Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:58 am BST

PDB ID	:	3UAU
Title	:	Crystal structure of the lipoprotein JlpA
Authors	:	Kawai, F.; Yeo, H.J.
Deposited on	:	2011-10-22
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

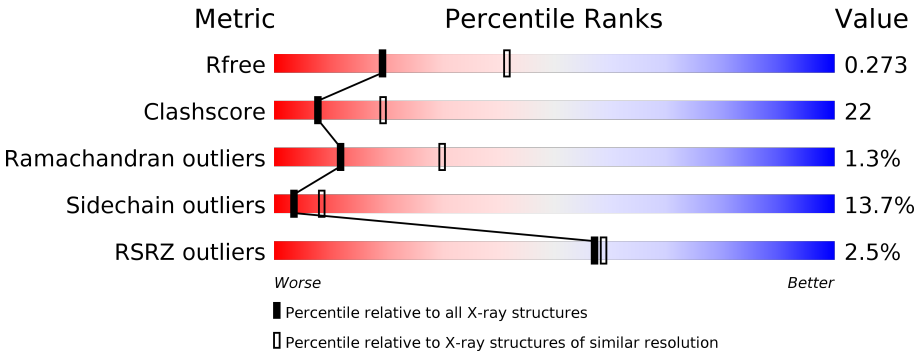
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	379	3% 56% 28% 6% 9%
1	B	379	2% 51% 31% 8% 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5510 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 Surface-exposed lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2766	1748	445	565	8			
1	B	341	Total	C	N	O	S	0	0	0
			2744	1736	441	560	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP A1VZX2
A	-5	GLY	-	EXPRESSION TAG	UNP A1VZX2
A	-4	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	-3	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	-2	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	-1	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	0	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	1	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	2	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	3	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	4	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	5	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	6	SER	-	EXPRESSION TAG	UNP A1VZX2
A	7	SER	-	EXPRESSION TAG	UNP A1VZX2
A	8	GLY	-	EXPRESSION TAG	UNP A1VZX2
A	9	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	10	ILE	-	EXPRESSION TAG	UNP A1VZX2
A	11	ASP	-	EXPRESSION TAG	UNP A1VZX2
A	12	ASP	-	EXPRESSION TAG	UNP A1VZX2
A	13	ASP	-	EXPRESSION TAG	UNP A1VZX2
A	14	ASP	-	EXPRESSION TAG	UNP A1VZX2
A	15	LYS	-	EXPRESSION TAG	UNP A1VZX2
A	16	HIS	-	EXPRESSION TAG	UNP A1VZX2
A	17	MET	-	EXPRESSION TAG	UNP A1VZX2
B	-6	MET	-	EXPRESSION TAG	UNP A1VZX2

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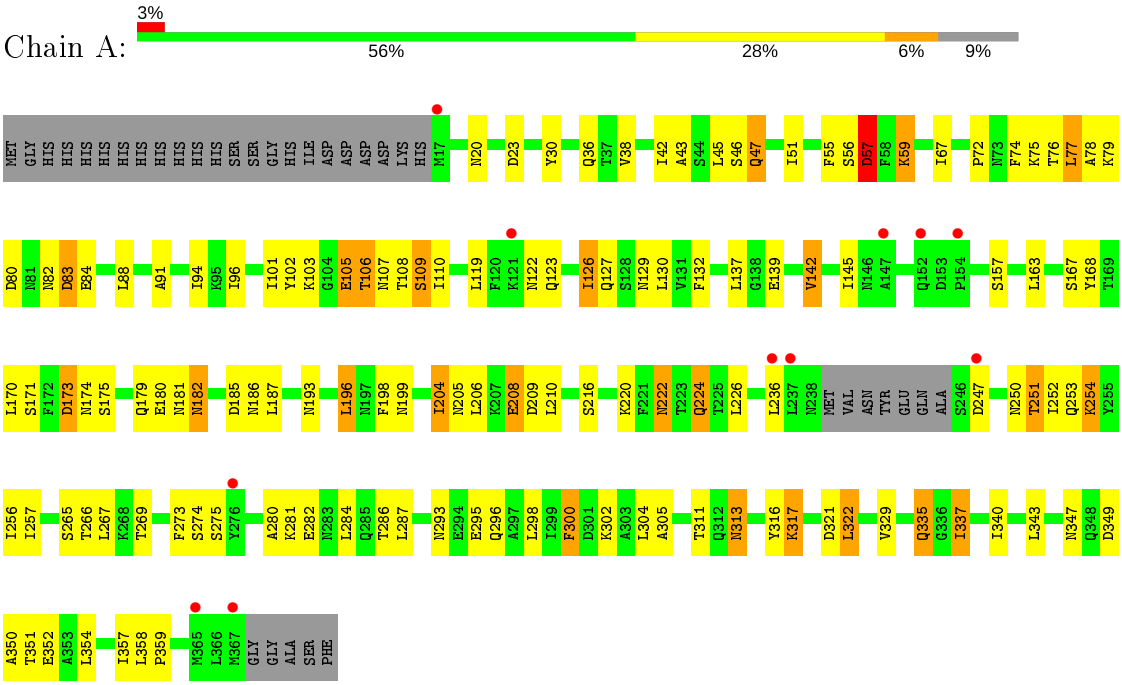
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	EXPRESSION TAG	UNP A1VZX2
B	-4	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	-3	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	-2	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	-1	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	0	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	1	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	2	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	3	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	4	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	5	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	6	SER	-	EXPRESSION TAG	UNP A1VZX2
B	7	SER	-	EXPRESSION TAG	UNP A1VZX2
B	8	GLY	-	EXPRESSION TAG	UNP A1VZX2
B	9	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	10	ILE	-	EXPRESSION TAG	UNP A1VZX2
B	11	ASP	-	EXPRESSION TAG	UNP A1VZX2
B	12	ASP	-	EXPRESSION TAG	UNP A1VZX2
B	13	ASP	-	EXPRESSION TAG	UNP A1VZX2
B	14	ASP	-	EXPRESSION TAG	UNP A1VZX2
B	15	LYS	-	EXPRESSION TAG	UNP A1VZX2
B	16	HIS	-	EXPRESSION TAG	UNP A1VZX2
B	17	MET	-	EXPRESSION TAG	UNP A1VZX2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

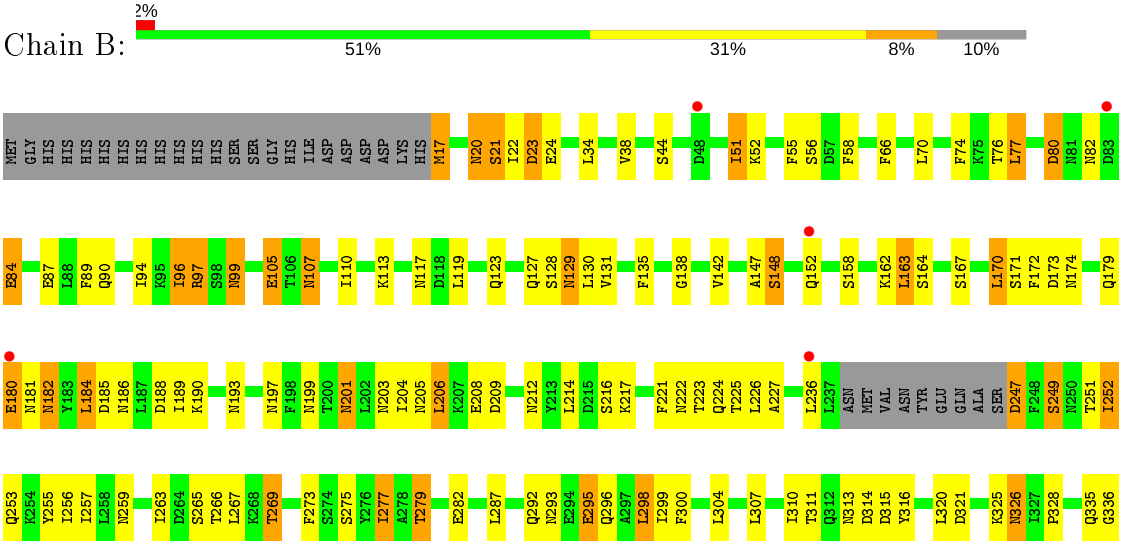
- Molecule 1: Surface-exposed lipoprotein

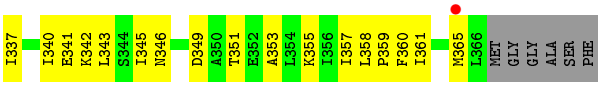
Chain A:



- Molecule 1: Surface-exposed lipoprotein

Chain B:




I337
I340
E341
K342
L343
S344
I345
N346
D349
A350
T351
E352
A353
L354
K355
I356
I357
L358
P359
F360
I361
M365
L366
MET
GLY
GLY
ALA
SER
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.63Å 111.63Å 170.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.70 19.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.90-2.70) 90.5 (19.90-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.272 0.243 , 0.273	Depositor DCC
R_{free} test set	1371 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.46% 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

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	0.84	2/2802 (0.1%)	0.81	1/3773 (0.0%)
1	B	0.90	2/2780 (0.1%)	0.85	1/3744 (0.0%)
All	All	0.87	4/5582 (0.1%)	0.83	2/7517 (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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	ASN	CB-CG	-7.45	1.33	1.51
1	A	91	ALA	CA-CB	-7.43	1.36	1.52
1	B	66	PHE	CB-CG	-5.18	1.42	1.51
1	A	208	GLU	CB-CG	5.04	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ILE	CB-CA-C	-7.27	97.05	111.60
1	B	206	LEU	CB-CG-CD2	-6.26	100.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	ILE	Peptide

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	2766	0	2732	102	0
1	B	2744	0	2712	137	0
All	All	5510	0	5444	238	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 22.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:THR:HG21	1:B:316:TYR:CE2	1.83	1.13
1:B:307:LEU:O	1:B:311:THR:HG22	1.59	1.01
1:B:349:ASP:OD2	1:B:351:THR:HG23	1.64	0.98
1:B:128:SER:C	1:B:129:ASN:HD22	1.67	0.96
1:A:337:ILE:HD11	1:A:358:LEU:HB3	1.50	0.94
1:B:107:ASN:HD21	1:B:224:GLN:HB2	1.32	0.93
1:A:80:ASP:HB2	1:A:84:GLU:O	1.69	0.91
1:A:80:ASP:HB3	1:A:82:ASN:O	1.71	0.91
1:B:343:LEU:H	1:B:351:THR:HG22	1.37	0.89
1:B:269:THR:HG21	1:B:316:TYR:CD2	2.12	0.84
1:B:287:LEU:HD23	1:B:287:LEU:C	2.00	0.82
1:B:129:ASN:HD22	1:B:129:ASN:N	1.75	0.81
1:A:204:ILE:HG22	1:A:205:ASN:N	1.95	0.81
1:B:269:THR:HG21	1:B:316:TYR:HE2	1.44	0.80
1:B:307:LEU:O	1:B:311:THR:CG2	2.29	0.80
1:A:204:ILE:CG2	1:A:205:ASN:N	2.45	0.79
1:B:358:LEU:O	1:B:361:ILE:HG22	1.81	0.79
1:A:354:LEU:HD11	1:A:358:LEU:HD13	1.64	0.79
1:A:280:ALA:O	1:A:284:LEU:HD22	1.83	0.79
1:B:181:ASN:C	1:B:182:ASN:HD22	1.86	0.78
1:A:313:ASN:HD22	1:A:313:ASN:N	1.80	0.78
1:A:256:ILE:O	1:A:329:VAL:HG23	1.83	0.77
1:A:349:ASP:OD2	1:A:351:THR:HG22	1.85	0.77
1:B:269:THR:CG2	1:B:316:TYR:CD2	2.67	0.77
1:B:17:MET:HE2	1:B:17:MET:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:PHE:O	1:B:277:ILE:HG23	1.84	0.76
1:A:204:ILE:HG21	1:A:206:LEU:HD21	1.69	0.75
1:B:287:LEU:HD23	1:B:287:LEU:O	1.87	0.75
1:B:76:THR:HG22	1:B:89:PHE:O	1.87	0.74
1:B:292:GLN:HB3	1:B:293:ASN:HA	1.69	0.73
1:B:201:ASN:HD22	1:B:201:ASN:C	1.90	0.73
1:A:80:ASP:CB	1:A:84:GLU:O	2.34	0.73
1:A:210:LEU:O	1:A:210:LEU:HD12	1.88	0.73
1:A:322:LEU:HD21	1:A:340:ILE:HG23	1.70	0.72
1:B:201:ASN:ND2	1:B:201:ASN:C	2.43	0.72
1:B:269:THR:HG23	1:B:314:ASP:O	1.89	0.72
1:B:247:ASP:O	1:B:251:THR:HG22	1.88	0.72
1:B:269:THR:CG2	1:B:316:TYR:CE2	2.70	0.71
1:B:181:ASN:O	1:B:208:GLU:CG	2.39	0.71
1:A:42:ILE:HG13	1:A:43:ALA:N	2.07	0.70
1:B:74:PHE:CD1	1:B:94:ILE:HD11	2.28	0.69
1:A:311:THR:HG22	1:A:316:TYR:CD1	2.29	0.68
1:B:138:GLY:O	1:B:142:VAL:HG23	1.94	0.67
1:B:358:LEU:HA	1:B:361:ILE:HG22	1.77	0.67
1:B:76:THR:HG21	1:B:89:PHE:CZ	2.30	0.66
1:B:128:SER:C	1:B:129:ASN:ND2	2.44	0.66
1:A:182:ASN:OD1	1:A:205:ASN:ND2	2.28	0.65
1:A:295:GLU:O	1:A:298:LEU:HG	1.97	0.65
1:B:257:ILE:HD13	1:B:326:ASN:ND2	2.12	0.65
1:A:269:THR:HG21	1:A:316:TYR:CD2	2.32	0.65
1:A:273:PHE:O	1:A:275:SER:N	2.30	0.64
1:A:205:ASN:N	1:A:257:ILE:O	2.29	0.64
1:A:168:TYR:HE1	1:A:196:LEU:HD23	1.62	0.64
1:A:43:ALA:O	1:A:47:GLN:HG3	1.99	0.62
1:B:190:LYS:HG3	1:B:199:ASN:HD22	1.63	0.62
1:B:181:ASN:O	1:B:208:GLU:HG3	1.99	0.62
1:B:266:THR:HA	1:B:316:TYR:O	1.99	0.62
1:B:87:GLU:CD	1:B:90:GLN:HE21	2.03	0.62
1:A:204:ILE:HG21	1:A:206:LEU:CD2	2.29	0.61
1:A:78:ALA:HB2	1:A:88:LEU:HD11	1.81	0.60
1:B:184:LEU:HD23	1:B:185:ASP:N	2.16	0.60
1:B:34:LEU:O	1:B:38:VAL:HG23	2.01	0.59
1:A:80:ASP:CB	1:A:82:ASN:O	2.45	0.59
1:A:79:LYS:NZ	1:A:83:ASP:OD2	2.30	0.59
1:B:163:LEU:HD23	1:B:164:SER:N	2.17	0.59
1:B:298:LEU:O	1:B:298:LEU:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:HB3	1:A:84:GLU:H	1.67	0.59
1:B:337:ILE:CD1	1:B:359:PRO:HG3	2.33	0.59
1:A:173:ASP:C	1:A:173:ASP:OD1	2.41	0.58
1:A:102:TYR:OH	1:A:106:THR:OG1	2.22	0.58
1:A:142:VAL:O	1:A:145:ILE:HG22	2.04	0.58
1:B:181:ASN:C	1:B:182:ASN:ND2	2.56	0.58
1:B:257:ILE:HD13	1:B:326:ASN:HD21	1.68	0.57
1:B:130:LEU:HD12	1:B:131:VAL:N	2.19	0.57
1:B:184:LEU:C	1:B:184:LEU:CD2	2.72	0.57
1:A:313:ASN:ND2	1:A:313:ASN:N	2.52	0.57
1:B:287:LEU:CD2	1:B:287:LEU:C	2.73	0.57
1:B:353:ALA:O	1:B:357:ILE:HG22	2.04	0.57
1:A:222:ASN:OD1	1:A:224:GLN:N	2.38	0.57
1:B:343:LEU:N	1:B:351:THR:HG22	2.16	0.57
1:B:129:ASN:ND2	1:B:129:ASN:N	2.47	0.56
1:A:354:LEU:CD1	1:A:358:LEU:HD13	2.34	0.56
1:A:76:THR:C	1:A:77:LEU:HD23	2.27	0.55
1:B:320:LEU:HD23	1:B:321:ASP:N	2.21	0.55
1:A:269:THR:HG21	1:A:316:TYR:CE2	2.42	0.54
1:A:354:LEU:HA	1:A:357:ILE:HG22	1.88	0.54
1:B:269:THR:CG2	1:B:316:TYR:HD2	2.18	0.54
1:B:76:THR:HG21	1:B:89:PHE:CE2	2.42	0.54
1:B:77:LEU:HD23	1:B:87:GLU:HA	1.88	0.54
1:A:20:ASN:HB2	1:B:97:ARG:NH1	2.23	0.54
1:A:322:LEU:CD2	1:A:340:ILE:HG23	2.37	0.54
1:B:225:THR:HG22	1:B:227:ALA:N	2.22	0.54
1:A:82:ASN:OD1	1:A:83:ASP:N	2.41	0.54
1:A:129:ASN:ND2	1:A:173:ASP:HB2	2.23	0.53
1:B:275:SER:O	1:B:279:THR:HG23	2.07	0.53
1:A:30:TYR:CE1	1:A:226:LEU:HD13	2.43	0.53
1:B:89:PHE:CD1	1:B:135:PHE:HE1	2.27	0.53
1:A:179:GLN:O	1:A:180:GLU:HG2	2.08	0.53
1:A:222:ASN:OD1	1:A:222:ASN:C	2.47	0.53
1:B:292:GLN:O	1:B:296:GLN:NE2	2.42	0.52
1:B:204:ILE:HG22	1:B:205:ASN:N	2.22	0.52
1:B:287:LEU:HD21	1:B:300:PHE:CZ	2.44	0.52
1:A:282:GLU:O	1:A:286:THR:HG23	2.08	0.52
1:A:322:LEU:HD21	1:A:340:ILE:CG2	2.37	0.52
1:B:206:LEU:CD2	1:B:256:ILE:HG12	2.40	0.52
1:A:329:VAL:O	1:A:329:VAL:HG12	2.09	0.52
1:B:181:ASN:CG	1:B:208:GLU:HG3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HD21	1:B:300:PHE:CE1	2.44	0.52
1:B:256:ILE:O	1:B:328:PRO:HA	2.09	0.52
1:B:89:PHE:CD1	1:B:135:PHE:CE1	2.98	0.51
1:A:59:LYS:HE2	1:A:59:LYS:HA	1.92	0.51
1:B:130:LEU:HD12	1:B:131:VAL:H	1.74	0.51
1:A:321:ASP:C	1:A:321:ASP:OD1	2.49	0.51
1:A:80:ASP:C	1:A:82:ASN:O	2.48	0.51
1:B:257:ILE:HG21	1:B:326:ASN:ND2	2.26	0.51
1:A:74:PHE:CD1	1:A:94:ILE:HD11	2.46	0.51
1:B:188:ASP:OD1	1:B:199:ASN:ND2	2.41	0.50
1:A:204:ILE:HG22	1:A:205:ASN:CA	2.41	0.50
1:B:337:ILE:HD11	1:B:359:PRO:HG3	1.94	0.50
1:A:313:ASN:H	1:A:313:ASN:HD22	1.56	0.50
1:A:300:PHE:HD1	1:A:300:PHE:N	2.10	0.50
1:B:358:LEU:HB3	1:B:359:PRO:CD	2.42	0.50
1:A:38:VAL:HG11	1:A:55:PHE:CE1	2.46	0.50
1:A:80:ASP:O	1:A:82:ASN:O	2.29	0.50
1:A:163:LEU:C	1:A:163:LEU:HD23	2.32	0.50
1:A:300:PHE:CD1	1:A:300:PHE:N	2.80	0.50
1:A:347:ASN:O	1:A:347:ASN:OD1	2.30	0.50
1:B:51:ILE:O	1:B:51:ILE:HG22	2.11	0.50
1:A:96:ILE:HA	1:A:129:ASN:O	2.12	0.50
1:B:203:ASN:O	1:B:259:ASN:HB2	2.11	0.49
1:A:108:THR:O	1:A:109:SER:C	2.50	0.49
1:B:197:ASN:O	1:B:265:SER:HA	2.12	0.49
1:A:181:ASN:ND2	1:A:208:GLU:OE1	2.46	0.49
1:B:185:ASP:OD1	1:B:186:ASN:N	2.46	0.49
1:B:185:ASP:C	1:B:185:ASP:OD1	2.51	0.49
1:B:76:THR:HG21	1:B:89:PHE:CE1	2.47	0.49
1:A:251:THR:HA	1:A:254:LYS:HD2	1.94	0.48
1:B:184:LEU:HD21	1:B:203:ASN:OD1	2.13	0.48
1:A:343:LEU:HD23	1:A:350:ALA:HB3	1.94	0.48
1:B:181:ASN:O	1:B:208:GLU:HG2	2.14	0.48
1:A:119:LEU:O	1:A:123:GLN:HG2	2.13	0.48
1:B:209:ASP:HB3	1:B:255:TYR:CE1	2.49	0.48
1:A:204:ILE:CG2	1:A:206:LEU:CD2	2.91	0.48
1:B:107:ASN:ND2	1:B:224:GLN:HB2	2.15	0.48
1:A:250:ASN:O	1:A:253:GLN:HB2	2.14	0.48
1:B:131:VAL:HG22	1:B:171:SER:CB	2.44	0.48
1:B:249:SER:O	1:B:253:GLN:HG3	2.14	0.48
1:A:139:GLU:O	1:A:142:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASN:HD21	1:A:295:GLU:CG	2.27	0.47
1:B:249:SER:O	1:B:252:ILE:HG22	2.15	0.47
1:B:320:LEU:C	1:B:320:LEU:HD23	2.35	0.47
1:B:94:ILE:CG2	1:B:130:LEU:HD11	2.44	0.47
1:A:74:PHE:CG	1:A:94:ILE:HD11	2.49	0.47
1:B:221:PHE:CZ	1:B:226:LEU:HA	2.50	0.47
1:A:105:GLU:O	1:A:107:ASN:ND2	2.48	0.47
1:A:167:SER:O	1:A:193:ASN:ND2	2.47	0.47
1:A:266:THR:HG22	1:A:317:LYS:HB2	1.96	0.47
1:B:105:GLU:HG3	1:B:105:GLU:O	2.14	0.47
1:B:358:LEU:CA	1:B:361:ILE:HG22	2.44	0.47
1:B:119:LEU:O	1:B:123:GLN:HG2	2.15	0.47
1:B:99:ASN:CB	1:B:127:GLN:H	2.28	0.47
1:A:293:ASN:ND2	1:A:295:GLU:CG	2.78	0.46
1:B:204:ILE:CG2	1:B:205:ASN:N	2.78	0.46
1:A:304:LEU:O	1:A:305:ALA:C	2.53	0.46
1:B:179:GLN:O	1:B:180:GLU:C	2.53	0.46
1:B:337:ILE:HD13	1:B:359:PRO:HG3	1.97	0.46
1:B:172:PHE:CD1	1:B:189:ILE:HG12	2.51	0.45
1:A:354:LEU:HD12	1:A:358:LEU:HB2	1.98	0.45
1:B:117:ASN:HD22	1:B:117:ASN:N	2.14	0.45
1:B:131:VAL:HG22	1:B:171:SER:HB2	1.98	0.45
1:B:236:LEU:O	1:B:236:LEU:HD23	2.17	0.45
1:B:87:GLU:OE2	1:B:90:GLN:NE2	2.49	0.45
1:A:179:GLN:O	1:A:182:ASN:O	2.35	0.45
1:B:267:LEU:O	1:B:315:ASP:HA	2.16	0.45
1:B:158:SER:O	1:B:162:LYS:HB2	2.16	0.45
1:A:351:THR:HG23	1:A:352:GLU:N	2.32	0.45
1:A:119:LEU:HD13	1:A:126:ILE:HD12	1.99	0.45
1:A:337:ILE:HD13	1:A:359:PRO:HG3	1.99	0.45
1:B:163:LEU:HD23	1:B:163:LEU:C	2.38	0.44
1:B:52:LYS:HD2	1:B:77:LEU:CD1	2.47	0.44
1:A:168:TYR:CE1	1:A:196:LEU:HD23	2.49	0.44
1:B:23:ASP:O	1:B:24:GLU:C	2.55	0.44
1:B:21:SER:C	1:B:22:ILE:HG13	2.37	0.44
1:A:181:ASN:O	1:A:208:GLU:HB2	2.18	0.44
1:B:190:LYS:HG3	1:B:199:ASN:ND2	2.32	0.44
1:B:223:THR:O	1:B:223:THR:HG22	2.18	0.44
1:B:94:ILE:HG22	1:B:130:LEU:HD11	1.98	0.44
1:A:132:PHE:HB2	1:A:170:LEU:HB3	2.00	0.44
1:A:287:LEU:HB3	1:A:300:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLU:OE1	1:B:90:GLN:NE2	2.47	0.44
1:B:222:ASN:OD1	1:B:222:ASN:C	2.56	0.44
1:B:55:PHE:CD2	1:B:55:PHE:O	2.71	0.43
1:B:20:ASN:N	1:B:20:ASN:OD1	2.51	0.43
1:B:298:LEU:HD12	1:B:298:LEU:C	2.38	0.43
1:B:345:ILE:O	1:B:346:ASN:C	2.55	0.43
1:A:280:ALA:O	1:A:284:LEU:CD2	2.59	0.43
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.70	0.43
1:B:325:LYS:HG2	1:B:341:GLU:HB2	2.00	0.43
1:B:184:LEU:C	1:B:184:LEU:HD23	2.38	0.43
1:B:147:ALA:O	1:B:148:SER:C	2.56	0.43
1:B:74:PHE:CG	1:B:94:ILE:HD11	2.53	0.43
1:A:269:THR:CG2	1:A:316:TYR:CD2	3.01	0.43
1:A:358:LEU:N	1:A:359:PRO:CD	2.82	0.43
1:B:257:ILE:HG21	1:B:326:ASN:HD22	1.83	0.43
1:B:223:THR:CG2	1:B:223:THR:O	2.67	0.42
1:B:355:LYS:O	1:B:359:PRO:HG2	2.18	0.42
1:A:209:ASP:O	1:A:210:LEU:C	2.56	0.42
1:B:360:PHE:CD2	1:B:360:PHE:C	2.92	0.42
1:B:94:ILE:HD13	1:B:94:ILE:HG21	1.76	0.42
1:A:126:ILE:HD13	1:A:126:ILE:HG21	1.64	0.42
1:B:99:ASN:HB3	1:B:127:GLN:H	1.85	0.42
1:B:170:LEU:HD13	1:B:172:PHE:CE2	2.54	0.42
1:A:174:ASN:ND2	1:A:185:ASP:OD1	2.44	0.42
1:A:335:GLN:HE21	1:A:335:GLN:HB2	1.64	0.42
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.86	0.42
1:B:58:PHE:CE1	1:B:96:ILE:HG13	2.55	0.42
1:A:110:ILE:HD13	1:A:110:ILE:HG21	1.80	0.42
1:A:74:PHE:CD2	1:A:74:PHE:C	2.93	0.42
1:A:354:LEU:O	1:A:357:ILE:N	2.53	0.42
1:B:193:ASN:OD1	1:B:193:ASN:C	2.58	0.42
1:B:252:ILE:CG2	1:B:253:GLN:N	2.83	0.42
1:A:293:ASN:HD21	1:A:295:GLU:HG2	1.86	0.41
1:B:295:GLU:OE1	1:B:295:GLU:N	2.53	0.41
1:B:17:MET:HE2	1:B:17:MET:CA	2.42	0.41
1:B:299:ILE:N	1:B:299:ILE:HD13	2.36	0.41
1:A:198:PHE:HA	1:A:265:SER:HB2	2.02	0.41
1:B:225:THR:HG22	1:B:227:ALA:H	1.84	0.41
1:B:358:LEU:HB3	1:B:359:PRO:HD3	2.03	0.41
1:B:80:ASP:HB2	1:B:84:GLU:O	2.19	0.41
1:B:263:ILE:HB	1:B:320:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LYS:HA	1:A:302:LYS:HD2	1.84	0.41
1:A:281:LYS:HA	1:A:284:LEU:HD23	2.03	0.41
1:A:46:SER:OG	1:A:47:GLN:N	2.54	0.41
1:A:56:SER:O	1:A:57:ASP:C	2.59	0.41
1:A:77:LEU:HD23	1:A:77:LEU:N	2.36	0.41
1:A:67:ILE:HG13	1:A:101:ILE:HG13	2.03	0.40
1:B:113:LYS:CE	1:B:212:ASN:OD1	2.69	0.40
1:B:110:ILE:O	1:B:221:PHE:N	2.53	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	340/379 (90%)	314 (92%)	22 (6%)	4 (1%)	13	32
1	B	337/379 (89%)	314 (93%)	18 (5%)	5 (2%)	10	26
All	All	677/758 (89%)	628 (93%)	40 (6%)	9 (1%)	12	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	SER
1	B	148	SER
1	B	336	GLY
1	A	57	ASP
1	A	109	SER
1	B	105	GLU
1	B	180	GLU
1	B	217	LYS
1	A	72	PRO

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	319/348 (92%)	274 (86%)	45 (14%)	3 8
1	B	316/348 (91%)	274 (87%)	42 (13%)	4 9
All	All	635/696 (91%)	548 (86%)	87 (14%)	3 8

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	36	GLN
1	A	45	LEU
1	A	47	GLN
1	A	51	ILE
1	A	57	ASP
1	A	59	LYS
1	A	75	LYS
1	A	77	LEU
1	A	83	ASP
1	A	103	LYS
1	A	105	GLU
1	A	106	THR
1	A	122	ASN
1	A	126	ILE
1	A	127	GLN
1	A	130	LEU
1	A	137	LEU
1	A	142	VAL
1	A	157	SER
1	A	171	SER
1	A	173	ASP
1	A	175	SER
1	A	182	ASN
1	A	186	ASN
1	A	187	LEU
1	A	196	LEU

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Mol	Chain	Res	Type
1	A	199	ASN
1	A	216	SER
1	A	220	LYS
1	A	222	ASN
1	A	224	GLN
1	A	236	LEU
1	A	247	ASP
1	A	251	THR
1	A	252	ILE
1	A	254	LYS
1	A	267	LEU
1	A	296	GLN
1	A	300	PHE
1	A	313	ASN
1	A	317	LYS
1	A	322	LEU
1	A	335	GLN
1	A	337	ILE
1	B	17	MET
1	B	20	ASN
1	B	21	SER
1	B	23	ASP
1	B	44	SER
1	B	51	ILE
1	B	56	SER
1	B	70	LEU
1	B	77	LEU
1	B	80	ASP
1	B	82	ASN
1	B	84	GLU
1	B	96	ILE
1	B	97	ARG
1	B	107	ASN
1	B	129	ASN
1	B	152	GLN
1	B	163	LEU
1	B	167	SER
1	B	170	LEU
1	B	173	ASP
1	B	174	ASN
1	B	182	ASN
1	B	184	LEU

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Mol	Chain	Res	Type
1	B	201	ASN
1	B	216	SER
1	B	247	ASP
1	B	249	SER
1	B	252	ILE
1	B	269	THR
1	B	277	ILE
1	B	279	THR
1	B	282	GLU
1	B	295	GLU
1	B	298	LEU
1	B	304	LEU
1	B	313	ASN
1	B	326	ASN
1	B	335	GLN
1	B	340	ILE
1	B	342	LYS
1	B	365	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	81	ASN
1	A	107	ASN
1	A	122	ASN
1	A	127	GLN
1	A	129	ASN
1	A	181	ASN
1	A	182	ASN
1	A	199	ASN
1	A	205	ASN
1	A	293	ASN
1	A	313	ASN
1	A	319	ASN
1	A	335	GLN
1	B	61	ASN
1	B	86	GLN
1	B	90	GLN
1	B	107	ASN
1	B	117	ASN
1	B	129	ASN

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	174	ASN
1	B	177	ASN
1	B	182	ASN
1	B	197	ASN
1	B	199	ASN
1	B	260	ASN
1	B	296	GLN
1	B	313	ASN
1	B	326	ASN
1	B	347	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	344/379 (90%)	-0.11	11 (3%) 47 48	35, 78, 135, 170	0
1	B	341/379 (89%)	-0.18	6 (1%) 68 70	34, 71, 139, 183	0
All	All	685/758 (90%)	-0.15	17 (2%) 57 59	34, 74, 138, 183	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	MET	4.0
1	A	237	LEU	3.8
1	B	236	LEU	3.6
1	B	152	GLN	3.5
1	A	236	LEU	3.1
1	A	152	GLN	3.0
1	A	147	ALA	2.7
1	A	17	MET	2.7
1	B	365	MET	2.6
1	A	247	ASP	2.6
1	A	121	LYS	2.6
1	B	48	ASP	2.5
1	B	83	ASP	2.5
1	B	180	GLU	2.3
1	A	367	MET	2.3
1	A	154	PRO	2.3
1	A	276	TYR	2.1

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.