W O R L D W I D E

wwPDB

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

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:32 am GMT

PDB ID	:	5HZG
Title	:	The crystal structure of the strigolactone-induced AtD14-D3-ASK1 complex
Authors	:	Yao, R.F.; Ming, Z.H.; Yan, L.M.; Rao, Z.H.; Lou, Z.Y.; Xie, D.X.
Deposited on	:	2016-02-02
Resolution	:	3.30 Å(reported)

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

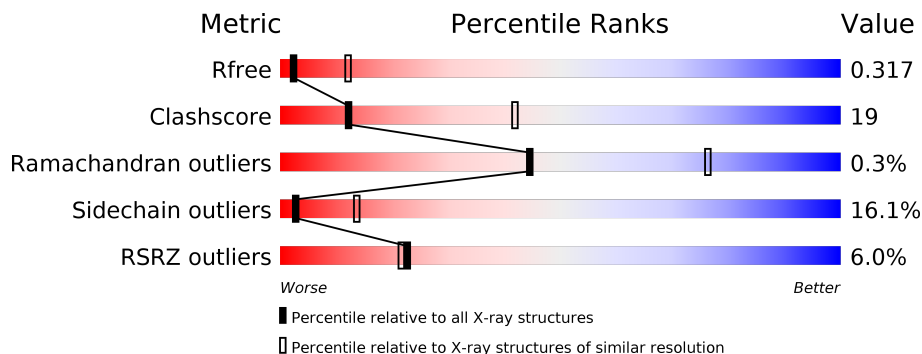|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.317
Clashscore		19
Ramachandran outliers		0.3%
Sidechain outliers		16.1%
RSRZ outliers		6.0%

Worse   *Better*

▌Percentile relative to all X-ray structures

🯄 Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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. 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	267	% 66% 25% · ·
1	E	267	3% 70% 22% 5% ·
2	B	740	2% 50% 24% 8% · 17%
2	F	740	3% 49% 24% 9% · 17%
3	C	169	27% 56% 17% · · 23%
3	G	169	19% 59% 18% · 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	6OM	A	301	-	X	X	X
4	6OM	E	301	-	X	X	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15676 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 Strigolactone esterase D14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2001	1285	341	369	6			
1	E	257	Total	C	N	O	S	0	0	0
			2001	1285	341	369	6			

- Molecule 2 is a protein called F-box/LRR-repeat MAX2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	615	Total	C	N	O	S	0	0	0
			4791	3055	842	862	32			
2	F	614	Total	C	N	O	S	0	0	0
			4782	3048	840	862	32			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP Q5VMP0
B	-18	ALA	-	expression tag	UNP Q5VMP0
B	-17	MET	-	expression tag	UNP Q5VMP0
B	-16	GLY	-	expression tag	UNP Q5VMP0
B	-15	SER	-	expression tag	UNP Q5VMP0
B	-14	GLY	-	expression tag	UNP Q5VMP0
B	-13	ILE	-	expression tag	UNP Q5VMP0
B	-12	GLN	-	expression tag	UNP Q5VMP0
B	-11	ARG	-	expression tag	UNP Q5VMP0
B	-10	PRO	-	expression tag	UNP Q5VMP0
B	-9	THR	-	expression tag	UNP Q5VMP0
B	-8	SER	-	expression tag	UNP Q5VMP0
B	-7	THR	-	expression tag	UNP Q5VMP0
B	-6	SER	-	expression tag	UNP Q5VMP0
B	-5	SER	-	expression tag	UNP Q5VMP0
B	-4	LEU	-	expression tag	UNP Q5VMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	VAL	-	expression tag	UNP Q5VMP0
B	-2	ALA	-	expression tag	UNP Q5VMP0
B	-1	ALA	-	expression tag	UNP Q5VMP0
B	0	ALA	-	expression tag	UNP Q5VMP0
F	-19	GLY	-	expression tag	UNP Q5VMP0
F	-18	ALA	-	expression tag	UNP Q5VMP0
F	-17	MET	-	expression tag	UNP Q5VMP0
F	-16	GLY	-	expression tag	UNP Q5VMP0
F	-15	SER	-	expression tag	UNP Q5VMP0
F	-14	GLY	-	expression tag	UNP Q5VMP0
F	-13	ILE	-	expression tag	UNP Q5VMP0
F	-12	GLN	-	expression tag	UNP Q5VMP0
F	-11	ARG	-	expression tag	UNP Q5VMP0
F	-10	PRO	-	expression tag	UNP Q5VMP0
F	-9	THR	-	expression tag	UNP Q5VMP0
F	-8	SER	-	expression tag	UNP Q5VMP0
F	-7	THR	-	expression tag	UNP Q5VMP0
F	-6	SER	-	expression tag	UNP Q5VMP0
F	-5	SER	-	expression tag	UNP Q5VMP0
F	-4	LEU	-	expression tag	UNP Q5VMP0
F	-3	VAL	-	expression tag	UNP Q5VMP0
F	-2	ALA	-	expression tag	UNP Q5VMP0
F	-1	ALA	-	expression tag	UNP Q5VMP0
F	0	ALA	-	expression tag	UNP Q5VMP0

- Molecule 3 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1024	645	168	207	4			
3	G	132	Total	C	N	O	S	0	0	0
			1039	655	170	210	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	MET	-	expression tag	UNP Q39255
C	-7	ASP	-	expression tag	UNP Q39255
C	-6	TYR	-	expression tag	UNP Q39255
C	-5	LYS	-	expression tag	UNP Q39255
C	-4	ASP	-	expression tag	UNP Q39255
C	-3	ASP	-	expression tag	UNP Q39255

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ASP	-	expression tag	UNP Q39255
C	-1	ASP	-	expression tag	UNP Q39255
C	0	LYS	-	expression tag	UNP Q39255
G	-8	MET	-	expression tag	UNP Q39255
G	-7	ASP	-	expression tag	UNP Q39255
G	-6	TYR	-	expression tag	UNP Q39255
G	-5	LYS	-	expression tag	UNP Q39255
G	-4	ASP	-	expression tag	UNP Q39255
G	-3	ASP	-	expression tag	UNP Q39255
G	-2	ASP	-	expression tag	UNP Q39255
G	-1	ASP	-	expression tag	UNP Q39255
G	0	LYS	-	expression tag	UNP Q39255

- Molecule 4 is (2Z)-2-methylbut-2-ene-1,4-diol (three-letter code: 6OM) (formula: $C_5H_{10}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 5	O 2	0	0
4	E	1	Total 7	C 5	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total 5	O 5	0	0
5	E	2	Total 2	O 2	0	0
5	F	10	Total 10	O 10	0	0
5	G	4	Total 4	O 4	0	0

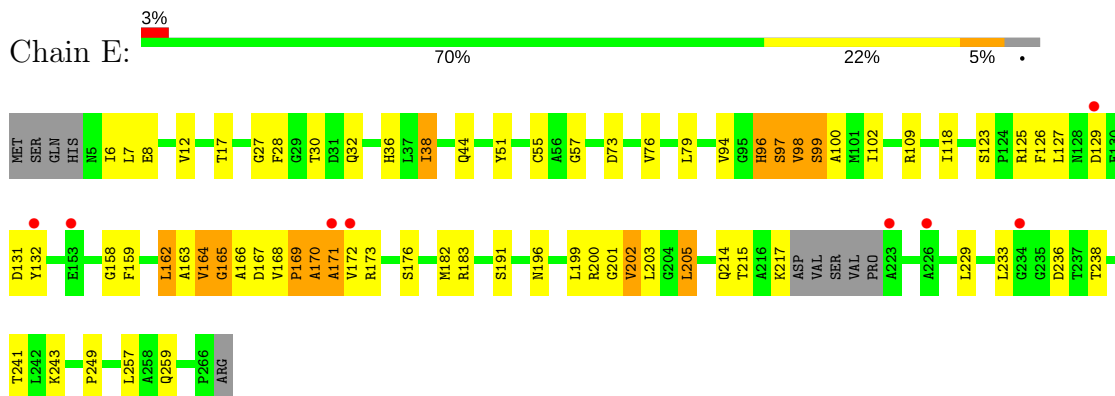# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
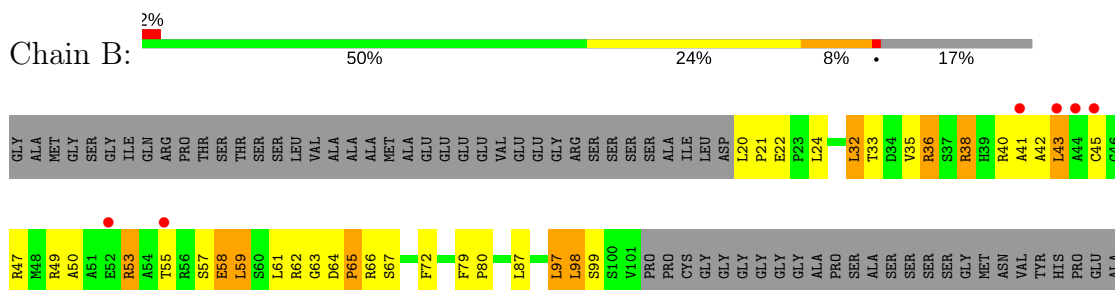
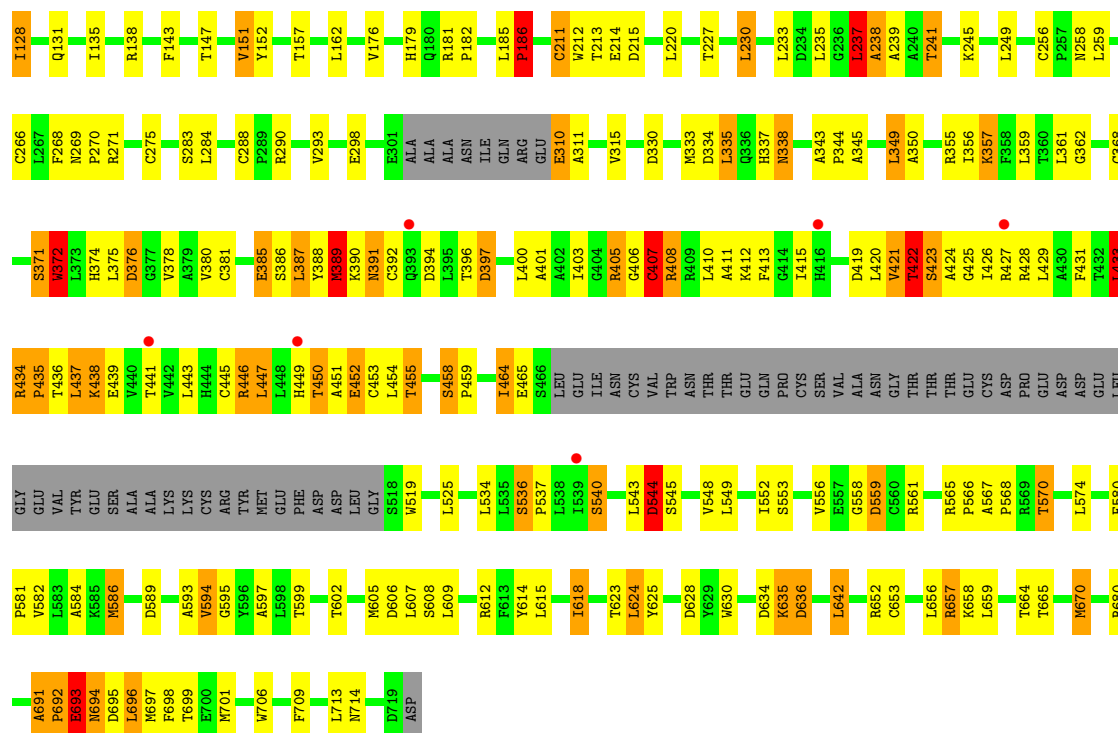• Molecule 1: Strigolactone esterase D14
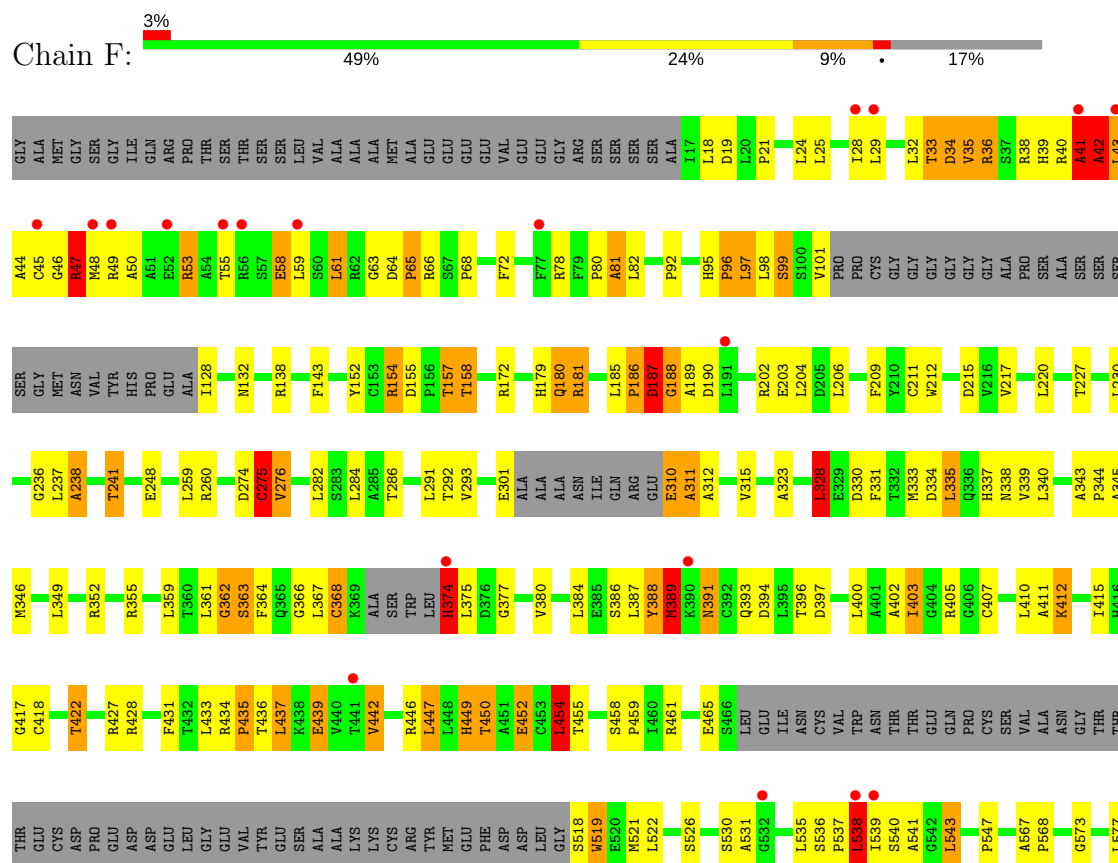
Chain A:

• Molecule 1: Strigolactone esterase D14
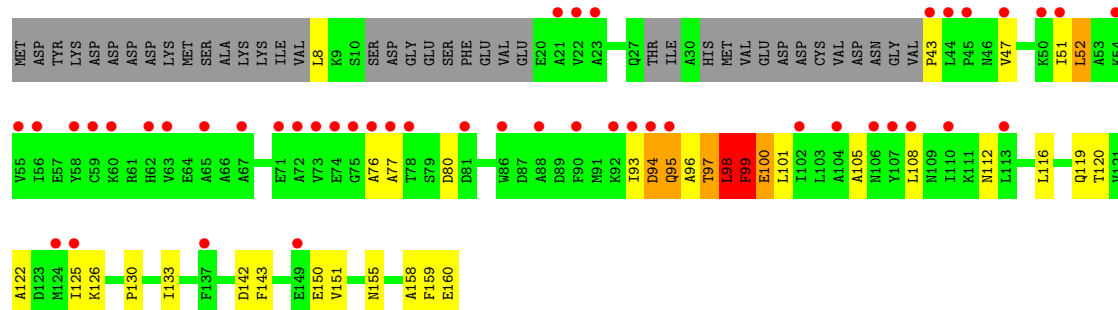
Chain E:

• Molecule 2: F-box/LRR-repeat MAX2 homolog

Chain B:

I128 Q131 I135 R138 F143 T147 V151 Y152 T157 L162 V176 H179 Q180 R181 P182 L185 P186 C211 W212 T213 E214 D215 L220 T227 L230 L233 D234 L235 G236 L237 A238 A239 A240 T241 K245 L249 C256 P257 N258 L259

C266 L267 F268 N269 P270 R271 C275 S283 L284 C288 P289 R290 V293 E298 E301 ALA ALA ALA ASN ILE GLN ARG GLU E310 A311 V315 D330 M333 D334 L335 Q336 H337 N338 A343 P344 A345 L349 A350 R355 I356 K357 F358 L359 L360 L361 G362 C368

S371 W372 L373 H374 L375 D376 G377 V378 A379 V380 C381 E385 S386 L387 Y388 M389 K390 N391 C392 Q393 D394 L395 T396 D397 L400 A401 A402 I403 G404 R405 G406 C407 R408 R409 L410 A411 K412 F413 G414 I415 H416 D419 L420 V421 T422 S423 A424 G425 I426 R427 R428 L429 A430 F431 T432 L433

R434 P435 T436 L437 K438 E439 V440 T441 V442 L443 H444 C445 R446 L447 L448 H449 T450 A451 E452 C453 L454 T455 S458 P459 I464 E465 S466 LEU GLU ILE ASN CYS VAL TRP ASN THR GLU GLN PRO CYS SER VAL ALA ASN GLY THR THR GLU CYS ASP PRO GLU ASP GLU LEU

GLY GLU VAL TYR SER ALA ALA LYS LYS CYS ARG MET GLU ASP ASP LEU GLY S518 W519 L525 L534 L535 S536 P537 L538 I539 S540 L543 D544 S545 V548 L549 I552 S553 V556 E557 G558 D559 C560 R561 R565 P566 A567 P568 R569 T570 L574 F580

P581 V582 L583 A584 K585 M586 D589 A593 V594 G595 Y596 A597 L598 T599 T602 M605 D606 L607 S608 L609 R612 F613 Y614 L615 I618 T623 L624 Y625 D628 Y629 W630 D634 K635 D636 L642 R652 C653 L656 R657 K658 L659 T664 T665 M670 R680

A691 P692 E693 N694 D695 L696 M697 F698 T699 E700 M701 W706 F709 L713 N714 D719 ASP

• Molecule 2: F-box/LRR-repeat MAX2 homolog

Chain F:

3%

49%   24%   9%   •   17%

GLY ALA MET GLY SER GLY ILE GLN ARG PRO THR SER THR SER LEU VAL ALA ALA ALA MET ALA GLU GLU GLU VAL GLU GLU GLY ARG SER SER SER ALA I17 L18 D19 L20 P21 L24 L25 I28 L29 L32 T33 D34 V35 R36 S37 R38 H39 R40 A41 A42 L43

A44 C45 G46 R47 M48 R49 A50 A51 E52 R53 A54 T55 R56 S57 E58 L59 S60 L61 R62 G63 D64 P65 R66 S67 P68 F72 F77 R78 F79 P80 A81 L82 P92 H95 P96 L97 L98 S99 S100 V101 PRO PRO CYS GLY GLY GLY GLY GLY ALA PRO SER SER ALA SER SER SER

SER GLY MET ASN VAL TYR HIS PRO GLU ALA I128 N132 R138 F143 Y152 C153 R154 D155 P156 T157 T158 R172 H179 Q180 R181 L185 P186 D187 G188 A189 D190 L191 R202 E203 L204 D205 L206 F209 Y210 C211 W212 D215 V216 V217 L220 T227 L230

G236 L237 A238 T241 E248 L259 R260 D274 C275 V276 L282 S283 L284 A285 T286 L291 T292 V293 E301 ALA ALA ALA ASN ILE GLN ARG GLU E310 A311 A312 V315 A323 L328 E329 D330 F331 T332 M333 D334 L335 Q336 H337 N338 V339 L340 A343 P344 A345

M346 L349 R352 R355 L359 T360 L361 G362 S363 F364 Q365 G366 L367 C368 K369 ALA SER TRP LEU H374 L375 D376 G377 V380 L384 E385 S386 L387 Y388 M389 K390 N391 C392 Q393 D394 L395 T396 D397 L400 A401 A402 I403 G404 R405 G406 C407 L410 A411 K412 I415 H416

G417 C418 T422 R427 R428 F431 T432 L433 R434 P435 T436 L437 K438 E439 V440 T441 V442 R446 L447 L448 H449 T450 A451 E452 C453 L454 T455 S458 P459 I460 R461 E465 S466 LEU GLU ILE ASN CYS VAL TRP ASN THR GLU GLU THR GLU GLN PRO CYS SER SER VAL ALA ASN GLY THR THR

THR GLU CYS ASP PRO GLU ASP GLU GLU LEU GLY GLU GLU VAL TYR GLU SER ALA ALA LYS LYS CYS ARG MET GLU PHE ASP ASP LEU GLY S518 W519 E520 M521 L522 S526 S530 A531 G532 L535 S536 P537 L538 I539 S540 A541 G542 L543 P547 A567 P568 G573 L577

• Molecule 3: SKP1-like protein 1A

Chain C:

• Molecule 3: SKP1-like protein 1A

Chain G:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.40Å 172.98Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.30 49.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.07-3.30) 99.5 (49.07-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.246 , 0.316 0.256 , 0.317	Depositor DCC
R_{free} test set	2669 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	81.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 60.6	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	15676	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality   (i)

5.1   Standard geometry   (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6OM

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	0.56	0/2046	1.05	8/2785 (0.3%)
1	E	0.56	0/2046	1.17	22/2785 (0.8%)
2	B	0.64	2/4904 (0.0%)	1.27	53/6669 (0.8%)
2	F	0.63	3/4892 (0.1%)	1.31	72/6650 (1.1%)
3	C	0.52	0/1036	0.99	8/1397 (0.6%)
3	G	0.53	0/1052	0.85	6/1421 (0.4%)
All	All	0.60	5/15976 (0.0%)	1.20	169/21707 (0.8%)

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	A	0	2
1	E	0	1
2	B	0	9
2	F	0	15
3	G	0	1
All	All	0	28

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	435	PRO	N-CD	13.99	1.67	1.47
2	B	186	PRO	N-CD	6.95	1.57	1.47
2	F	435	PRO	N-CD	6.95	1.57	1.47
2	F	568	PRO	N-CD	6.09	1.56	1.47
2	F	186	PRO	N-CD	5.12	1.55	1.47

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	597	ALA	CB-CA-C	-24.47	73.39	110.10
1	A	170	ALA	CB-CA-C	22.46	143.79	110.10
2	B	692	PRO	N-CA-CB	-18.29	81.35	103.30
2	F	656	LEU	CB-CA-C	-17.40	77.14	110.20
2	F	42	ALA	N-CA-C	16.11	154.50	111.00

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	TRP	Peptide
1	A	96	HIS	Peptide
2	B	186	PRO	Peptide
2	B	241	THR	Peptide
2	B	400	LEU	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	2001	0	1972	45	0
1	E	2001	0	1972	52	0
2	B	4791	0	4814	226	0
2	F	4782	0	4808	218	0
3	C	1024	0	1011	75	0
3	G	1039	0	1030	33	0
4	A	7	0	0	4	0
4	E	7	0	0	5	0
5	A	3	0	0	0	0
5	B	5	0	0	2	0
5	E	2	0	0	0	0
5	F	10	0	0	0	0
5	G	4	0	0	0	0
All	All	15676	0	15607	595	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 19.

The worst 5 of 595 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)
2:F:92:PRO:HB2	2:F:95:HIS:CD2	1.26	1.61
2:B:389:MET:CE	2:B:392:CYS:HB2	1.32	1.59
1:E:170:ALA:CB	1:E:172:VAL:HB	1.36	1.52
2:B:389:MET:HE1	2:B:392:CYS:CA	1.36	1.52
2:B:389:MET:CE	2:B:392:CYS:CB	1.88	1.52

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/267 (95%)	224 (88%)	28 (11%)	1 (0%)	38	71
1	E	253/267 (95%)	221 (87%)	32 (13%)	0	100	100
2	B	607/740 (82%)	517 (85%)	89 (15%)	1 (0%)	51	81
2	F	604/740 (82%)	516 (85%)	86 (14%)	2 (0%)	44	76
3	C	123/169 (73%)	101 (82%)	20 (16%)	2 (2%)	11	43
3	G	126/169 (75%)	108 (86%)	18 (14%)	0	100	100
All	All	1966/2352 (84%)	1687 (86%)	273 (14%)	6 (0%)	44	76

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	PRO
3	C	98	LEU
2	F	598	LEU
3	C	99	PHE
2	F	65	PRO

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	214/226 (95%)	183 (86%)	31 (14%)	4	18
1	E	214/226 (95%)	185 (86%)	29 (14%)	4	20
2	B	519/615 (84%)	420 (81%)	99 (19%)	2	7
2	F	519/615 (84%)	425 (82%)	94 (18%)	2	9
3	C	110/146 (75%)	103 (94%)	7 (6%)	20	55
3	G	112/146 (77%)	101 (90%)	11 (10%)	9	34
All	All	1688/1974 (86%)	1417 (84%)	271 (16%)	3	14

5 of 271 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	695	ASP
1	E	162	LEU
2	F	693	GLU
2	B	699	THR
1	E	6	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	533	GLN
1	E	196	ASN
3	G	46	ASN
2	B	683	GLN
2	F	95	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	#$|Z| > 2$
4	6OM	A	301	1	5,6,6	3.68	5 (100%)	2,6,6	0.87	0
4	6OM	E	301	-	5,6,6	3.68	5 (100%)	2,6,6	0.89	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
4	6OM	A	301	1	-	1/5/5/5	0/0/0/0
4	6OM	E	301	-	-	1/5/5/5	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	6OM	C3-C2	-3.66	1.45	1.50
4	E	301	6OM	C3-C2	-3.63	1.45	1.50
4	E	301	6OM	C4-C1	-3.60	1.41	1.50
4	A	301	6OM	C4-C1	-3.58	1.41	1.50
4	E	301	6OM	O2-C5	-2.91	1.31	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	6OM	O1-C3-C2-C1
4	A	301	6OM	O1-C3-C2-C1

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	6OM	4	0
4	E	301	6OM	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	257/267 (96%)	-0.12	2 (0%)	86	85	41, 65, 119, 148	0
1	E	257/267 (96%)	0.15	8 (3%)	49	48	53, 86, 155, 192	0
2	B	615/740 (83%)	0.06	12 (1%)	65	63	40, 78, 124, 159	0
2	F	614/740 (82%)	0.13	20 (3%)	47	44	41, 74, 126, 171	0
3	C	130/169 (76%)	1.64	46 (35%)	0	1	77, 152, 200, 232	0
3	G	132/169 (78%)	1.12	32 (24%)	1	1	77, 140, 182, 210	0
All	All	2005/2352 (85%)	0.24	120 (5%)	23	21	40, 80, 158, 232	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	73	VAL	10.5
3	G	73	VAL	7.9
3	C	90	PHE	7.2
3	C	76	ALA	6.5
3	C	77	ALA	6.4

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	6OM	A	301	7/7	0.75	0.36	3.44	50,51,55,55	0
4	6OM	E	301	7/7	0.80	0.42	2.23	50,51,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.