Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:58 PM EDT

PDB ID	:	3I38
Title	:	Structure of a putative chaperone protein dnaj from klebsiella pneumoniae subsp. pneumoniae mgh 78578
Authors	:	Filippova, E.V.; Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Bearden, J.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-06-30
Resolution	:	2.30 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 (i)) were used in the production of this report:

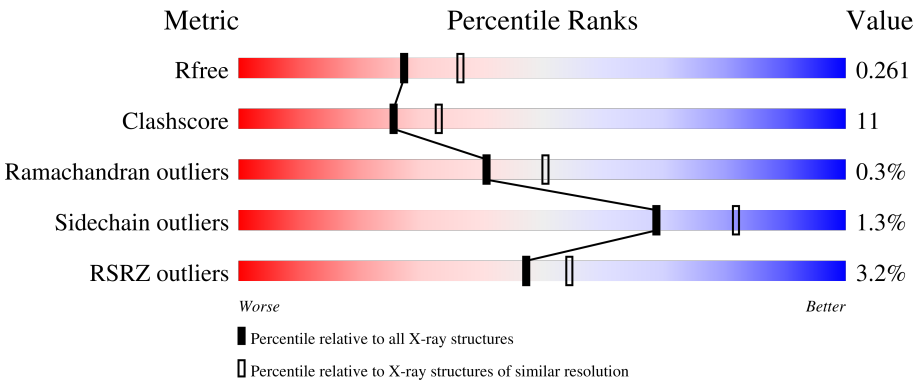
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	109	3%, 76%, 17%, • 6%
1	B	109	3%, 83%, 9%, 7%
1	C	109	3%, 72%, 17%, • 10%
1	D	109	87%, 7%, 6%

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Mol	Chain	Length	Quality of chain
1	E	109	6% 66% 24% 10%
1	F	109	3% 73% 16% • 8%
1	G	109	83% 11% • 6%
1	H	109	4% 67% 23% • 9%
1	I	109	4% 65% 23% 12%
1	J	109	7% 66% 25% • 7%
1	K	109	2% 83% 13% 5%
1	L	109	% 75% 13% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9501 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 Putative chaperone DnaJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	103	795	517	138	139	1	0	0	0
1	B	101	793	516	139	137	1	0	2	0
1	C	98	753	492	128	132	1	0	0	0
1	D	103	804	522	140	141	1	0	1	0
1	E	98	753	492	128	132	1	0	0	0
1	F	100	773	504	134	134	1	0	0	0
1	G	103	795	517	138	139	1	0	0	0
1	H	99	771	501	132	137	1	0	1	0
1	I	96	737	481	126	129	1	0	0	0
1	J	101	780	508	135	136	1	0	0	0
1	K	104	799	520	139	139	1	0	0	0
1	L	98	762	497	130	134	1	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	SER	-	expression tag	UNP A6TH30
A	198	ASN	-	expression tag	UNP A6TH30
A	199	ALA	-	expression tag	UNP A6TH30
B	197	SER	-	expression tag	UNP A6TH30
B	198	ASN	-	expression tag	UNP A6TH30

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	ALA	-	expression tag	UNP A6TH30
C	197	SER	-	expression tag	UNP A6TH30
C	198	ASN	-	expression tag	UNP A6TH30
C	199	ALA	-	expression tag	UNP A6TH30
D	197	SER	-	expression tag	UNP A6TH30
D	198	ASN	-	expression tag	UNP A6TH30
D	199	ALA	-	expression tag	UNP A6TH30
E	197	SER	-	expression tag	UNP A6TH30
E	198	ASN	-	expression tag	UNP A6TH30
E	199	ALA	-	expression tag	UNP A6TH30
F	197	SER	-	expression tag	UNP A6TH30
F	198	ASN	-	expression tag	UNP A6TH30
F	199	ALA	-	expression tag	UNP A6TH30
G	197	SER	-	expression tag	UNP A6TH30
G	198	ASN	-	expression tag	UNP A6TH30
G	199	ALA	-	expression tag	UNP A6TH30
H	197	SER	-	expression tag	UNP A6TH30
H	198	ASN	-	expression tag	UNP A6TH30
H	199	ALA	-	expression tag	UNP A6TH30
I	197	SER	-	expression tag	UNP A6TH30
I	198	ASN	-	expression tag	UNP A6TH30
I	199	ALA	-	expression tag	UNP A6TH30
J	197	SER	-	expression tag	UNP A6TH30
J	198	ASN	-	expression tag	UNP A6TH30
J	199	ALA	-	expression tag	UNP A6TH30
K	-2	SER	-	expression tag	UNP A6TH30
K	-1	ASN	-	expression tag	UNP A6TH30
K	0	ALA	-	expression tag	UNP A6TH30
L	197	SER	-	expression tag	UNP A6TH30
L	198	ASN	-	expression tag	UNP A6TH30
L	199	ALA	-	expression tag	UNP A6TH30

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	21	21	21	0	0
			Total	O		
2	B	26	26	26	0	0
			Total	O		
2	C	9	9	9	0	0
			Total	O		
2	D	19	19	19	0	0

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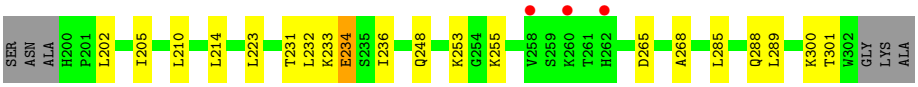
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	E	3	3	3	0	0
			Total	O		
2	F	12	12	12	0	0
			Total	O		
2	G	27	27	27	0	0
			Total	O		
2	H	11	11	11	0	0
			Total	O		
2	I	3	3	3	0	0
			Total	O		
2	J	8	8	8	0	0
			Total	O		
2	K	20	20	20	0	0
			Total	O		
2	L	27	27	27	0	0

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 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.

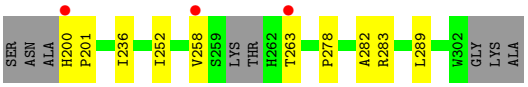
• Molecule 1: Putative chaperone DnaJ

Chain A:



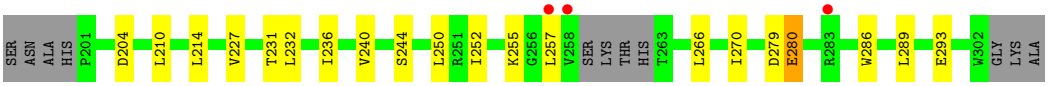
• Molecule 1: Putative chaperone DnaJ

Chain B:



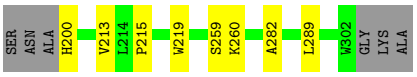
• Molecule 1: Putative chaperone DnaJ

Chain C:



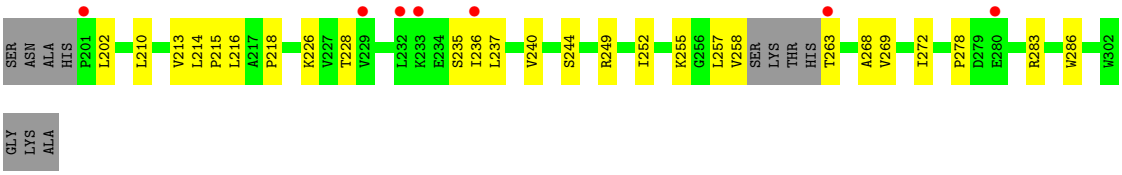
• Molecule 1: Putative chaperone DnaJ

Chain D:



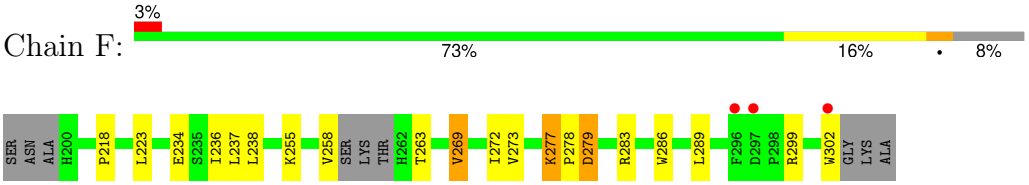
• Molecule 1: Putative chaperone DnaJ

Chain E:



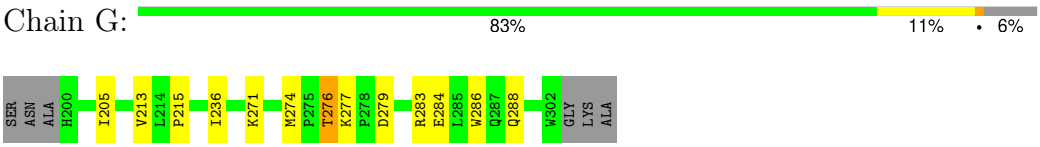
• Molecule 1: Putative chaperone DnaJ

Chain F:



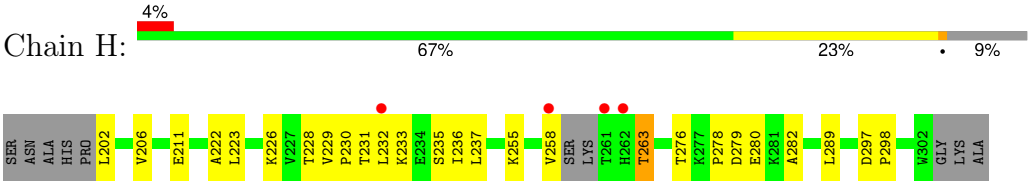
• Molecule 1: Putative chaperone DnaJ

Chain G:



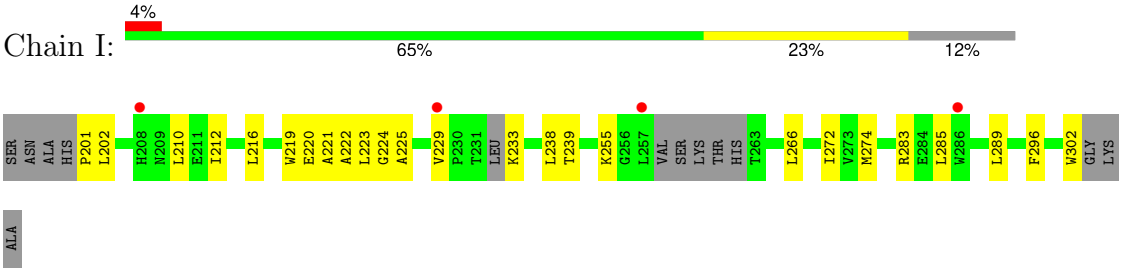
• Molecule 1: Putative chaperone DnaJ

Chain H:



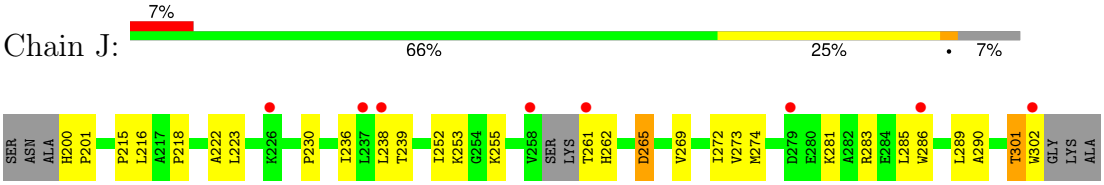
• Molecule 1: Putative chaperone DnaJ

Chain I:



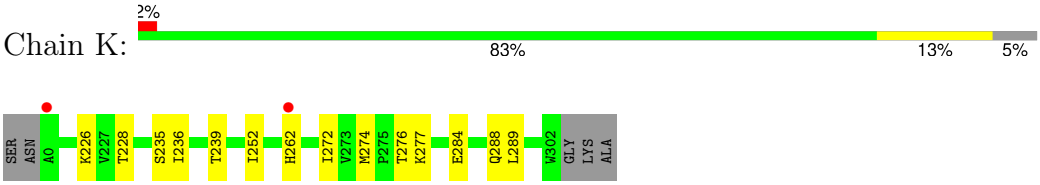
• Molecule 1: Putative chaperone DnaJ

Chain J:



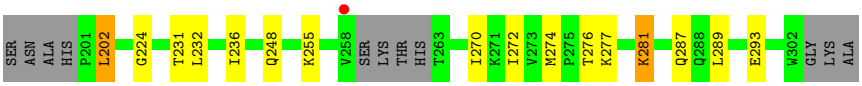
• Molecule 1: Putative chaperone DnaJ

Chain K:



• Molecule 1: Putative chaperone DnaJ

Chain L:


SER
ASN
ALA
HIS
P201
L202
G224
T231
L232
I236
Q248
K255
V258
SER
LYS
THR
HIS
T263
I270
K271
I272
V273
M274
P275
T276
K277
K281
Q287
Q288
L289
E293
W302
GLY
LYS
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.80Å 61.63Å 92.91Å 81.75° 78.71° 83.79°	Depositor
Resolution (Å)	90.54 – 2.30 38.66 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.1 (90.54-2.30) 97.6 (38.66-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0051	Depositor
R, R_{free}	0.217 , 0.262 0.228 , 0.261	Depositor DCC
R_{free} test set	3350 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9501	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 14.74% 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	0.68	0/814	0.81	0/1107
1	B	0.70	0/817	0.84	0/1109
1	C	0.57	0/769	0.79	0/1044
1	D	0.68	0/823	0.83	0/1119
1	E	0.48	0/769	0.78	0/1044
1	F	0.54	0/791	0.80	0/1075
1	G	0.67	0/814	0.84	1/1107 (0.1%)
1	H	0.52	0/787	0.76	0/1069
1	I	0.47	0/752	0.74	0/1019
1	J	0.57	0/798	0.77	0/1085
1	K	0.61	0/818	0.83	0/1113
1	L	0.67	0/778	0.89	1/1056 (0.1%)
All	All	0.60	0/9530	0.81	2/12947 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	279	ASP	CB-CG-OD2	5.85	123.56	118.30
1	L	224	GLY	N-CA-C	-5.21	100.06	113.10

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	795	0	834	17	0
1	B	793	0	834	12	0
1	C	753	0	795	24	0
1	D	804	0	841	10	0
1	E	753	0	795	26	0
1	F	773	0	808	24	0
1	G	795	0	834	12	0
1	H	771	0	804	19	0
1	I	737	0	771	30	0
1	J	780	0	815	37	0
1	K	799	0	839	19	0
1	L	762	0	802	23	0
2	A	21	0	0	1	0
2	B	26	0	0	0	0
2	C	9	0	0	0	0
2	D	19	0	0	1	0
2	E	3	0	0	0	0
2	F	12	0	0	0	0
2	G	27	0	0	0	0
2	H	11	0	0	0	0
2	I	3	0	0	0	0
2	J	8	0	0	1	0
2	K	20	0	0	2	0
2	L	27	0	0	3	0
All	All	9501	0	9772	202	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 11.

All (202) 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:236:ILE:HG21	1:C:252:ILE:HD13	1.28	1.12
1:J:238:LEU:HD23	1:J:239:THR:N	1.74	1.01
1:I:201:PRO:HB2	1:I:212:ILE:HD11	1.43	0.96
1:A:231:THR:HG23	2:A:118:HOH:O	1.73	0.89
1:C:231:THR:HG22	1:C:232:LEU:H	1.37	0.89
1:C:289:LEU:O	1:C:289:LEU:HD23	1.76	0.85
1:C:236:ILE:CG2	1:C:252:ILE:HD13	2.06	0.85
1:I:201:PRO:HB2	1:I:212:ILE:CD1	2.06	0.84
1:A:231:THR:HG22	1:A:233:LYS:H	1.43	0.83
1:C:231:THR:HG22	1:C:232:LEU:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:HG23	1:B:263:THR:HG22	1.63	0.79
1:I:201:PRO:CB	1:I:212:ILE:HD11	2.13	0.78
1:E:258:VAL:HA	1:E:263:THR:HG22	1.64	0.78
1:F:236:ILE:HD12	1:F:236:ILE:O	1.86	0.75
1:E:286:TRP:CZ2	1:F:289:LEU:HD21	2.22	0.74
1:K:262:HIS:ND1	2:K:159:HOH:O	2.22	0.71
1:I:221:ALA:HB3	1:J:274:MSE:HE2	1.74	0.70
1:F:234:GLU:OE2	1:F:255:LYS:NZ	2.24	0.70
1:I:272:ILE:HB	1:J:272:ILE:HB	1.74	0.70
1:J:265:ASP:OD1	1:J:265:ASP:N	2.25	0.69
1:B:236:ILE:HD11	1:B:252:ILE:HD13	1.76	0.68
1:I:210:LEU:O	1:I:266:LEU:HD12	1.94	0.66
1:F:236:ILE:HD12	1:F:236:ILE:C	2.16	0.66
1:F:258:VAL:HA	1:F:263:THR:HG22	1.78	0.66
1:D:200:HIS:N	2:D:155:HOH:O	2.29	0.65
1:B:258:VAL:HG13	1:B:258:VAL:O	1.96	0.65
1:C:289:LEU:HD22	1:D:219:TRP:CE3	2.32	0.65
1:E:236:ILE:HD11	1:E:255:LYS:HE3	1.78	0.64
1:J:236:ILE:HD11	1:J:255:LYS:HE2	1.79	0.64
1:J:281:LYS:HE3	1:J:285:LEU:HD11	1.80	0.64
1:L:236:ILE:HD12	1:L:236:ILE:C	2.18	0.64
1:C:231:THR:CG2	1:C:232:LEU:H	2.10	0.64
1:G:236:ILE:C	1:G:236:ILE:HD12	2.18	0.64
1:I:224:GLY:O	1:I:225:ALA:HB2	1.98	0.63
1:F:237:LEU:C	1:F:237:LEU:HD23	2.19	0.63
1:E:202:LEU:CD2	1:H:202:LEU:N	2.62	0.62
1:A:231:THR:HG22	1:A:232:LEU:N	2.14	0.62
1:F:258:VAL:HG13	1:F:263:THR:HG22	1.80	0.62
1:A:236:ILE:HD12	1:A:236:ILE:C	2.19	0.62
1:H:226:LYS:HB3	1:H:237:LEU:HD11	1.81	0.61
1:J:261:THR:N	2:J:140:HOH:O	2.34	0.61
1:E:236:ILE:HD12	1:E:252:ILE:HG21	1.82	0.60
1:J:238:LEU:HD12	1:J:252:ILE:HD11	1.82	0.60
1:K:274:MSE:HG2	1:L:272:ILE:HD13	1.84	0.59
1:I:238:LEU:HD12	1:I:239:THR:N	2.17	0.59
1:L:236:ILE:HD12	1:L:236:ILE:O	2.03	0.59
1:L:287:GLN:HG3	2:L:148:HOH:O	2.01	0.59
1:B:236:ILE:HD12	1:B:236:ILE:O	2.02	0.58
1:C:231:THR:HG21	1:C:255:LYS:HD2	1.84	0.58
1:K:274:MSE:HG2	1:L:272:ILE:CD1	2.32	0.58
1:C:231:THR:CG2	1:C:232:LEU:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LEU:HD23	1:C:289:LEU:C	2.23	0.58
1:H:236:ILE:HD11	1:H:255:LYS:HE3	1.86	0.58
1:E:249:ARG:HG2	1:E:269:VAL:HG12	1.86	0.57
1:I:229:VAL:HG21	1:I:238:LEU:HD23	1.85	0.57
1:A:205:ILE:HD13	1:A:210:LEU:CD2	2.35	0.57
1:A:231:THR:CG2	1:A:232:LEU:N	2.68	0.57
1:E:286:TRP:CH2	1:F:289:LEU:HD21	2.40	0.57
1:E:236:ILE:CD1	1:E:252:ILE:HG21	2.35	0.56
1:G:236:ILE:HD12	1:G:236:ILE:O	2.05	0.56
1:I:289:LEU:HD21	1:J:286:TRP:CZ2	2.41	0.56
1:J:269:VAL:O	1:J:269:VAL:HG23	2.05	0.56
1:L:202:LEU:HD12	1:L:202:LEU:N	2.20	0.56
1:G:276:THR:HG23	1:G:277:LYS:N	2.21	0.55
1:E:210:LEU:HD21	1:E:257:LEU:HD21	1.89	0.55
1:F:237:LEU:HD23	1:F:238:LEU:N	2.21	0.55
1:I:238:LEU:HD12	1:I:239:THR:H	1.70	0.55
1:C:286:TRP:CH2	1:D:289:LEU:HD21	2.42	0.55
1:K:236:ILE:HD11	1:K:252:ILE:HD13	1.89	0.54
1:L:276:THR:HG22	1:L:277:LYS:N	2.21	0.54
1:J:253:LYS:HA	1:J:265:ASP:HB3	1.89	0.54
1:J:236:ILE:HD11	1:J:255:LYS:CE	2.37	0.54
1:I:285:LEU:HB2	1:J:289:LEU:HD13	1.90	0.54
1:H:231:THR:HG22	1:H:232:LEU:N	2.23	0.54
1:K:274:MSE:CG	1:L:272:ILE:HD13	2.38	0.54
1:E:269:VAL:HG23	1:E:269:VAL:O	2.08	0.54
1:I:255:LYS:O	1:I:266:LEU:HB2	2.08	0.54
1:L:287:GLN:CG	2:L:148:HOH:O	2.57	0.53
1:A:234:GLU:OE2	1:A:255:LYS:NZ	2.42	0.53
1:C:293:GLU:OE2	1:D:282:ALA:HB2	2.09	0.53
1:J:215:PRO:O	1:J:216:LEU:HD23	2.08	0.53
1:J:218:PRO:HD3	1:J:273:VAL:O	2.09	0.53
1:A:231:THR:HG22	1:A:233:LYS:N	2.19	0.53
1:F:299:ARG:HD2	1:F:302:TRP:CZ3	2.44	0.52
1:E:202:LEU:HD23	1:H:202:LEU:N	2.24	0.52
1:E:226:LYS:HB3	1:E:237:LEU:HD11	1.92	0.52
1:I:283:ARG:HG3	1:J:223:LEU:HD22	1.91	0.52
1:A:231:THR:HG21	1:A:255:LYS:HD2	1.91	0.52
1:I:274:MSE:CE	1:J:222:ALA:HB2	2.40	0.52
1:I:289:LEU:HD21	1:J:286:TRP:CE2	2.44	0.52
1:D:259:SER:OG	1:D:260:LYS:N	2.42	0.52
1:J:238:LEU:HD23	1:J:239:THR:H	1.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:HIS:HB2	1:B:201:PRO:CD	2.40	0.51
1:F:279:ASP:O	1:F:283:ARG:HD3	2.10	0.51
1:L:231:THR:HB	2:L:46:HOH:O	2.09	0.51
1:E:240:VAL:HG12	1:E:244:SER:OG	2.11	0.51
1:E:286:TRP:CE2	1:F:289:LEU:HD21	2.45	0.51
1:I:222:ALA:HB1	1:J:286:TRP:CD1	2.45	0.51
1:G:283:ARG:HG3	1:H:223:LEU:CD2	2.41	0.50
1:F:277:LYS:H	1:F:277:LYS:HD2	1.76	0.50
1:J:238:LEU:HD23	1:J:238:LEU:C	2.32	0.50
1:C:286:TRP:CZ2	1:D:289:LEU:HD21	2.47	0.50
1:F:258:VAL:HG13	1:F:263:THR:CG2	2.40	0.50
1:A:289:LEU:HD12	1:B:289:LEU:HD22	1.93	0.50
1:K:276:THR:CG2	1:K:277:LYS:N	2.75	0.50
1:E:213:VAL:O	1:E:215:PRO:HD3	2.12	0.49
1:F:236:ILE:C	1:F:236:ILE:CD1	2.81	0.49
1:K:289:LEU:CD2	1:L:289:LEU:CD1	2.90	0.49
1:B:236:ILE:HD12	1:B:236:ILE:C	2.33	0.49
1:C:214:LEU:HD11	1:C:227:VAL:HG11	1.94	0.49
1:H:206:VAL:HG21	1:H:211:GLU:OE2	2.13	0.49
1:L:248[B]:GLN:HB3	1:L:270:ILE:HD12	1.95	0.49
1:H:229:VAL:HG13	1:H:230:PRO:HD2	1.94	0.49
1:I:233:LYS:HA	1:I:233:LYS:HE2	1.95	0.49
1:K:226:LYS:HG2	1:K:239:THR:HG22	1.95	0.49
1:J:236:ILE:HD11	1:J:255:LYS:NZ	2.28	0.48
1:A:253:LYS:HA	1:A:265:ASP:OD1	2.12	0.48
1:K:272:ILE:HD13	1:L:274:MSE:HG2	1.94	0.48
1:K:274:MSE:CG	1:L:272:ILE:CD1	2.92	0.48
1:C:236:ILE:HG21	1:C:252:ILE:CD1	2.21	0.48
1:K:276:THR:HG22	1:K:277:LYS:N	2.28	0.48
1:E:213:VAL:O	1:E:213:VAL:HG23	2.15	0.47
1:K:289:LEU:HD22	1:L:289:LEU:CD1	2.43	0.47
1:E:278:PRO:HG2	1:E:283:ARG:HD2	1.96	0.47
1:I:302:TRP:CE3	1:J:230:PRO:HD3	2.49	0.47
1:I:285:LEU:HD13	1:J:289:LEU:HA	1.97	0.47
1:H:231:THR:C	1:H:233:LYS:N	2.68	0.47
1:E:278:PRO:HG2	1:E:283:ARG:CD	2.44	0.47
1:F:237:LEU:C	1:F:237:LEU:CD2	2.83	0.47
1:K:272:ILE:CD1	1:L:274:MSE:HG2	2.45	0.46
1:A:300:LYS:O	1:A:301:THR:C	2.53	0.46
1:D:213:VAL:O	1:D:215:PRO:HD3	2.15	0.46
1:G:284:GLU:OE2	1:G:288:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:HIS:N	1:J:201:PRO:CD	2.79	0.46
1:B:258:VAL:HG23	1:B:263:THR:CG2	2.39	0.46
1:E:210:LEU:HD11	1:E:257:LEU:HD23	1.97	0.46
1:C:289:LEU:HD22	1:D:219:TRP:CZ3	2.51	0.46
1:K:289:LEU:HD22	1:L:289:LEU:HD12	1.98	0.45
1:B:278:PRO:HB2	1:B:282:ALA:HB3	1.98	0.45
1:L:276:THR:CG2	1:L:277:LYS:N	2.80	0.45
1:L:281:LYS:HA	1:L:281:LYS:HE2	1.97	0.45
1:G:274:MSE:CE	1:H:222:ALA:HB2	2.47	0.45
1:I:296:PHE:HZ	1:J:273:VAL:HG12	1.82	0.45
1:K:228:THR:HG23	1:K:235:SER:OG	2.17	0.45
1:J:239:THR:O	1:J:239:THR:HG23	2.17	0.44
1:J:261:THR:O	1:J:262:HIS:CG	2.70	0.44
1:B:200:HIS:CB	1:B:201:PRO:CD	2.96	0.44
1:C:240:VAL:HG22	1:C:250:LEU:CD1	2.47	0.44
1:I:223:LEU:HD23	1:J:283:ARG:HG3	1.98	0.44
1:K:262:HIS:CE1	2:K:159:HOH:O	2.68	0.44
1:C:289:LEU:CD2	1:D:219:TRP:CZ3	3.01	0.44
1:A:236:ILE:C	1:A:236:ILE:CD1	2.85	0.43
1:G:215:PRO:HA	1:G:271:LYS:O	2.18	0.43
1:C:204:ASP:HB2	1:I:202:LEU:HD22	2.00	0.43
1:F:277:LYS:H	1:F:277:LYS:CD	2.32	0.43
1:I:289:LEU:HD21	1:J:286:TRP:CH2	2.52	0.43
1:F:279:ASP:N	1:F:279:ASP:OD1	2.52	0.43
1:I:216:LEU:HB3	1:I:220:GLU:HB3	2.00	0.43
1:C:244:SER:HB3	1:C:270:ILE:CD1	2.49	0.43
1:E:218:PRO:HB2	1:F:286:TRP:CZ3	2.53	0.43
1:E:272:ILE:HB	1:F:272:ILE:HB	1.99	0.43
1:F:278:PRO:HG2	1:F:283:ARG:HG3	2.01	0.43
1:B:200:HIS:CB	1:B:201:PRO:HD3	2.48	0.43
1:I:219:TRP:CD1	1:J:290:ALA:HB2	2.53	0.43
1:J:281:LYS:NZ	1:J:285:LEU:HD21	2.33	0.43
1:K:289:LEU:CD2	1:L:289:LEU:HD12	2.49	0.43
1:H:228:THR:HG22	1:H:235:SER:HB3	1.99	0.43
1:E:202:LEU:HD21	1:H:202:LEU:N	2.33	0.43
1:G:286:TRP:CZ2	1:H:289:LEU:HD21	2.54	0.43
1:J:302:TRP:N	1:J:302:TRP:CD1	2.85	0.43
1:K:284:GLU:O	1:K:288:GLN:HG3	2.20	0.42
1:C:210:LEU:HD13	1:C:257:LEU:HG	2.00	0.42
1:C:279:ASP:O	1:C:280:GLU:C	2.58	0.42
1:L:202:LEU:N	1:L:202:LEU:CD1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:VAL:O	1:F:269:VAL:CG2	2.67	0.42
1:E:215:PRO:O	1:E:216:LEU:HD23	2.20	0.42
1:A:214:LEU:HD22	1:A:268:ALA:HB1	2.02	0.42
1:E:228:THR:HG23	1:E:235:SER:HB3	2.01	0.42
1:J:238:LEU:HD23	1:J:239:THR:CA	2.49	0.42
1:K:289:LEU:CD2	1:L:289:LEU:HD11	2.50	0.42
1:E:214:LEU:HD22	1:E:268:ALA:HB1	2.02	0.42
1:H:258:VAL:HG23	1:H:263:THR:HB	2.02	0.41
1:A:285:LEU:HD23	1:A:288:GLN:NE2	2.35	0.41
1:G:283:ARG:HB2	1:G:283:ARG:NH1	2.35	0.41
1:I:272:ILE:HG21	1:J:272:ILE:HG21	2.02	0.41
1:A:223:LEU:HD23	1:B:283[B]:ARG:HG2	2.01	0.41
1:G:205:ILE:HD12	1:L:232:LEU:HD21	2.02	0.41
1:E:286:TRP:HB2	1:F:223:LEU:HD21	2.03	0.41
1:H:278:PRO:HB2	1:H:282:ALA:HB3	2.02	0.41
1:H:297:ASP:HA	1:H:298:PRO:HD2	1.92	0.41
1:I:233:LYS:HA	1:I:233:LYS:CE	2.50	0.41
1:J:301:THR:HB	1:J:302:TRP:HD1	1.86	0.41
1:H:279[B]:ASP:OD1	1:H:280:GLU:N	2.41	0.41
1:C:286:TRP:CZ3	1:D:289:LEU:HD21	2.56	0.40
1:F:218:PRO:HD3	1:F:273:VAL:O	2.20	0.40
1:G:277:LYS:HE3	1:G:277:LYS:HB2	1.97	0.40
1:A:202:LEU:N	1:A:202:LEU:HD12	2.37	0.40
1:C:204:ASP:HB2	1:I:202:LEU:CD2	2.50	0.40
1:G:213:VAL:O	1:G:215:PRO:HD3	2.21	0.40
1:I:274:MSE:HE1	1:J:222:ALA:HB2	2.04	0.40
1:H:231:THR:C	1:H:233:LYS:H	2.24	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	101/109 (93%)	95 (94%)	6 (6%)	0	100	100
1	B	99/109 (91%)	95 (96%)	4 (4%)	0	100	100
1	C	94/109 (86%)	88 (94%)	5 (5%)	1 (1%)	14	15
1	D	102/109 (94%)	95 (93%)	7 (7%)	0	100	100
1	E	94/109 (86%)	84 (89%)	10 (11%)	0	100	100
1	F	96/109 (88%)	87 (91%)	9 (9%)	0	100	100
1	G	101/109 (93%)	94 (93%)	6 (6%)	1 (1%)	15	17
1	H	96/109 (88%)	91 (95%)	5 (5%)	0	100	100
1	I	90/109 (83%)	79 (88%)	11 (12%)	0	100	100
1	J	97/109 (89%)	88 (91%)	8 (8%)	1 (1%)	15	17
1	K	102/109 (94%)	94 (92%)	8 (8%)	0	100	100
1	L	95/109 (87%)	94 (99%)	1 (1%)	0	100	100
All	All	1167/1308 (89%)	1084 (93%)	80 (7%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	301	THR
1	C	280	GLU
1	G	276	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	85/87 (98%)	83 (98%)	2 (2%)	49	66
1	B	85/87 (98%)	85 (100%)	0	100	100
1	C	80/87 (92%)	79 (99%)	1 (1%)	69	82
1	D	86/87 (99%)	86 (100%)	0	100	100
1	E	80/87 (92%)	80 (100%)	0	100	100
1	F	82/87 (94%)	79 (96%)	3 (4%)	34	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	85/87 (98%)	85 (100%)	0	100	100
1	H	82/87 (94%)	80 (98%)	2 (2%)	49	66
1	I	77/87 (88%)	77 (100%)	0	100	100
1	J	83/87 (95%)	82 (99%)	1 (1%)	71	84
1	K	84/87 (97%)	84 (100%)	0	100	100
1	L	81/87 (93%)	77 (95%)	4 (5%)	25	35
All	All	990/1044 (95%)	977 (99%)	13 (1%)	69	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	GLU
1	A	248	GLN
1	C	266	LEU
1	F	269	VAL
1	F	277	LYS
1	F	279	ASP
1	H	263	THR
1	H	276	THR
1	J	265	ASP
1	L	202	LEU
1	L	255	LYS
1	L	281	LYS
1	L	293	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	GLN
1	F	245	GLN
1	I	287	GLN
1	J	262	HIS
1	K	200	HIS
1	K	245	GLN
1	K	287	GLN
1	L	245	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)

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	102/109 (93%)	0.02	3 (2%)	51	58	17, 27, 44, 61	0
1	B	100/109 (91%)	0.12	3 (3%)	50	57	15, 26, 42, 60	0
1	C	97/109 (88%)	0.24	3 (3%)	49	56	16, 28, 37, 69	0
1	D	102/109 (93%)	-0.13	0	100	100	15, 29, 39, 69	0
1	E	97/109 (88%)	0.53	7 (7%)	15	20	22, 32, 37, 68	0
1	F	99/109 (90%)	0.15	3 (3%)	50	57	24, 31, 38, 72	0
1	G	102/109 (93%)	-0.13	0	100	100	19, 28, 39, 66	0
1	H	98/109 (89%)	0.23	4 (4%)	37	44	20, 30, 37, 62	0
1	I	95/109 (87%)	0.53	4 (4%)	36	43	23, 31, 46, 79	0
1	J	100/109 (91%)	0.54	8 (8%)	12	16	23, 32, 46, 79	0
1	K	103/109 (94%)	-0.02	2 (1%)	66	73	18, 28, 42, 70	0
1	L	97/109 (88%)	-0.01	1 (1%)	82	86	18, 28, 37, 68	0
All	All	1192/1308 (91%)	0.17	38 (3%)	47	54	15, 30, 42, 79	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	237	LEU	4.6
1	H	262	HIS	4.0
1	A	258	VAL	3.9
1	F	302	TRP	3.7
1	B	258	VAL	3.7
1	E	201	PRO	3.5
1	H	232	LEU	3.5
1	F	296	PHE	3.1
1	K	0	ALA	2.8
1	I	257	LEU	2.7
1	E	280	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	263	THR	2.7
1	C	258	VAL	2.7
1	H	261	THR	2.7
1	J	286	TRP	2.7
1	E	233	LYS	2.7
1	I	208	HIS	2.6
1	J	226	LYS	2.6
1	J	261	THR	2.5
1	A	262	HIS	2.5
1	E	236	ILE	2.5
1	E	232	LEU	2.5
1	L	258	VAL	2.5
1	J	258	VAL	2.4
1	I	286	TRP	2.4
1	F	297	ASP	2.3
1	C	283	ARG	2.3
1	B	263	THR	2.3
1	E	229	VAL	2.3
1	H	258	VAL	2.3
1	I	229	VAL	2.2
1	K	262	HIS	2.2
1	B	200	HIS	2.2
1	C	257	LEU	2.2
1	A	260	LYS	2.1
1	J	238	LEU	2.1
1	J	279	ASP	2.1
1	J	302	TRP	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.