



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2021 – 08:05 am BST

PDB ID : 6SWU
Title : Crystal structure of the TPR domain of KLC1 in complex with an engineered high-affinity cargo peptide.
Authors : Chegkazi, M.S.; Steiner, R.A.
Deposited on : 2019-09-23
Resolution : 2.85 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 ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

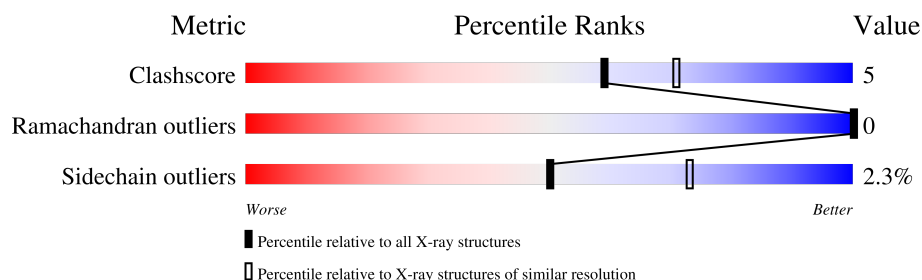
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	343	<div> <div>74%</div> <div>11%</div> <div>14%</div> </div>
1	B	343	<div> <div>76%</div> <div>7%</div> <div>16%</div> </div>
1	C	343	<div> <div>73%</div> <div>10%</div> <div>16%</div> </div>
1	D	343	<div> <div>73%</div> <div>10%</div> <div>16%</div> </div>
1	E	343	<div> <div>72%</div> <div>10%</div> <div>18%</div> </div>
1	F	343	<div> <div>74%</div> <div>8%</div> <div>18%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27765 atoms, of which 13832 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 Kinesin light chain 1, Kinesin light chain 1, TPR domain of kinesin light chain 1 in complex with an engineered high-affinity cargo peptide of sequence TVFTTEDIYEWDDSAI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	H	N	O	S	117	0	0
			4709	1479	2352	418	451	9			
1	B	288	Total	C	H	N	O	S	113	1	0
			4639	1456	2322	412	440	9			
1	C	287	Total	C	H	N	O	S	114	0	0
			4588	1446	2289	404	440	9			
1	D	287	Total	C	H	N	O	S	114	0	0
			4602	1449	2297	407	440	9			
1	E	281	Total	C	H	N	O	S	112	0	0
			4501	1416	2246	400	431	8			
1	F	281	Total	C	H	N	O	S	112	0	0
			4510	1419	2252	400	431	8			

There are 24 discrepancies between the modelled and reference sequences:

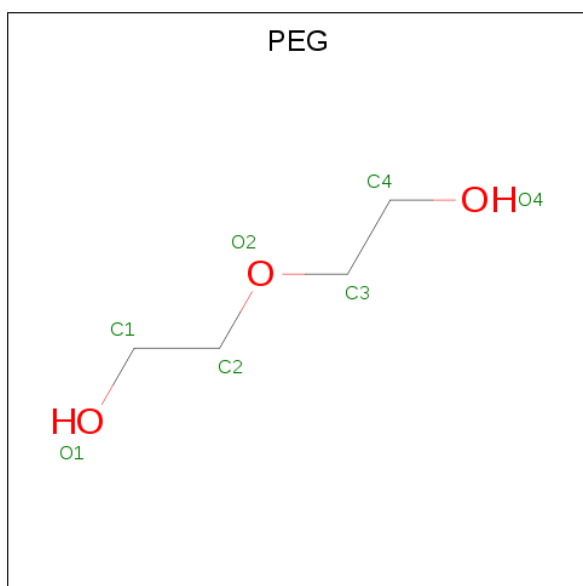
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLY	-	expression tag	UNP Q5UE59
A	202	SER	-	expression tag	UNP Q5UE59
A	203	HIS	-	expression tag	UNP Q5UE59
A	204	MET	-	expression tag	UNP Q5UE59
B	201	GLY	-	expression tag	UNP Q5UE59
B	202	SER	-	expression tag	UNP Q5UE59
B	203	HIS	-	expression tag	UNP Q5UE59
B	204	MET	-	expression tag	UNP Q5UE59
C	201	GLY	-	expression tag	UNP Q5UE59
C	202	SER	-	expression tag	UNP Q5UE59
C	203	HIS	-	expression tag	UNP Q5UE59
C	204	MET	-	expression tag	UNP Q5UE59
D	201	GLY	-	expression tag	UNP Q5UE59
D	202	SER	-	expression tag	UNP Q5UE59
D	203	HIS	-	expression tag	UNP Q5UE59

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Chain	Residue	Modelled	Actual	Comment	Reference
D	204	MET	-	expression tag	UNP Q5UE59
E	201	GLY	-	expression tag	UNP Q5UE59
E	202	SER	-	expression tag	UNP Q5UE59
E	203	HIS	-	expression tag	UNP Q5UE59
E	204	MET	-	expression tag	UNP Q5UE59
F	201	GLY	-	expression tag	UNP Q5UE59
F	202	SER	-	expression tag	UNP Q5UE59
F	203	HIS	-	expression tag	UNP Q5UE59
F	204	MET	-	expression tag	UNP Q5UE59

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	1	0
			17	4	10	3		
2	A	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	D	1	Total	C	H	O	1	0
			10	2	6	2		
3	D	1	Total	C	H	O	1	0
			10	2	6	2		
3	D	1	Total	C	H	O	1	0
			10	2	6	2		
3	E	1	Total	C	H	O	1	0
			10	2	6	2		
3	F	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	19	Total	O	0	0
			19	19		
4	C	18	Total	O	0	0
			18	18		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	13	Total 13	O 13	0	0
4	E	3	Total 3	O 3	0	0
4	F	13	Total 13	O 13	0	0

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.73Å 107.53Å 222.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.33 – 2.85	Depositor
% Data completeness (in resolution range)	99.2 (111.33-2.85)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.202 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27765	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.67	0/2398	0.82	0/3233
1	B	0.69	0/2359	0.82	0/3180
1	C	0.68	0/2340	0.81	1/3160 (0.0%)
1	D	0.66	0/2346	0.79	1/3167 (0.0%)
1	E	0.65	0/2294	0.78	1/3094 (0.0%)
1	F	0.65	0/2297	0.78	0/3099
All	All	0.67	0/14034	0.80	3/18933 (0.0%)

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	D	0	1
1	E	0	2
1	F	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	433	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	475	ARG	CG-CD-NE	-6.02	99.15	111.80
1	C	542	ALA	CA-C-O	5.30	131.23	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	312	LYS	Mainchain
1	E	311	GLY	Peptide
1	E	332	GLY	Mainchain
1	F	311	GLY	Peptide

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	2357	2352	2343	26	0
1	B	2317	2322	2312	16	0
1	C	2299	2289	2279	24	0
1	D	2305	2297	2287	21	0
1	E	2255	2246	2236	24	0
1	F	2258	2252	2241	22	0
2	A	14	20	20	0	0
3	C	16	24	24	0	0
3	D	12	18	18	0	0
3	E	4	6	6	0	0
3	F	4	6	6	0	0
4	A	26	0	0	0	0
4	B	19	0	0	1	0
4	C	18	0	0	0	0
4	D	13	0	0	0	0
4	E	3	0	0	0	0
4	F	13	0	0	0	0
All	All	13933	13832	13772	129	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 5.

The worst 5 of 129 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:E:412:HIS:HE1	1:E:423:ASN:OD1	1.35	1.09
1:B:236:CYS:SG	1:B:257:MET:HE1	1.96	1.05
1:E:412:HIS:CE1	1:E:423:ASN:OD1	2.13	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:CYS:SG	1:B:257:MET:CE	2.50	0.99
1:D:313:TYR:OH	1:D:351:ASN:ND2	1.96	0.97

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	288/343 (84%)	286 (99%)	2 (1%)	0	100	100
1	B	281/343 (82%)	277 (99%)	4 (1%)	0	100	100
1	C	281/343 (82%)	279 (99%)	2 (1%)	0	100	100
1	D	281/343 (82%)	278 (99%)	3 (1%)	0	100	100
1	E	273/343 (80%)	270 (99%)	3 (1%)	0	100	100
1	F	273/343 (80%)	271 (99%)	2 (1%)	0	100	100
All	All	1677/2058 (82%)	1661 (99%)	16 (1%)	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	247/279 (88%)	244 (99%)	3 (1%)	71	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	243/279 (87%)	236 (97%)	7 (3%)	42	67
1	C	241/279 (86%)	235 (98%)	6 (2%)	47	71
1	D	242/279 (87%)	236 (98%)	6 (2%)	47	71
1	E	236/279 (85%)	231 (98%)	5 (2%)	53	75
1	F	237/279 (85%)	231 (98%)	6 (2%)	47	71
All	All	1446/1674 (86%)	1413 (98%)	33 (2%)	50	73

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	243	LEU
1	F	247	SER
1	F	537	GLU
1	C	263	LEU
1	C	247	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	226	GLN
1	F	385	ASN
1	D	363	GLN
1	F	259	ASN
1	D	351	ASN

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

11 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	$\# Z > 2$
3	EDO	F	601	-	3,3,3	0.18	0	2,2,2	0.33	0
3	EDO	D	603	-	3,3,3	0.12	0	2,2,2	0.27	0
3	EDO	C	602	-	3,3,3	0.17	0	2,2,2	0.34	0
3	EDO	C	603	-	3,3,3	0.12	0	2,2,2	0.17	0
3	EDO	C	604	-	3,3,3	0.18	0	2,2,2	0.43	0
3	EDO	E	601	-	3,3,3	0.09	0	2,2,2	0.23	0
3	EDO	C	601	-	3,3,3	0.14	0	2,2,2	0.33	0
3	EDO	D	602	-	3,3,3	0.07	0	2,2,2	0.18	0
3	EDO	D	601	-	3,3,3	0.10	0	2,2,2	0.24	0
2	PEG	A	601	-	6,6,6	0.18	0	5,5,5	0.08	0
2	PEG	A	602	-	6,6,6	0.24	0	5,5,5	0.13	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
3	EDO	F	601	-	-	0/1/1/1	-
3	EDO	D	603	-	-	0/1/1/1	-
3	EDO	C	602	-	-	0/1/1/1	-
3	EDO	C	603	-	-	1/1/1/1	-
3	EDO	C	604	-	-	0/1/1/1	-
3	EDO	E	601	-	-	0/1/1/1	-
3	EDO	C	601	-	-	0/1/1/1	-
3	EDO	D	602	-	-	1/1/1/1	-
3	EDO	D	601	-	-	0/1/1/1	-
2	PEG	A	601	-	-	3/4/4/4	-
2	PEG	A	602	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	PEG	O2-C3-C4-O4
2	A	601	PEG	O1-C1-C2-O2
2	A	601	PEG	O2-C3-C4-O4
2	A	602	PEG	O1-C1-C2-O2
3	C	603	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.