



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:35 AM UTC

PDB ID : 3QWZ / pdb_00003qwz
Title : Crystal structure of FAF1 UBX-p97N-domain complex
Authors : Park, J.K.; Jeon, H.; Lee, J.J.; Kim, K.H.; Lee, K.J.; Kim, E.E.
Deposited on : 2011-02-28
Resolution : 2.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

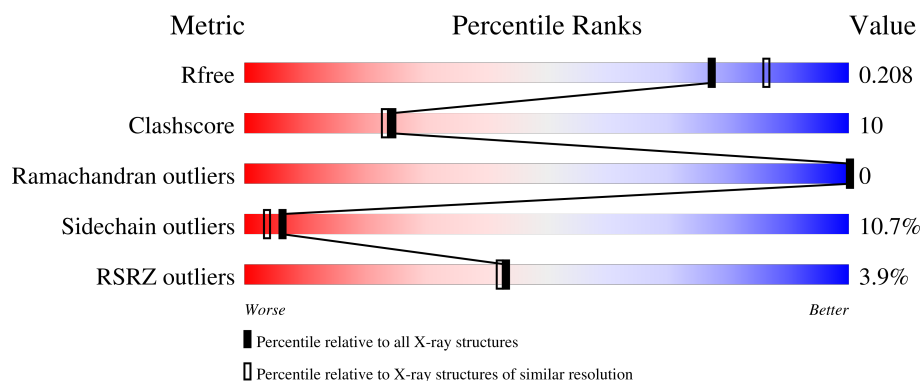
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	211	4% 46%28%10%16%
2	B	84	% 58%29%8%...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2258 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1416	891	248	269	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P55072
A	-1	SER	-	expression tag	UNP P55072
A	0	HIS	-	expression tag	UNP P55072

- Molecule 2 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total	C	N	O	S	0	0	0
			679	444	112	122	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	567	GLY	-	expression tag	UNP Q9UNN5
B	568	SER	-	expression tag	UNP Q9UNN5
B	569	HIS	-	expression tag	UNP Q9UNN5
B	570	MET	-	expression tag	UNP Q9UNN5

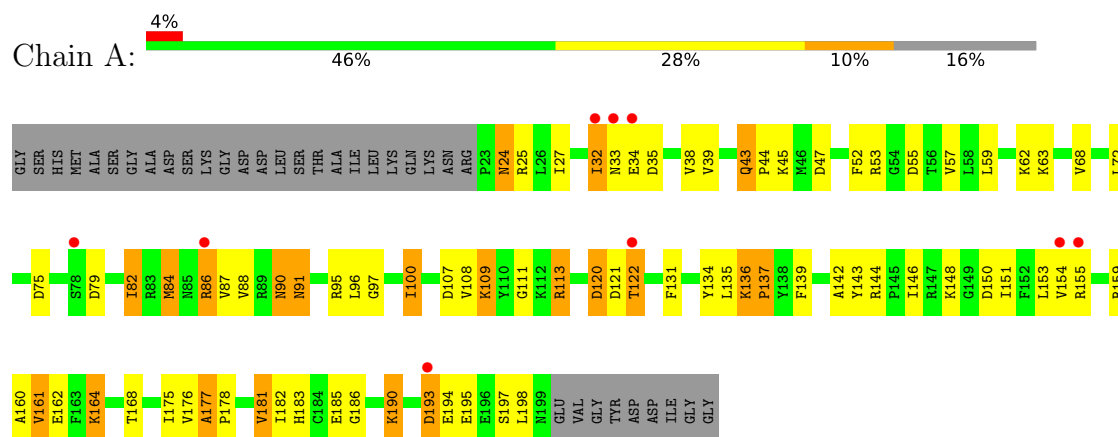
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	49	Total	O	0	0
			49	49		

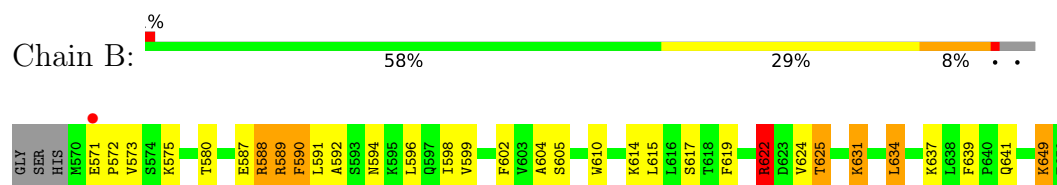
3 Residue-property plots [i](#)

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: Transitional endoplasmic reticulum ATPase



- Molecule 2: FAS-associated factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.49Å 59.94Å 75.54Å 90.00° 114.83° 90.00°	Depositor
Resolution (Å)	19.33 – 2.00 19.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.33-2.00) 96.4 (19.33-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.249 0.214 , 0.208	Depositor DCC
R_{free} test set	932 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2258	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	2.24	48/1416 (3.4%)	1.37	10/1916 (0.5%)
2	B	2.21	21/673 (3.1%)	1.24	0/908
All	All	2.23	69/2089 (3.3%)	1.33	10/2824 (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	1

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ARG	C-O	-9.02	1.15	1.24
1	A	160	ALA	CA-CB	-8.95	1.41	1.53
1	A	136	LYS	C-O	-8.82	1.16	1.24
1	A	161	VAL	C-O	-8.40	1.15	1.24
2	B	649	MLY	C-N	8.23	1.44	1.33
1	A	177	ALA	CA-CB	-7.91	1.41	1.53
2	B	602	PHE	C-O	-7.18	1.15	1.24
1	A	175	ILE	C-O	-7.12	1.16	1.24
1	A	153	LEU	C-O	-6.85	1.15	1.24
2	B	634	LEU	C-O	-6.81	1.16	1.24
2	B	604	ALA	CA-CB	-6.59	1.43	1.53
1	A	84	MET	C-N	6.52	1.42	1.33
1	A	90	ASN	C-O	-6.48	1.16	1.24
2	B	624	VAL	C-O	-6.44	1.16	1.24
2	B	625	THR	C-O	-6.43	1.14	1.24
1	A	24	ASN	N-CA	-6.23	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	VAL	C-O	-6.22	1.17	1.24
1	A	168	THR	C-O	-6.04	1.16	1.23
1	A	143	TYR	C-O	-5.99	1.16	1.24
1	A	108	VAL	C-O	-5.97	1.18	1.24
1	A	148	LYS	C-O	-5.97	1.16	1.23
1	A	159	ARG	C-O	-5.95	1.18	1.24
1	A	87	VAL	C-O	-5.95	1.17	1.24
2	B	592	ALA	CA-CB	-5.88	1.43	1.53
1	A	120	ASP	C-N	-5.84	1.24	1.33
1	A	142	ALA	C-O	-5.84	1.16	1.23
2	B	622	ARG	C-O	-5.82	1.17	1.23
1	A	197	SER	C-O	-5.80	1.16	1.23
1	A	131	PHE	C-O	-5.79	1.17	1.24
1	A	72	LEU	C-O	-5.75	1.16	1.23
2	B	625	THR	CB-CG2	-5.72	1.33	1.52
1	A	164	MLY	C-N	5.67	1.41	1.33
2	B	587	GLU	C-O	-5.67	1.17	1.23
2	B	625	THR	CB-OG1	-5.67	1.34	1.43
1	A	134	TYR	C-O	-5.61	1.16	1.23
1	A	57	VAL	C-O	-5.57	1.18	1.24
2	B	614	MLY	C-N	5.47	1.41	1.33
1	A	111	GLY	C-O	-5.46	1.18	1.23
2	B	605	SER	C-O	-5.46	1.17	1.24
1	A	137	PRO	CB-CG	-5.45	1.22	1.49
2	B	590	PHE	N-CA	-5.41	1.38	1.45
2	B	589	ARG	C-O	-5.40	1.17	1.23
1	A	43	GLN	C-O	-5.40	1.19	1.24
1	A	146	ILE	CB-CG2	-5.40	1.34	1.52
1	A	182	ILE	C-O	-5.39	1.18	1.24
2	B	631	LYS	C-O	-5.39	1.17	1.23
1	A	27	ILE	C-O	-5.38	1.17	1.24
1	A	97	GLY	C-O	-5.36	1.16	1.24
1	A	186	GLY	C-O	-5.35	1.18	1.23
1	A	185	GLU	C-O	-5.34	1.17	1.23
2	B	604	ALA	C-O	-5.34	1.17	1.24
1	A	150	ASP	C-O	-5.34	1.17	1.23
1	A	91	ASN	C-O	-5.32	1.17	1.24
1	A	181	VAL	C-O	-5.30	1.18	1.23
1	A	27	ILE	N-CA	-5.27	1.40	1.46
1	A	137	PRO	C-O	-5.27	1.17	1.24
1	A	95	ARG	CB-CG	-5.26	1.36	1.52
1	A	68	VAL	C-O	-5.22	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	625	THR	N-CA	-5.21	1.38	1.46
1	A	45	LYS	CD-CE	-5.21	1.36	1.52
1	A	135	LEU	C-O	-5.18	1.18	1.24
2	B	580	THR	C-O	-5.16	1.16	1.23
2	B	599	VAL	C-O	-5.14	1.18	1.24
1	A	53	ARG	C-O	-5.11	1.17	1.24
2	B	639	PHE	C-O	-5.10	1.17	1.24
1	A	88	VAL	C-O	-5.08	1.18	1.24
1	A	82	ILE	C-O	-5.07	1.18	1.24
1	A	47	ASP	C-O	-5.05	1.18	1.24
1	A	79	ASP	C-O	-5.04	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ARG	N-CA-C	7.85	122.85	113.28
1	A	24	ASN	N-CA-C	6.42	120.16	109.95
1	A	155	ARG	CB-CA-C	-6.26	97.69	109.72
1	A	181	VAL	N-CA-C	6.07	116.25	108.12
1	A	109	LYS	N-CA-C	5.93	119.75	110.32
1	A	38	VAL	N-CA-C	5.78	116.81	108.48
1	A	135	LEU	N-CA-C	5.75	117.35	111.14
1	A	154	VAL	O-C-N	5.38	128.72	122.97
1	A	159	ARG	N-CA-C	5.21	115.25	108.07
1	A	161	VAL	N-CA-C	5.08	116.23	109.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	84	MET	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1416	0	1440	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	679	0	694	10	0
3	A	114	0	0	2	0
3	B	49	0	0	1	0
All	All	2258	0	2134	42	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 10.

All (42) 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:A:122:THR:HG21	1:A:162:GLU:N	1.69	1.05
1:A:122:THR:HG21	1:A:162:GLU:H	0.88	1.04
1:A:122:THR:HG23	1:A:161:VAL:HA	1.45	0.98
1:A:122:THR:CG2	1:A:161:VAL:HA	1.94	0.96
1:A:113:ARG:HE	1:A:183:HIS:HE1	1.21	0.87
2:B:571:GLU:HG2	2:B:572:PRO:HD2	1.68	0.74
1:A:113:ARG:HE	1:A:183:HIS:CE1	2.07	0.72
1:A:122:THR:HG23	1:A:122:THR:O	1.91	0.69
2:B:575:LYS:HG3	3:B:72:HOH:O	1.91	0.69
1:A:113:ARG:NE	1:A:183:HIS:HE1	1.89	0.68
1:A:122:THR:CG2	1:A:122:THR:O	2.41	0.68
1:A:91:ASN:HD21	1:A:151:ILE:H	1.46	0.63
1:A:177:ALA:HB1	1:A:178:PRO:HD2	1.81	0.62
1:A:193:ASP:HB2	3:A:302:HOH:O	1.98	0.61
1:A:190:LYS:NZ	1:A:190:LYS:HB3	2.16	0.60
1:A:32:ILE:H	1:A:32:ILE:HD12	1.66	0.60
1:A:43:GLN:N	1:A:44:PRO:HD2	2.16	0.60
1:A:90:ASN:HD21	1:A:198:LEU:H	1.50	0.60
1:A:100:ILE:HD12	1:A:100:ILE:C	2.28	0.58
1:A:90:ASN:ND2	1:A:198:LEU:H	2.01	0.58
2:B:571:GLU:CG	2:B:572:PRO:HD2	2.35	0.56
1:A:164:MLY:HH23	3:A:246:HOH:O	2.07	0.54
1:A:107:ASP:O	1:A:109:LYS:HE2	2.06	0.54
1:A:122:THR:HG21	1:A:161:VAL:HA	1.82	0.53
1:A:136:LYS:N	1:A:137:PRO:CD	2.72	0.53
1:A:86:ARG:CZ	1:A:86:ARG:H	2.22	0.52
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.94	0.50
2:B:617:SER:OG	2:B:622:ARG:HG2	2.14	0.47
2:B:573:VAL:HG23	2:B:590:PHE:O	2.15	0.47
1:A:120:ASP:OD1	1:A:121:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:ASN:HB3	2:B:598:ILE:HD12	1.96	0.46
2:B:610:TRP:CH2	2:B:649:MLY:HH11	2.51	0.46
1:A:164:MLY:HH12	1:A:195:GLU:OE2	2.17	0.45
2:B:588:ARG:HG2	2:B:590:PHE:CZ	2.51	0.45
1:A:113:ARG:HG3	1:A:181:VAL:HB	1.98	0.45
2:B:588:ARG:HG3	2:B:589:ARG:N	2.32	0.44
1:A:177:ALA:HB1	1:A:178:PRO:CD	2.47	0.43
1:A:33:ASN:HD21	2:B:619:PHE:HE2	1.66	0.42
1:A:139:PHE:CD1	1:A:176:VAL:HG11	2.54	0.42
1:A:34:GLU:O	1:A:35:ASP:C	2.63	0.42
1:A:91:ASN:ND2	1:A:151:ILE:H	2.16	0.41
1:A:52:PHE:HB2	1:A:55:ASP:OD2	2.20	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	173/211 (82%)	162 (94%)	11 (6%)	0	100	100
2	B	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
All	All	250/295 (85%)	234 (94%)	16 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	160/185 (86%)	145 (91%)	15 (9%)	8	5
2	B	74/76 (97%)	64 (86%)	10 (14%)	4	2
All	All	234/261 (90%)	209 (89%)	25 (11%)	6	4

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	25	ARG
1	A	32	ILE
1	A	59	LEU
1	A	63	LYS
1	A	75	ASP
1	A	82	ILE
1	A	86	ARG
1	A	96	LEU
1	A	100	ILE
1	A	113	ARG
1	A	122	THR
1	A	190	LYS
1	A	193	ASP
1	A	194	GLU
2	B	588	ARG
2	B	591	LEU
2	B	596	LEU
2	B	615	LEU
2	B	622	ARG
2	B	625	THR
2	B	631	LYS
2	B	634	LEU
2	B	637	LYS
2	B	641	GLN

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	33	ASN
1	A	36	ASN
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	91	ASN
1	A	183	HIS
2	B	641	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	A	62	1	9,10,11	1.68	1 (11%)	6,11,13	3.99	2 (33%)
2	MLY	B	614	2	9,10,11	2.24	1 (11%)	6,11,13	2.36	1 (16%)
2	MLY	B	649	2	9,10,11	3.33	2 (22%)	6,11,13	5.45	3 (50%)
1	MLY	A	164	1	9,10,11	3.52	2 (22%)	6,11,13	6.35	3 (50%)

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	A	62	1	-	1/8/9/11	-
2	MLY	B	614	2	-	1/8/9/11	-
2	MLY	B	649	2	-	2/8/9/11	-
1	MLY	A	164	1	-	2/8/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	MLY	CH2-NZ	-9.87	1.15	1.46
2	B	649	MLY	CH1-NZ	-8.88	1.18	1.46
2	B	614	MLY	CH2-NZ	6.40	1.65	1.46
1	A	62	MLY	CH1-NZ	-4.08	1.33	1.46
2	B	649	MLY	CH2-NZ	3.40	1.56	1.46
1	A	164	MLY	CB-CA	-2.05	1.50	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	MLY	CH2-NZ-CH1	12.87	142.71	109.72
1	A	62	MLY	CH2-NZ-CH1	9.02	132.84	109.72
2	B	649	MLY	CH2-NZ-CH1	8.64	131.86	109.72
2	B	649	MLY	CH1-NZ-CE	7.79	141.63	110.75
1	A	164	MLY	CH1-NZ-CE	-6.54	84.81	110.75
2	B	649	MLY	CH2-NZ-CE	-6.23	86.04	110.75
1	A	164	MLY	CH2-NZ-CE	5.43	132.27	110.75
2	B	614	MLY	CH1-NZ-CE	5.29	131.71	110.75
1	A	62	MLY	CH1-NZ-CE	-3.46	97.05	110.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	614	MLY	O-C-CA-CB
2	B	649	MLY	O-C-CA-CB
1	A	164	MLY	CD-CE-NZ-CH2
2	B	649	MLY	CD-CE-NZ-CH1
1	A	62	MLY	CD-CE-NZ-CH2
1	A	164	MLY	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	649	MLY	1	0
1	A	164	MLY	2	0

5.5 Carbohydrates

There are no oligosaccharides 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 [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	175/211 (82%)	0.02	9 (5%) 33 32	11, 24, 45, 62	0
2	B	79/84 (94%)	0.04	1 (1%) 75 74	13, 25, 52, 69	0
All	All	254/295 (86%)	0.02	10 (3%) 43 42	11, 24, 47, 69	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ARG	6.3
1	A	154	VAL	3.1
2	B	571	GLU	2.8
1	A	34	GLU	2.7
1	A	32	ILE	2.4
1	A	86	ARG	2.3
1	A	193	ASP	2.3
1	A	33	ASN	2.2
1	A	78	SER	2.1
1	A	122	THR	2.0

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, 95th 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	164	11/12	0.88	0.11	21,22,32,32	0
2	MLY	B	614	11/12	0.93	0.09	12,15,21,29	0
2	MLY	B	649	11/12	0.94	0.07	17,20,27,27	0
1	MLY	A	62	11/12	0.97	0.05	15,17,20,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.