



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:07 AM UTC

PDB ID : 6OEC / pdb_00006oec
Title : Yeast Spc42 Trimeric Coiled-Coil Amino Acids 181-211 fused to PDB: 3H5I
Authors : Drennan, A.C.; Shivaani, K.; Seeger, M.A.; Andreas, M.P.; Gardner, J.M.;
Sether, E.K.R.; Jasperson, S.L.; Rayment, I.
Deposited on : 2019-03-27
Resolution : 2.51 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

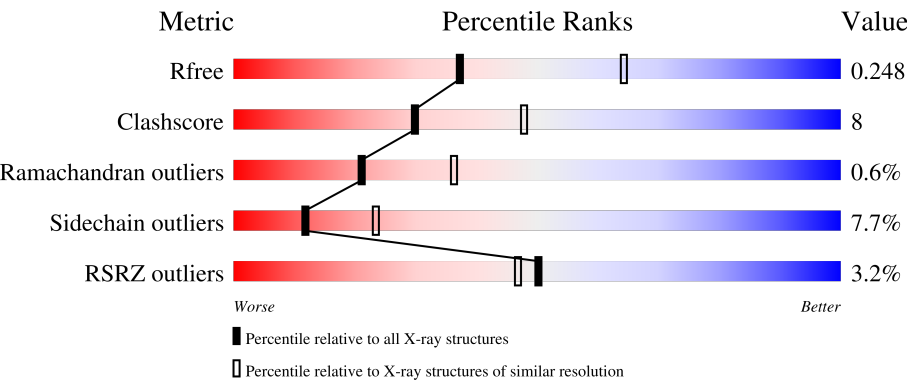
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.51 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 $\leq 5\%$. 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	162	% 77%18% ••
1	B	162	3% 77%19% ••
1	C	162	6% 67%24% •6%
1	D	162	% 72%23% ••
1	E	162	2% 75%19% ••

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Mol	Chain	Length	Quality of chain
1	F	162	
1	G	162	
1	H	162	
1	I	162	
1	J	162	
1	K	162	
1	L	162	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14397 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 Response regulator/sensory box protein/GGDEF domain protein, Spindle pole body component SPC42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1213	773	197	238	5			
1	B	158	Total	C	N	O	S	0	0	0
			1221	778	196	241	6			
1	C	153	Total	C	N	O	S	0	0	0
			1189	761	190	232	6			
1	D	156	Total	C	N	O	S	0	0	0
			1213	773	197	238	5			
1	E	157	Total	C	N	O	S	0	0	0
			1218	777	198	237	6			
1	F	149	Total	C	N	O	S	0	0	0
			1158	745	185	222	6			
1	G	149	Total	C	N	O	S	0	0	0
			1164	745	189	225	5			
1	H	150	Total	C	N	O	S	0	0	0
			1166	749	186	225	6			
1	I	153	Total	C	N	O	S	0	0	0
			1194	764	193	231	6			
1	J	152	Total	C	N	O	S	0	0	0
			1186	760	192	228	6			
1	K	151	Total	C	N	O	S	0	0	0
			1175	754	188	227	6			
1	L	162	Total	C	N	O	S	0	0	0
			1247	792	203	246	6			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q3ADQ4
A	-2	ALA	-	expression tag	UNP Q3ADQ4
A	-1	SER	-	expression tag	UNP Q3ADQ4
A	0	ALA	-	expression tag	UNP Q3ADQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q3ADQ4
A	2	SER	-	expression tag	UNP Q3ADQ4
A	3	LEU	-	expression tag	UNP Q3ADQ4
A	133	GLU	-	linker	UNP Q3ADQ4
A	134	GLY	-	linker	UNP Q3ADQ4
A	193	GLU	THR	engineered mutation	UNP P36094
A	195	GLU	SER	engineered mutation	UNP P36094
B	-3	GLY	-	expression tag	UNP Q3ADQ4
B	-2	ALA	-	expression tag	UNP Q3ADQ4
B	-1	SER	-	expression tag	UNP Q3ADQ4
B	0	ALA	-	expression tag	UNP Q3ADQ4
B	1	MET	-	expression tag	UNP Q3ADQ4
B	2	SER	-	expression tag	UNP Q3ADQ4
B	3	LEU	-	expression tag	UNP Q3ADQ4
B	133	GLU	-	linker	UNP Q3ADQ4
B	134	GLY	-	linker	UNP Q3ADQ4
B	193	GLU	THR	engineered mutation	UNP P36094
B	195	GLU	SER	engineered mutation	UNP P36094
C	-3	GLY	-	expression tag	UNP Q3ADQ4
C	-2	ALA	-	expression tag	UNP Q3ADQ4
C	-1	SER	-	expression tag	UNP Q3ADQ4
C	0	ALA	-	expression tag	UNP Q3ADQ4
C	1	MET	-	expression tag	UNP Q3ADQ4
C	2	SER	-	expression tag	UNP Q3ADQ4
C	3	LEU	-	expression tag	UNP Q3ADQ4
C	179	GLU	-	linker	UNP Q3ADQ4
C	180	GLY	-	linker	UNP Q3ADQ4
C	193	GLU	THR	engineered mutation	UNP P36094
C	195	GLU	SER	engineered mutation	UNP P36094
D	-3	GLY	-	expression tag	UNP Q3ADQ4
D	-2	ALA	-	expression tag	UNP Q3ADQ4
D	-1	SER	-	expression tag	UNP Q3ADQ4
D	0	ALA	-	expression tag	UNP Q3ADQ4
D	1	MET	-	expression tag	UNP Q3ADQ4
D	2	SER	-	expression tag	UNP Q3ADQ4
D	3	LEU	-	expression tag	UNP Q3ADQ4
D	133	GLU	-	linker	UNP Q3ADQ4
D	134	GLY	-	linker	UNP Q3ADQ4
D	193	GLU	THR	engineered mutation	UNP P36094
D	195	GLU	SER	engineered mutation	UNP P36094
E	-3	GLY	-	expression tag	UNP Q3ADQ4
E	-2	ALA	-	expression tag	UNP Q3ADQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q3ADQ4
E	0	ALA	-	expression tag	UNP Q3ADQ4
E	1	MET	-	expression tag	UNP Q3ADQ4
E	2	SER	-	expression tag	UNP Q3ADQ4
E	3	LEU	-	expression tag	UNP Q3ADQ4
E	133	GLU	-	linker	UNP Q3ADQ4
E	134	GLY	-	linker	UNP Q3ADQ4
E	193	GLU	THR	engineered mutation	UNP P36094
E	195	GLU	SER	engineered mutation	UNP P36094
F	-3	GLY	-	expression tag	UNP Q3ADQ4
F	-2	ALA	-	expression tag	UNP Q3ADQ4
F	-1	SER	-	expression tag	UNP Q3ADQ4
F	0	ALA	-	expression tag	UNP Q3ADQ4
F	1	MET	-	expression tag	UNP Q3ADQ4
F	2	SER	-	expression tag	UNP Q3ADQ4
F	3	LEU	-	expression tag	UNP Q3ADQ4
F	179	GLU	-	linker	UNP Q3ADQ4
F	180	GLY	-	linker	UNP Q3ADQ4
F	193	GLU	THR	engineered mutation	UNP P36094
F	195	GLU	SER	engineered mutation	UNP P36094
G	-3	GLY	-	expression tag	UNP Q3ADQ4
G	-2	ALA	-	expression tag	UNP Q3ADQ4
G	-1	SER	-	expression tag	UNP Q3ADQ4
G	0	ALA	-	expression tag	UNP Q3ADQ4
G	1	MET	-	expression tag	UNP Q3ADQ4
G	2	SER	-	expression tag	UNP Q3ADQ4
G	3	LEU	-	expression tag	UNP Q3ADQ4
G	133	GLU	-	linker	UNP Q3ADQ4
G	180	GLY	-	linker	UNP Q3ADQ4
G	193	GLU	THR	engineered mutation	UNP P36094
G	195	GLU	SER	engineered mutation	UNP P36094
H	-3	GLY	-	expression tag	UNP Q3ADQ4
H	-2	ALA	-	expression tag	UNP Q3ADQ4
H	-1	SER	-	expression tag	UNP Q3ADQ4
H	0	ALA	-	expression tag	UNP Q3ADQ4
H	1	MET	-	expression tag	UNP Q3ADQ4
H	2	SER	-	expression tag	UNP Q3ADQ4
H	3	LEU	-	expression tag	UNP Q3ADQ4
H	179	GLU	-	linker	UNP Q3ADQ4
H	180	GLY	-	linker	UNP Q3ADQ4
H	193	GLU	THR	engineered mutation	UNP P36094
H	195	GLU	SER	engineered mutation	UNP P36094

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	GLY	-	expression tag	UNP Q3ADQ4
I	-2	ALA	-	expression tag	UNP Q3ADQ4
I	-1	SER	-	expression tag	UNP Q3ADQ4
I	0	ALA	-	expression tag	UNP Q3ADQ4
I	1	MET	-	expression tag	UNP Q3ADQ4
I	2	SER	-	expression tag	UNP Q3ADQ4
I	3	LEU	-	expression tag	UNP Q3ADQ4
I	179	GLU	-	linker	UNP Q3ADQ4
I	180	GLY	-	linker	UNP Q3ADQ4
I	193	GLU	THR	engineered mutation	UNP P36094
I	195	GLU	SER	engineered mutation	UNP P36094
J	-3	GLY	-	expression tag	UNP Q3ADQ4
J	-2	ALA	-	expression tag	UNP Q3ADQ4
J	-1	SER	-	expression tag	UNP Q3ADQ4
J	0	ALA	-	expression tag	UNP Q3ADQ4
J	1	MET	-	expression tag	UNP Q3ADQ4
J	2	SER	-	expression tag	UNP Q3ADQ4
J	3	LEU	-	expression tag	UNP Q3ADQ4
J	179	GLU	-	linker	UNP Q3ADQ4
J	180	GLY	-	linker	UNP Q3ADQ4
J	193	GLU	THR	engineered mutation	UNP P36094
J	195	GLU	SER	engineered mutation	UNP P36094
K	-3	GLY	-	expression tag	UNP Q3ADQ4
K	-2	ALA	-	expression tag	UNP Q3ADQ4
K	-1	SER	-	expression tag	UNP Q3ADQ4
K	0	ALA	-	expression tag	UNP Q3ADQ4
K	1	MET	-	expression tag	UNP Q3ADQ4
K	2	SER	-	expression tag	UNP Q3ADQ4
K	3	LEU	-	expression tag	UNP Q3ADQ4
K	179	GLU	-	linker	UNP Q3ADQ4
K	180	GLY	-	linker	UNP Q3ADQ4
K	193	GLU	THR	engineered mutation	UNP P36094
K	195	GLU	SER	engineered mutation	UNP P36094
L	-3	GLY	-	expression tag	UNP Q3ADQ4
L	-2	ALA	-	expression tag	UNP Q3ADQ4
L	-1	SER	-	expression tag	UNP Q3ADQ4
L	0	ALA	-	expression tag	UNP Q3ADQ4
L	1	MET	-	expression tag	UNP Q3ADQ4
L	2	SER	-	expression tag	UNP Q3ADQ4
L	3	LEU	-	expression tag	UNP Q3ADQ4
L	133	GLU	-	linker	UNP Q3ADQ4
L	134	GLY	-	linker	UNP Q3ADQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	193	GLU	THR	engineered mutation	UNP P36094
L	195	GLU	SER	engineered mutation	UNP P36094

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	6	Total O 6 6	0	0
3	C	1	Total O 1 1	0	0
3	D	4	Total O 4 4	0	0
3	E	7	Total O 7 7	0	0
3	F	1	Total O 1 1	0	0
3	G	6	Total O 6 6	0	0
3	H	1	Total O 1 1	0	0
3	I	2	Total O 2 2	0	0

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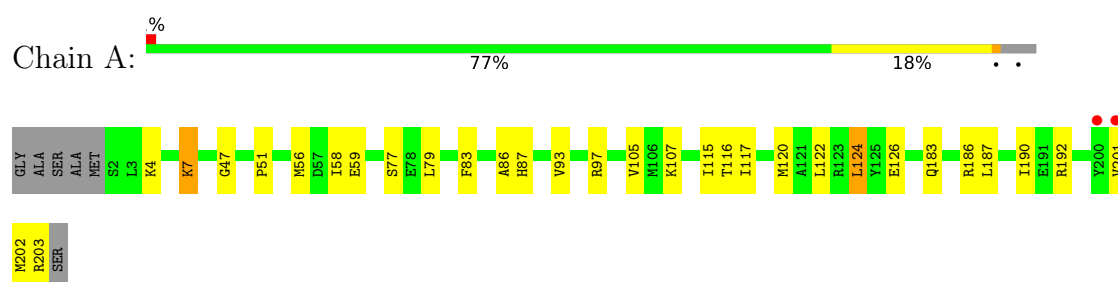
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	3	Total 3	O 3	0	0
3	K	1	Total 1	O 1	0	0
3	L	4	Total 4	O 4	0	0

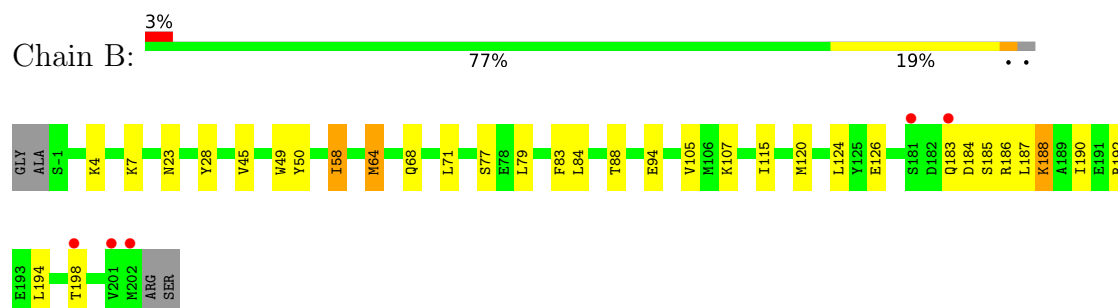
3 Residue-property plots

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.

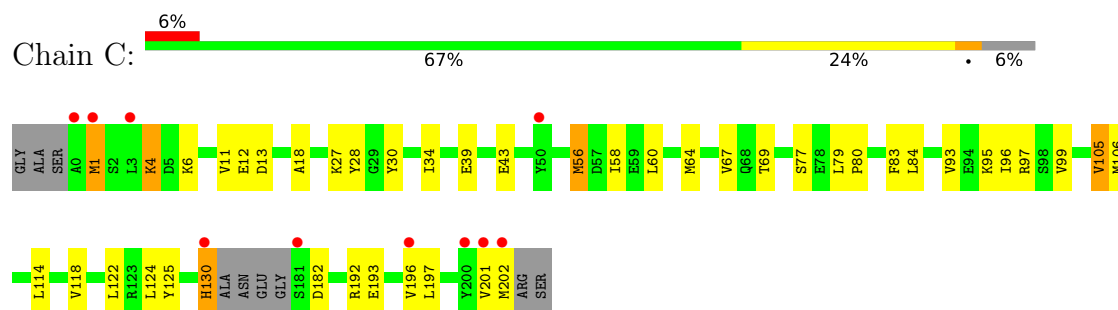
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

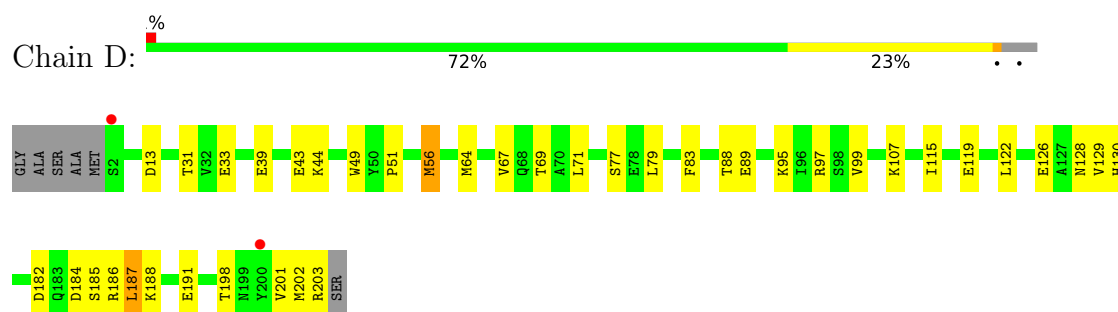


- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

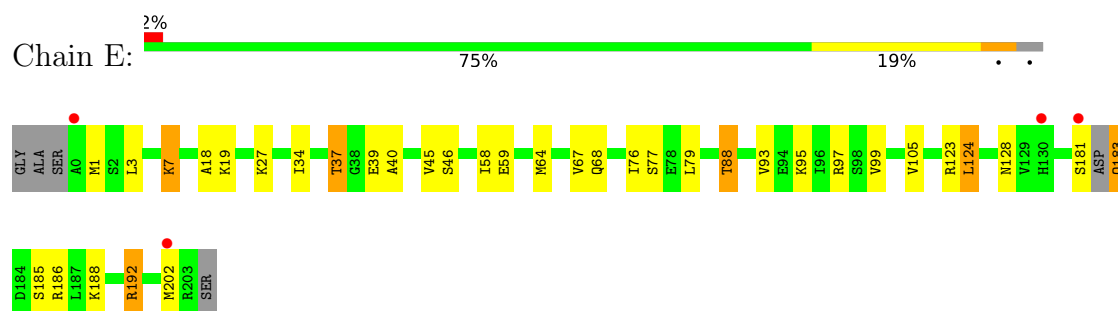


- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

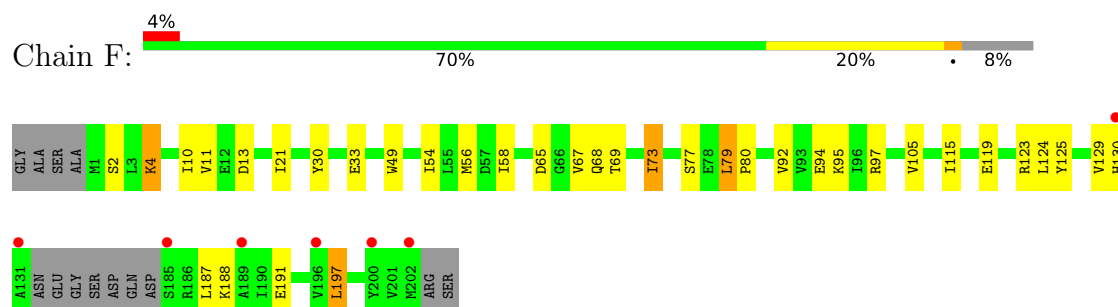




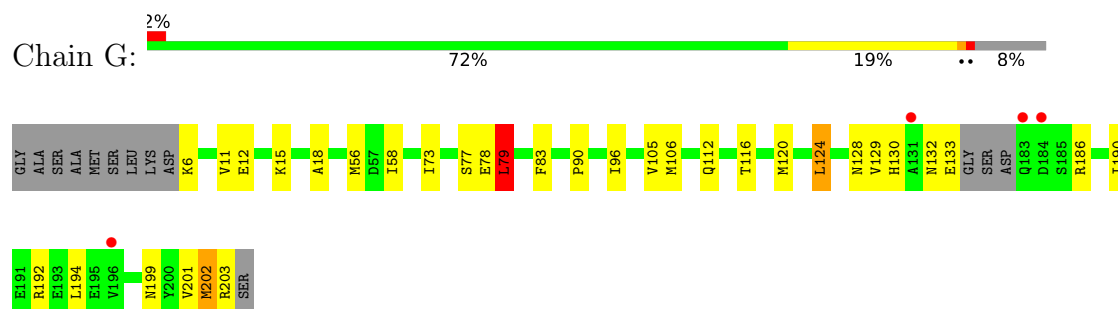
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

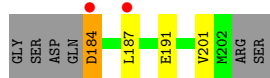


- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

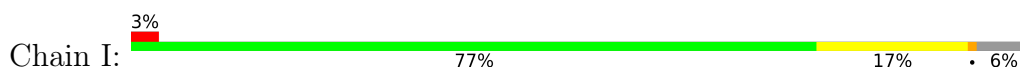


- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

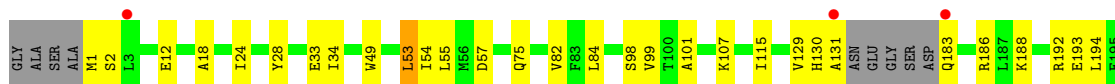




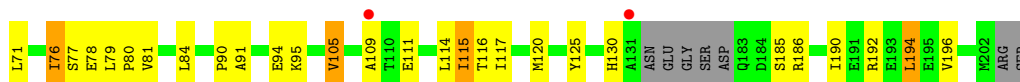
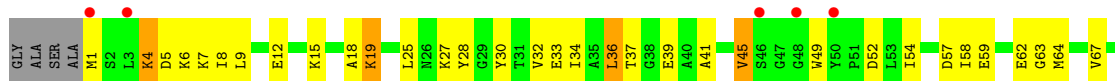
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



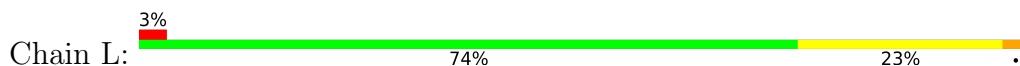
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.20Å 169.72Å 122.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.51 48.14 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.6 (48.14-2.51) 93.5 (48.14-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.195 , 0.249 0.195 , 0.248	Depositor DCC
R_{free} test set	4396 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14397	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 29.56 % 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 1.5186e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CA

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	0.47	0/1228	0.62	0/1663
1	B	0.44	0/1236	0.65	0/1674
1	C	0.42	0/1203	0.59	0/1628
1	D	0.49	0/1228	0.65	0/1663
1	E	0.47	0/1232	0.66	0/1666
1	F	0.45	0/1172	0.63	0/1586
1	G	0.51	0/1178	0.71	0/1595
1	H	0.45	0/1180	0.65	1/1597 (0.1%)
1	I	0.46	0/1208	0.64	0/1634
1	J	0.46	0/1200	0.58	0/1623
1	K	0.41	0/1189	0.58	0/1609
1	L	0.49	0/1262	0.67	0/1708
All	All	0.46	0/14516	0.64	1/19646 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	79	LEU	CA-CB-CG	5.41	135.23	116.30

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	1213	0	1242	18	0
1	B	1221	0	1251	19	0
1	C	1189	0	1225	26	0
1	D	1213	0	1242	22	0
1	E	1218	0	1254	20	0
1	F	1158	0	1204	24	0
1	G	1164	0	1196	23	0
1	H	1166	0	1208	20	0
1	I	1194	0	1233	20	0
1	J	1186	0	1229	21	0
1	K	1175	0	1216	36	0
1	L	1247	0	1277	27	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	I	1	0	0	0	0
2	L	1	0	0	0	0
3	A	10	0	0	0	0
3	B	6	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	0	0
3	E	7	0	0	0	0
3	F	1	0	0	0	0
3	G	6	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	3	0	0	0	0
3	K	1	0	0	0	0
3	L	4	0	0	0	0
All	All	14397	0	14777	246	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 8.

The worst 5 of 246 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:37:THR:HG22	1:E:40:ALA:H	1.18	1.03
1:L:37:THR:HG22	1:L:40:ALA:H	1.27	0.96
1:G:124:LEU:HD22	1:I:120:MET:HE2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HG22	1:A:120:MET:HE2	1.65	0.78
1:H:67:VAL:HG21	1:H:95:LYS:HB3	1.64	0.77

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	154/162 (95%)	147 (96%)	5 (3%)	2 (1%)	9	17
1	B	156/162 (96%)	151 (97%)	5 (3%)	0	100	100
1	C	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
1	D	154/162 (95%)	146 (95%)	7 (4%)	1 (1%)	21	36
1	E	153/162 (94%)	152 (99%)	1 (1%)	0	100	100
1	F	145/162 (90%)	140 (97%)	5 (3%)	0	100	100
1	G	145/162 (90%)	140 (97%)	3 (2%)	2 (1%)	9	16
1	H	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
1	I	149/162 (92%)	146 (98%)	3 (2%)	0	100	100
1	J	148/162 (91%)	143 (97%)	4 (3%)	1 (1%)	18	32
1	K	147/162 (91%)	138 (94%)	7 (5%)	2 (1%)	9	16
1	L	160/162 (99%)	155 (97%)	3 (2%)	2 (1%)	9	17
All	All	1806/1944 (93%)	1738 (96%)	58 (3%)	10 (1%)	21	36

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	MET
1	G	202	MET
1	K	76	ILE

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Mol	Chain	Res	Type
1	L	131	ALA
1	A	202	MET

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	132/135 (98%)	127 (96%)	5 (4%)	29	53
1	B	133/135 (98%)	122 (92%)	11 (8%)	10	21
1	C	130/135 (96%)	117 (90%)	13 (10%)	7	14
1	D	132/135 (98%)	120 (91%)	12 (9%)	9	17
1	E	132/135 (98%)	119 (90%)	13 (10%)	7	15
1	F	126/135 (93%)	119 (94%)	7 (6%)	19	37
1	G	126/135 (93%)	115 (91%)	11 (9%)	9	19
1	H	127/135 (94%)	117 (92%)	10 (8%)	11	22
1	I	130/135 (96%)	123 (95%)	7 (5%)	20	39
1	J	129/135 (96%)	125 (97%)	4 (3%)	35	60
1	K	128/135 (95%)	112 (88%)	16 (12%)	4	8
1	L	135/135 (100%)	124 (92%)	11 (8%)	11	22
All	All	1560/1620 (96%)	1440 (92%)	120 (8%)	12	23

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	79	LEU
1	L	37	THR
1	G	199	ASN
1	L	3	LEU
1	L	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	17	GLN
1	K	74	GLN
1	K	130	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	156/162 (96%)	-0.22	2 (1%) 75 72	24, 37, 75, 82	0
1	B	158/162 (97%)	-0.21	5 (3%) 50 47	25, 39, 84, 104	0
1	C	153/162 (94%)	0.18	10 (6%) 25 22	31, 46, 98, 111	0
1	D	156/162 (96%)	-0.27	2 (1%) 75 72	21, 33, 76, 89	0
1	E	157/162 (96%)	-0.24	4 (2%) 58 55	21, 35, 84, 95	0
1	F	149/162 (91%)	-0.01	7 (4%) 36 33	28, 42, 88, 97	0
1	G	149/162 (91%)	-0.35	4 (2%) 56 52	20, 29, 80, 99	0
1	H	150/162 (92%)	-0.14	4 (2%) 56 52	23, 42, 71, 84	0
1	I	153/162 (94%)	-0.20	5 (3%) 49 46	25, 38, 71, 99	0
1	J	152/162 (93%)	-0.12	4 (2%) 57 53	29, 42, 68, 86	0
1	K	151/162 (93%)	0.34	7 (4%) 37 34	32, 55, 78, 92	0
1	L	162/162 (100%)	-0.20	5 (3%) 51 48	22, 37, 83, 94	0
All	All	1846/1944 (94%)	-0.12	59 (3%) 50 47	20, 40, 81, 111	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	185	SER	5.8
1	B	202	MET	5.0
1	C	0	ALA	4.8
1	F	131	ALA	4.3
1	I	3	LEU	3.9

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 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, 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($\text{\AA}^2$)	Q<0.9
2	CA	C	301	1/1	0.91	0.08	72,72,72,72	0
2	CA	E	301	1/1	0.91	0.09	71,71,71,71	0
2	CA	L	301	1/1	0.91	0.08	72,72,72,72	0
2	CA	G	301	1/1	0.92	0.09	56,56,56,56	0
2	CA	B	301	1/1	0.92	0.09	68,68,68,68	0
2	CA	F	301	1/1	0.93	0.08	70,70,70,70	0
2	CA	I	301	1/1	0.96	0.06	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.