Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 05:02 AM EST

PDB ID	:	3O2T
Title	:	Crystal structure of the N-terminal domain of human Symplekin
Authors	:	Tong, L.; Xiang, K.; Xiang, S.
Deposited on	:	2010-07-22
Resolution	:	1.40 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 (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:

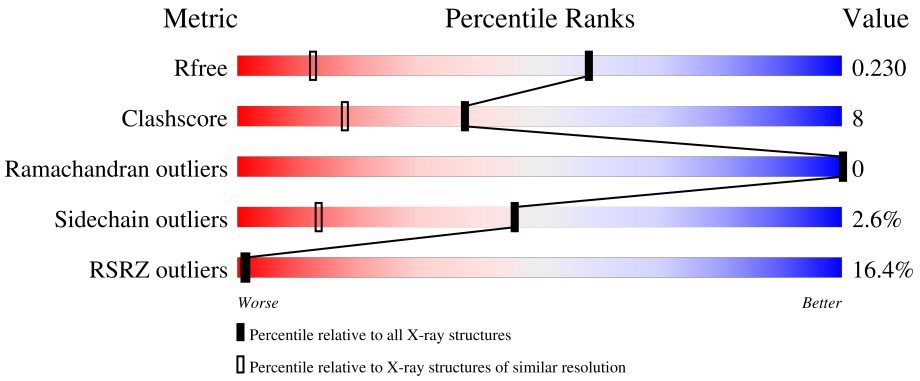
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	386	13% 68% 9% · 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2745 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.

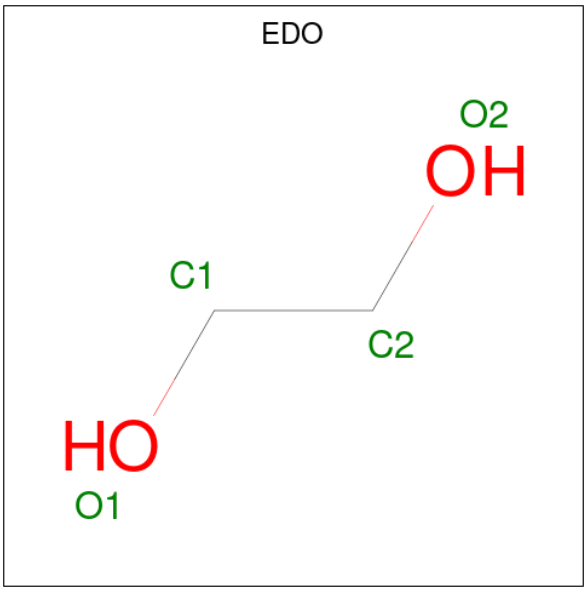
- Molecule 1 is a protein called Symplekin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2409	1535	412	449	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	expression tag	UNP Q92797
A	11	GLY	-	expression tag	UNP Q92797
A	12	SER	-	expression tag	UNP Q92797
A	13	SER	-	expression tag	UNP Q92797
A	14	HIS	-	expression tag	UNP Q92797
A	15	HIS	-	expression tag	UNP Q92797
A	16	HIS	-	expression tag	UNP Q92797
A	17	HIS	-	expression tag	UNP Q92797
A	18	HIS	-	expression tag	UNP Q92797
A	19	HIS	-	expression tag	UNP Q92797
A	20	SER	-	expression tag	UNP Q92797
A	21	SER	-	expression tag	UNP Q92797
A	22	GLY	-	expression tag	UNP Q92797
A	23	LEU	-	expression tag	UNP Q92797
A	24	VAL	-	expression tag	UNP Q92797
A	25	PRO	-	expression tag	UNP Q92797
A	26	ARG	-	expression tag	UNP Q92797
A	27	GLY	-	expression tag	UNP Q92797
A	28	SER	-	expression tag	UNP Q92797
A	29	HIS	-	expression tag	UNP Q92797

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0

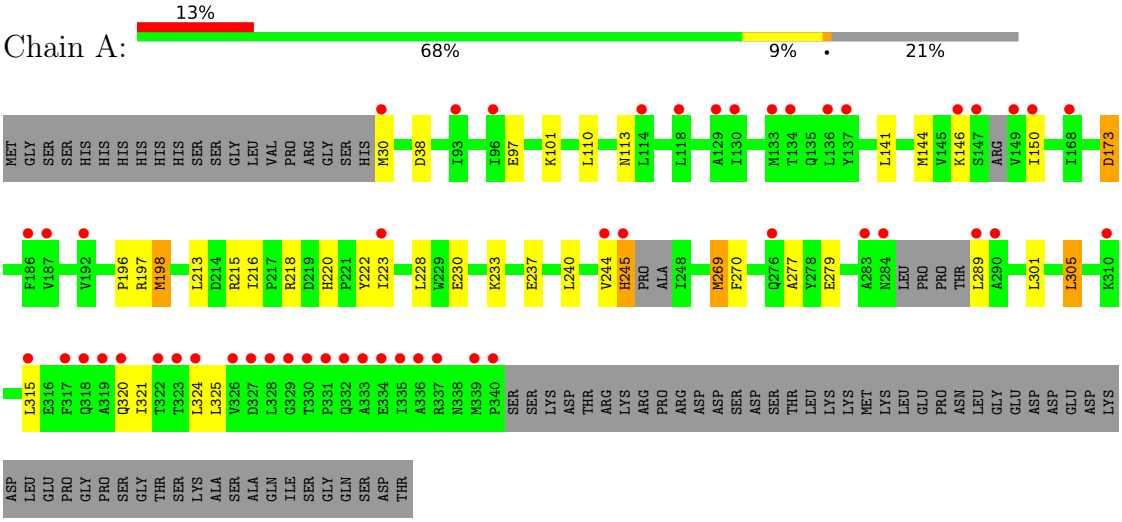
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	332	Total O 332 332	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: Symplekin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.60Å 63.03Å 62.28Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	30.00 – 1.40 28.12 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-1.40) 98.6 (28.12-1.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.159 , 0.192 0.202 , 0.230	Depositor DCC
R_{free} test set	3181 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.000 for -h,l,k 0.027 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2745	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: EDO

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	0.68	1/2439 (0.0%)	0.77	4/3298 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	ASP	CB-CG	-6.89	1.37	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	198	MET	CG-SD-CE	-8.13	87.20	100.20
1	A	218	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	218	ARG	CG-CD-NE	-5.22	100.84	111.80

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	2409	0	2506	38	0
2	A	4	0	6	0	0
3	A	332	0	0	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2745	0	2512	38	1

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 8.

All (38) 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:150:ILE:HD11	3:A:696:HOH:O	1.33	1.25
1:A:245:HIS:HD2	3:A:505:HOH:O	1.16	1.21
1:A:220:HIS:CD2	1:A:223:ILE:HG22	1.91	1.04
1:A:245:HIS:CD2	3:A:505:HOH:O	1.94	1.03
1:A:144:MET:SD	3:A:696:HOH:O	2.34	0.85
1:A:146:LYS:HD3	3:A:397:HOH:O	1.78	0.82
1:A:30:MET:N	3:A:661:HOH:O	2.12	0.81
1:A:220:HIS:HD2	1:A:223:ILE:H	1.37	0.70
1:A:233:LYS:HE3	1:A:270:PHE:HE1	1.57	0.69
1:A:230:GLU:HG2	3:A:463:HOH:O	1.95	0.66
1:A:220:HIS:CG	1:A:223:ILE:HG22	2.30	0.66
1:A:223:ILE:HD11	1:A:228:LEU:HD11	1.81	0.62
1:A:101:LYS:HG2	3:A:542:HOH:O	2.00	0.62
1:A:233:LYS:HE3	1:A:270:PHE:CE1	2.35	0.62
1:A:150:ILE:CD1	3:A:696:HOH:O	2.09	0.60
1:A:244:VAL:O	1:A:244:VAL:HG12	2.01	0.59
1:A:146:LYS:HG3	3:A:492:HOH:O	2.03	0.58
1:A:305:LEU:HD22	1:A:321:ILE:HG23	1.86	0.57
1:A:97:GLU:O	1:A:101:LYS:HG3	2.07	0.55
1:A:305:LEU:HD13	1:A:325:LEU:HG	1.88	0.55
1:A:220:HIS:CD2	1:A:223:ILE:H	2.21	0.54
1:A:240:LEU:HD22	1:A:277:ALA:HB2	1.89	0.53
1:A:233:LYS:O	1:A:237:GLU:HG3	2.10	0.52
1:A:198:MET:SD	1:A:269:MET:HG3	2.53	0.48
1:A:213:LEU:HD12	1:A:216:ILE:HD12	1.96	0.46
1:A:141:LEU:HD22	3:A:399:HOH:O	2.15	0.46
1:A:146:LYS:CD	3:A:397:HOH:O	2.50	0.45
1:A:244:VAL:O	1:A:244:VAL:CG1	2.64	0.44
1:A:197:ARG:HD3	1:A:215:ARG:HH12	1.83	0.44
1:A:233:LYS:HD3	3:A:617:HOH:O	2.18	0.44
1:A:289:LEU:HD12	1:A:289:LEU:O	2.18	0.44
1:A:289:LEU:HD12	1:A:289:LEU:C	2.39	0.42
1:A:279:GLU:CD	1:A:320:GLN:HE21	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD11	3:A:398:HOH:O	2.20	0.41
1:A:110:LEU:HA	1:A:113:ASN:HD22	1.85	0.41
1:A:141:LEU:CD1	1:A:223:ILE:HD13	2.51	0.41
1:A:196:PRO:HD2	1:A:269:MET:CE	2.52	0.40
1:A:220:HIS:CD2	1:A:222:TYR:H	2.39	0.40

All (1) 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:A:468:HOH:O	3:A:657:HOH:O[2_655]	1.88	0.32

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	296/386 (77%)	295 (100%)	1 (0%)	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	272/344 (79%)	265 (97%)	7 (3%)	46	13

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	173	ASP
1	A	245	HIS
1	A	269	MET
1	A	305	LEU
1	A	315	LEU
1	A	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	113	ASN
1	A	142	GLN
1	A	220	HIS
1	A	245	HIS
1	A	282	HIS
1	A	318	GLN
1	A	320	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	EDO	A	1	-	3,3,3	0.76	0	2,2,2	0.19	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	EDO	A	1	-	-	0/1/1/1	-

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 (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

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	304/386 (78%)	0.76	50 (16%) 1 1	5, 14, 26, 30	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	VAL	8.3
1	A	289	LEU	6.8
1	A	336	ALA	6.0
1	A	315	LEU	5.9
1	A	245	HIS	5.1
1	A	340	PRO	4.8
1	A	150	ILE	4.8
1	A	326	VAL	4.8
1	A	333	ALA	4.8
1	A	332	GLN	4.7
1	A	244	VAL	4.7
1	A	322	THR	4.6
1	A	337	ARG	4.3
1	A	290	ALA	4.0
1	A	319	ALA	3.9
1	A	331	PRO	3.7
1	A	284	ASN	3.6
1	A	130	ILE	3.3
1	A	335	ILE	3.3
1	A	147	SER	3.2
1	A	328	LEU	3.1
1	A	318	GLN	3.0
1	A	93	ILE	3.0
1	A	283	ALA	3.0
1	A	30	MET	3.0
1	A	330	THR	2.9
1	A	223	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	327	ASP	2.8
1	A	146	LYS	2.8
1	A	114	LEU	2.8
1	A	323	THR	2.8
1	A	96	ILE	2.8
1	A	339	MET	2.7
1	A	187	VAL	2.6
1	A	334	GLU	2.6
1	A	310	LYS	2.6
1	A	129	ALA	2.6
1	A	192	VAL	2.6
1	A	186	PHE	2.5
1	A	320	GLN	2.5
1	A	276	GLN	2.4
1	A	317	PHE	2.3
1	A	133	MET	2.3
1	A	324	LEU	2.3
1	A	137	TYR	2.3
1	A	118	LEU	2.2
1	A	329	GLY	2.2
1	A	136	LEU	2.2
1	A	168	ILE	2.2
1	A	134	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	1	4/4	0.96	0.23	15,16,16,17	0

6.5 Other polymers (i)

There are no such residues in this entry.