WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2023 – 12:17 pm GMT

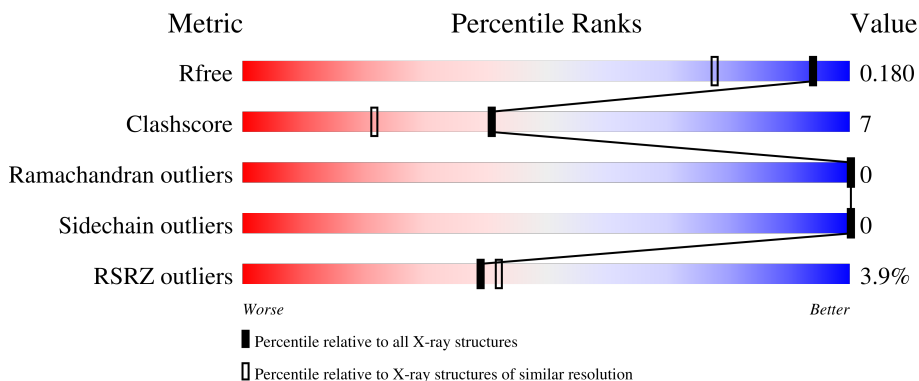|		
PDB ID	:	7NFN
Title	:	A heptameric barrel state of a de novo coiled-coil assembly: CC-Type2-(LaId)4-L21N-I24N.
Authors	:	Rhys, G.G.; Dawson, W.M.; Brady, R.L.; Woolfson, D.N.
Deposited on	:	2021-02-07
Resolution	:	1.45 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
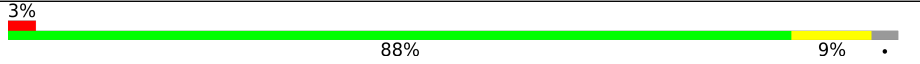*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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.
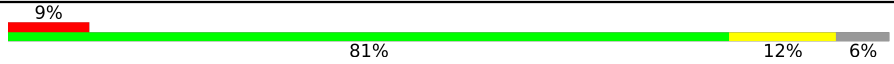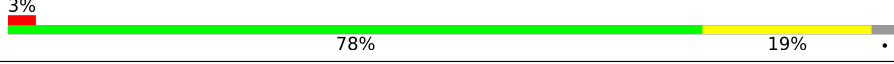
Metric	Percentile Ranks	Value
Rfree		0.180
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		3.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
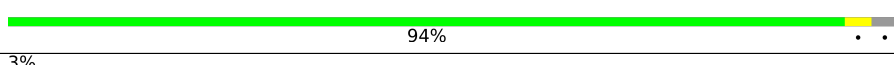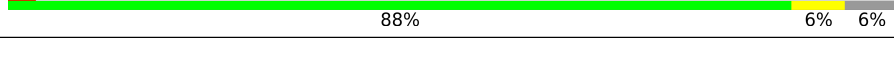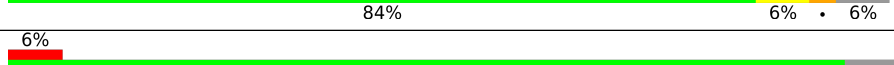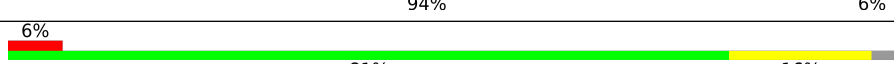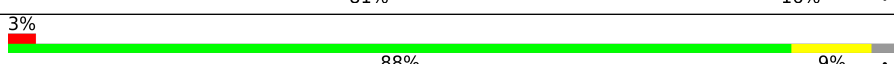
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	32	3% / 88% 9% ·
1	B	32	3% / 88% 9% ·
1	C	32	6% / 88% 9% ·
1	D	32	3% / 81% 12% 6%
1	E	32	78% 16% 6%

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Mol	Chain	Length	Quality of chain
1	F	32	9% / 81% / 12% / 6%
1	G	32	3% / 78% / 19%
1	H	32	94%
1	I	32	3% / 84% / 12%
1	J	32	3% / 88% / 6% / 6%
1	K	32	84% / 6% / 6%
1	L	32	6% / 94% / 6%
1	M	32	6% / 81% / 16%
1	N	32	3% / 88% / 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard 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
2	HEZ	G	101	-	-	X	-
2	HEZ	H	101	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3993 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 CC-Type2-(LaId)4-L21N-I24N.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	31	Total 267	C 164	N 53	O 50	0	4	0
1	B	31	Total 266	C 163	N 53	O 50	0	4	0
1	C	31	Total 273	C 167	N 56	O 50	0	4	0
1	D	30	Total 259	C 162	N 52	O 45	0	3	0
1	E	30	Total 252	C 157	N 49	O 46	0	3	0
1	F	30	Total 238	C 149	N 48	O 41	0	1	0
1	G	31	Total 258	C 159	N 51	O 48	0	3	0
1	H	31	Total 247	C 153	N 47	O 47	0	2	0
1	I	31	Total 255	C 157	N 54	O 44	0	2	0
1	J	30	Total 250	C 155	N 49	O 46	0	2	0
1	K	30	Total 252	C 157	N 49	O 46	0	3	0
1	L	30	Total 250	C 155	N 49	O 46	0	2	0
1	M	31	Total 254	C 157	N 50	O 47	0	2	0
1	N	31	Total 238	C 148	N 47	O 43	0	1	0

- Molecule 2 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).

HEZ
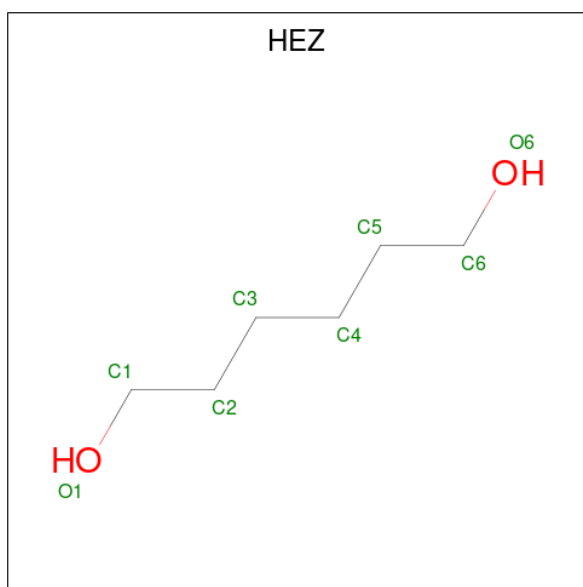
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 8	C 6	O 2	0	0
2	C	1	Total 8	C 6	O 2	0	0
2	D	1	Total 8	C 6	O 2	0	0
2	F	1	Total 8	C 6	O 2	0	0
2	G	1	Total 8	C 6	O 2	0	0
2	H	1	Total 8	C 6	O 2	0	0
2	M	1	Total 8	C 6	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	31	Total 31	O 31	0	0
3	C	27	Total 27	O 27	0	0
3	D	24	Total 24	O 24	0	0
3	E	30	Total 30	O 30	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	17	Total 17	O 17	0	0
3	G	22	Total 22	O 22	0	0
3	H	27	Total 27	O 27	0	0
3	I	34	Total 34	O 34	0	0
3	J	27	Total 27	O 27	0	0
3	K	30	Total 30	O 30	0	0
3	L	26	Total 26	O 26	0	0
3	M	25	Total 25	O 25	0	0
3	N	29	Total 29	O 29	0	0

3 Residue-property plots ⓘ

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: CC-Type2-(LaId)4-L21N-I24N
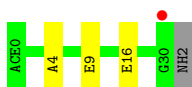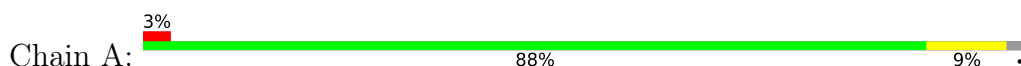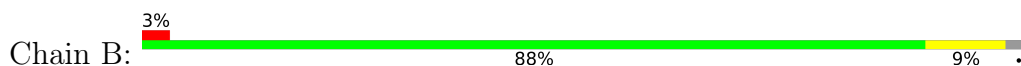
Chain A:

- Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain B:

- Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain C:

- Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain D:

- Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain E:

- Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain F:

9%

81% 12% 6%

ACE0 G1 E2 W19 A25 K26 A27 L28 R29 GLY NH2

• Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain G:

3%

78% 19%

ACE0 G1 E2 I3 A4 R8 E9 W19 R22 G30 NH2

• Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain H:

94%

ACE0 E9 G30 NH2

• Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain I:

3%

84% 12%

ACE0 K5 R8 A11 R29 G30 NH2

• Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain J:

3%

88% 6% 6%

ACE0 E9 R29 GLY NH2

• Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain K:

84% 6% 6%

ACE0 K5 R8 E9 R29 GLY NH2

• Molecule 1: CC-Type2-(LaId)4-L21N-I24N
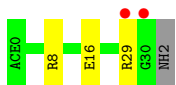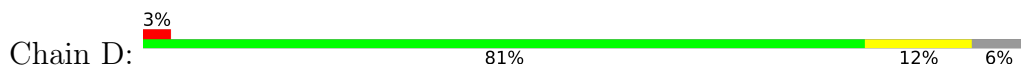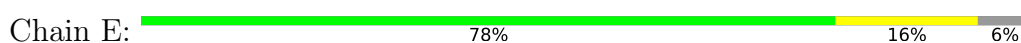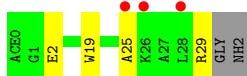
Chain L:

6%

94% 6%

ACE0 L28 R29 GLY NH2

• Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain M:
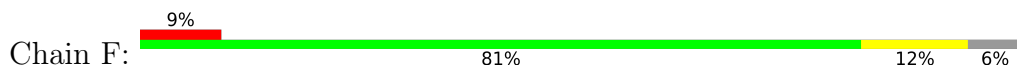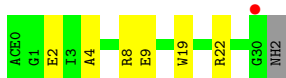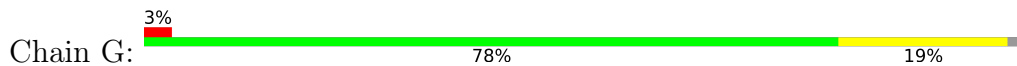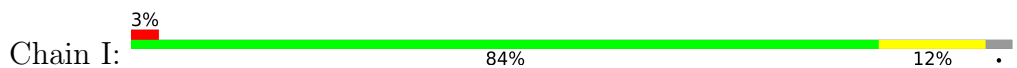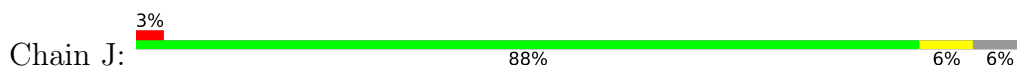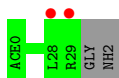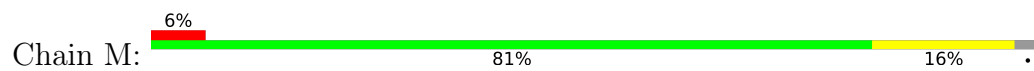
• Molecule 1: CC-Type2-(LaId)4-L21N-I24N

Chain N:
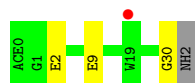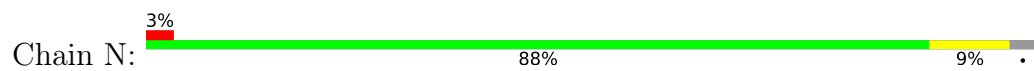
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.90Å 47.91Å 62.28Å 67.39° 67.49° 77.73°	Depositor
Resolution (Å)	44.16 – 1.45 44.12 – 1.45	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.16-1.45) 90.4 (44.12-1.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.134 , 0.178 0.137 , 0.180	Depositor DCC
R_{free} test set	3975 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.4	EDS
L-test for twinning[2]	$< |L| > = 0.54, < L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.430 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3993	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6387e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: HEZ, ACE

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	0.87	0/266	0.89	0/355
1	B	0.78	0/265	0.77	0/353
1	C	0.87	0/272	0.95	1/362 (0.3%)
1	D	0.89	1/258 (0.4%)	0.95	1/342 (0.3%)
1	E	0.81	0/251	0.85	0/335
1	F	0.75	0/237	0.91	0/316
1	G	0.85	0/257	0.84	1/342 (0.3%)
1	H	0.80	0/246	0.83	0/328
1	I	0.78	0/254	0.85	0/338
1	J	0.83	0/249	0.81	0/332
1	K	0.75	0/251	0.87	2/335 (0.6%)
1	L	0.75	0/249	0.89	0/332
1	M	0.78	0/253	0.89	1/337 (0.3%)
1	N	0.92	1/237 (0.4%)	0.94	0/317
All	All	0.82	2/3545 (0.1%)	0.88	6/4724 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	GLU	CD-OE2	5.29	1.31	1.25
1	N	9	GLU	CD-OE2	-5.02	1.20	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	8	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	C	29	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	K	8	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	M	22	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	22	ARG	NE-CZ-NH1	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

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	267	0	269	3	0
1	B	266	0	268	4	0
1	C	273	0	280	1	1
1	D	259	0	278	1	0
1	E	252	0	260	5	0
1	F	238	0	252	5	0
1	G	258	0	263	7	1
1	H	247	0	250	3	0
1	I	255	0	269	4	0
1	J	250	0	259	4	0
1	K	252	0	260	3	0
1	L	250	0	259	0	0
1	M	254	0	262	4	0
1	N	238	0	246	2	0
2	B	8	0	14	0	0
2	C	8	0	14	1	0
2	D	8	0	14	1	0
2	F	8	0	14	3	0
2	G	8	0	13	7	0
2	H	8	0	14	8	0
2	M	8	0	14	2	0
3	A	29	0	0	1	0
3	B	31	0	0	2	0
3	C	27	0	0	0	1
3	D	24	0	0	0	0
3	E	30	0	0	3	1
3	F	17	0	0	2	0
3	G	22	0	0	3	0
3	H	27	0	0	4	0
3	I	34	0	0	3	0
3	J	27	0	0	3	1
3	K	30	0	0	2	0
3	L	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	25	0	0	1	3
3	N	29	0	0	2	0
All	All	3993	0	3772	53	4

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 7.

The worst 5 of 53 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:9[B]:GLU:OE1	1:B:8[B]:ARG:NH1	1.87	1.07
1:I:29:ARG:NH1	3:I:101:HOH:O	1.83	1.00
1:M:9[A]:GLU:OE2	3:M:201:HOH:O	1.80	0.99
1:G:9[B]:GLU:OE2	3:G:201:HOH:O	1.89	0.89
2:H:101:HEZ:H11	3:H:210:HOH:O	1.81	0.80

All (4) 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)
3:E:127:HOH:O	3:M:223:HOH:O[1_455]	1.35	0.85
3:C:223:HOH:O	3:M:215:HOH:O[1_455]	1.88	0.32
1:C:16:GLU:OE2	3:M:215:HOH:O[1_455]	1.97	0.23
1:G:8[B]:ARG:NH1	3:J:125:HOH:O[1_545]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	33/32 (103%)	33 (100%)	0	0	100	100
1	B	33/32 (103%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	33/32 (103%)	33 (100%)	0	0	100	100
1	D	31/32 (97%)	31 (100%)	0	0	100	100
1	E	31/32 (97%)	31 (100%)	0	0	100	100
1	F	29/32 (91%)	29 (100%)	0	0	100	100
1	G	32/32 (100%)	32 (100%)	0	0	100	100
1	H	31/32 (97%)	31 (100%)	0	0	100	100
1	I	31/32 (97%)	31 (100%)	0	0	100	100
1	J	30/32 (94%)	30 (100%)	0	0	100	100
1	K	31/32 (97%)	31 (100%)	0	0	100	100
1	L	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
1	M	31/32 (97%)	30 (97%)	1 (3%)	0	100	100
1	N	30/32 (94%)	30 (100%)	0	0	100	100
All	All	436/448 (97%)	434 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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	23/20 (115%)	23 (100%)	0	100	100
1	B	23/20 (115%)	23 (100%)	0	100	100
1	C	24/20 (120%)	24 (100%)	0	100	100
1	D	23/20 (115%)	23 (100%)	0	100	100
1	E	22/20 (110%)	22 (100%)	0	100	100
1	F	20/20 (100%)	20 (100%)	0	100	100
1	G	22/20 (110%)	22 (100%)	0	100	100
1	H	21/20 (105%)	21 (100%)	0	100	100
1	I	22/20 (110%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	22/20 (110%)	22 (100%)	0	100	100
1	K	22/20 (110%)	22 (100%)	0	100	100
1	L	22/20 (110%)	22 (100%)	0	100	100
1	M	22/20 (110%)	22 (100%)	0	100	100
1	N	20/20 (100%)	20 (100%)	0	100	100
All	All	308/280 (110%)	308 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

7 ligands 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	$\#\|Z\| > 2$
2	HEZ	H	101	-	7,7,7	0.55	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	HEZ	C	101	-	7,7,7	0.27	0	6,6,6	0.24	0
2	HEZ	B	101	-	7,7,7	0.30	0	6,6,6	0.32	0
2	HEZ	D	101	-	7,7,7	0.27	0	6,6,6	0.83	0
2	HEZ	M	101	-	7,7,7	0.38	0	6,6,6	0.81	0
2	HEZ	F	101	-	7,7,7	0.20	0	6,6,6	0.16	0
2	HEZ	G	101	-	7,7,7	0.81	0	6,6,6	0.64	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
2	HEZ	H	101	-	-	3/5/5/5	-
2	HEZ	C	101	-	-	4/5/5/5	-
2	HEZ	B	101	-	-	2/5/5/5	-
2	HEZ	D	101	-	-	2/5/5/5	-
2	HEZ	M	101	-	-	5/5/5/5	-
2	HEZ	F	101	-	-	1/5/5/5	-
2	HEZ	G	101	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	101	HEZ	C3-C4-C5-C6
2	M	101	HEZ	C4-C5-C6-O6
2	M	101	HEZ	C2-C3-C4-C5
2	C	101	HEZ	C3-C4-C5-C6
2	C	101	HEZ	C2-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	101	HEZ	8	0
2	C	101	HEZ	1	0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	101	HEZ	1	0
2	M	101	HEZ	2	0
2	F	101	HEZ	3	0
2	G	101	HEZ	7	0

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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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, 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	30/32 (93%)	0.07	1 (3%)	46	48	12, 17, 37, 60	0
1	B	30/32 (93%)	0.07	1 (3%)	46	48	11, 16, 35, 59	0
1	C	30/32 (93%)	0.12	2 (6%)	17	19	11, 18, 35, 48	0
1	D	29/32 (90%)	-0.13	1 (3%)	45	48	12, 15, 26, 60	0
1	E	29/32 (90%)	-0.16	0	100	100	13, 18, 32, 44	0
1	F	29/32 (90%)	0.25	3 (10%)	6	7	13, 20, 45, 72	0
1	G	30/32 (93%)	-0.08	1 (3%)	46	48	12, 17, 44, 64	0
1	H	30/32 (93%)	-0.15	0	100	100	11, 16, 34, 57	0
1	I	30/32 (93%)	0.05	1 (3%)	46	48	11, 20, 34, 55	0
1	J	29/32 (90%)	-0.13	1 (3%)	45	48	12, 16, 28, 72	0
1	K	29/32 (90%)	-0.19	0	100	100	13, 18, 32, 44	1 (3%)
1	L	29/32 (90%)	0.23	2 (6%)	16	18	13, 20, 42, 64	0
1	M	30/32 (93%)	0.13	2 (6%)	17	19	12, 17, 44, 66	0
1	N	30/32 (93%)	0.10	1 (3%)	46	48	12, 18, 34, 59	0
All	All	414/448 (92%)	0.01	16 (3%)	39	42	11, 18, 44, 72	1 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	30	GLY	6.9
1	B	30	GLY	6.4
1	J	29	ARG	5.5
1	L	28	LEU	4.7
1	D	29	ARG	3.9

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	HEZ	G	101	8/8	0.74	0.29	31,37,47,49	0
2	HEZ	D	101	8/8	0.79	0.13	29,37,45,62	0
2	HEZ	C	101	8/8	0.86	0.16	32,39,56,59	0
2	HEZ	H	101	8/8	0.87	0.15	29,35,47,56	0
2	HEZ	M	101	8/8	0.88	0.14	22,40,67,73	0
2	HEZ	F	101	8/8	0.90	0.19	28,38,60,68	0
2	HEZ	B	101	8/8	0.93	0.09	32,42,50,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.