W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2023 – 09:21 am GMT

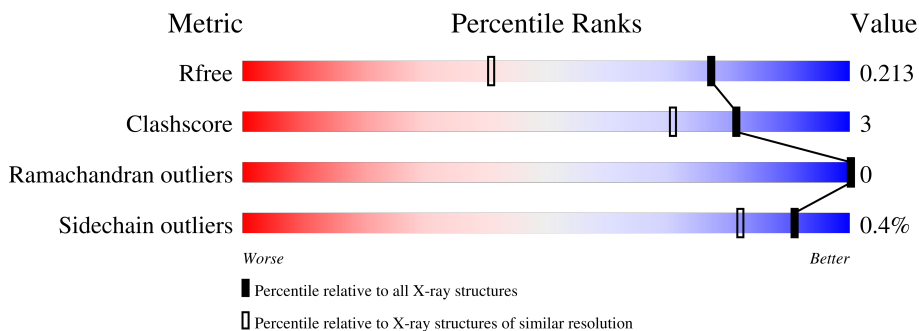|		
PDB ID	:	6IAM
Title	:	Modulating Protein-Protein Interactions with Visible Light Peptide Backbone Switches
Authors	:	Werel, L.; Essen, L.-O.
Deposited on	:	2018-11-27
Resolution	:	1.51 Å(reported)

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 1.51 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		0.213
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.4%

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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)

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%

Mol	Chain	Length	Quality of chain
1	A	306	95% 5%
2	B	12	75% 17% 8%
3	C	4	100%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5458 atoms, of which 2509 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 WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total 4765	C 1524	H 2374	N 400	O 456	S 11	0	4	0

- Molecule 2 is a protein called SER-ALA-ARG-ALA-XY5-VAL-HIS-LEU-ARG-LYS-SER-ALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total 202	C 63	H 102	N 24	O 13	0	0	1

- Molecule 3 is a protein called Small ubiquitin-related modifier 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	4	Total 63	C 19	H 33	N 5	O 6	0	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	K 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Na 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	395	Total 395	O 395	0	0
6	B	19	Total 19	O 19	0	0
6	C	9	Total 9	O 9	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. 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. 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: WD repeat-containing protein 5

Chain A:

95%   5%

T29 P30 V31   L41   G57   C195   Q204   I210 D211   V217   I229   Y243   F263   E322   I327   C334

• Molecule 2: SER-ALA-ARG-ALA-XY5-VAL-HIS-LEU-ARG-LYS-SER-ALA

Chain B:

75%   17%   8%

S1   A4 XY55 V6   A12
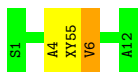
• Molecule 3: Small ubiquitin-related modifier 5

Chain C:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.53Å 46.56Å 66.17Å 90.00° 107.22° 90.00°	Depositor
Resolution (Å)	37.49 – 1.51 44.44 – 1.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.49-1.51) 99.3 (44.44-1.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 1.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.148 , 0.170 0.207 , 0.213	Depositor DCC
R_{free} test set	2053 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	11.3	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.0	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	0.95	EDS
Total number of atoms	5458	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: NA, K, XY5

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	0.38	0/2460	0.67	0/3336
2	B	1.19	2/78 (2.6%)	2.15	3/101 (3.0%)
3	C	0.55	0/30	0.65	0/39
All	All	0.43	2/2568 (0.1%)	0.75	3/3476 (0.1%)

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
2	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	VAL	CA-CB	7.05	1.69	1.54
2	B	6	VAL	CA-C	-6.79	1.35	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6	VAL	N-CA-C	15.17	151.97	111.00
2	B	6	VAL	CB-CA-C	-9.07	94.17	111.40
2	B	6	VAL	CA-C-N	-7.96	99.70	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	4	ALA	Peptide
2	B	5	XY5	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	2391	2374	2373	12	0
2	B	100	102	88	1	0
3	C	30	33	33	0	0
4	A	3	0	0	0	0
5	A	2	0	0	0	0
6	A	395	0	0	8	2
6	B	19	0	0	0	0
6	C	9	0	0	0	0
All	All	2949	2509	2494	13	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 3.

The worst 5 of 13 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:322:GLU:OE2	6:A:501:HOH:O	1.76	1.02
1:A:204:GLN:OE1	6:A:502:HOH:O	1.78	0.99
1:A:195[B]:CYS:SG	1:A:217:VAL:HG11	2.25	0.77
1:A:211:ASP:OD2	6:A:504:HOH:O	2.13	0.66
1:A:229:ILE:HD12	1:A:243:TYR:HB3	1.84	0.58

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)
6:A:659:HOH:O	6:A:803:HOH:O[2_444]	1.96	0.24
6:A:713:HOH:O	6:A:853:HOH:O[2_444]	2.04	0.16

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	308/306 (101%)	296 (96%)	12 (4%)	0	100	100
2	B	9/12 (75%)	9 (100%)	0	0	100	100
3	C	2/4 (50%)	2 (100%)	0	0	100	100
All	All	319/322 (99%)	307 (96%)	12 (4%)	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	272/268 (102%)	271 (100%)	1 (0%)	91	82
2	B	8/8 (100%)	8 (100%)	0	100	100
3	C	3/3 (100%)	3 (100%)	0	100	100
All	All	283/279 (101%)	282 (100%)	1 (0%)	91	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ILE

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 ⓘ

Of 5 ligands modelled in this entry, 5 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.