Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 05:24 PM EDT

PDB ID	:	2G9N
Title	:	Structure of the DEAD domain of Human eukaryotic initiation factor 4A, eIF4A
Authors	:	Hogbom, M.; Ogg, D.; Arrowsmith, C.; Berglund, H.; Collins, R.; Edwards, A.; Ehn, M.; Flodin, S.; Flores, A.; Graslund, S.; Hallberg, B.M.; Hammarstrom, M.; Kotenyova, T.; Nilsson-Ehle, P.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Thorsell, A.G.; Uppenberg, J.; Van Den Berg, S.; Weigelt, J.; Holmberg-Schiavone, L.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-03-07
Resolution	:	2.25 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

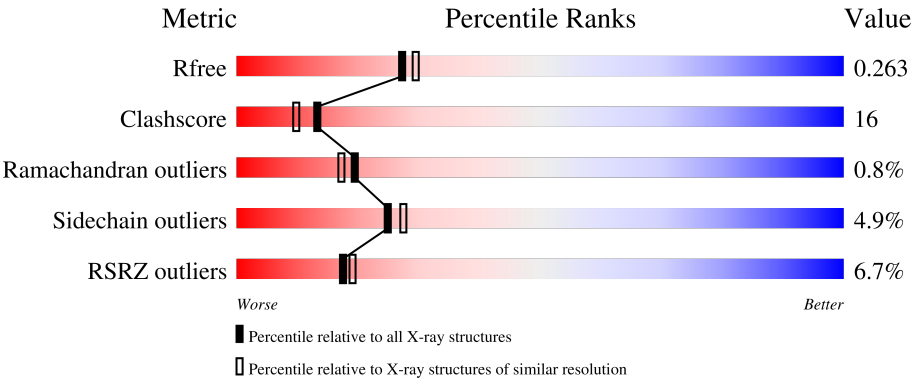
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	221	6% 67% 26%
1	B	221	6% 69% 21% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	146	-	-	-	X
1	MLY	B	146	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3657 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 Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1721	1107	287	315	12			
1	B	215	Total	C	N	O	S	0	0	0
			1710	1098	285	315	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	cloning artifact	UNP P60842
A	19	MET	-	cloning artifact	UNP P60842
A	54	MLY	LYS	modified residue	UNP P60842
A	68	MLY	LYS	modified residue	UNP P60842
A	82	MLY	LYS	modified residue	UNP P60842
A	99	MLY	LYS	modified residue	UNP P60842
A	118	MLY	LYS	modified residue	UNP P60842
A	146	MLY	LYS	modified residue	UNP P60842
A	174	MLY	LYS	modified residue	UNP P60842
A	177	MLY	LYS	modified residue	UNP P60842
A	193	MLY	LYS	modified residue	UNP P60842
A	202	MLY	LYS	modified residue	UNP P60842
A	225	MLY	LYS	modified residue	UNP P60842
A	226	MLY	LYS	modified residue	UNP P60842
A	237	MLY	LYS	modified residue	UNP P60842
A	238	MLY	LYS	modified residue	UNP P60842
B	18	SER	-	cloning artifact	UNP P60842
B	19	MET	-	cloning artifact	UNP P60842
B	54	MLY	LYS	modified residue	UNP P60842
B	68	MLY	LYS	modified residue	UNP P60842
B	82	MLY	LYS	modified residue	UNP P60842
B	99	MLY	LYS	modified residue	UNP P60842
B	118	MLY	LYS	modified residue	UNP P60842
B	146	MLY	LYS	modified residue	UNP P60842
B	174	MLY	LYS	modified residue	UNP P60842

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Chain	Residue	Modelled	Actual	Comment	Reference
B	177	MLY	LYS	modified residue	UNP P60842
B	193	MLY	LYS	modified residue	UNP P60842
B	202	MLY	LYS	modified residue	UNP P60842
B	225	MLY	LYS	modified residue	UNP P60842
B	226	MLY	LYS	modified residue	UNP P60842
B	237	MLY	LYS	modified residue	UNP P60842
B	238	MLY	LYS	modified residue	UNP P60842

- Molecule 2 is water.

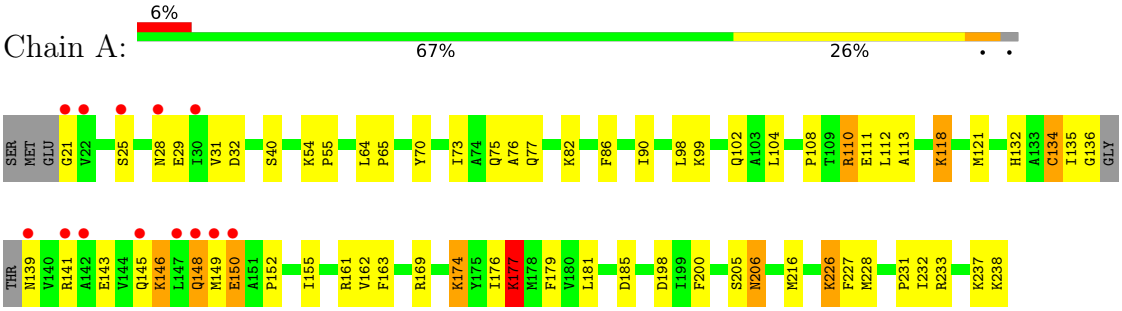
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total	O	0	0
			123	123		
2	B	103	Total	O	0	0
			103	103		

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.

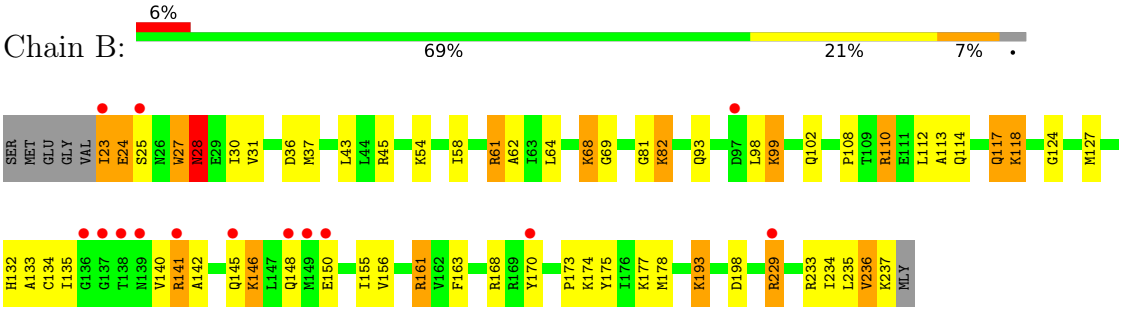
• Molecule 1: Eukaryotic initiation factor 4A-I

Chain A:



• Molecule 1: Eukaryotic initiation factor 4A-I

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.80Å 78.25Å 59.09Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.25) 99.8 (20.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.257 0.190 , 0.263	Depositor DCC
R_{free} test set	1026 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3657	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MLY

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	2/1592 (0.1%)	1.02	7/2163 (0.3%)
1	B	0.80	0/1593	1.08	10/2166 (0.5%)
All	All	0.82	2/3185 (0.1%)	1.05	17/4329 (0.4%)

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	9
1	B	0	15
All	All	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	GLU	CG-CD	6.09	1.61	1.51
1	A	111	GLU	CB-CG	5.34	1.62	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	146	MLY	O-C-N	-16.77	95.87	122.70
1	A	146	MLY	O-C-N	-15.51	97.88	122.70
1	A	146	MLY	C-N-CA	15.34	160.05	121.70
1	B	146	MLY	C-N-CA	12.71	153.49	121.70
1	B	146	MLY	CA-C-N	10.96	141.32	117.20
1	B	99	MLY	O-C-N	-10.72	105.55	122.70
1	B	82	MLY	O-C-N	-8.51	109.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	193	MLY	CA-C-N	8.28	135.41	117.20
1	A	177	MLY	O-C-N	-7.97	109.94	122.70
1	A	146	MLY	CA-C-N	7.83	134.43	117.20
1	B	193	MLY	O-C-N	-6.56	112.21	122.70
1	A	118	MLY	O-C-N	-5.80	113.43	122.70
1	B	118	MLY	CA-C-N	5.62	129.55	117.20
1	B	118	MLY	O-C-N	-5.46	113.96	122.70
1	B	118	MLY	C-N-CA	5.33	135.01	121.70
1	A	174	MLY	C-N-CA	5.18	134.65	121.70
1	A	185	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	MLY	Mainchain
1	A	145	GLN	Mainchain,Peptide
1	A	146	MLY	Mainchain
1	A	148	GLN	Peptide
1	A	176	ILE	Mainchain
1	A	177	MLY	Mainchain
1	A	226	MLY	Mainchain
1	A	98	LEU	Mainchain
1	B	117	GLN	Mainchain
1	B	134	CYS	Peptide
1	B	146	MLY	Mainchain,Peptide
1	B	173	PRO	Mainchain
1	B	236	VAL	Mainchain
1	B	24	GLU	Peptide
1	B	27	TRP	Peptide
1	B	28	ASN	Peptide
1	B	54	MLY	Mainchain
1	B	68	MLY	Mainchain
1	B	81	GLY	Mainchain
1	B	82	MLY	Mainchain
1	B	98	LEU	Mainchain
1	B	99	MLY	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	1721	0	1773	57	1
1	B	1710	0	1753	56	1
2	A	123	0	0	4	1
2	B	103	0	0	13	0
All	All	3657	0	3526	113	2

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 16.

All (113) 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:93:GLN:HE22	1:B:178:MET:CE	1.62	1.12
1:B:113:ALA:HB3	1:B:135:ILE:HD11	1.29	1.09
1:B:113:ALA:CB	1:B:135:ILE:HD11	1.84	1.07
1:B:124:GLY:HA2	1:B:127:MET:HE3	1.36	1.07
1:B:93:GLN:NE2	1:B:178:MET:HE3	1.71	1.05
1:B:93:GLN:HE22	1:B:178:MET:HE3	0.89	1.05
1:A:77:GLN:HG3	1:A:238:MLY:HD3	1.35	1.01
1:A:31:VAL:HG21	1:A:64:LEU:CD1	1.91	1.00
1:A:110:ARG:HH11	1:A:110:ARG:HG3	1.27	0.99
1:B:43:LEU:HD13	1:B:127:MET:HE1	1.47	0.95
1:B:93:GLN:NE2	1:B:178:MET:CE	2.28	0.93
1:A:31:VAL:HG21	1:A:64:LEU:HD12	1.47	0.92
1:B:124:GLY:HA2	1:B:127:MET:CE	2.08	0.83
1:A:228:MET:HE3	1:A:231:PRO:HB3	1.65	0.79
1:A:73:ILE:HG13	1:A:228:MET:HE1	1.64	0.76
1:B:25:SER:HA	1:B:233:ARG:O	1.86	0.76
1:A:21:GLY:O	1:A:75:GLN:NE2	2.19	0.74
1:B:175:TYR:O	1:B:177:MLY:HH12	1.90	0.71
1:A:110:ARG:HH11	1:A:110:ARG:CG	2.03	0.71
1:B:25:SER:HB3	1:B:27:TRP:H	1.56	0.70
1:B:229:ARG:CG	1:B:229:ARG:HH11	2.05	0.69
1:A:31:VAL:CG2	1:A:64:LEU:HD12	2.21	0.68
1:A:31:VAL:HG21	1:A:64:LEU:HD11	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLY:CA	1:B:127:MET:HE3	2.18	0.66
1:B:118:MLY:HH12	2:B:337:HOH:O	1.94	0.66
1:B:93:GLN:NE2	1:B:178:MET:HE1	2.13	0.64
1:B:113:ALA:HB1	1:B:135:ILE:HD11	1.79	0.64
1:A:228:MET:CE	1:A:231:PRO:HB3	2.27	0.64
1:A:113:ALA:CB	1:A:135:ILE:HD11	2.28	0.64
1:A:113:ALA:HB1	1:A:135:ILE:HD11	1.82	0.62
1:A:238:MLY:HE2	2:B:321:HOH:O	2.00	0.61
1:A:228:MET:CE	1:A:231:PRO:CB	2.81	0.59
1:B:43:LEU:HD13	1:B:127:MET:CE	2.26	0.59
1:B:24:GLU:HA	1:B:235:LEU:HB3	1.85	0.59
1:A:132:HIS:CD2	1:A:152:PRO:HB3	2.38	0.58
1:B:102:GLN:HG2	1:B:177:MLY:HH11	1.83	0.58
1:B:161:ARG:HG3	2:B:298:HOH:O	2.01	0.58
1:B:23:ILE:N	2:B:330:HOH:O	2.37	0.58
1:B:45:ARG:HD3	2:B:308:HOH:O	2.04	0.57
1:B:229:ARG:HH11	1:B:229:ARG:HG3	1.69	0.57
1:A:121:MET:HG3	2:A:347:HOH:O	2.04	0.56
1:B:110:ARG:HD2	2:B:323:HOH:O	2.06	0.56
1:A:238:MLY:HG2	2:B:321:HOH:O	2.04	0.56
1:A:205:SER:HA	2:A:299:HOH:O	2.06	0.55
1:B:237:MLY:HE2	1:B:237:MLY:C	2.36	0.55
1:B:114:GLN:CD	2:B:282:HOH:O	2.44	0.54
1:A:143:GLU:OE1	1:A:161:ARG:NH2	2.41	0.54
1:B:25:SER:CB	1:B:27:TRP:H	2.19	0.54
1:A:135:ILE:CG2	1:A:136:GLY:N	2.71	0.54
1:A:73:ILE:CG1	1:A:228:MET:HE1	2.36	0.53
1:A:110:ARG:HG3	1:A:110:ARG:NH1	2.08	0.53
1:B:133:ALA:HA	1:B:156:VAL:O	2.09	0.53
1:B:108:PRO:HD2	1:B:112:LEU:HD23	1.91	0.52
1:A:77:GLN:CG	1:A:238:MLY:HD3	2.25	0.52
1:B:237:MLY:HE2	1:B:237:MLY:O	2.10	0.52
1:A:110:ARG:HB2	1:A:135:ILE:HG21	1.92	0.52
1:A:177:MLY:HH22	2:A:340:HOH:O	2.08	0.52
1:A:177:MLY:CH2	2:A:340:HOH:O	2.58	0.52
1:B:132:HIS:HB3	1:B:155:ILE:HD13	1.92	0.51
1:B:163:PHE:CE1	1:B:198:ASP:HB3	2.45	0.51
1:B:24:GLU:HG3	1:B:235:LEU:O	2.11	0.51
1:A:102:GLN:HB3	1:A:177:MLY:HH23	1.93	0.51
1:A:65:PRO:HB3	1:A:232:ILE:HD13	1.94	0.50
1:A:149:MET:HG3	1:A:150:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG11	1:B:37:MET:HG2	1.95	0.49
1:B:114:GLN:NE2	2:B:282:HOH:O	2.44	0.49
1:A:206:ASN:C	1:A:206:ASN:OD1	2.52	0.48
1:A:76:ALA:O	1:A:82:MLY:HH12	2.14	0.48
1:B:31:VAL:CG2	1:B:36:ASP:HB2	2.44	0.47
1:B:168:ARG:HB3	1:B:170:TYR:CE2	2.50	0.47
1:A:179:PHE:CZ	1:A:181:LEU:HD21	2.49	0.47
1:A:99:MLY:HD2	1:A:99:MLY:H	1.80	0.46
1:A:134:CYS:C	1:A:135:ILE:HD12	2.35	0.46
1:B:163:PHE:HE1	1:B:198:ASP:HB3	1.81	0.45
1:A:104:LEU:HD11	1:A:162:VAL:HG11	1.99	0.45
1:B:118:MLY:HD2	2:B:337:HOH:O	2.16	0.45
1:A:226:MLY:HG3	1:A:227:PHE:CZ	2.52	0.45
1:B:229:ARG:HH11	1:B:229:ARG:HG2	1.81	0.45
1:B:229:ARG:CG	1:B:229:ARG:NH1	2.73	0.45
1:A:135:ILE:HG22	1:A:136:GLY:N	2.32	0.45
1:A:135:ILE:CG2	1:A:136:GLY:H	2.29	0.44
1:B:114:GLN:CG	2:B:282:HOH:O	2.64	0.44
1:A:110:ARG:CG	1:A:110:ARG:NH1	2.68	0.44
1:A:70:TYR:CD2	1:A:232:ILE:CD1	3.01	0.44
1:A:32:ASP:O	1:A:55:PRO:HD2	2.18	0.43
1:B:58:ILE:HB	1:B:236:VAL:HG21	1.99	0.43
1:A:25:SER:HA	1:A:233:ARG:O	2.18	0.43
1:A:150:GLU:HG3	1:A:150:GLU:H	1.63	0.43
1:A:228:MET:HE1	1:A:231:PRO:CB	2.49	0.43
1:A:228:MET:HE3	1:A:228:MET:HB3	1.60	0.43
1:A:135:ILE:HG23	1:A:136:GLY:H	1.83	0.43
1:B:68:MLY:HA	1:B:68:MLY:HD3	1.82	0.42
1:B:28:ASN:HD22	1:B:61:ARG:HG2	1.84	0.42
1:A:86:PHE:O	1:A:90:ILE:HG13	2.20	0.42
1:A:152:PRO:HG2	1:A:155:ILE:HD11	2.01	0.42
1:B:193:MLY:HH13	2:B:328:HOH:O	2.18	0.42
1:A:163:PHE:CE1	1:A:198:ASP:HB3	2.55	0.42
1:A:200:PHE:CE1	1:A:227:PHE:HB3	2.54	0.42
1:B:141:ARG:O	1:B:145:GLN:HG3	2.19	0.42
1:B:31:VAL:CG1	1:B:64:LEU:HD11	2.50	0.42
1:B:142:ALA:HA	1:B:145:GLN:HE21	1.84	0.42
1:A:148:GLN:OE1	1:A:148:GLN:HA	2.19	0.42
1:A:21:GLY:N	1:A:216:MET:H	2.18	0.41
1:B:148:GLN:HA	1:B:148:GLN:OE1	2.21	0.41
1:B:110:ARG:HA	1:B:135:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:MLY:HH13	1:A:174:MLY:HD3	1.68	0.41
1:B:62:ALA:HB2	1:B:234:ILE:CD1	2.51	0.41
1:B:135:ILE:O	1:B:135:ILE:HG23	2.20	0.41
1:B:175:TYR:O	1:B:177:MLY:CH1	2.66	0.41
1:A:108:PRO:HD2	1:A:112:LEU:HD23	2.03	0.41
1:B:110:ARG:NH1	2:B:306:HOH:O	2.52	0.40
1:A:110:ARG:CB	1:A:135:ILE:HG21	2.50	0.40
1:A:226:MLY:HG3	1:A:227:PHE:CE2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:283:HOH:O	2:A:335:HOH:O[2_745]	2.08	0.12
1:A:169:ARG:NH1	1:B:69:GLY:O[1_656]	2.18	0.02

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	199/221 (90%)	191 (96%)	8 (4%)	0	100 100
1	B	201/221 (91%)	191 (95%)	7 (4%)	3 (2%)	10 6
All	All	400/442 (90%)	382 (96%)	15 (4%)	3 (1%)	19 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	ASN
1	B	150	GLU
1	B	140	VAL

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	172/176 (98%)	163 (95%)	9 (5%)	23	24
1	B	172/176 (98%)	164 (95%)	8 (5%)	26	29
All	All	344/352 (98%)	327 (95%)	17 (5%)	25	27

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	29	GLU
1	A	40	SER
1	A	110	ARG
1	A	134	CYS
1	A	139	ASN
1	A	141	ARG
1	A	150	GLU
1	A	206	ASN
1	B	23	ILE
1	B	30	ILE
1	B	61	ARG
1	B	110	ARG
1	B	117	GLN
1	B	141	ARG
1	B	161	ARG
1	B	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	132	HIS
1	A	139	ASN
1	B	93	GLN
1	B	114	GLN

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Mol	Chain	Res	Type
1	B	145	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

27 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	B	225	1	9,10,11	0.69	0	6,11,13	0.68	0
1	MLY	A	54	1	9,10,11	1.35	1 (11%)	6,11,13	1.00	0
1	MLY	A	202	1	9,10,11	0.75	0	6,11,13	0.46	0
1	MLY	B	174	1	9,10,11	0.98	0	6,11,13	1.05	1 (16%)
1	MLY	A	193	1	9,10,11	0.67	0	6,11,13	0.44	0
1	MLY	B	99	1	9,10,11	0.97	0	6,11,13	0.54	0
1	MLY	A	238	1	9,10,11	0.88	0	6,11,13	0.50	0
1	MLY	A	146	1	9,10,11	0.87	0	6,11,13	0.50	0
1	MLY	B	193	1	9,10,11	1.03	0	6,11,13	0.82	0
1	MLY	A	68	1	9,10,11	0.72	0	6,11,13	0.70	0
1	MLY	A	99	1	9,10,11	1.14	0	6,11,13	0.38	0
1	MLY	B	118	1	9,10,11	1.20	0	6,11,13	0.85	0
1	MLY	A	237	1	9,10,11	1.08	1 (11%)	6,11,13	0.60	0
1	MLY	A	177	1	9,10,11	0.97	0	6,11,13	1.12	0
1	MLY	B	237	1	9,10,11	1.06	0	6,11,13	0.91	0
1	MLY	A	226	1	9,10,11	0.59	0	6,11,13	0.80	0
1	MLY	B	146	1	9,10,11	0.67	0	6,11,13	0.46	0
1	MLY	A	82	1	9,10,11	0.86	0	6,11,13	0.65	0
1	MLY	B	226	1	9,10,11	0.70	0	6,11,13	0.82	0
1	MLY	B	82	1	9,10,11	1.09	1 (11%)	6,11,13	0.79	0
1	MLY	A	225	1	9,10,11	0.91	0	6,11,13	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	B	68	1	9,10,11	0.66	0	6,11,13	0.94	0
1	MLY	B	177	1	9,10,11	0.96	0	6,11,13	1.20	0
1	MLY	B	202	1	9,10,11	0.83	0	6,11,13	0.52	0
1	MLY	A	118	1	9,10,11	0.88	0	6,11,13	0.37	0
1	MLY	A	174	1	9,10,11	1.07	1 (11%)	6,11,13	0.84	0
1	MLY	B	54	1	9,10,11	0.81	0	6,11,13	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	225	1	-	3/8/9/11	-
1	MLY	A	54	1	-	5/8/9/11	-
1	MLY	A	202	1	-	3/8/9/11	-
1	MLY	B	174	1	-	2/8/9/11	-
1	MLY	A	193	1	-	0/8/9/11	-
1	MLY	B	99	1	-	5/8/9/11	-
1	MLY	A	238	1	-	2/8/9/11	-
1	MLY	A	146	1	-	5/8/9/11	-
1	MLY	B	193	1	-	2/8/9/11	-
1	MLY	A	68	1	-	5/8/9/11	-
1	MLY	A	99	1	-	3/8/9/11	-
1	MLY	B	118	1	-	3/8/9/11	-
1	MLY	A	237	1	-	3/8/9/11	-
1	MLY	A	177	1	-	5/8/9/11	-
1	MLY	B	237	1	-	4/8/9/11	-
1	MLY	A	226	1	-	1/8/9/11	-
1	MLY	B	146	1	-	2/8/9/11	-
1	MLY	A	82	1	-	2/8/9/11	-
1	MLY	B	226	1	-	1/8/9/11	-
1	MLY	B	82	1	-	2/8/9/11	-
1	MLY	A	225	1	-	1/8/9/11	-
1	MLY	B	68	1	-	2/8/9/11	-
1	MLY	B	177	1	-	5/8/9/11	-
1	MLY	B	202	1	-	4/8/9/11	-
1	MLY	A	118	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	174	1	-	3/8/9/11	-
1	MLY	B	54	1	-	7/8/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	MLY	CB-CA	3.52	1.58	1.53
1	B	82	MLY	CB-CA	2.58	1.57	1.53
1	A	174	MLY	CB-CA	-2.56	1.50	1.53
1	A	237	MLY	O-C	2.02	1.28	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	174	MLY	CH1-NZ-CE	2.21	119.50	110.74

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	54	MLY	O-C-CA-CB
1	A	68	MLY	N-CA-CB-CG
1	A	68	MLY	C-CA-CB-CG
1	A	68	MLY	O-C-CA-CB
1	A	202	MLY	N-CA-CB-CG
1	A	202	MLY	C-CA-CB-CG
1	B	54	MLY	N-CA-CB-CG
1	B	54	MLY	C-CA-CB-CG
1	B	54	MLY	O-C-CA-CB
1	B	99	MLY	N-CA-CB-CG
1	B	99	MLY	C-CA-CB-CG
1	B	99	MLY	O-C-CA-CB
1	B	146	MLY	N-CA-CB-CG
1	B	146	MLY	C-CA-CB-CG
1	A	54	MLY	CD-CE-NZ-CH2
1	A	82	MLY	CD-CE-NZ-CH1
1	A	146	MLY	CD-CE-NZ-CH1
1	A	146	MLY	CD-CE-NZ-CH2
1	A	177	MLY	CD-CE-NZ-CH1
1	A	177	MLY	CD-CE-NZ-CH2
1	B	54	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	B	54	MLY	CD-CE-NZ-CH2
1	B	82	MLY	CD-CE-NZ-CH2
1	B	177	MLY	CD-CE-NZ-CH1
1	B	202	MLY	CD-CE-NZ-CH1
1	B	225	MLY	CD-CE-NZ-CH2
1	B	237	MLY	CD-CE-NZ-CH1
1	B	237	MLY	CD-CE-NZ-CH2
1	B	237	MLY	CG-CD-CE-NZ
1	A	68	MLY	CG-CD-CE-NZ
1	B	68	MLY	CG-CD-CE-NZ
1	A	238	MLY	CG-CD-CE-NZ
1	A	82	MLY	CD-CE-NZ-CH2
1	B	177	MLY	CD-CE-NZ-CH2
1	B	202	MLY	CD-CE-NZ-CH2
1	B	225	MLY	CD-CE-NZ-CH1
1	A	202	MLY	CA-CB-CG-CD
1	A	174	MLY	CD-CE-NZ-CH1
1	B	82	MLY	CD-CE-NZ-CH1
1	B	174	MLY	CD-CE-NZ-CH1
1	B	193	MLY	CD-CE-NZ-CH1
1	A	237	MLY	CA-CB-CG-CD
1	B	237	MLY	CA-CB-CG-CD
1	A	54	MLY	CG-CD-CE-NZ
1	B	202	MLY	CG-CD-CE-NZ
1	A	54	MLY	CD-CE-NZ-CH1
1	B	118	MLY	CD-CE-NZ-CH1
1	B	118	MLY	CD-CE-NZ-CH2
1	B	54	MLY	CA-CB-CG-CD
1	A	177	MLY	CG-CD-CE-NZ
1	B	226	MLY	CA-CB-CG-CD
1	B	177	MLY	CE-CD-CG-CB
1	B	177	MLY	CG-CD-CE-NZ
1	A	68	MLY	CE-CD-CG-CB
1	A	174	MLY	CG-CD-CE-NZ
1	A	237	MLY	CE-CD-CG-CB
1	A	226	MLY	CA-CB-CG-CD
1	B	202	MLY	CA-CB-CG-CD
1	B	54	MLY	CE-CD-CG-CB
1	A	99	MLY	CE-CD-CG-CB
1	A	237	MLY	CG-CD-CE-NZ
1	A	146	MLY	C-CA-CB-CG
1	A	177	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	A	174	MLY	CD-CE-NZ-CH2
1	A	146	MLY	CE-CD-CG-CB
1	B	225	MLY	CE-CD-CG-CB
1	A	99	MLY	CD-CE-NZ-CH1
1	A	146	MLY	CG-CD-CE-NZ
1	B	68	MLY	CA-CB-CG-CD
1	B	174	MLY	CD-CE-NZ-CH2
1	A	238	MLY	N-CA-CB-CG
1	A	177	MLY	CA-CB-CG-CD
1	B	118	MLY	CG-CD-CE-NZ
1	A	54	MLY	CA-CB-CG-CD
1	B	193	MLY	CD-CE-NZ-CH2
1	A	99	MLY	CD-CE-NZ-CH2
1	A	118	MLY	CD-CE-NZ-CH2
1	B	177	MLY	C-CA-CB-CG
1	B	99	MLY	CE-CD-CG-CB
1	B	99	MLY	CA-CB-CG-CD
1	A	225	MLY	CE-CD-CG-CB

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	238	MLY	4	0
1	B	193	MLY	1	0
1	A	99	MLY	1	0
1	B	118	MLY	2	0
1	A	177	MLY	3	0
1	B	237	MLY	2	0
1	A	226	MLY	2	0
1	A	82	MLY	1	0
1	B	68	MLY	1	0
1	B	177	MLY	3	0
1	A	174	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	202/221 (91%)	0.19	13 (6%)	19	21	4, 11, 34, 56	0
1	B	202/221 (91%)	0.15	14 (6%)	16	18	3, 11, 37, 44	0
All	All	404/442 (91%)	0.17	27 (6%)	17	19	3, 11, 37, 56	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	GLY	5.6
1	A	139	ASN	5.4
1	A	149	MET	4.9
1	A	21	GLY	4.5
1	A	22	VAL	4.2
1	A	147	LEU	3.9
1	B	141	ARG	3.8
1	B	139	ASN	3.6
1	B	149	MET	3.5
1	A	142	ALA	3.1
1	A	148	GLN	3.0
1	A	30	ILE	3.0
1	A	28	ASN	3.0
1	B	136	GLY	2.9
1	B	138	THR	2.8
1	B	23	ILE	2.8
1	A	145	GLN	2.7
1	A	141	ARG	2.4
1	A	150	GLU	2.4
1	B	97	ASP	2.4
1	B	229	ARG	2.3
1	A	25	SER	2.3
1	B	25	SER	2.3
1	B	148	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	170	TYR	2.2
1	B	145	GLN	2.1
1	B	150	GLU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	A	146	11/12	0.66	0.42	50,51,55,55	0
1	MLY	B	237	11/12	0.76	0.33	18,20,36,36	0
1	MLY	B	146	11/12	0.77	0.42	40,41,45,45	0
1	MLY	A	99	11/12	0.80	0.30	11,13,28,29	0
1	MLY	A	225	11/12	0.80	0.27	11,12,26,27	0
1	MLY	A	237	11/12	0.83	0.22	17,21,30,30	0
1	MLY	A	238	11/12	0.84	0.33	25,27,36,37	0
1	MLY	B	177	11/12	0.89	0.19	7,9,24,25	0
1	MLY	B	54	11/12	0.89	0.22	11,12,21,23	0
1	MLY	B	226	11/12	0.90	0.16	13,14,22,22	0
1	MLY	A	177	11/12	0.90	0.18	9,13,25,26	0
1	MLY	B	68	11/12	0.91	0.16	14,16,24,25	0
1	MLY	B	193	11/12	0.91	0.17	8,10,23,24	0
1	MLY	B	99	11/12	0.92	0.18	10,12,27,29	0
1	MLY	B	202	11/12	0.93	0.13	9,10,24,24	0
1	MLY	A	118	11/12	0.93	0.17	6,8,24,25	0
1	MLY	A	68	11/12	0.93	0.14	12,14,25,25	0
1	MLY	B	225	11/12	0.94	0.17	11,13,28,29	0
1	MLY	A	174	11/12	0.94	0.11	5,6,9,10	0
1	MLY	B	118	11/12	0.94	0.15	4,5,25,26	0
1	MLY	A	202	11/12	0.95	0.13	9,11,25,26	0
1	MLY	B	174	11/12	0.95	0.11	2,4,6,7	0
1	MLY	A	226	11/12	0.96	0.12	11,12,18,20	0
1	MLY	B	82	11/12	0.96	0.15	5,9,13,14	0
1	MLY	A	54	11/12	0.96	0.12	7,8,20,20	0
1	MLY	A	82	11/12	0.97	0.14	6,8,15,17	0
1	MLY	A	193	11/12	0.97	0.10	8,9,18,18	0

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.