



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 8GRE / pdb_00008gre
Title : F-box protein in complex with skp1(FL) and substrate
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Deposited on : 2022-09-01
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

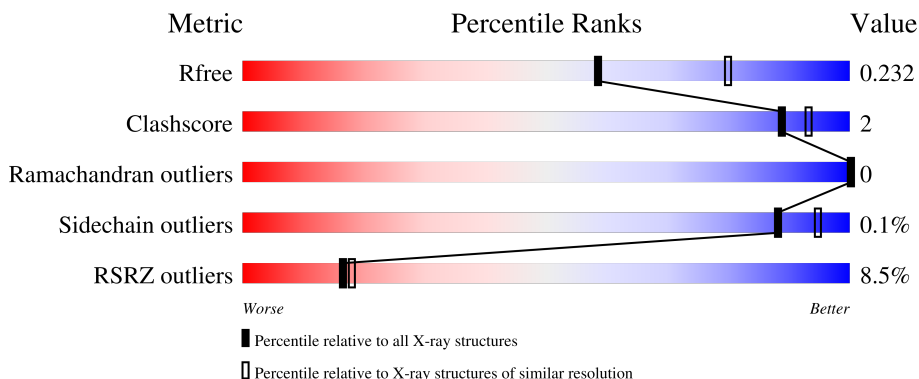
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	460	
1	B	460	
2	C	369	
3	D	194	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10749 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3460	2213	582	658	7	0	0	0
1	B	438	3460	2212	583	658	7	0	0	0

- Molecule 2 is a protein called F-box protein UCC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	338	2785	1817	456	501	11	0	0	0

- Molecule 3 is a protein called E3 ubiquitin ligase complex SCF subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	94	776	489	134	150	3	0	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	73	Total O 73 73	0	0
5	B	68	Total O 68 68	0	0
5	C	93	Total O 93 93	0	0
5	D	10	Total O 10 10	0	0

ASP	ASP	SER	SER	S113	S113
ASN	ASN	V86	V86	A114	A114
ASN	ASN	L87	L87	P115	P115
ASN	ASN	Q88	Q88	V116	V116
GLY	GLY	K89	K89	D117	D117
ASP	ASP	V90	V90	S118	S118
ASP	ASP	I91	I91	W119	W119
ASP	ASP	E92	E92	D120	D120
ASP	ASP	W93	W93		
ASP	ASP	A94	A94		
GLU	GLU	E95	E95		
ASP	ASP	H96	H96		
GLU	GLU	HIS	HIS		
ASP	ASP	ARG	ARG		
ASP	ASP	ASP	ASP		
ASP	ASP	SER	SER		
ASP	ASP	ASN	ASN		
ASP	ASP	PHE	PHE		
ASP	ASP	PRO	PRO		
ASP	ASP	ASP	ASP		
ASP	ASP	ASP	ASP		
ASP	ASP	ASP	ASP		
ASP	ASP	SER	SER		
ASP	ASP	ARG	ARG		
ASP	ASP	ARG	ARG		
ASP	ASP	LYS	LYS		
R121	R121	L145	L145		
E122	E122	L146	L146		
F123	F123	L147	L147		
L124	L124	D148	D148		
K125	K125	A149	A149		
V126	V126	G150	G150		
D127	D127	C151	C151		
M130	M130	K152	K152		
L131	L131	V153	V153		
Y132	Y132	V154	V154		
E133	E133	A155	A155		
I134	I134	E156	E156		
I135	I135	R168	R168		
L136	L136	T169	T169		
A137	A137	F170	F170		
A138	A138	M171	M171		
M139	M139				
Y140	Y140				
L141	L141				
M142	M142				
I143	I143				
K144	K144				
P145	P145				
L146	L146				
L147	L147				
D148	D148				
A149	A149				
G150	G150				
C151	C151				
K152	K152				
V153	V153				
V154	V154				
A155	A155				
E156	E156				
R168	R168				
T169	T169				
F170	F170				
M171	M171				
R194	R194				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.59Å 150.94Å 160.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.71 – 2.30 37.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.71-2.30) 92.8 (37.71-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.232 0.207 , 0.232	Depositor DCC
R_{free} test set	1986 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10749	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.09	0/3541	0.26	0/4795
1	B	0.08	0/3541	0.25	0/4796
2	C	0.10	0/2864	0.27	0/3896
3	D	0.09	0/790	0.29	0/1067
All	All	0.09	0/10736	0.26	0/14554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3460	0	3434	13	0
1	B	3460	0	3431	11	0
2	C	2785	0	2773	10	0
3	D	776	0	754	5	0
4	A	12	0	16	0	0
4	C	12	0	16	0	0
5	A	73	0	0	0	0
5	B	68	0	0	0	0
5	C	93	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	0	0	0
All	All	10749	0	10424	39	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 2.

The worst 5 of 39 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:C:293:ALA:HB1	2:C:338:LEU:HD11	1.83	0.60
1:B:272:SER:HB2	1:B:438:ILE:HA	1.92	0.51
2:C:219:ILE:HG13	2:C:287:PRO:HA	1.93	0.51
1:A:211:ARG:HG3	1:A:219:MET:HG2	1.93	0.51
1:A:272:SER:HB2	1:A:438:ILE:HA	1.92	0.51

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	436/460 (95%)	426 (98%)	10 (2%)	0	100	100
1	B	436/460 (95%)	428 (98%)	8 (2%)	0	100	100
2	C	332/369 (90%)	325 (98%)	7 (2%)	0	100	100
3	D	90/194 (46%)	87 (97%)	3 (3%)	0	100	100
All	All	1294/1483 (87%)	1266 (98%)	28 (2%)	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	375/396 (95%)	374 (100%)	1 (0%)	86	93
1	B	375/396 (95%)	375 (100%)	0	100	100
2	C	309/337 (92%)	309 (100%)	0	100	100
3	D	83/179 (46%)	83 (100%)	0	100	100
All	All	1142/1308 (87%)	1141 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	305	GLN
2	C	211	ASN
1	B	383	HIS
1	B	234	ASN
2	C	25	ASN

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](#)

4 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	GOL	C	402	-	5,5,5	0.91	0	5,5,5	1.10	0
4	GOL	A	501	-	5,5,5	0.93	0	5,5,5	1.10	0
4	GOL	C	401	-	5,5,5	0.92	0	5,5,5	1.07	0
4	GOL	A	502	-	5,5,5	0.94	0	5,5,5	1.08	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	GOL	C	402	-	-	0/4/4/4	-
4	GOL	A	501	-	-	2/4/4/4	-
4	GOL	C	401	-	-	2/4/4/4	-
4	GOL	A	502	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GOL	O1-C1-C2-C3
4	C	401	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	501	GOL	O1-C1-C2-O2
4	C	401	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	438/460 (95%)	0.51	20 (4%) 37 39	25, 48, 72, 86	0
1	B	438/460 (95%)	0.59	21 (4%) 35 37	27, 50, 79, 96	0
2	C	338/369 (91%)	0.41	23 (6%) 23 25	26, 41, 71, 91	0
3	D	94/194 (48%)	2.28	47 (50%) 0 0	33, 88, 121, 129	0
All	All	1308/1483 (88%)	0.64	111 (8%) 16 18	25, 48, 83, 129	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	114	ALA	8.5
3	D	86	VAL	6.3
3	D	123	PHE	6.3
3	D	93	TRP	6.1
3	D	85	SER	5.8

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(\AA^2)	Q<0.9
4	GOL	A	502	6/6	0.68	0.16	68,74,75,76	0
4	GOL	C	402	6/6	0.71	0.21	55,59,62,64	0
4	GOL	A	501	6/6	0.88	0.15	36,46,50,51	0
4	GOL	C	401	6/6	0.89	0.14	56,58,61,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.