



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:59 PM BST

PDB ID : 6OEC
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 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

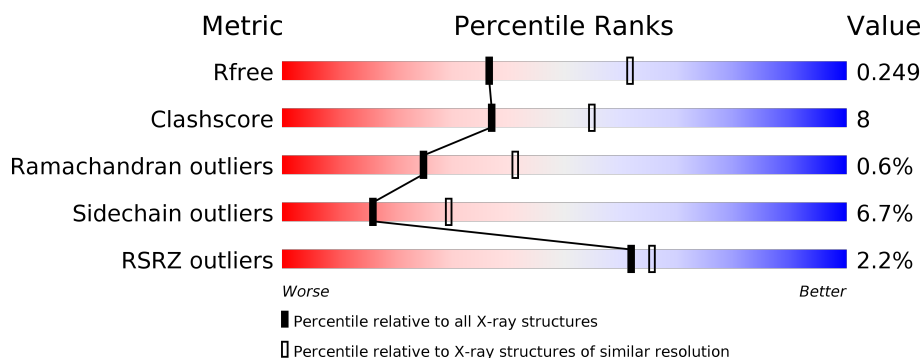
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (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 on 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	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	162	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	162	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• 6%</div> </div> </div>
1	D	162	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	E	162	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>
1	F	162	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 8%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	162	<div> <div></div> <div>72%</div> <div>19%</div> <div>8%</div> </div>
1	H	162	<div> <div></div> <div>74%</div> <div>17%</div> <div>7%</div> </div>
1	I	162	<div> <div></div> <div>77%</div> <div>15%</div> <div>6%</div> </div>
1	J	162	<div> <div></div> <div>71%</div> <div>22%</div> <div>6%</div> </div>
1	K	162	<div> <div></div> <div>57%</div> <div>31%</div> <div>7%</div> </div>
1	L	162	<div> <div></div> <div>73%</div> <div>24%</div> <div></div> </div>

2 Entry composition [i](#)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (three-letter code: CA) (formula: Ca).

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

Continued on next page...

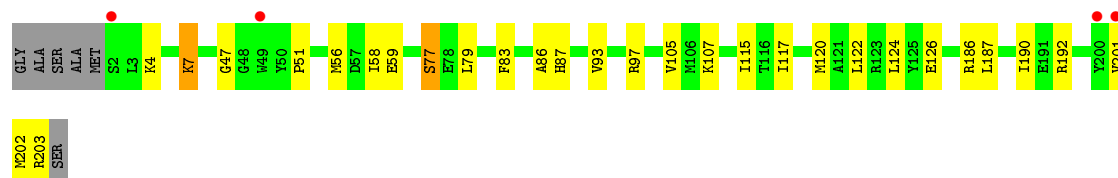
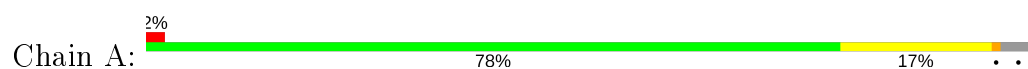
Continued from previous page...

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

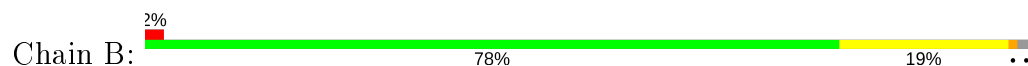
3 Residue-property plots [i](#)

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.

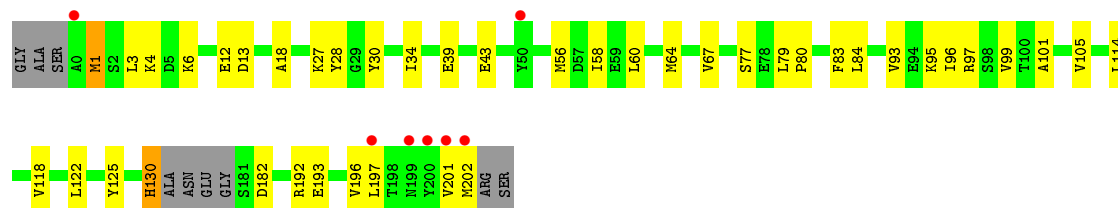
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



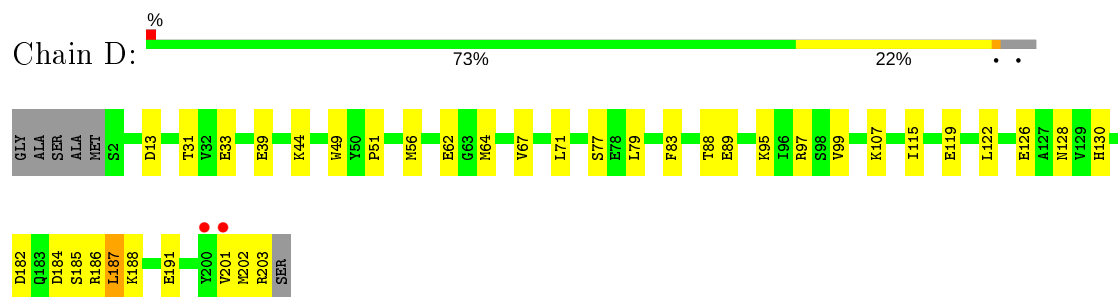
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



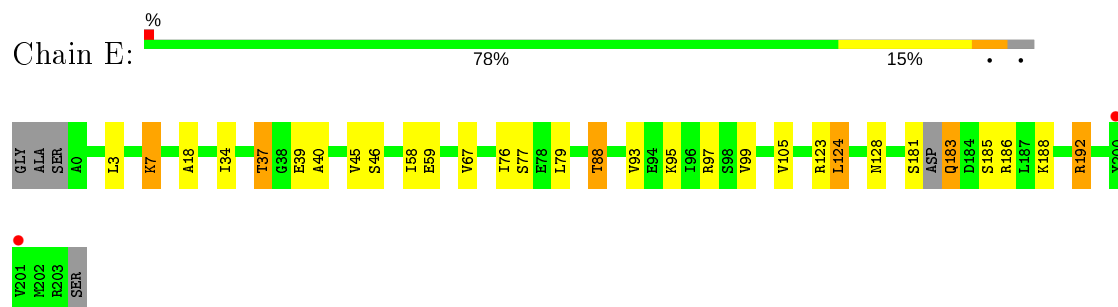
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



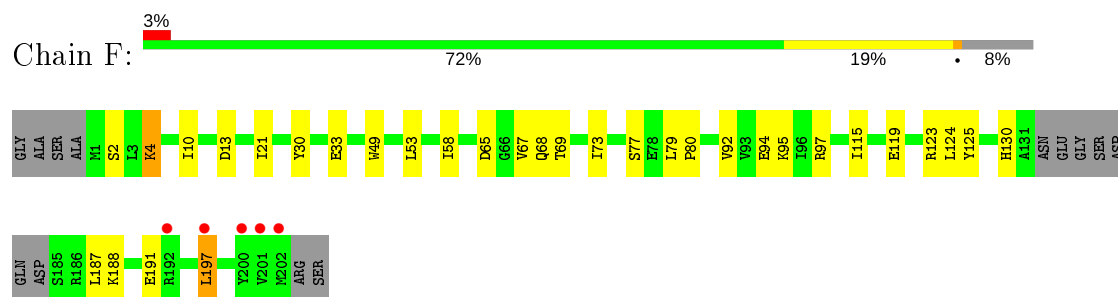
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



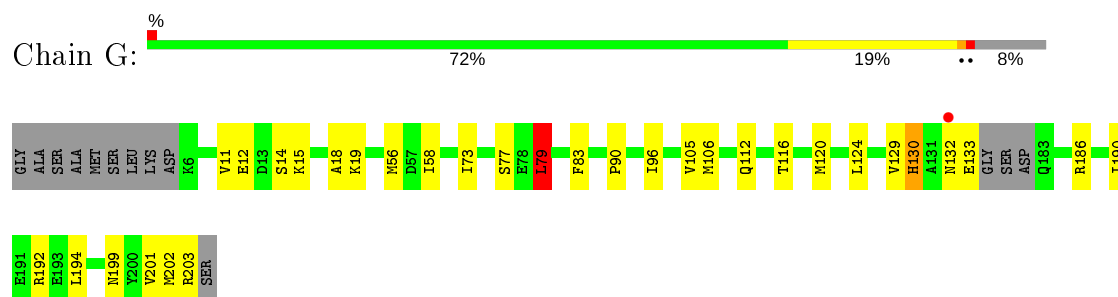
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



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

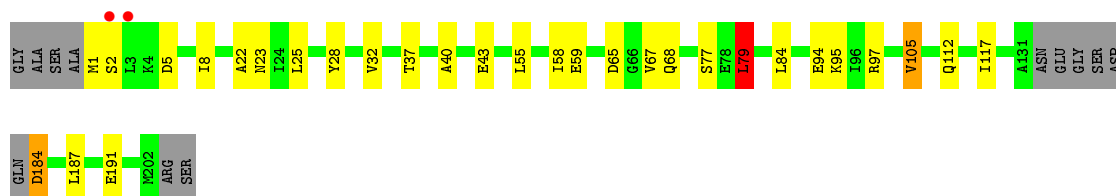


- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

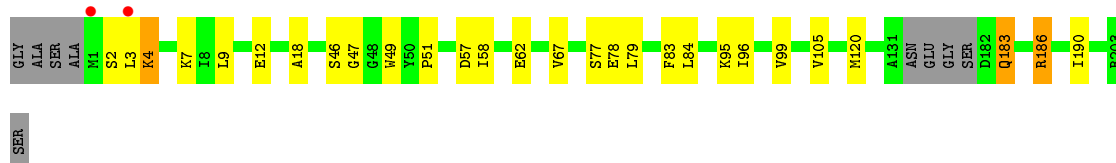
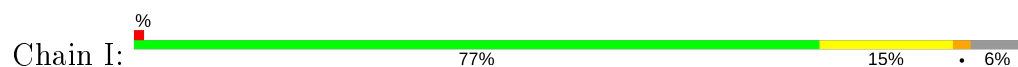


- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42

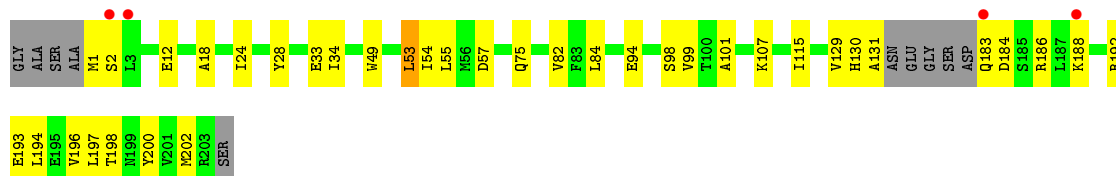




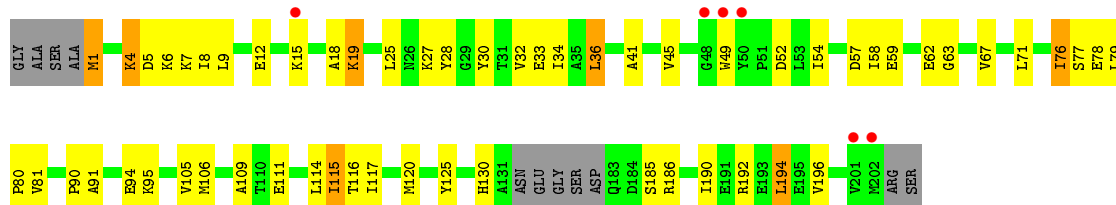
- Molecule 1: Response regulator/sensory box protein/GGDEF domain protein,Spindle pole body component SPC42



- 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



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



D184	
I187	
K188	
A189	
I190	
E191	
R192	
E193	
L194	
T198	
V201	
P202	
R203	
S204	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	133.20 Å 169.72 Å 122.03 Å 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) 93.6 (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 2.51 Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.195 , 0.249 0.195 , 0.249	Depositor DCC
R_{free} test set	4392 reflections (4.96%)	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)	0.32 , 45.9	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.55	0/1228	0.63	0/1663
1	B	0.49	0/1236	0.65	0/1674
1	C	0.50	0/1203	0.61	0/1628
1	D	0.56	0/1228	0.65	0/1663
1	E	0.51	0/1232	0.63	0/1666
1	F	0.51	0/1172	0.63	0/1586
1	G	0.56	0/1178	0.69	0/1595
1	H	0.51	0/1180	0.69	1/1597 (0.1%)
1	I	0.51	0/1208	0.64	0/1634
1	J	0.52	0/1200	0.61	0/1623
1	K	0.47	0/1189	0.59	0/1609
1	L	0.53	0/1262	0.64	0/1708
All	All	0.52	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	8.66	135.23	115.30

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	18	0
1	C	1189	0	1225	22	0
1	D	1213	0	1242	21	0
1	E	1218	0	1254	17	0
1	F	1158	0	1204	21	0
1	G	1164	0	1196	19	0
1	H	1166	0	1208	18	0
1	I	1194	0	1233	19	0
1	J	1186	0	1229	22	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	228	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.

All (228) 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:H:67:VAL:HG21	1:H:95:LYS:HB3	1.64	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:LYS:NZ	1:K:111:GLU:OE2	2.19	0.75
1:G:186:ARG:NH1	1:H:184:ASP:OD2	2.19	0.75
1:E:37:THR:HG22	1:E:40:ALA:N	2.00	0.71
1:D:185:SER:HA	1:D:188:LYS:HE3	1.71	0.71
1:K:105:VAL:HG22	1:K:117:ILE:HG21	1.73	0.71
1:A:187:LEU:HD11	1:B:183:GLN:HG3	1.75	0.69
1:H:37:THR:HG23	1:H:40:ALA:H	1.57	0.69
1:H:37:THR:CG2	1:H:40:ALA:H	2.06	0.68
1:L:120:MET:O	1:L:124:LEU:HG	1.93	0.68
1:L:37:THR:HG22	1:L:40:ALA:N	2.06	0.67
1:G:186:ARG:NH2	1:H:191:GLU:OE1	2.27	0.66
1:E:181:SER:HG	1:E:183:GLN:N	1.94	0.65
1:D:77:SER:OG	1:D:79:LEU:HG	1.97	0.64
1:C:67:VAL:HG13	1:C:99:VAL:HG11	1.80	0.64
1:A:186:ARG:O	1:A:190:ILE:HG13	1.99	0.62
1:G:77:SER:OG	1:G:79:LEU:HD13	2.02	0.60
1:B:184:ASP:OD1	1:B:188:LYS:HE2	2.01	0.60
1:C:18:ALA:HB1	1:C:34:ILE:HD13	1.83	0.59
1:B:185:SER:HA	1:B:188:LYS:HG3	1.83	0.58
1:K:116:THR:O	1:K:120:MET:HG3	2.04	0.58
1:A:7:LYS:HD2	1:A:51:PRO:HA	1.85	0.57
1:J:197:LEU:HD11	1:L:198:THR:HG22	1.84	0.57
1:C:84:LEU:HD23	1:C:105:VAL:HG13	1.87	0.57
1:A:58:ILE:HG23	1:A:59:GLU:HG3	1.88	0.56
1:J:24:ILE:HG22	1:J:115:ILE:HD11	1.87	0.56
1:C:130:HIS:O	1:C:130:HIS:ND1	2.38	0.56
1:E:18:ALA:HB1	1:E:34:ILE:HD13	1.87	0.56
1:K:15:LYS:HE3	1:K:36:LEU:HD11	1.88	0.55
1:L:203:ARG:O	1:L:204:SER:OG	2.22	0.55
1:B:183:GLN:HA	1:B:186:ARG:HD3	1.87	0.55
1:G:201:VAL:O	1:G:203:ARG:N	2.40	0.55
1:E:58:ILE:HG23	1:E:59:GLU:HG3	1.89	0.55
1:I:183:GLN:HA	1:I:186:ARG:HE	1.72	0.55
1:D:201:VAL:O	1:D:203:ARG:N	2.38	0.55
1:F:115:ILE:O	1:F:119:GLU:HG3	2.06	0.55
1:F:67:VAL:HG21	1:F:95:LYS:HD2	1.88	0.54
1:I:62:GLU:OE2	1:I:62:GLU:HA	2.08	0.54
1:F:10:ILE:HD13	1:F:21:ILE:HG22	1.88	0.54
1:A:192:ARG:NH2	1:J:75:GLN:OE1	2.40	0.54
1:I:67:VAL:HG13	1:I:99:VAL:HG11	1.89	0.54
1:D:186:ARG:HD3	1:F:187:LEU:HD13	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:18:ALA:HB1	1:J:34:ILE:HD13	1.89	0.54
1:K:9:LEU:HB2	1:K:49:TRP:HZ3	1.73	0.54
1:E:37:THR:HG23	1:E:39:GLU:OE1	2.07	0.54
1:C:67:VAL:HG21	1:C:95:LYS:HB3	1.89	0.54
1:B:88:THR:HG22	1:B:88:THR:O	2.08	0.53
1:H:105:VAL:HG22	1:H:117:ILE:HG21	1.91	0.53
1:J:55:LEU:HD22	1:J:84:LEU:HD21	1.90	0.53
1:D:115:ILE:O	1:D:119:GLU:HG3	2.09	0.53
1:K:54:ILE:HB	1:K:81:VAL:HG22	1.91	0.53
1:L:80:PRO:HD3	1:L:125:TYR:CD1	2.44	0.53
1:A:190:ILE:CG2	1:B:190:ILE:HD11	2.39	0.53
1:C:1:MET:HB3	1:C:28:TYR:CD2	2.44	0.52
1:E:128:ASN:OD1	1:F:123:ARG:NH2	2.36	0.52
1:F:65:ASP:OD1	1:F:68:GLN:HG3	2.08	0.52
1:D:187:LEU:HG	1:F:187:LEU:HD21	1.90	0.52
1:G:201:VAL:C	1:G:203:ARG:H	2.12	0.52
1:G:194:LEU:HD22	1:I:190:ILE:HG23	1.92	0.52
1:A:77:SER:OG	1:A:79:LEU:HG	2.09	0.52
1:J:1:MET:HA	1:J:28:TYR:HA	1.92	0.52
1:K:78:GLU:OE2	1:L:112:GLN:HG2	2.10	0.52
1:B:64:MET:HG2	1:B:68:GLN:HB3	1.91	0.51
1:B:84:LEU:HD23	1:B:105:VAL:HG13	1.92	0.51
1:D:39:GLU:OE2	1:D:64:MET:HG3	2.11	0.51
1:H:105:VAL:HG13	1:H:117:ILE:HD12	1.92	0.51
1:J:194:LEU:HD11	1:K:190:ILE:HG23	1.93	0.51
1:C:193:GLU:O	1:C:196:VAL:HB	2.11	0.51
1:F:80:PRO:HD3	1:F:125:TYR:CD1	2.46	0.51
1:F:187:LEU:O	1:F:191:GLU:HG3	2.10	0.51
1:I:77:SER:OG	1:I:79:LEU:HG	2.10	0.51
1:L:116:THR:HG22	1:L:120:MET:CE	2.40	0.51
1:L:77:SER:OG	1:L:79:LEU:HG	2.10	0.51
1:F:13:ASP:OD1	1:F:13:ASP:N	2.40	0.50
1:C:13:ASP:OD1	1:C:13:ASP:N	2.44	0.50
1:K:1:MET:HG2	1:K:28:TYR:HD1	1.75	0.50
1:G:186:ARG:HD3	1:H:187:LEU:HD13	1.94	0.50
1:K:90:PRO:O	1:K:94:GLU:HG3	2.11	0.50
1:L:51:PRO:HG2	1:L:79:LEU:HD13	1.93	0.50
1:D:201:VAL:C	1:D:203:ARG:H	2.15	0.50
1:J:193:GLU:HG2	1:L:198:THR:HG21	1.92	0.50
1:K:33:GLU:HB2	1:K:49:TRP:CH2	2.45	0.50
1:D:51:PRO:O	1:D:79:LEU:HD22	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MET:HE3	1:H:28:TYR:HD2	1.77	0.49
1:B:187:LEU:HA	1:B:190:ILE:HG22	1.95	0.49
1:B:50:TYR:HE1	1:B:77:SER:HB2	1.77	0.49
1:H:58:ILE:HG23	1:H:59:GLU:HG2	1.94	0.49
1:J:33:GLU:HG3	1:J:49:TRP:CH2	2.48	0.49
1:K:67:VAL:HG21	1:K:95:LYS:HB3	1.93	0.49
1:I:183:GLN:HA	1:I:186:ARG:HH21	1.78	0.49
1:F:58:ILE:HG12	1:F:92:VAL:HG13	1.95	0.48
1:K:7:LYS:N	1:K:52:ASP:OD2	2.29	0.48
1:H:55:LEU:HD13	1:H:84:LEU:HD21	1.95	0.48
1:L:116:THR:HG22	1:L:120:MET:HE2	1.96	0.48
1:C:114:LEU:O	1:C:118:VAL:HG23	2.14	0.48
1:J:53:LEU:HG	1:J:54:ILE:N	2.28	0.48
1:K:80:PRO:HD3	1:K:125:TYR:CD1	2.49	0.48
1:K:94:GLU:OE2	1:L:87:HIS:HB3	2.14	0.48
1:D:67:VAL:HG13	1:D:99:VAL:HG11	1.94	0.48
1:C:77:SER:OG	1:C:79:LEU:HG	2.14	0.47
1:F:4:LYS:HD3	1:F:30:TYR:CZ	2.49	0.47
1:C:80:PRO:HD3	1:C:125:TYR:CD2	2.50	0.47
1:L:90:PRO:O	1:L:94:GLU:HG3	2.13	0.47
1:D:184:ASP:O	1:D:188:LYS:HG3	2.15	0.47
1:J:12:GLU:OE1	1:J:57:ASP:OD2	2.32	0.47
1:L:113:VAL:O	1:L:117:ILE:HG13	2.15	0.47
1:I:9:LEU:HB2	1:I:49:TRP:HZ3	1.79	0.46
1:G:12:GLU:HB3	1:G:18:ALA:HB2	1.97	0.46
1:K:57:ASP:OD1	1:K:58:ILE:N	2.49	0.46
1:L:62:GLU:HG3	1:L:62:GLU:H	1.38	0.46
1:C:4:LYS:HD2	1:C:30:TYR:CZ	2.51	0.46
1:F:130:HIS:O	1:F:130:HIS:ND1	2.48	0.46
1:I:67:VAL:HG21	1:I:95:LYS:HB3	1.97	0.46
1:J:183:GLN:HA	1:J:186:ARG:HD3	1.98	0.46
1:J:192:ARG:O	1:J:196:VAL:HG23	2.16	0.46
1:J:188:LYS:HD2	1:K:186:ARG:HH22	1.81	0.46
1:C:12:GLU:HB3	1:C:18:ALA:HB2	1.97	0.46
1:I:79:LEU:HA	1:I:79:LEU:HD23	1.66	0.46
1:A:115:ILE:HA	1:A:115:ILE:HD13	1.67	0.46
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.75	0.46
1:I:12:GLU:OE1	1:I:57:ASP:OD2	2.33	0.46
1:J:53:LEU:HD11	1:J:82:VAL:HG23	1.98	0.46
1:A:56:MET:O	1:A:83:PHE:HA	2.16	0.45
1:H:22:ALA:HA	1:H:32:VAL:HG11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:ALA:HB1	1:K:34:ILE:HD13	1.97	0.45
1:A:201:VAL:C	1:A:203:ARG:H	2.19	0.45
1:G:58:ILE:HD13	1:G:96:ILE:HG12	1.98	0.45
1:J:198:THR:O	1:J:202:MET:HG2	2.16	0.45
1:I:84:LEU:HD23	1:I:105:VAL:HG13	1.97	0.45
1:B:4:LYS:HD3	1:B:4:LYS:HA	1.72	0.45
1:E:77:SER:OG	1:E:79:LEU:HG	2.17	0.45
1:F:69:THR:HG22	1:F:73:ILE:HD12	1.98	0.45
1:C:93:VAL:HG13	1:C:97:ARG:HE	1.81	0.45
1:E:45:VAL:HG12	1:E:76:ILE:HG21	1.99	0.45
1:G:201:VAL:C	1:G:203:ARG:N	2.69	0.45
1:L:96:ILE:O	1:L:100:THR:HG22	2.17	0.45
1:A:120:MET:HE1	1:C:101:ALA:HB1	1.98	0.45
1:A:93:VAL:CG1	1:A:97:ARG:HE	2.30	0.45
1:D:128:ASN:HB2	1:E:123:ARG:NH1	2.32	0.45
1:E:183:GLN:O	1:E:183:GLN:HG3	2.15	0.45
1:G:124:LEU:HD22	1:I:120:MET:HE2	1.98	0.45
1:J:129:VAL:O	1:J:131:ALA:N	2.46	0.45
1:K:41:ALA:O	1:K:45:VAL:HG12	2.17	0.45
1:L:57:ASP:HA	1:L:84:LEU:HB2	1.99	0.45
1:H:37:THR:HG22	1:H:40:ALA:CB	2.47	0.44
1:K:45:VAL:HA	1:K:49:TRP:O	2.17	0.44
1:C:193:GLU:O	1:C:197:LEU:HG	2.17	0.44
1:J:101:ALA:HB1	1:K:120:MET:HE1	1.99	0.44
1:L:33:GLU:HG3	1:L:49:TRP:CZ2	2.51	0.44
1:C:6:LYS:HG3	1:C:122:LEU:HD13	1.99	0.44
1:E:7:LYS:HD3	1:I:47:GLY:C	2.38	0.44
1:L:184:ASP:OD1	1:L:188:LYS:HE3	2.18	0.44
1:F:77:SER:OG	1:F:79:LEU:HG	2.17	0.44
1:A:86:ALA:O	1:A:87:HIS:ND1	2.51	0.44
1:B:50:TYR:HD1	1:B:79:LEU:HD21	1.82	0.44
1:H:65:ASP:OD1	1:H:68:GLN:HG3	2.18	0.44
1:C:130:HIS:C	1:C:130:HIS:HD1	2.20	0.44
1:I:49:TRP:CZ3	1:I:51:PRO:HB3	2.53	0.44
1:A:58:ILE:HA	1:A:58:ILE:HD12	1.82	0.44
1:C:39:GLU:OE2	1:C:64:MET:HG3	2.17	0.44
1:D:122:LEU:HA	1:D:122:LEU:HD23	1.73	0.44
1:K:192:ARG:O	1:K:196:VAL:HG23	2.17	0.44
1:G:116:THR:HG22	1:G:120:MET:HE2	2.00	0.44
1:J:200:TYR:CE2	1:L:201:VAL:HG13	2.53	0.44
1:K:194:LEU:HD12	1:L:190:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HG23	1:B:83:PHE:CD2	2.52	0.43
1:G:11:VAL:HG11	1:G:56:MET:HE2	1.99	0.43
1:G:56:MET:O	1:G:83:PHE:HA	2.18	0.43
1:F:188:LYS:HE3	1:F:188:LYS:HB3	1.78	0.43
1:F:33:GLU:HG3	1:F:49:TRP:CH2	2.53	0.43
1:G:186:ARG:O	1:G:190:ILE:HG13	2.17	0.43
1:D:56:MET:O	1:D:83:PHE:HA	2.18	0.43
1:K:58:ILE:HG23	1:K:59:GLU:HG3	1.99	0.43
1:B:185:SER:HA	1:B:188:LYS:HE3	1.99	0.43
1:I:12:GLU:HB3	1:I:18:ALA:HB2	2.00	0.43
1:L:80:PRO:HB3	1:L:102:TYR:CZ	2.54	0.43
1:A:124:LEU:HD22	1:B:120:MET:SD	2.59	0.43
1:B:45:VAL:HA	1:B:49:TRP:O	2.19	0.43
1:E:124:LEU:HA	1:E:124:LEU:HD23	1.94	0.42
1:G:130:HIS:O	1:G:133:GLU:HG2	2.19	0.42
1:K:115:ILE:HD13	1:K:115:ILE:HA	1.65	0.42
1:L:194:LEU:O	1:L:198:THR:HG23	2.18	0.42
1:K:4:LYS:HB2	1:K:6:LYS:HG2	2.01	0.42
1:D:130:HIS:HB3	1:D:182:ASP:HB3	2.02	0.42
1:D:33:GLU:HG3	1:D:49:TRP:CZ2	2.54	0.42
1:B:28:TYR:CD1	1:B:115:ILE:HG13	2.55	0.42
1:D:13:ASP:N	1:D:13:ASP:OD1	2.53	0.42
1:E:67:VAL:HG13	1:E:99:VAL:HG11	2.01	0.42
1:L:3:LEU:HD23	1:L:3:LEU:HA	1.77	0.42
1:D:187:LEU:O	1:D:191:GLU:HG3	2.20	0.42
1:D:88:THR:HG23	1:F:94:GLU:HG2	2.00	0.42
1:K:91:ALA:O	1:K:95:LYS:HG3	2.20	0.42
1:H:8:ILE:HD12	1:H:25:LEU:HD13	2.02	0.41
1:J:98:SER:HB2	1:K:109:ALA:HA	2.02	0.41
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.83	0.41
1:E:93:VAL:O	1:E:97:ARG:HG3	2.19	0.41
1:F:124:LEU:HA	1:F:124:LEU:HD23	1.86	0.41
1:I:51:PRO:HG2	1:I:79:LEU:HD13	2.02	0.41
1:K:8:ILE:HG21	1:K:25:LEU:HD13	2.02	0.41
1:A:105:VAL:HG22	1:A:117:ILE:HG21	2.03	0.41
1:I:2:SER:O	1:I:4:LYS:HG2	2.20	0.41
1:K:19:LYS:HD2	1:K:19:LYS:HA	1.63	0.41
1:E:88:THR:O	1:E:88:THR:HG23	2.20	0.41
1:H:77:SER:OG	1:H:79:LEU:HB3	2.20	0.41
1:K:190:ILE:O	1:K:194:LEU:HB2	2.20	0.41
1:C:39:GLU:OE1	1:C:39:GLU:N	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD23	1:C:60:LEU:HA	1.93	0.41
1:F:197:LEU:HD12	1:F:197:LEU:HA	1.87	0.41
1:I:77:SER:OG	1:I:78:GLU:N	2.53	0.41
1:L:33:GLU:HG3	1:L:49:TRP:CH2	2.55	0.41
1:H:112:GLN:N	1:H:112:GLN:OE1	2.48	0.41
1:D:97:ARG:NH2	1:F:97:ARG:HH22	2.19	0.41
1:G:112:GLN:OE1	1:G:112:GLN:N	2.43	0.41
1:J:101:ALA:HB1	1:K:120:MET:CE	2.51	0.41
1:K:76:ILE:HG22	1:K:77:SER:N	2.35	0.41
1:A:122:LEU:O	1:A:126:GLU:HG3	2.21	0.41
1:G:129:VAL:HG12	1:G:130:HIS:ND1	2.36	0.41
1:I:83:PHE:CD1	1:I:96:ILE:HG23	2.56	0.41
1:K:12:GLU:OE1	1:K:57:ASP:HB2	2.20	0.41
1:L:190:ILE:HA	1:L:193:GLU:HB2	2.03	0.41
1:A:51:PRO:HD2	1:A:79:LEU:HD11	2.03	0.40
1:J:94:GLU:HG2	1:K:106:MET:HE1	2.02	0.40
1:G:106:MET:HE2	1:H:94:GLU:HG2	2.03	0.40
1:K:30:TYR:O	1:K:32:VAL:HG23	2.21	0.40
1:C:83:PHE:CD1	1:C:96:ILE:HG23	2.57	0.40
1:E:188:LYS:HE3	1:E:192:ARG:HD3	2.04	0.40

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%)	12	20
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%)	25	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	11	19
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%)	22	37
1	K	147/162 (91%)	138 (94%)	7 (5%)	2 (1%)	11	19
1	L	160/162 (99%)	155 (97%)	3 (2%)	2 (1%)	12	20
All	All	1806/1944 (93%)	1738 (96%)	58 (3%)	10 (1%)	25	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	MET
1	G	202	MET
1	K	76	ILE
1	L	131	ALA
1	A	202	MET
1	J	130	HIS
1	L	132	ASN
1	G	79	LEU
1	K	63	GLY
1	A	47	GLY

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%)	128 (97%)	4 (3%)	41	66
1	B	133/135 (98%)	124 (93%)	9 (7%)	16	29
1	C	130/135 (96%)	119 (92%)	11 (8%)	10	19
1	D	132/135 (98%)	123 (93%)	9 (7%)	16	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	132/135 (98%)	120 (91%)	12 (9%)	9	17
1	F	126/135 (93%)	122 (97%)	4 (3%)	39	63
1	G	126/135 (93%)	115 (91%)	11 (9%)	10	19
1	H	127/135 (94%)	119 (94%)	8 (6%)	18	32
1	I	130/135 (96%)	123 (95%)	7 (5%)	22	40
1	J	129/135 (96%)	124 (96%)	5 (4%)	32	55
1	K	128/135 (95%)	115 (90%)	13 (10%)	7	13
1	L	135/135 (100%)	124 (92%)	11 (8%)	11	21
All	All	1560/1620 (96%)	1456 (93%)	104 (7%)	16	29

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	LYS
1	A	77	SER
1	A	107	LYS
1	B	7	LYS
1	B	23	ASN
1	B	107	LYS
1	B	124	LEU
1	B	130	HIS
1	B	188	LYS
1	B	192	ARG
1	B	194	LEU
1	B	198	THR
1	C	1	MET
1	C	3	LEU
1	C	27	LYS
1	C	43	GLU
1	C	56	MET
1	C	58	ILE
1	C	130	HIS
1	C	182	ASP
1	C	192	ARG
1	C	201	VAL
1	C	202	MET
1	D	31	THR
1	D	44	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	62	GLU
1	D	71	LEU
1	D	89	GLU
1	D	95	LYS
1	D	107	LYS
1	D	126	GLU
1	D	187	LEU
1	E	3	LEU
1	E	7	LYS
1	E	37	THR
1	E	46	SER
1	E	88	THR
1	E	95	LYS
1	E	105	VAL
1	E	124	LEU
1	E	183	GLN
1	E	185	SER
1	E	186	ARG
1	E	192	ARG
1	F	2	SER
1	F	4	LYS
1	F	53	LEU
1	F	197	LEU
1	G	14	SER
1	G	15	LYS
1	G	19	LYS
1	G	73	ILE
1	G	79	LEU
1	G	90	PRO
1	G	105	VAL
1	G	130	HIS
1	G	132	ASN
1	G	192	ARG
1	G	199	ASN
1	H	2	SER
1	H	5	ASP
1	H	23	ASN
1	H	43	GLU
1	H	79	LEU
1	H	97	ARG
1	H	105	VAL
1	H	184	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	3	LEU
1	I	4	LYS
1	I	7	LYS
1	I	46	SER
1	I	58	ILE
1	I	183	GLN
1	I	186	ARG
1	J	2	SER
1	J	53	LEU
1	J	99	VAL
1	J	107	LYS
1	J	184	ASP
1	K	1	MET
1	K	4	LYS
1	K	5	ASP
1	K	19	LYS
1	K	36	LEU
1	K	62	GLU
1	K	71	LEU
1	K	79	LEU
1	K	114	LEU
1	K	115	ILE
1	K	130	HIS
1	K	185	SER
1	K	194	LEU
1	L	3	LEU
1	L	37	THR
1	L	59	GLU
1	L	62	GLU
1	L	64	MET
1	L	65	ASP
1	L	98	SER
1	L	130	HIS
1	L	187	LEU
1	L	192	ARG
1	L	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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 ⓘ

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, 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%)	-0.16	4 (2%) 56 59	24, 37, 75, 82	0
1	B	158/162 (97%)	-0.17	4 (2%) 57 61	25, 39, 84, 104	0
1	C	153/162 (94%)	0.17	7 (4%) 32 35	31, 46, 98, 112	0
1	D	156/162 (96%)	-0.24	2 (1%) 77 79	21, 33, 76, 89	0
1	E	157/162 (96%)	-0.23	2 (1%) 77 79	21, 35, 84, 95	0
1	F	149/162 (91%)	-0.01	5 (3%) 45 49	28, 42, 88, 97	0
1	G	149/162 (91%)	-0.28	1 (0%) 87 89	20, 29, 80, 99	0
1	H	150/162 (92%)	-0.26	2 (1%) 77 79	23, 42, 71, 84	0
1	I	153/162 (94%)	-0.30	2 (1%) 77 79	25, 38, 71, 99	0
1	J	152/162 (93%)	-0.24	4 (2%) 56 59	29, 42, 68, 86	0
1	K	151/162 (93%)	0.10	6 (3%) 38 42	32, 55, 78, 92	0
1	L	162/162 (100%)	-0.21	1 (0%) 89 90	22, 37, 83, 94	0
All	All	1846/1944 (94%)	-0.15	40 (2%) 62 65	20, 40, 81, 112	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	TYR	5.7
1	C	201	VAL	5.0
1	C	199	ASN	3.9
1	F	202	MET	3.9
1	F	200	TYR	3.8
1	A	201	VAL	3.7
1	A	2	SER	3.4
1	E	201	VAL	3.4
1	I	3	LEU	3.2
1	C	202	MET	3.2
1	B	201	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	49	TRP	3.1
1	H	2	SER	3.1
1	A	200	TYR	3.0
1	F	201	VAL	3.0
1	F	192	ARG	3.0
1	H	3	LEU	2.9
1	G	132	ASN	2.8
1	B	200	TYR	2.8
1	D	201	VAL	2.8
1	J	2	SER	2.8
1	C	50	TYR	2.8
1	C	0	ALA	2.8
1	I	1	MET	2.7
1	C	197	LEU	2.7
1	L	183	GLN	2.6
1	K	48	GLY	2.5
1	K	201	VAL	2.5
1	A	49	TRP	2.5
1	B	202	MET	2.5
1	K	202	MET	2.4
1	B	196	VAL	2.3
1	J	183	GLN	2.3
1	K	50	TYR	2.2
1	E	200	TYR	2.1
1	J	188	LYS	2.1
1	K	15	LYS	2.1
1	J	3	LEU	2.1
1	D	200	TYR	2.1
1	F	197	LEU	2.0

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 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, 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(Å ²)	Q<0.9
2	CA	L	301	1/1	0.86	0.10	72,72,72,72	0
2	CA	G	301	1/1	0.92	0.10	56,56,56,56	0
2	CA	C	301	1/1	0.93	0.06	72,72,72,72	0
2	CA	B	301	1/1	0.94	0.04	68,68,68,68	0
2	CA	E	301	1/1	0.94	0.06	71,71,71,71	0
2	CA	F	301	1/1	0.95	0.07	70,70,70,70	0
2	CA	I	301	1/1	0.97	0.06	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.