:SG	2.59	0.43
1:H:180:ASN:O	1:H:181:LYS:HB3	2.17	0.43
2:O:18:ASN:HB3	2:O:84:LEU:HD21	2.01	0.43
1:A:185:LEU:N	1:A:185:LEU:CD2	2.82	0.43
1:C:172:LYS:NZ	1:C:183:SER:O	2.51	0.43
1:E:130:CYS:HA	1:E:164:LYS:HG3	2.01	0.43
1:H:114:PHE:CE1	1:H:118:ILE:HG21	2.54	0.43
1:H:178:GLU:OE1	2:P:37:ARG:NH2	2.52	0.43
1:B:100:LEU:HD22	1:B:167:TRP:NE1	2.34	0.43
1:B:180:ASN:O	1:B:181:LYS:CB	2.67	0.43
1:C:75:ASP:O	1:C:79:HIS:ND1	2.43	0.43
2:I:26:LYS:HD3	2:L:52:ARG:HH21	1.83	0.43
1:B:33:PHE:CE1	1:B:64:LEU:HD11	2.52	0.42
2:J:5:GLU:HB2	2:J:69:VAL:HG23	2.00	0.42
1:F:110:LEU:HD22	1:F:185:LEU:HD23	2.01	0.42
1:C:167:TRP:CG	1:C:168:PRO:HD3	2.54	0.42
1:D:117:ARG:NE	1:D:180:ASN:O	2.52	0.42
1:E:84:GLY:HA2	1:E:87:GLU:HB2	2.01	0.42
1:G:25:ILE:HD11	1:G:77:LEU:HD13	2.01	0.42
2:J:5:GLU:HB2	2:J:69:VAL:CG2	2.49	0.42
1:C:10:GLN:O	1:C:13:GLN:HB2	2.19	0.42
1:F:61:LEU:HD12	1:F:64:LEU:CD1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:GLN:HG2	1:F:66:GLU:N	2.35	0.42
2:P:65:ARG:N	2:P:65:ARG:HD2	2.34	0.42
1:F:79:HIS:CD2	3:U:46:ALA:HB2	2.55	0.42
2:K:19:PHE:CD1	2:K:19:PHE:N	2.88	0.42
2:K:3:PHE:HB3	3:S:54:ARG:HE	1.84	0.42
1:G:2:THR:HB	1:G:69:TRP:HE1	1.85	0.42
1:F:180:ASN:O	1:F:181:LYS:HB3	2.20	0.42
1:H:167:TRP:N	1:H:168:PRO:HD2	2.35	0.42
1:C:2:THR:HB	1:C:69:TRP:HE1	1.84	0.42
1:E:111:GLN:N	1:E:112:PRO:CD	2.83	0.42
1:B:187:ILE:HD12	1:B:187:ILE:O	2.20	0.41
3:T:44:ILE:HB	3:T:68:HIS:HB3	2.02	0.41
3:X:50:LEU:HD22	3:X:59:TYR:CD2	2.54	0.41
2:N:2:PRO:HA	2:N:5:GLU:HG2	2.03	0.41
1:B:65:GLN:HG2	1:B:66:GLU:N	2.35	0.41
1:D:5:GLN:O	1:D:9:LEU:HB2	2.20	0.41
1:E:1:MET:SD	1:E:3:THR:HG22	2.60	0.41
1:H:30:ALA:HB3	1:H:31:PRO:HD3	2.02	0.41
1:H:32:TRP:HB3	1:H:64:LEU:HD21	2.01	0.41
2:K:77:ARG:NH1	2:K:82:VAL:HG13	2.34	0.41
2:K:80:LYS:CG	2:K:81:LEU:H	2.33	0.41
1:H:25:ILE:HD12	1:H:25:ILE:HA	1.96	0.41
2:K:22:VAL:HG23	2:K:55:LEU:HD21	2.03	0.41
1:A:111:GLN:N	1:A:112:PRO:CD	2.84	0.41
1:C:20:LEU:HD11	1:C:25:ILE:HD12	2.01	0.41
1:C:44:GLU:HG3	1:C:56:LEU:HD22	2.02	0.41
1:D:180:ASN:O	1:D:181:LYS:HB3	2.19	0.41
1:D:32:TRP:HB3	1:D:64:LEU:HD21	2.02	0.41
2:M:52:ARG:HG2	2:M:52:ARG:HH11	1.86	0.41
2:M:72:PHE:O	2:M:75:ALA:HB3	2.20	0.41
1:D:172:LYS:O	1:D:176:GLU:HB2	2.21	0.41
1:G:104:ARG:NH1	1:G:160:LEU:O	2.48	0.41
2:K:70:GLU:HG3	2:K:92:TYR:HE2	1.85	0.41
3:T:23:ILE:HD12	3:T:50:LEU:HD13	2.03	0.41
1:F:181:LYS:N	2:N:66:PRO:HG3	2.35	0.41
1:H:117:ARG:HG2	1:H:181:LYS:NZ	2.36	0.41
1:C:63:GLU:HG2	1:F:34:ARG:NH2	2.37	0.40
1:D:30:ALA:HB3	1:D:31:PRO:HD3	2.02	0.40
1:F:106:LEU:HD23	1:F:109:ARG:NH2	2.36	0.40
2:O:76:LEU:HB3	2:O:85:ALA:HB2	2.03	0.40
1:F:180:ASN:OD1	1:F:183:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:27:LYS:CB	3:S:41:GLN:OE1	2.69	0.40
1:D:119:ILE:HG23	1:D:148:MET:SD	2.60	0.40
2:L:65:ARG:N	2:L:65:ARG:HD2	2.36	0.40
1:A:9:LEU:HD13	1:A:70:PHE:HE1	1.87	0.40
1:D:167:TRP:N	1:D:168:PRO:HD2	2.35	0.40
1:E:26:LEU:HD13	1:E:38:VAL:HG23	2.02	0.40
1:E:108:LYS:NZ	1:F:35:GLU:OE1	2.49	0.40
1:F:33:PHE:CE1	1:F:64:LEU:HD11	2.56	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	186/205 (91%)	180 (97%)	5 (3%)	1 (0%)	29	61
1	B	187/205 (91%)	182 (97%)	5 (3%)	0	100	100
1	C	187/205 (91%)	184 (98%)	2 (1%)	1 (0%)	29	61
1	D	186/205 (91%)	176 (95%)	8 (4%)	2 (1%)	14	44
1	E	186/205 (91%)	179 (96%)	6 (3%)	1 (0%)	29	61
1	F	187/205 (91%)	182 (97%)	5 (3%)	0	100	100
1	G	187/205 (91%)	184 (98%)	2 (1%)	1 (0%)	29	61
1	H	186/205 (91%)	177 (95%)	7 (4%)	2 (1%)	14	44
2	I	95/108 (88%)	90 (95%)	4 (4%)	1 (1%)	14	44
2	J	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	K	95/108 (88%)	91 (96%)	3 (3%)	1 (1%)	14	44
2	L	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	M	95/108 (88%)	88 (93%)	5 (5%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	O	95/108 (88%)	93 (98%)	2 (2%)	0	100	100
2	P	95/108 (88%)	94 (99%)	1 (1%)	0	100	100
3	S	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
3	T	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
3	U	70/79 (89%)	68 (97%)	2 (3%)	0	100	100
3	W	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
3	X	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
All	All	2602/2899 (90%)	2523 (97%)	67 (3%)	12 (0%)	29	61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	LYS
1	D	115	LYS
2	K	82	VAL
2	M	48	LEU
1	E	186	TRP
1	G	181	LYS
1	H	115	LYS
1	D	114	PHE
2	M	47	THR
1	A	179	ARG
1	H	114	PHE
2	I	47	THR

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	169/182 (93%)	160 (95%)	9 (5%)	22	52
1	B	170/182 (93%)	160 (94%)	10 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	170/182 (93%)	157 (92%)	13 (8%)	13	41
1	D	169/182 (93%)	154 (91%)	15 (9%)	9	33
1	E	166/182 (91%)	156 (94%)	10 (6%)	19	49
1	F	167/182 (92%)	155 (93%)	12 (7%)	14	43
1	G	168/182 (92%)	156 (93%)	12 (7%)	14	44
1	H	169/182 (93%)	154 (91%)	15 (9%)	9	33
2	I	87/94 (93%)	85 (98%)	2 (2%)	50	74
2	J	87/94 (93%)	85 (98%)	2 (2%)	50	74
2	K	87/94 (93%)	82 (94%)	5 (6%)	20	50
2	L	87/94 (93%)	81 (93%)	6 (7%)	15	45
2	M	87/94 (93%)	84 (97%)	3 (3%)	37	65
2	N	87/94 (93%)	84 (97%)	3 (3%)	37	65
2	O	87/94 (93%)	83 (95%)	4 (5%)	27	57
2	P	87/94 (93%)	81 (93%)	6 (7%)	15	45
3	S	65/69 (94%)	62 (95%)	3 (5%)	27	57
3	T	67/69 (97%)	63 (94%)	4 (6%)	19	49
3	U	64/69 (93%)	62 (97%)	2 (3%)	40	68
3	W	63/69 (91%)	61 (97%)	2 (3%)	39	67
3	X	67/69 (97%)	63 (94%)	4 (6%)	19	49
All	All	2370/2553 (93%)	2228 (94%)	142 (6%)	19	49

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLU
1	A	25	ILE
1	A	64	LEU
1	A	105	LEU
1	A	108	LYS
1	A	110	LEU
1	A	121	THR
1	A	185	LEU
1	B	14	ASP
1	B	25	ILE

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Mol	Chain	Res	Type
1	B	27	SER
1	B	65	GLN
1	B	77	LEU
1	B	85	LEU
1	B	105	LEU
1	B	113	GLU
1	B	116	THR
1	B	140	LEU
1	C	4	GLU
1	C	13	GLN
1	C	58	LEU
1	C	74	LEU
1	C	85	LEU
1	C	104	ARG
1	C	105	LEU
1	C	106	LEU
1	C	109	ARG
1	C	110	LEU
1	C	153	GLU
1	C	179	ARG
1	C	185	LEU
1	D	1	MET
1	D	25	ILE
1	D	27	SER
1	D	36	GLU
1	D	37	GLU
1	D	40	TYR
1	D	58	LEU
1	D	117	ARG
1	D	124	ILE
1	D	155	LEU
1	D	159	LEU
1	D	173	LEU
1	D	175	LEU
1	D	177	LYS
1	D	180	ASN
1	E	1	MET
1	E	4	GLU
1	E	25	ILE
1	E	38	VAL
1	E	58	LEU
1	E	64	LEU

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Mol	Chain	Res	Type
1	E	105	LEU
1	E	108	LYS
1	E	110	LEU
1	E	121	THR
1	F	13	GLN
1	F	14	ASP
1	F	25	ILE
1	F	27	SER
1	F	40	TYR
1	F	58	LEU
1	F	65	GLN
1	F	77	LEU
1	F	85	LEU
1	F	113	GLU
1	F	116	THR
1	F	140	LEU
1	G	58	LEU
1	G	74	LEU
1	G	85	LEU
1	G	104	ARG
1	G	105	LEU
1	G	106	LEU
1	G	109	ARG
1	G	110	LEU
1	G	153	GLU
1	G	155	LEU
1	G	179	ARG
1	G	185	LEU
1	H	1	MET
1	H	25	ILE
1	H	27	SER
1	H	36	GLU
1	H	37	GLU
1	H	40	TYR
1	H	58	LEU
1	H	65	GLN
1	H	117	ARG
1	H	124	ILE
1	H	155	LEU
1	H	173	LEU
1	H	175	LEU
1	H	177	LYS

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Mol	Chain	Res	Type
1	H	180	ASN
2	I	1	MET
2	I	83	ASP
2	J	3	PHE
2	J	14	ARG
2	K	37	ARG
2	K	47	THR
2	K	63	GLN
2	K	76	LEU
2	K	80	LYS
2	L	3	PHE
2	L	35	THR
2	L	62	LEU
2	L	65	ARG
2	L	84	LEU
2	L	93	GLN
2	N	1	MET
2	N	3	PHE
2	N	14	ARG
2	O	37	ARG
2	O	63	GLN
2	O	76	LEU
2	O	81	LEU
2	P	3	PHE
2	P	35	THR
2	P	62	LEU
2	P	65	ARG
2	P	93	GLN
2	P	96	GLN
3	S	13	ILE
3	S	57	SER
3	S	60	ASN
3	T	14	THR
3	T	31	GLN
3	T	39	ASP
3	T	73	LEU
3	U	57	SER
3	U	60	ASN
3	W	57	SER
3	W	60	ASN
3	X	14	THR
3	X	31	GLN

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Mol	Chain	Res	Type
3	X	39	ASP
3	X	73	LEU
2	M	1	MET
2	M	83	ASP
2	M	96	GLN

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

Mol	Chain	Res	Type
1	E	79	HIS
3	S	41	GLN
3	U	41	GLN
3	X	60	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 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)

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	188/205 (91%)	0.29	5 (2%)	54	53	59, 90, 139, 156	0
1	B	189/205 (92%)	0.32	4 (2%)	63	62	57, 93, 147, 180	0
1	C	189/205 (92%)	0.26	4 (2%)	63	62	57, 90, 156, 243	0
1	D	188/205 (91%)	0.38	6 (3%)	47	46	55, 83, 122, 155	0
1	E	188/205 (91%)	0.34	5 (2%)	54	53	71, 108, 153, 196	0
1	F	189/205 (92%)	0.33	1 (0%)	91	90	69, 113, 159, 194	0
1	G	189/205 (92%)	0.29	6 (3%)	47	46	56, 88, 134, 168	0
1	H	188/205 (91%)	0.41	9 (4%)	30	31	60, 95, 138, 182	0
2	I	97/108 (89%)	0.10	1 (1%)	82	81	54, 80, 135, 187	0
2	J	97/108 (89%)	0.17	1 (1%)	82	81	54, 82, 139, 152	0
2	K	97/108 (89%)	0.08	1 (1%)	82	81	55, 79, 113, 223	0
2	L	97/108 (89%)	0.08	2 (2%)	63	62	76, 107, 151, 169	0
2	M	97/108 (89%)	0.43	10 (10%)	6	8	94, 145, 199, 219	0
2	N	97/108 (89%)	0.57	8 (8%)	11	13	109, 151, 198, 216	0
2	O	97/108 (89%)	0.83	14 (14%)	2	3	104, 158, 196, 240	0
2	P	97/108 (89%)	0.66	12 (12%)	4	5	121, 154, 185, 217	0
3	S	71/79 (89%)	0.80	12 (16%)	1	2	70, 112, 154, 189	0
3	T	73/79 (92%)	1.48	15 (20%)	1	1	94, 143, 182, 201	1 (1%)
3	U	72/79 (91%)	1.07	19 (26%)	0	0	123, 181, 218, 231	0
3	W	71/79 (89%)	1.57	22 (30%)	0	0	108, 150, 177, 208	0
3	X	73/79 (92%)	1.07	12 (16%)	1	2	82, 116, 157, 183	0
All	All	2644/2899 (91%)	0.46	169 (6%)	19	20	54, 104, 178, 243	1 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	33	CYS	5.7
3	W	43	LEU	5.5
2	O	72	PHE	5.3
2	O	76	LEU	5.1
3	U	5	VAL	5.1
3	U	13	ILE	5.1
3	X	43	LEU	4.7
3	U	69	LEU	4.6
3	U	15	LEU	4.6
3	T	73	LEU	4.4
2	P	72	PHE	4.3
2	O	31	LEU	4.2
3	T	50	LEU	4.0
2	P	84	LEU	4.0
3	T	61	ILE	4.0
3	T	41	GLN	4.0
2	O	95	TYR	3.9
2	N	34	LEU	3.9
3	W	39	ASP	3.9
2	N	65	ARG	3.8
3	T	15	LEU	3.8
3	U	12	THR	3.8
3	X	30	ILE	3.7
3	X	69	LEU	3.7
2	O	92	TYR	3.7
2	N	64	ARG	3.7
3	W	26	VAL	3.7
3	W	15	LEU	3.7
3	U	50	LEU	3.7
2	M	72	PHE	3.7
3	U	67	LEU	3.6
3	W	13	ILE	3.6
3	U	43	LEU	3.6
3	W	50	LEU	3.6
1	C	89	ILE	3.4
3	T	26	VAL	3.3
2	O	97	PRO	3.3
3	T	23	ILE	3.3
3	U	6	LYS	3.3
3	T	56	LEU	3.3
3	W	56	LEU	3.3
3	W	52	ASP	3.2
3	W	23	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	X	3	ILE	3.2
2	P	79	CYS	3.2
3	X	41	GLN	3.2
1	E	143	CYS	3.2
2	M	76	LEU	3.1
1	A	103	TYR	3.1
3	T	40	GLN	3.1
3	U	34	GLU	3.1
3	U	59	TYR	3.0
1	E	144	SER	3.0
2	P	55	LEU	3.0
3	W	69	LEU	3.0
2	N	73	ILE	3.0
2	M	97	PRO	3.0
3	W	41	GLN	3.0
2	K	81	LEU	3.0
1	F	188	VAL	2.9
1	H	42	GLN	2.9
1	E	97	ILE	2.8
2	M	88	VAL	2.8
3	W	38	PRO	2.8
2	P	88	VAL	2.8
3	T	43	LEU	2.8
2	O	74	ALA	2.8
2	M	31	LEU	2.7
1	H	46	ASN	2.7
3	X	71	LEU	2.7
3	W	44	ILE	2.7
2	O	62	LEU	2.7
1	A	179	ARG	2.7
2	P	95	TYR	2.7
3	T	3	ILE	2.7
2	I	97	PRO	2.7
1	G	185	LEU	2.7
3	W	30	ILE	2.6
3	X	73	LEU	2.6
3	W	42	ARG	2.6
2	P	97	PRO	2.6
3	S	13	ILE	2.6
3	U	30	ILE	2.6
3	W	3	ILE	2.6
3	T	52	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	88	VAL	2.6
1	B	188	VAL	2.6
1	H	143	CYS	2.6
1	G	2	THR	2.6
3	U	4	PHE	2.5
3	X	5	VAL	2.5
1	H	133	ASN	2.5
1	H	144	SER	2.5
2	P	67	GLY	2.5
1	H	138	GLU	2.5
1	D	46	ASN	2.5
2	L	97	PRO	2.5
3	T	22	THR	2.4
1	H	89	ILE	2.4
1	B	89	ILE	2.4
1	G	46	ASN	2.4
2	P	11	TYR	2.4
3	U	33	LYS	2.4
2	N	30	TYR	2.4
1	D	117	ARG	2.4
2	O	33	CYS	2.4
2	P	62	LEU	2.4
2	M	79	CYS	2.4
3	T	30	ILE	2.4
3	S	15	LEU	2.4
1	D	27	SER	2.3
2	J	2	PRO	2.3
3	U	3	ILE	2.3
3	W	14	THR	2.3
3	X	1	MET	2.3
2	M	27	ILE	2.3
2	M	84	LEU	2.3
3	W	70	VAL	2.3
1	C	85	LEU	2.3
2	O	88	VAL	2.3
1	D	133	ASN	2.3
2	O	4	ALA	2.3
1	D	42	GLN	2.3
1	C	9	LEU	2.2
1	A	188	VAL	2.2
1	G	182	PHE	2.2
3	W	34	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	U	11	LYS	2.2
3	S	36	ILE	2.2
1	D	128	SER	2.2
1	E	32	TRP	2.2
3	S	43	LEU	2.2
3	W	16	GLU	2.2
3	S	26	VAL	2.2
1	G	150	ALA	2.2
3	S	23	ILE	2.2
1	G	147	GLY	2.2
3	T	67	LEU	2.2
2	O	68	TRP	2.2
3	S	52	ASP	2.2
2	P	1	MET	2.2
1	H	23	THR	2.2
1	H	129	GLU	2.1
1	B	144	SER	2.1
2	N	72	PHE	2.1
3	W	12	THR	2.1
3	U	1	MET	2.1
1	A	9	LEU	2.1
2	O	75	ALA	2.1
3	U	70	VAL	2.1
2	N	1	MET	2.1
3	S	38	PRO	2.1
3	S	61	ILE	2.1
3	S	27	LYS	2.1
2	M	73	ILE	2.1
1	C	46	ASN	2.1
1	E	20	LEU	2.1
3	X	15	LEU	2.1
2	M	80	LYS	2.1
3	X	67	LEU	2.1
3	S	40	GLN	2.0
2	O	69	VAL	2.0
3	X	56	LEU	2.0
3	U	72	ARG	2.0
3	W	5	VAL	2.0
3	S	30	ILE	2.0
1	A	100	LEU	2.0
2	P	92	TYR	2.0
1	B	5	GLN	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 monosaccharides 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.