



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:02 PM UTC

PDB ID : 6GN0 / pdb_00006gn0
Title : Exoenzyme S from *Pseudomonas aeruginosa* in complex with human 14-3-3 protein beta, tetrameric crystal form
Authors : Karlberg, T.; Pinto, A.F.; Hornyak, P.; Nareoja, K.; Schuler, H.
Deposited on : 2018-05-29
Resolution : 3.24 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

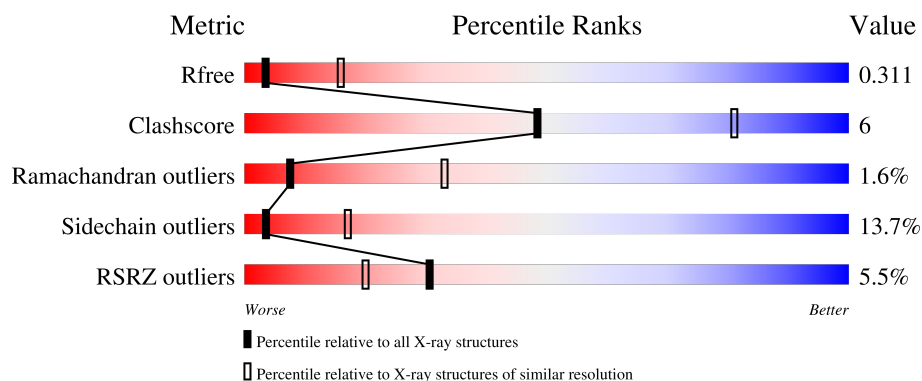
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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.



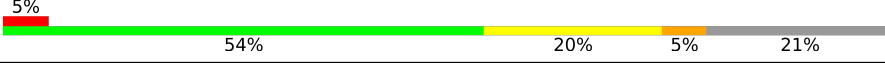
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	248	2% 74%18%••
1	B	248	4% 74%18%•6%
1	C	248	4% 76%17%•5%
1	D	248	4% 77%18%••
2	E	244	5% 58%16%5%•20%

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Mol	Chain	Length	Quality of chain
2	F	244	 8% 51% 22% 5% 21%
2	G	244	 6% 53% 20% 7% 20%
2	H	244	 5% 54% 20% 5% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13303 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 14-3-3 protein beta/alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1919	1195	324	391	9			
1	B	233	Total	C	N	O	S	0	0	0
			1863	1164	312	378	9			
1	C	236	Total	C	N	O	S	0	0	0
			1895	1185	316	385	9			
1	D	237	Total	C	N	O	S	0	0	0
			1887	1178	315	385	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLU	-	expression tag	UNP P31946
A	241	ASN	-	expression tag	UNP P31946
A	242	LEU	-	expression tag	UNP P31946
A	243	TYR	-	expression tag	UNP P31946
A	244	PHE	-	expression tag	UNP P31946
A	245	GLN	-	expression tag	UNP P31946
A	246	SER	-	expression tag	UNP P31946
A	247	LEU	-	expression tag	UNP P31946
A	248	GLU	-	expression tag	UNP P31946
B	240	GLU	-	expression tag	UNP P31946
B	241	ASN	-	expression tag	UNP P31946
B	242	LEU	-	expression tag	UNP P31946
B	243	TYR	-	expression tag	UNP P31946
B	244	PHE	-	expression tag	UNP P31946
B	245	GLN	-	expression tag	UNP P31946
B	246	SER	-	expression tag	UNP P31946
B	247	LEU	-	expression tag	UNP P31946
B	248	GLU	-	expression tag	UNP P31946
C	240	GLU	-	expression tag	UNP P31946
C	241	ASN	-	expression tag	UNP P31946
C	242	LEU	-	expression tag	UNP P31946

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Chain	Residue	Modelled	Actual	Comment	Reference
C	243	TYR	-	expression tag	UNP P31946
C	244	PHE	-	expression tag	UNP P31946
C	245	GLN	-	expression tag	UNP P31946
C	246	SER	-	expression tag	UNP P31946
C	247	LEU	-	expression tag	UNP P31946
C	248	GLU	-	expression tag	UNP P31946
D	240	GLU	-	expression tag	UNP P31946
D	241	ASN	-	expression tag	UNP P31946
D	242	LEU	-	expression tag	UNP P31946
D	243	TYR	-	expression tag	UNP P31946
D	244	PHE	-	expression tag	UNP P31946
D	245	GLN	-	expression tag	UNP P31946
D	246	SER	-	expression tag	UNP P31946
D	247	LEU	-	expression tag	UNP P31946
D	248	GLU	-	expression tag	UNP P31946

- Molecule 2 is a protein called Exoenzyme S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	194	Total	C	N	O	S	0	0	0
			1438	887	256	292	3			
2	F	192	Total	C	N	O	S	0	0	0
			1423	876	256	288	3			
2	G	195	Total	C	N	O	S	0	0	0
			1446	892	258	293	3			
2	H	193	Total	C	N	O	S	0	0	0
			1432	882	258	289	3			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	210	MET	-	initiating methionine	UNP Q51451
E	211	GLY	-	expression tag	UNP Q51451
E	212	SER	-	expression tag	UNP Q51451
E	213	SER	-	expression tag	UNP Q51451
E	214	HIS	-	expression tag	UNP Q51451
E	215	HIS	-	expression tag	UNP Q51451
E	216	HIS	-	expression tag	UNP Q51451
E	217	HIS	-	expression tag	UNP Q51451
E	218	HIS	-	expression tag	UNP Q51451
E	219	HIS	-	expression tag	UNP Q51451
E	220	SER	-	expression tag	UNP Q51451

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Chain	Residue	Modelled	Actual	Comment	Reference
E	221	GLN	-	expression tag	UNP Q51451
E	222	ASP	-	expression tag	UNP Q51451
E	223	PRO	-	expression tag	UNP Q51451
E	224	ASN	-	expression tag	UNP Q51451
E	225	SER	-	expression tag	UNP Q51451
E	226	GLU	-	expression tag	UNP Q51451
E	227	ASN	-	expression tag	UNP Q51451
E	228	LEU	-	expression tag	UNP Q51451
E	229	TYR	-	expression tag	UNP Q51451
E	230	PHE	-	expression tag	UNP Q51451
E	231	GLN	-	expression tag	UNP Q51451
E	232	GLY	-	expression tag	UNP Q51451
E	233	ALA	-	expression tag	UNP Q51451
E	379	ALA	GLU	engineered mutation	UNP Q51451
E	381	ALA	GLU	engineered mutation	UNP Q51451
E	415	LEU	GLN	conflict	UNP Q51451
E	434	PRO	ARG	conflict	UNP Q51451
F	210	MET	-	initiating methionine	UNP Q51451
F	211	GLY	-	expression tag	UNP Q51451
F	212	SER	-	expression tag	UNP Q51451
F	213	SER	-	expression tag	UNP Q51451
F	214	HIS	-	expression tag	UNP Q51451
F	215	HIS	-	expression tag	UNP Q51451
F	216	HIS	-	expression tag	UNP Q51451
F	217	HIS	-	expression tag	UNP Q51451
F	218	HIS	-	expression tag	UNP Q51451
F	219	HIS	-	expression tag	UNP Q51451
F	220	SER	-	expression tag	UNP Q51451
F	221	GLN	-	expression tag	UNP Q51451
F	222	ASP	-	expression tag	UNP Q51451
F	223	PRO	-	expression tag	UNP Q51451
F	224	ASN	-	expression tag	UNP Q51451
F	225	SER	-	expression tag	UNP Q51451
F	226	GLU	-	expression tag	UNP Q51451
F	227	ASN	-	expression tag	UNP Q51451
F	228	LEU	-	expression tag	UNP Q51451
F	229	TYR	-	expression tag	UNP Q51451
F	230	PHE	-	expression tag	UNP Q51451
F	231	GLN	-	expression tag	UNP Q51451
F	232	GLY	-	expression tag	UNP Q51451
F	233	ALA	-	expression tag	UNP Q51451
F	379	ALA	GLU	engineered mutation	UNP Q51451

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Chain	Residue	Modelled	Actual	Comment	Reference
F	381	ALA	GLU	engineered mutation	UNP Q51451
F	415	LEU	GLN	conflict	UNP Q51451
F	434	PRO	ARG	conflict	UNP Q51451
G	210	MET	-	initiating methionine	UNP Q51451
G	211	GLY	-	expression tag	UNP Q51451
G	212	SER	-	expression tag	UNP Q51451
G	213	SER	-	expression tag	UNP Q51451
G	214	HIS	-	expression tag	UNP Q51451
G	215	HIS	-	expression tag	UNP Q51451
G	216	HIS	-	expression tag	UNP Q51451
G	217	HIS	-	expression tag	UNP Q51451
G	218	HIS	-	expression tag	UNP Q51451
G	219	HIS	-	expression tag	UNP Q51451
G	220	SER	-	expression tag	UNP Q51451
G	221	GLN	-	expression tag	UNP Q51451
G	222	ASP	-	expression tag	UNP Q51451
G	223	PRO	-	expression tag	UNP Q51451
G	224	ASN	-	expression tag	UNP Q51451
G	225	SER	-	expression tag	UNP Q51451
G	226	GLU	-	expression tag	UNP Q51451
G	227	ASN	-	expression tag	UNP Q51451
G	228	LEU	-	expression tag	UNP Q51451
G	229	TYR	-	expression tag	UNP Q51451
G	230	PHE	-	expression tag	UNP Q51451
G	231	GLN	-	expression tag	UNP Q51451
G	232	GLY	-	expression tag	UNP Q51451
G	233	ALA	-	expression tag	UNP Q51451
G	379	ALA	GLU	engineered mutation	UNP Q51451
G	381	ALA	GLU	engineered mutation	UNP Q51451
G	415	LEU	GLN	conflict	UNP Q51451
G	434	PRO	ARG	conflict	UNP Q51451
H	210	MET	-	initiating methionine	UNP Q51451
H	211	GLY	-	expression tag	UNP Q51451
H	212	SER	-	expression tag	UNP Q51451
H	213	SER	-	expression tag	UNP Q51451
H	214	HIS	-	expression tag	UNP Q51451
H	215	HIS	-	expression tag	UNP Q51451
H	216	HIS	-	expression tag	UNP Q51451
H	217	HIS	-	expression tag	UNP Q51451
H	218	HIS	-	expression tag	UNP Q51451
H	219	HIS	-	expression tag	UNP Q51451
H	220	SER	-	expression tag	UNP Q51451

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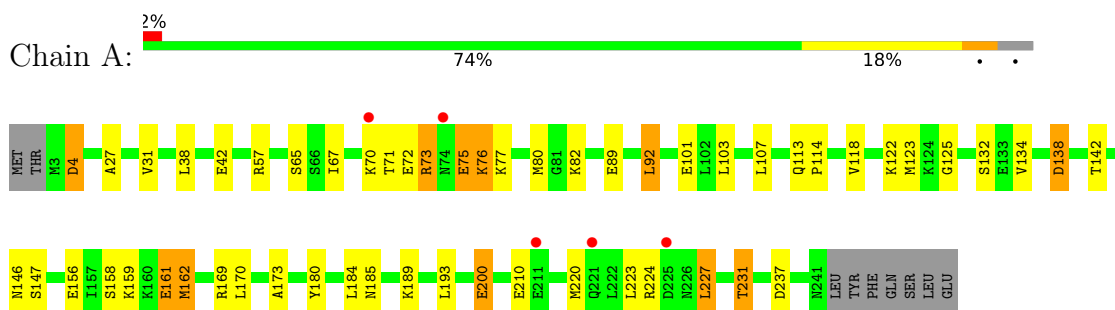
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Chain	Residue	Modelled	Actual	Comment	Reference
H	221	GLN	-	expression tag	UNP Q51451
H	222	ASP	-	expression tag	UNP Q51451
H	223	PRO	-	expression tag	UNP Q51451
H	224	ASN	-	expression tag	UNP Q51451
H	225	SER	-	expression tag	UNP Q51451
H	226	GLU	-	expression tag	UNP Q51451
H	227	ASN	-	expression tag	UNP Q51451
H	228	LEU	-	expression tag	UNP Q51451
H	229	TYR	-	expression tag	UNP Q51451
H	230	PHE	-	expression tag	UNP Q51451
H	231	GLN	-	expression tag	UNP Q51451
H	232	GLY	-	expression tag	UNP Q51451
H	233	ALA	-	expression tag	UNP Q51451
H	379	ALA	GLU	engineered mutation	UNP Q51451
H	381	ALA	GLU	engineered mutation	UNP Q51451
H	415	LEU	GLN	conflict	UNP Q51451
H	434	PRO	ARG	conflict	UNP Q51451

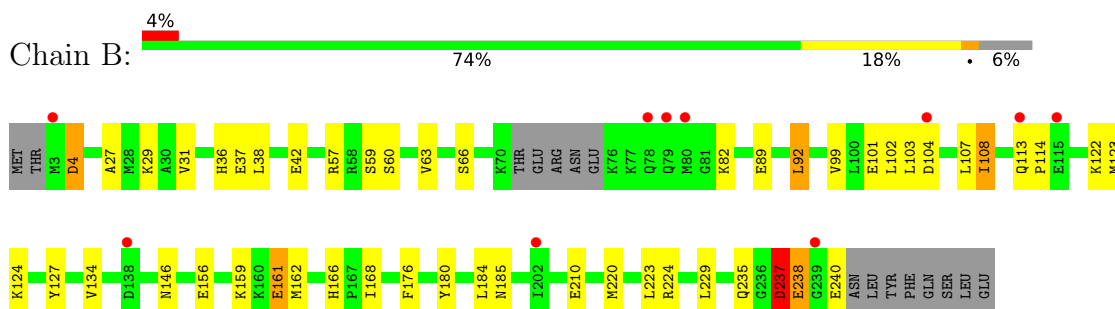
3 Residue-property plots [i](#)

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.

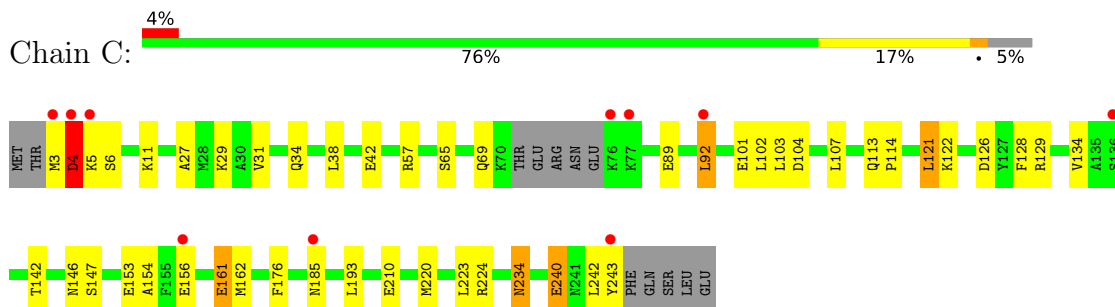
- Molecule 1: 14-3-3 protein beta/alpha



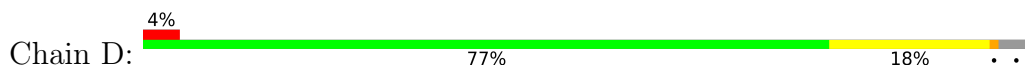
- Molecule 1: 14-3-3 protein beta/alpha

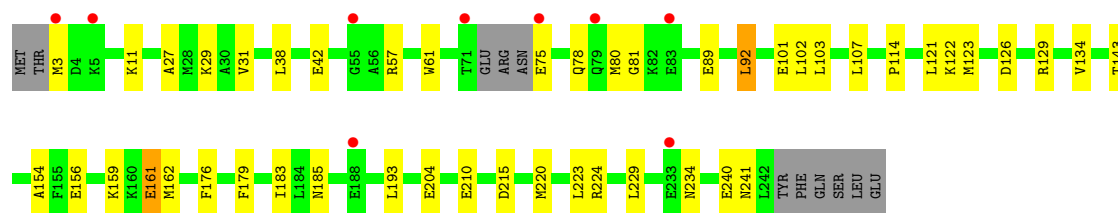


- Molecule 1: 14-3-3 protein beta/alpha

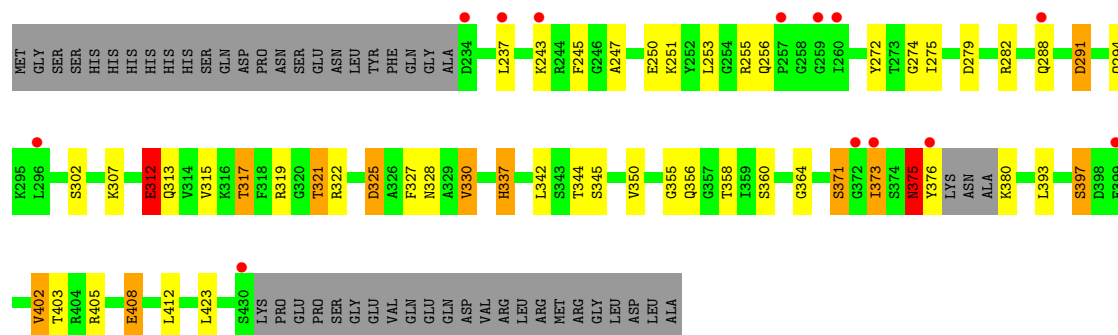


- Molecule 1: 14-3-3 protein beta/alpha

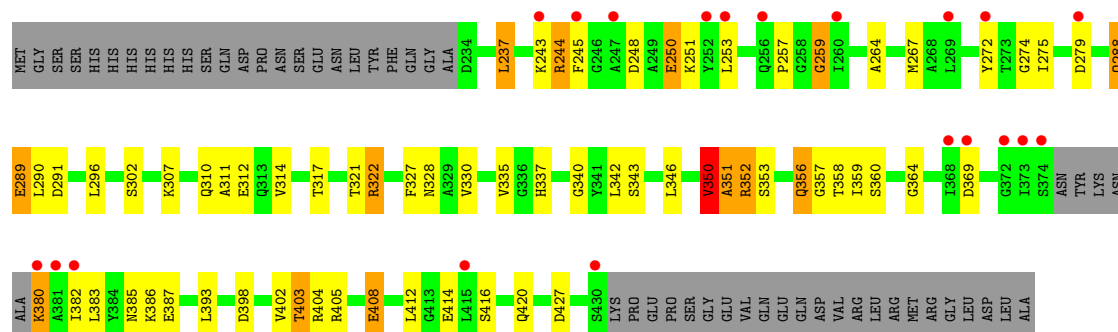




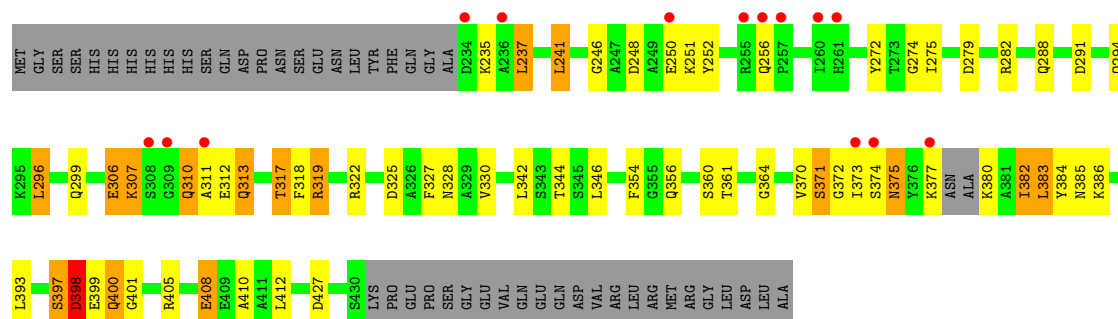
• Molecule 2: Exoenzyme S



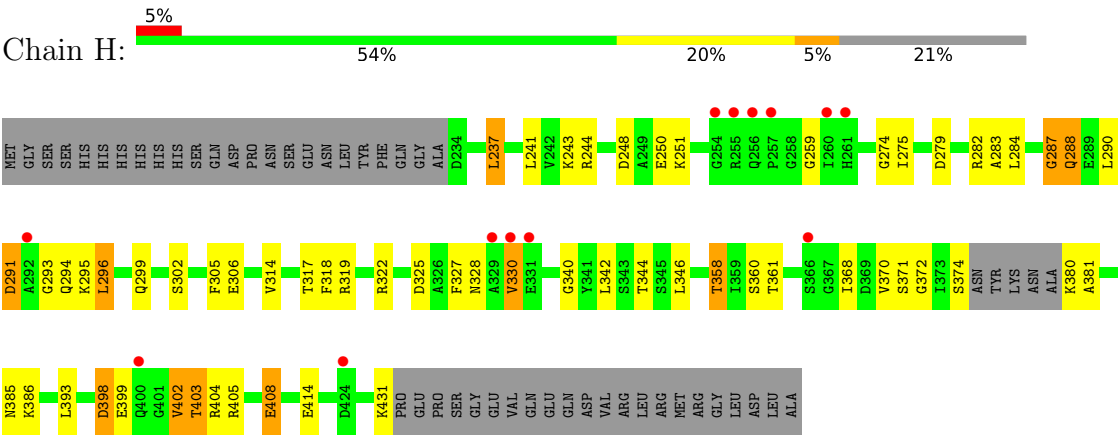
• Molecule 2: Exoenzyme S



• Molecule 2: Exoenzyme S



● Molecule 2: Exoenzyme S



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.20Å 168.76Å 82.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.05 – 3.24 118.05 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.0 (118.05-3.24) 99.0 (118.05-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.243 , 0.294 0.256 , 0.311	Depositor DCC
R_{free} test set	1842 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13303	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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](#)

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	0.90	0/1946	1.57	11/2619 (0.4%)
1	B	0.87	1/1889 (0.1%)	1.49	9/2542 (0.4%)
1	C	0.87	1/1922 (0.1%)	1.53	10/2587 (0.4%)
1	D	0.86	2/1913 (0.1%)	1.55	11/2577 (0.4%)
2	E	0.90	1/1454 (0.1%)	1.52	21/1953 (1.1%)
2	F	0.87	0/1438	1.54	21/1930 (1.1%)
2	G	0.92	0/1462	1.53	28/1963 (1.4%)
2	H	0.88	1/1447 (0.1%)	1.48	12/1941 (0.6%)
All	All	0.88	6/13471 (0.0%)	1.53	123/18112 (0.7%)

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	C	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	240	GLU	CA-C	6.94	1.61	1.53
1	B	108	ILE	CA-C	6.50	1.58	1.52
1	D	240	GLU	CA-CB	5.47	1.58	1.53
2	E	312	GLU	CA-C	5.38	1.59	1.52
2	H	358	THR	CA-C	5.21	1.58	1.52

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	240	GLU	CA-C-N	12.29	143.83	121.70
1	D	240	GLU	C-N-CA	12.29	143.83	121.70
1	C	240	GLU	CA-C-N	11.23	141.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	GLU	C-N-CA	11.23	141.91	121.70
1	A	138	ASP	CA-CB-CG	8.64	121.25	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	240	GLU	Peptide

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	1919	0	1879	16	0
1	B	1863	0	1823	17	0
1	C	1895	0	1853	15	0
1	D	1887	0	1836	16	0
2	E	1438	0	1401	18	0
2	F	1423	0	1395	27	0
2	G	1446	0	1412	20	0
2	H	1432	0	1408	20	0
All	All	13303	0	13007	145	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.

The worst 5 of 145 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:B:237:ASP:HB2	1:B:238:GLU:HB3	1.55	0.86
1:D:204:GLU:HG2	2:F:352:ARG:NH1	1.91	0.85
1:C:4:ASP:HA	1:C:34:GLN:HE22	1.42	0.83
1:D:204:GLU:HG2	2:F:352:ARG:HH12	1.45	0.81
2:H:385:ASN:HD22	2:H:386:LYS:H	1.31	0.79

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	237/248 (96%)	221 (93%)	15 (6%)	1 (0%)	30	60
1	B	229/248 (92%)	214 (93%)	13 (6%)	2 (1%)	14	44
1	C	232/248 (94%)	219 (94%)	12 (5%)	1 (0%)	30	60
1	D	233/248 (94%)	222 (95%)	11 (5%)	0	100	100
2	E	190/244 (78%)	161 (85%)	22 (12%)	7 (4%)	2	16
2	F	188/244 (77%)	164 (87%)	17 (9%)	7 (4%)	2	16
2	G	191/244 (78%)	171 (90%)	15 (8%)	5 (3%)	4	23
2	H	189/244 (78%)	163 (86%)	22 (12%)	4 (2%)	5	27
All	All	1689/1968 (86%)	1535 (91%)	127 (8%)	27 (2%)	7	33

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	5	LYS
2	E	256	GLN
2	F	257	PRO
2	G	398	ASP
2	H	288	GLN

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	210/220 (96%)	182 (87%)	28 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	203/220 (92%)	183 (90%)	20 (10%)	7	29
1	C	207/220 (94%)	188 (91%)	19 (9%)	8	31
1	D	205/220 (93%)	186 (91%)	19 (9%)	8	31
2	E	145/189 (77%)	122 (84%)	23 (16%)	2	12
2	F	144/189 (76%)	115 (80%)	29 (20%)	1	6
2	G	146/189 (77%)	118 (81%)	28 (19%)	1	7
2	H	145/189 (77%)	119 (82%)	26 (18%)	2	8
All	All	1405/1636 (86%)	1213 (86%)	192 (14%)	3	17

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	275	ILE
2	G	256	GLN
2	F	296	LEU
2	F	356	GLN
2	G	307	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	152	GLN
2	F	385	ASN
2	H	256	GLN
2	F	299	GLN
2	G	286	GLN

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 [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 [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	239/248 (96%)	0.23	5 (2%) 63 43	18, 38, 74, 101	0
1	B	233/248 (93%)	0.35	10 (4%) 40 25	15, 37, 66, 104	0
1	C	236/248 (95%)	0.65	10 (4%) 40 26	33, 56, 84, 100	0
1	D	237/248 (95%)	0.55	9 (3%) 44 28	25, 54, 91, 115	0
2	E	194/244 (79%)	0.63	13 (6%) 24 16	23, 55, 90, 98	0
2	F	192/244 (78%)	0.91	20 (10%) 11 8	28, 61, 101, 122	0
2	G	195/244 (79%)	0.63	14 (7%) 21 14	15, 53, 95, 110	0
2	H	193/244 (79%)	0.70	13 (6%) 24 16	35, 59, 90, 123	0
All	All	1719/1968 (87%)	0.57	94 (5%) 30 20	15, 52, 90, 123	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	374	SER	4.3
2	H	257	PRO	4.1
2	H	260	ILE	3.8
2	F	245	PHE	3.8
2	F	247	ALA	3.7

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.