wwPDB X-ray Structure Validation Summary Report (i)

Mar 6, 2026 – 06:40 PM UTC

PDB ID	:	6UGC / pdb_00006ugc
Title	:	C3 symmetric peptide design number 3
Authors	:	Mulligan, V.K.; Kang, C.S.; Antselovich, I.; Sawaya, M.R.; Yeates, T.O.; Baker, D.
Deposited on	:	2019-09-26
Resolution	:	0.90 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

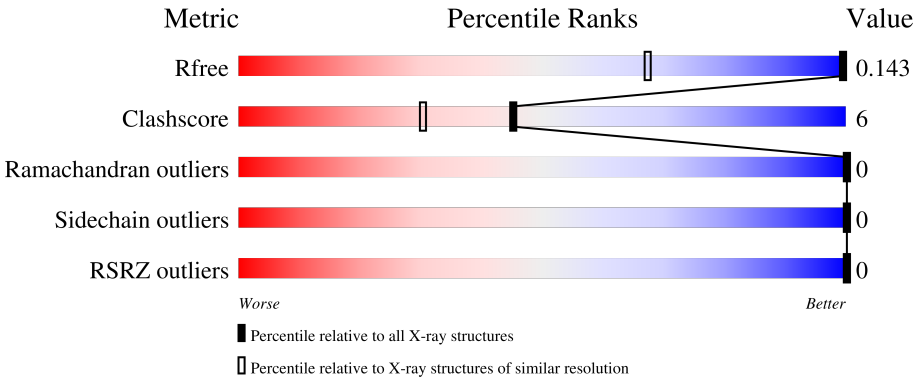
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 0.90 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	1366 (1.00-0.80)
Clashscore	190562	1416 (1.00-0.80)
Ramachandran outliers	187476	1341 (1.00-0.80)
Sidechain outliers	187428	1342 (1.00-0.80)
RSRZ outliers	180081	1363 (1.00-0.80)

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	9	100%
1	B	9	100%
1	C	9	67% 33%
1	D	9	89% 11%
1	E	9	89% 11%

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Mol	Chain	Length	Quality of chain
1	F	9	89% 11%
1	G	9	44% 56%
1	H	9	89% 11%
1	I	9	33% 67%
1	J	9	33% 67%
1	K	9	33% 67%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1284 atoms, of which 444 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 C3-3 cyclic peptide design.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	9	Total	C	H	N	O	0	1	0
			114	39	45	9	21			
1	B	9	Total	C	H	N	O	0	0	0
			114	39	45	9	21			
1	C	9	Total	C	H	N	O	0	3	0
			150	51	57	12	30			
1	D	9	Total	C	H	N	O	0	1	0
			126	43	49	10	24			
1	E	9	Total	C	H	N	O	0	1	0
			126	43	49	10	24			
1	F	9	Total	C	H	N	O	0	1	0
			114	39	45	9	21			
1	G	9	Total	C	H	N	O	0	4	0
			158	54	60	12	32			
1	H	9	Total	C	H	N	O	0	1	0
			126	43	49	10	24			
1	I	3	Total	C	H	N	O	0	0	0
			38	13	15	3	7			
1	J	3	Total	C	H	N	O	0	0	0
			38	13	15	3	7			
1	K	3	Total	C	H	N	O	0	0	0
			38	13	15	3	7			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Na	0	1
			4	4		
2	B	3	Total	Na	0	0
			3	3		
2	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Na 2 2	0	0
2	E	5	Total Na 8 8	0	2
2	F	2	Total Na 2 2	0	0
2	G	1	Total Na 1 1	0	0
2	H	2	Total Na 2 2	0	0
2	I	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0
2	K	1	Total Na 1 1	0	0

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cd 1 1	0	0
3	B	1	Total Cd 1 1	0	0
3	D	1	Total Cd 1 1	0	0
3	E	1	Total Cd 1 1	0	0
3	F	1	Total Cd 1 1	0	0
3	H	1	Total Cd 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 14 14	0	2
4	B	12	Total O 12 12	0	0
4	C	5	Total O 5 5	0	0

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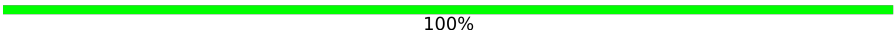
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	16	Total O 17 17	0	1
4	E	12	Total O 12 12	0	0
4	F	12	Total O 12 12	0	0
4	G	5	Total O 5 5	0	0
4	H	8	Total O 8 8	0	0
4	I	8	Total O 9 9	0	1
4	J	7	Total O 7 7	0	0
4	K	9	Total O 9 9	0	0

3 Residue-property plots (i)

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

- Molecule 1: C3-3 cyclic peptide design

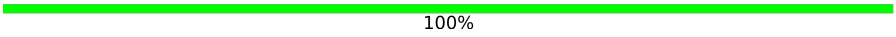
Chain A:



There are no outlier residues recorded for this chain.

- Molecule 1: C3-3 cyclic peptide design

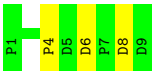
Chain B:



There are no outlier residues recorded for this chain.

- Molecule 1: C3-3 cyclic peptide design

Chain C:



- Molecule 1: C3-3 cyclic peptide design

Chain D:

- Molecule 1: C3-3 cyclic peptide design

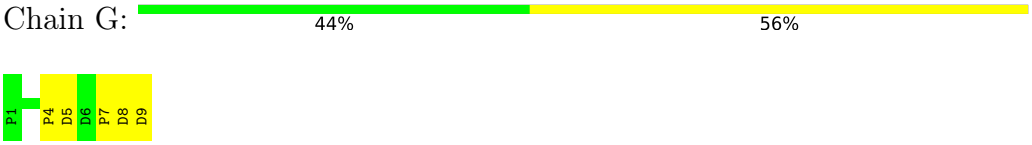
Chain E:

- Molecule 1: C3-3 cyclic peptide design

Chain F:

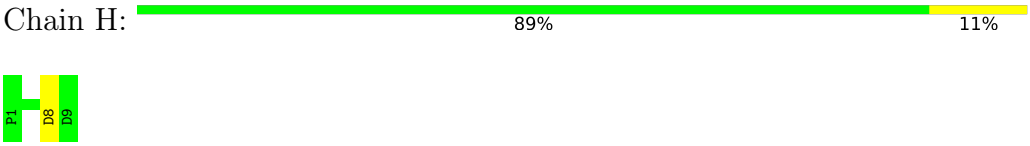
• Molecule 1: C3-3 cyclic peptide design

Chain G:



• Molecule 1: C3-3 cyclic peptide design

Chain H:



• Molecule 1: C3-3 cyclic peptide design

Chain I:

• Molecule 1: C3-3 cyclic peptide design

Chain J:

• Molecule 1: C3-3 cyclic peptide design

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 1 c	Depositor
Cell constants a, b, c, α, β, γ	51.03Å 51.03Å 36.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.51 – 0.90 25.51 – 0.90	Depositor EDS
% Data completeness (in resolution range)	78.7 (25.51-0.90) 78.7 (25.51-0.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.118 , 0.143 0.118 , 0.143	Depositor DCC
R_{free} test set	3065 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 53.1	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	1284	wwPDB-VP
Average B, all atoms (Å^2)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]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: NA, CD

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	0.73	0/71	0.93	0/98
1	B	0.78	0/71	0.96	0/98
1	C	0.58	0/95	0.83	0/131
1	D	0.68	0/79	0.98	0/109
1	E	0.62	0/79	0.90	0/109
1	F	0.82	0/71	1.10	0/98
1	G	0.57	0/103	0.94	0/143
1	H	0.67	0/79	0.92	0/109
1	I	0.85	0/23	0.92	0/30
1	J	0.74	0/23	0.89	0/30
1	K	0.64	0/23	0.96	0/30
All	All	0.68	0/717	0.94	0/985

There are no bond length outliers.

There are no bond angle outliers.

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	69	45	43	0	0
1	B	69	45	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	93	57	53	2	0
1	D	77	49	48	1	0
1	E	77	49	48	1	0
1	F	69	45	43	1	0
1	G	98	60	57	5	0
1	H	77	49	48	1	0
1	I	23	15	17	0	0
1	J	23	15	17	0	0
1	K	23	15	17	0	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	8	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	14	0	0	0	0
4	B	12	0	0	0	0
4	C	5	0	0	0	0
4	D	17	0	0	0	0
4	E	12	0	0	0	0
4	F	12	0	0	0	0
4	G	5	0	0	0	0
4	H	8	0	0	0	0
4	I	9	0	0	0	0
4	J	7	0	0	0	0
4	K	9	0	0	0	0
All	All	840	444	436	7	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 6.

The worst 5 of 7 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:G:7:PRO:C	1:G:8[B]:ASP:CA	2.53	0.80
1:E:2[A]:ASP:OD2	1:G:5[A]:ASP:OD2	2.15	0.65
1:C:4:PRO:HG2	1:D:8[B]:ASP:OD1	2.06	0.56
1:G:8[B]:ASP:CA	1:G:9:ASP:N	2.69	0.55
1:F:1:PRO:HG2	1:G:8[B]:ASP:OD2	2.17	0.45

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	7/9 (78%)	7 (100%)	0	0	100	100
1	B	7/9 (78%)	7 (100%)	0	0	100	100
1	C	10/9 (111%)	10 (100%)	0	0	100	100
1	D	8/9 (89%)	8 (100%)	0	0	100	100
1	E	8/9 (89%)	8 (100%)	0	0	100	100
1	F	7/9 (78%)	7 (100%)	0	0	100	100
1	G	11/9 (122%)	11 (100%)	0	0	100	100
1	H	8/9 (89%)	8 (100%)	0	0	100	100
1	I	1/9 (11%)	1 (100%)	0	0	100	100
1	J	1/9 (11%)	1 (100%)	0	0	100	100
1	K	1/9 (11%)	1 (100%)	0	0	100	100
All	All	69/99 (70%)	69 (100%)	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	9/9 (100%)	9 (100%)	0	100	100
1	B	9/9 (100%)	9 (100%)	0	100	100
1	C	12/9 (133%)	12 (100%)	0	100	100
1	D	10/9 (111%)	10 (100%)	0	100	100
1	E	10/9 (111%)	10 (100%)	0	100	100
1	F	9/9 (100%)	9 (100%)	0	100	100
1	G	13/9 (144%)	13 (100%)	0	100	100
1	H	10/9 (111%)	10 (100%)	0	100	100
1	I	3/9 (33%)	3 (100%)	0	100	100
1	J	3/9 (33%)	3 (100%)	0	100	100
1	K	3/9 (33%)	3 (100%)	0	100	100
All	All	91/99 (92%)	91 (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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	9/9 (100%)	-0.27	0	100	100	5, 6, 8, 9	0
1	B	9/9 (100%)	-0.13	0	100	100	5, 6, 9, 9	0
1	C	9/9 (100%)	0.30	0	100	100	2, 5, 9, 9	2 (22%)
1	D	9/9 (100%)	-0.24	0	100	100	3, 6, 8, 8	1 (11%)
1	E	9/9 (100%)	-0.27	0	100	100	3, 5, 8, 9	1 (11%)
1	F	9/9 (100%)	-0.21	0	100	100	5, 6, 9, 9	0
1	G	9/9 (100%)	0.14	0	100	100	2, 5, 8, 11	3 (33%)
1	H	9/9 (100%)	-0.14	0	100	100	3, 6, 6, 14	1 (11%)
1	I	3/9 (33%)	-0.70	0	100	100	5, 5, 6, 7	0
1	J	3/9 (33%)	-0.39	0	100	100	6, 6, 7, 8	0
1	K	3/9 (33%)	-0.45	0	100	100	6, 6, 6, 7	0
All	All	81/99 (81%)	-0.15	0	100	100	2, 6, 9, 14	8 (9%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands (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
2	NA	B	103	1/1	0.91	0.20	19,19,19,19	0
2	NA	F	102	1/1	0.94	0.20	17,17,17,17	0
2	NA	A	103	1/1	0.95	0.16	13,13,13,13	0
2	NA	E	104	1/1	0.96	0.15	14,14,14,14	0
2	NA	D	102	1/1	0.97	0.23	13,13,13,13	0
2	NA	A	102[B]	1/1	0.98	0.21	4,4,4,4	1
2	NA	A	102[A]	1/1	0.98	0.21	11,11,11,11	1
2	NA	H	102	1/1	0.98	0.21	15,15,15,15	0
2	NA	E	103[A]	1/1	0.99	0.08	1,1,1,1	1
2	NA	E	103[B]	1/1	0.99	0.08	1,1,1,1	1
2	NA	E	103[C]	1/1	0.99	0.08	3,3,3,3	1
2	NA	E	102	1/1	1.00	0.03	2,2,2,2	0
2	NA	B	102	1/1	1.00	0.04	2,2,2,2	0
2	NA	A	101	1/1	1.00	0.01	3,3,3,3	0
2	NA	C	101	1/1	1.00	0.01	5,5,5,5	0
2	NA	D	101	1/1	1.00	0.01	4,4,4,4	0
2	NA	E	105[A]	1/1	1.00	0.08	7,7,7,7	1
2	NA	E	105[B]	1/1	1.00	0.08	9,9,9,9	1
2	NA	F	101	1/1	1.00	0.01	4,4,4,4	0
2	NA	B	101	1/1	1.00	0.01	5,5,5,5	0
2	NA	G	101	1/1	1.00	0.01	5,5,5,5	0
2	NA	H	101	1/1	1.00	0.01	5,5,5,5	0
2	NA	E	101	1/1	1.00	0.01	4,4,4,4	0
2	NA	I	101	1/1	1.00	0.01	4,4,4,4	1
2	NA	J	101	1/1	1.00	0.03	4,4,4,4	1
2	NA	K	101	1/1	1.00	0.07	4,4,4,4	1
3	CD	A	104	1/1	1.00	0.01	4,4,4,4	0
3	CD	B	104	1/1	1.00	0.00	5,5,5,5	0
3	CD	D	103	1/1	1.00	0.01	4,4,4,4	0
3	CD	E	106	1/1	1.00	0.01	5,5,5,5	0
3	CD	F	103	1/1	1.00	0.01	4,4,4,4	0
3	CD	H	103	1/1	1.00	0.01	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.