



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:42 PM UTC

PDB ID : 5XGC / pdb_00005xgc
Title : Crystal structure of SmgGDS-558
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Deposited on : 2017-04-13
Resolution : 2.10 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 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

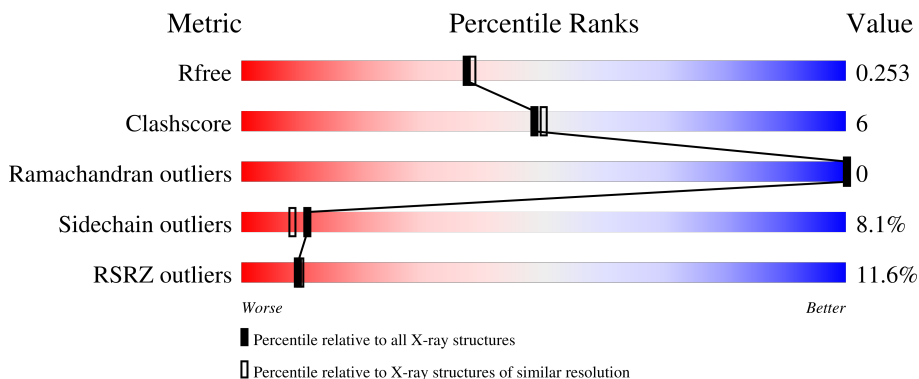
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	503	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3531 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 Rap1 GTPase-GDP dissociation stimulator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3457	2178	602	656	21			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	GLY	-	expression tag	UNP P52306
A	57	PRO	-	expression tag	UNP P52306
A	58	LEU	-	expression tag	UNP P52306
A	59	GLY	-	expression tag	UNP P52306
A	60	SER	-	expression tag	UNP P52306

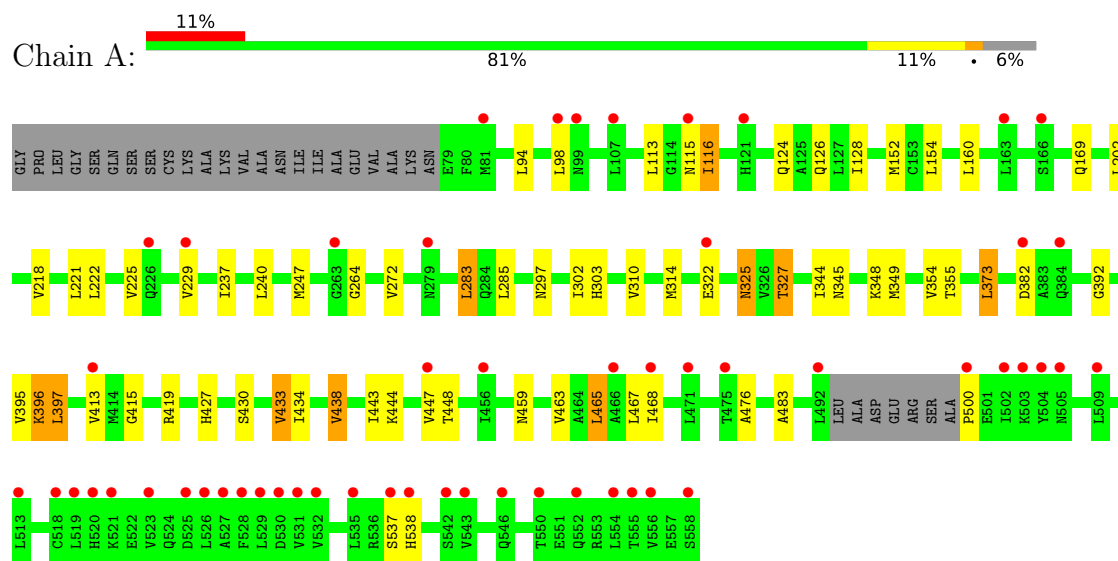
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		

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: Rap1 GTPase-GDP dissociation stimulator 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.33Å 51.12Å 52.44Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	49.43 – 2.10 49.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.43-2.10) 99.9 (49.43-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.215 , 0.252 (Not available) , 0.253	Depositor DCC
R_{free} test set	1546 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3531	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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

5.1 Standard geometry

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	0.60	0/3490	0.87	1/4724 (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	A	500	PRO	N-CA-CB	6.29	109.92	103.00

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	3457	0	3415	38	0
2	A	74	0	0	1	0
All	All	3531	0	3415	38	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 6.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG12	1:A:314:MET:HE3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:HD21	1:A:327:THR:HB	1.48	0.76
1:A:310:VAL:CG1	1:A:314:MET:HE3	2.17	0.75
1:A:537:SER:HA	1:A:538:HIS:C	2.18	0.68
1:A:382:ASP:O	1:A:427:HIS:CE1	2.48	0.67
1:A:325:ASN:ND2	1:A:327:THR:HB	2.12	0.64
1:A:225:VAL:O	1:A:229:VAL:HG23	1.97	0.63
1:A:373:LEU:C	1:A:373:LEU:HD12	2.24	0.62
1:A:264:GLY:HA3	1:A:303:HIS:CE1	2.36	0.60
1:A:438:VAL:HG12	1:A:443:ILE:HD11	1.84	0.60
1:A:438:VAL:HG12	1:A:443:ILE:CD1	2.36	0.56
1:A:128:ILE:HD12	1:A:169:GLN:HG3	1.88	0.56
1:A:222:LEU:HD23	1:A:247:MET:HE1	1.88	0.55
1:A:240:LEU:HD21	1:A:283:LEU:HD13	1.89	0.55
1:A:314:MET:HE2	1:A:354:VAL:CB	2.37	0.54
1:A:285:LEU:HD13	1:A:327:THR:CG2	2.37	0.54
1:A:397:LEU:C	1:A:397:LEU:HD23	2.33	0.54
1:A:218:VAL:HG22	2:A:604:HOH:O	2.08	0.52
1:A:285:LEU:HD13	1:A:327:THR:HG23	1.91	0.51
1:A:314:MET:HE2	1:A:354:VAL:CA	2.42	0.50
1:A:468:ILE:HD11	1:A:476:ALA:HB2	1.93	0.50
1:A:444:LYS:O	1:A:448:THR:HG23	2.12	0.50
1:A:314:MET:HE2	1:A:354:VAL:HB	1.93	0.49
1:A:124:GLN:O	1:A:128:ILE:HG12	2.13	0.49
1:A:113:LEU:HD23	1:A:116:ILE:HD11	1.95	0.48
1:A:344:ILE:HG22	1:A:348:LYS:HE3	1.96	0.48
1:A:325:ASN:C	1:A:325:ASN:HD22	2.22	0.48
1:A:434:ILE:O	1:A:438:VAL:HG13	2.14	0.47
1:A:310:VAL:HG21	1:A:349:MET:HG2	1.97	0.46
1:A:415:GLY:O	1:A:419:ARG:HG3	2.16	0.46
1:A:392:GLY:HA3	1:A:433:VAL:HB	1.98	0.45
1:A:302:ILE:HA	1:A:345:ASN:HD21	1.81	0.44
1:A:314:MET:HE2	1:A:354:VAL:HA	1.99	0.44
1:A:537:SER:CA	1:A:538:HIS:C	2.90	0.43
1:A:459:ASN:O	1:A:463:VAL:HG23	2.19	0.43
1:A:447:VAL:HG11	1:A:483:ALA:HB1	2.02	0.42
1:A:396:LYS:HE3	1:A:396:LYS:O	2.21	0.41
1:A:465:LEU:HA	1:A:468:ILE:HG22	2.03	0.41

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	469/503 (93%)	451 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	347/426 (82%)	319 (92%)	28 (8%)	11	8

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	98	LEU
1	A	115	ASN
1	A	116	ILE
1	A	126	GLN
1	A	152	MET
1	A	154	LEU
1	A	160	LEU
1	A	202	LEU
1	A	221	LEU
1	A	237	ILE
1	A	272	VAL
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	297	ASN
1	A	322	GLU
1	A	325	ASN
1	A	327	THR
1	A	355	THR
1	A	373	LEU
1	A	395	VAL
1	A	396	LYS
1	A	397	LEU
1	A	413	VAL
1	A	430	SER
1	A	433	VAL
1	A	438	VAL
1	A	465	LEU
1	A	467	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	186	GLN
1	A	211	GLN
1	A	258	GLN
1	A	282	GLN
1	A	297	ASN
1	A	303	HIS
1	A	307	ASN
1	A	325	ASN
1	A	330	HIS
1	A	345	ASN
1	A	390	GLN
1	A	445	HIS
1	A	458	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	473/503 (94%)	0.79	55 (11%) 9 10	39, 59, 124, 157	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	4.5
1	A	526	LEU	4.1
1	A	550	THR	4.1
1	A	527	ALA	4.0
1	A	531	VAL	3.9
1	A	535	LEU	3.8
1	A	500	PRO	3.6
1	A	492	LEU	3.6
1	A	505	ASN	3.6
1	A	519	LEU	3.6
1	A	518	CYS	3.5
1	A	532	VAL	3.4
1	A	504	TYR	3.4
1	A	468	ILE	3.2
1	A	502	ILE	3.1
1	A	229	VAL	3.0
1	A	503	LYS	3.0
1	A	546	GLN	2.9
1	A	521	LYS	2.9
1	A	523	VAL	2.9
1	A	509	LEU	2.9
1	A	529	LEU	2.8
1	A	456	ILE	2.8
1	A	115	ASN	2.7
1	A	538	HIS	2.7
1	A	554	LEU	2.6
1	A	558	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	543	VAL	2.6
1	A	471	LEU	2.6
1	A	530	ASP	2.6
1	A	263	GLY	2.5
1	A	382	ASP	2.5
1	A	322	GLU	2.5
1	A	520	HIS	2.5
1	A	99	ASN	2.5
1	A	81	MET	2.5
1	A	166	SER	2.4
1	A	384	GLN	2.4
1	A	525	ASP	2.4
1	A	537	SER	2.3
1	A	556	VAL	2.3
1	A	475	THR	2.3
1	A	552	GLN	2.3
1	A	542	SER	2.2
1	A	528	PHE	2.2
1	A	413	VAL	2.2
1	A	226	GLN	2.1
1	A	513	LEU	2.1
1	A	279	ASN	2.1
1	A	98	LEU	2.1
1	A	555	THR	2.1
1	A	447	VAL	2.0
1	A	466	ALA	2.0
1	A	107	LEU	2.0
1	A	121	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.