



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:03 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 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

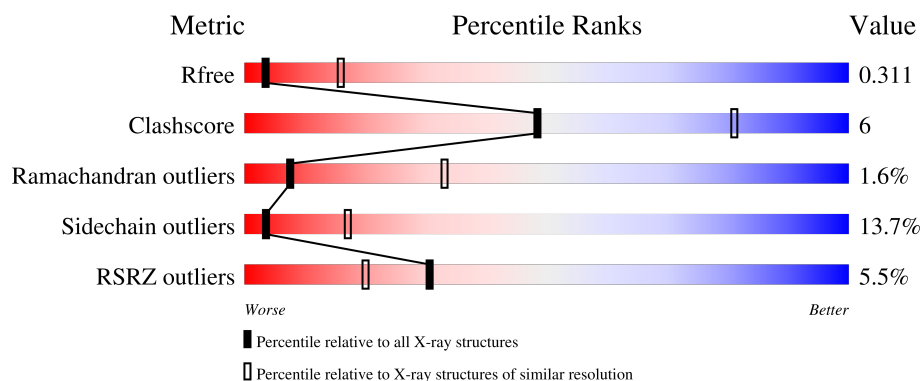
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



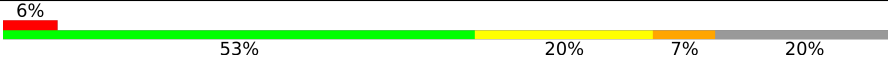
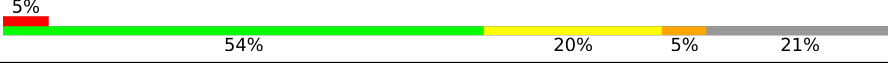
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

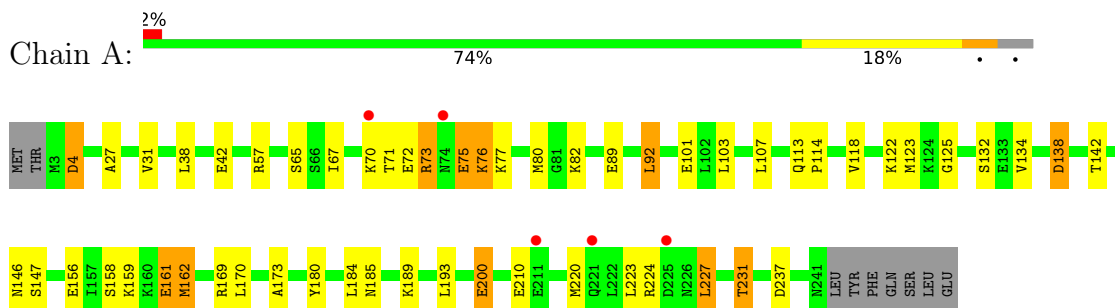
Continued from previous page...

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

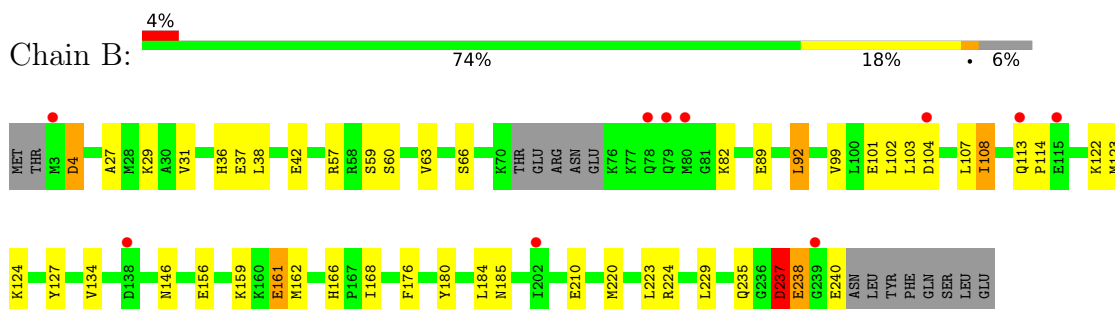
3 Residue-property plots [i](#)

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.

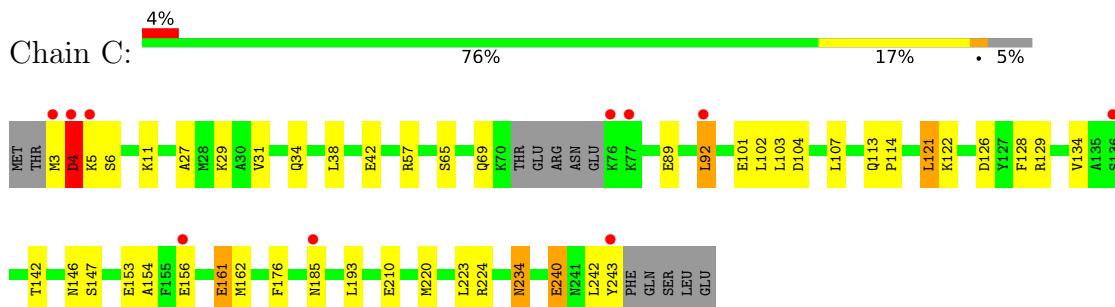
- Molecule 1: 14-3-3 protein beta/alpha



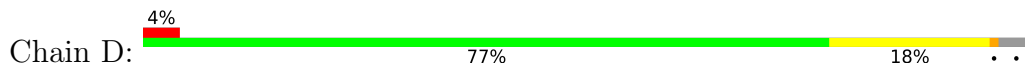
- Molecule 1: 14-3-3 protein beta/alpha

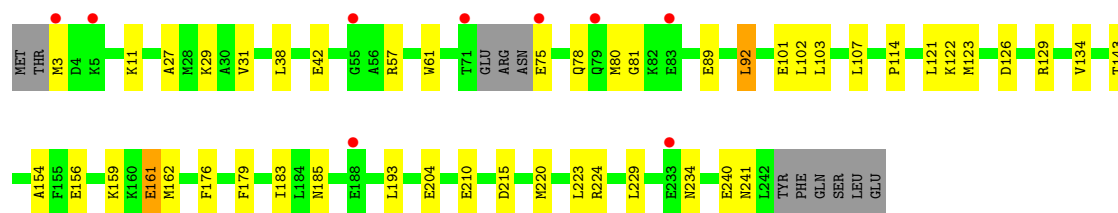


- Molecule 1: 14-3-3 protein beta/alpha

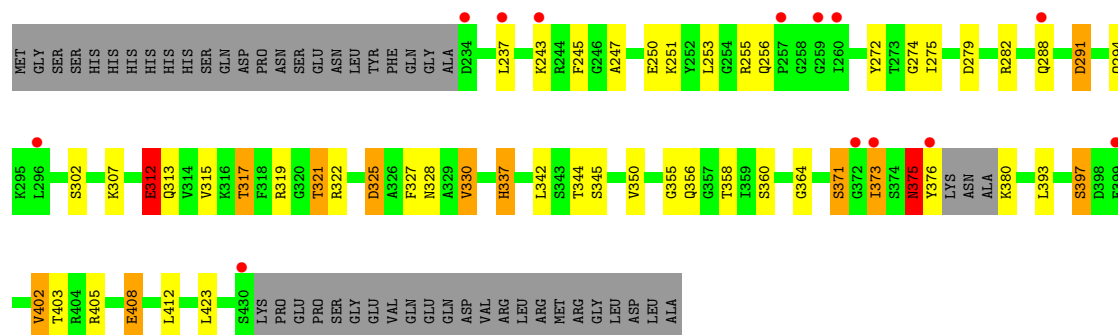


- Molecule 1: 14-3-3 protein beta/alpha

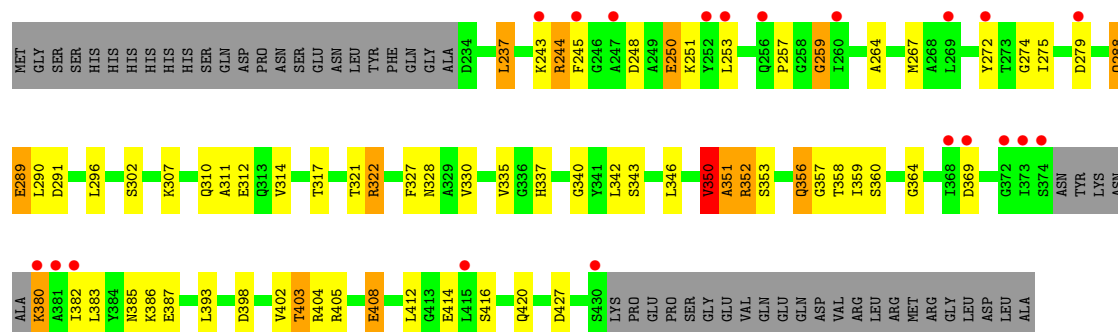




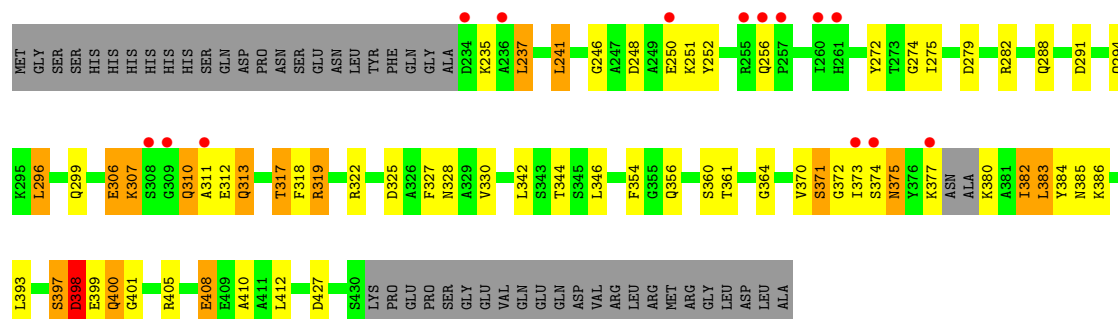
• Molecule 2: Exoenzyme S



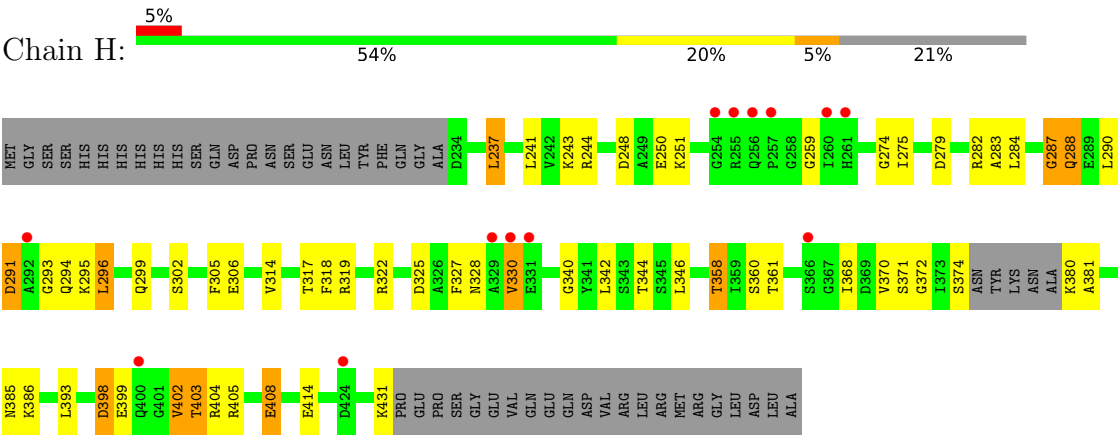
• Molecule 2: Exoenzyme S



• 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

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	0.90	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

All (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
1	D	240	GLU	CA-C	5.18	1.59	1.53

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	GLU	CA-C-N	11.23	141.91	121.70
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
2	H	291	ASP	CA-CB-CG	8.43	121.03	112.60
2	G	398	ASP	CA-CB-CG	8.27	120.87	112.60
1	A	4	ASP	CA-CB-CG	7.60	120.20	112.60
2	F	245	PHE	CA-C-N	7.32	134.88	121.70
2	F	245	PHE	C-N-CA	7.32	134.88	121.70
1	C	234	ASN	CA-CB-CG	7.18	119.78	112.60
2	H	287	GLY	CA-C-N	7.01	134.92	121.54
2	H	287	GLY	C-N-CA	7.01	134.92	121.54
2	E	291	ASP	CA-CB-CG	6.93	119.53	112.60
1	B	237	ASP	CA-C-N	6.71	133.79	121.70
1	B	237	ASP	C-N-CA	6.71	133.79	121.70
2	E	245	PHE	CA-CB-CG	-6.57	107.23	113.80
2	E	325	ASP	CA-CB-CG	6.37	118.97	112.60
2	E	375	ASN	CA-C-N	6.21	132.87	121.70
2	E	375	ASN	C-N-CA	6.21	132.87	121.70
2	G	397	SER	CA-C-N	6.14	133.27	121.54
2	G	397	SER	C-N-CA	6.14	133.27	121.54
1	B	4	ASP	CA-CB-CG	6.13	118.73	112.60
2	F	398	ASP	CA-C-N	6.12	128.81	120.54
2	F	398	ASP	C-N-CA	6.12	128.81	120.54
1	D	126	ASP	CA-CB-CG	6.10	118.70	112.60
2	F	245	PHE	CA-CB-CG	-6.09	107.71	113.80
2	H	372	GLY	CA-C-N	6.06	129.08	120.53
2	H	372	GLY	C-N-CA	6.06	129.08	120.53
2	E	397	SER	CA-C-N	5.99	132.49	121.70
2	E	397	SER	C-N-CA	5.99	132.49	121.70
2	F	288	GLN	CA-C-N	5.99	129.79	120.75
2	F	288	GLN	C-N-CA	5.99	129.79	120.75
2	E	294	GLN	CA-C-N	5.93	128.23	120.28
2	E	294	GLN	C-N-CA	5.93	128.23	120.28
1	A	75	GLU	CA-C-N	5.92	129.70	120.82
1	A	75	GLU	C-N-CA	5.92	129.70	120.82
2	F	427	ASP	CA-CB-CG	5.92	118.52	112.60
2	G	372	GLY	CA-C-N	5.88	127.90	120.72
2	G	372	GLY	C-N-CA	5.88	127.90	120.72
1	D	241	ASN	CA-CB-CG	5.84	118.44	112.60
2	E	371	SER	CA-C-N	5.69	127.44	120.22
2	E	371	SER	C-N-CA	5.69	127.44	120.22
2	H	283	ALA	CA-C-N	5.64	127.77	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	283	ALA	C-N-CA	5.64	127.77	120.44
2	F	350	VAL	N-CA-CB	5.63	116.67	110.53
2	G	306	GLU	CA-C-N	5.63	132.29	121.54
2	G	306	GLU	C-N-CA	5.63	132.29	121.54
2	G	310	GLN	CA-C-N	5.56	131.71	121.70
2	G	310	GLN	C-N-CA	5.56	131.71	121.70
2	E	375	ASN	CA-CB-CG	5.56	118.16	112.60
2	E	245	PHE	CA-C-N	5.56	131.70	121.70
2	E	245	PHE	C-N-CA	5.56	131.70	121.70
2	G	272	TYR	CA-C-N	5.55	128.49	120.38
2	G	272	TYR	C-N-CA	5.55	128.49	120.38
1	B	237	ASP	CA-CB-CG	5.53	118.13	112.60
2	G	427	ASP	CA-CB-CG	5.51	118.11	112.60
2	F	250	GLU	CA-C-N	5.49	129.05	120.82
2	F	250	GLU	C-N-CA	5.49	129.05	120.82
1	C	176	PHE	CA-CB-CG	5.47	119.27	113.80
2	H	288	GLN	CA-C-N	5.47	128.86	120.82
2	H	288	GLN	C-N-CA	5.47	128.86	120.82
1	A	147	SER	CA-C-N	5.46	127.54	120.44
1	A	147	SER	C-N-CA	5.46	127.54	120.44
1	D	229	LEU	CA-C-N	5.46	127.59	120.28
1	D	229	LEU	C-N-CA	5.46	127.59	120.28
2	G	250	GLU	CA-C-N	5.43	128.97	120.82
2	G	250	GLU	C-N-CA	5.43	128.97	120.82
2	G	311	ALA	CA-C-N	5.43	131.91	121.54
2	G	311	ALA	C-N-CA	5.43	131.91	121.54
2	E	272	TYR	CA-C-N	5.40	128.27	120.38
2	E	272	TYR	C-N-CA	5.40	128.27	120.38
2	H	399	GLU	N-CA-C	-5.37	105.59	111.82
2	G	325	ASP	CA-CB-CG	5.36	117.95	112.60
1	D	176	PHE	CA-CB-CG	5.34	119.14	113.80
2	E	250	GLU	CA-C-N	5.31	128.78	120.82
2	E	250	GLU	C-N-CA	5.31	128.78	120.82
1	A	189	LYS	CA-C-N	5.29	127.32	120.44
1	A	189	LYS	C-N-CA	5.29	127.32	120.44
1	B	229	LEU	CA-C-N	5.29	127.37	120.28
1	B	229	LEU	C-N-CA	5.29	127.37	120.28
2	G	401	GLY	CA-C-N	5.29	128.18	120.98
2	G	401	GLY	C-N-CA	5.29	128.18	120.98
1	C	4	ASP	CA-C-N	5.29	131.64	121.54
1	C	4	ASP	C-N-CA	5.29	131.64	121.54
2	E	247	ALA	CA-C-N	5.29	128.35	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	247	ALA	C-N-CA	5.29	128.35	120.31
2	F	272	TYR	CA-C-N	5.27	128.08	120.38
2	F	272	TYR	C-N-CA	5.27	128.08	120.38
2	G	375	ASN	CA-CB-CG	5.26	117.86	112.60
2	F	244	ARG	CA-C-N	-5.22	114.33	122.42
2	F	244	ARG	C-N-CA	-5.22	114.33	122.42
1	C	11	LYS	CA-C-N	5.22	127.27	120.28
1	C	11	LYS	C-N-CA	5.22	127.27	120.28
2	G	313	GLN	CA-C-N	5.20	129.50	121.71
2	G	313	GLN	C-N-CA	5.20	129.50	121.71
1	D	81	GLY	CA-C-N	5.19	127.23	120.28
1	D	81	GLY	C-N-CA	5.19	127.23	120.28
2	F	416	SER	N-CA-C	5.18	116.61	110.97
2	E	245	PHE	N-CA-C	5.17	116.60	111.07
1	A	125	GLY	CA-C-N	5.13	127.47	120.54
1	A	125	GLY	C-N-CA	5.13	127.47	120.54
2	G	354	PHE	CA-C-N	5.13	127.86	120.11
2	G	354	PHE	C-N-CA	5.13	127.86	120.11
1	B	176	PHE	CA-CB-CG	5.13	118.93	113.80
2	F	259	GLY	CA-C-N	5.13	128.71	120.30
2	F	259	GLY	C-N-CA	5.13	128.71	120.30
1	C	6	SER	CA-C-N	5.12	127.41	120.65
1	C	6	SER	C-N-CA	5.12	127.41	120.65
1	A	200	GLU	CB-CG-CD	5.11	121.28	112.60
2	G	410	ALA	CA-C-N	5.11	127.43	120.54
2	G	410	ALA	C-N-CA	5.11	127.43	120.54
2	H	250	GLU	CA-C-N	5.09	128.46	120.82
2	H	250	GLU	C-N-CA	5.09	128.46	120.82
2	F	289	GLU	CA-C-N	5.08	130.84	121.70
2	F	289	GLU	C-N-CA	5.08	130.84	121.70
2	G	246	GLY	CA-C-N	5.08	127.04	120.44
2	G	246	GLY	C-N-CA	5.08	127.04	120.44
1	D	215	ASP	CA-C-N	5.07	127.03	120.44
1	D	215	ASP	C-N-CA	5.07	127.03	120.44
2	F	352	ARG	N-CA-C	-5.02	106.40	112.88
1	B	146	ASN	CA-C-N	5.00	127.43	120.63
1	B	146	ASN	C-N-CA	5.00	127.43	120.63

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.

All (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
2:F:385:ASN:HD22	2:F:386:LYS:H	1.31	0.76
2:G:385:ASN:HD22	2:G:386:LYS:H	1.33	0.72
2:F:250:GLU:HA	2:F:267:MET:HE2	1.70	0.72
1:B:237:ASP:HB2	1:B:238:GLU:CB	2.22	0.70
2:E:322:ARG:HA	2:E:322:ARG:HE	1.55	0.70
2:H:319:ARG:HB2	2:H:344:THR:HG22	1.75	0.68
1:B:114:PRO:HG3	1:B:161:GLU:HG2	1.75	0.67
2:E:371:SER:OG	2:E:380:LYS:HA	1.95	0.66
2:F:351:ALA:HA	2:F:359:ILE:HG21	1.78	0.66
2:E:317:THR:HB	2:E:344:THR:HB	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:393:LEU:HD21	2:G:408:GLU:HG2	1.79	0.63
1:A:76:LYS:O	1:A:80:MET:HG2	1.99	0.63
2:F:350:VAL:HA	2:F:353:SER:HB2	1.81	0.63
1:A:227:LEU:O	1:A:231:THR:HB	1.99	0.62
1:A:114:PRO:HG3	1:A:161:GLU:HG2	1.82	0.62
1:D:114:PRO:HG3	1:D:161:GLU:HG2	1.80	0.62
2:E:321:THR:HG21	2:E:325:ASP:HB2	1.82	0.62
2:E:393:LEU:HD21	2:E:408:GLU:HG2	1.82	0.61
2:G:371:SER:HG	2:G:380:LYS:N	1.99	0.61
1:C:121:LEU:HB3	1:C:154:ALA:HB2	1.82	0.61
2:H:241:LEU:HD12	2:H:296:LEU:HD23	1.83	0.61
2:E:321:THR:HB	2:E:358:THR:OG1	2.02	0.58
2:G:319:ARG:HB3	2:G:344:THR:HG22	1.84	0.58
1:A:118:VAL:HG21	1:A:162:MET:HE1	1.86	0.57
2:H:393:LEU:HD21	2:H:408:GLU:HG2	1.85	0.56
2:F:393:LEU:HD21	2:F:408:GLU:HG2	1.88	0.55
1:D:121:LEU:HB2	1:D:154:ALA:HB2	1.89	0.55
1:B:237:ASP:HB2	1:B:238:GLU:CA	2.37	0.54
2:E:397:SER:HB3	2:E:403:THR:HA	1.88	0.54
1:D:38:LEU:HD22	1:D:42:GLU:HB3	1.90	0.54
2:H:346:LEU:HB2	2:H:380:LYS:HB3	1.89	0.54
1:D:103:LEU:HA	1:D:107:LEU:HB2	1.90	0.54
1:C:38:LEU:HD22	1:C:42:GLU:HB3	1.90	0.54
2:G:370:VAL:HG11	2:G:383:LEU:HD23	1.90	0.54
2:G:397:SER:O	2:G:398:ASP:O	2.26	0.53
2:F:289:GLU:HB3	2:F:290:LEU:HB2	1.89	0.53
1:A:170:LEU:O	1:A:173:ALA:HB3	2.09	0.52
2:E:322:ARG:HA	2:E:322:ARG:NE	2.21	0.52
1:C:114:PRO:HG3	1:C:161:GLU:HG3	1.91	0.52
1:B:103:LEU:HA	1:B:107:LEU:HB2	1.90	0.52
2:H:327:PHE:HA	2:H:330:VAL:HG23	1.92	0.52
1:A:38:LEU:HD22	1:A:42:GLU:HB3	1.92	0.52
1:B:99:VAL:HG11	1:B:127:TYR:CD2	2.45	0.52
2:H:328:ASN:HA	2:H:405:ARG:NH2	2.25	0.52
2:G:317:THR:HG21	2:G:382:ILE:HB	1.92	0.51
2:G:364:GLY:HA2	2:G:412:LEU:HD11	1.91	0.51
2:E:345:SER:HB3	2:E:350:VAL:HG21	1.92	0.51
1:A:89:GLU:HG2	1:A:134:VAL:HB	1.93	0.51
1:D:204:GLU:CG	2:F:352:ARG:HH12	2.20	0.51
2:H:237:LEU:HD11	2:H:299:GLN:HB3	1.91	0.51
1:C:103:LEU:HA	1:C:107:LEU:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:385:ASN:HD22	2:F:386:LYS:N	2.05	0.50
2:H:325:ASP:H	2:H:328:ASN:ND2	2.09	0.50
2:F:322:ARG:HG2	2:F:357:GLY:H	1.77	0.50
2:G:291:ASP:HB2	2:G:294:GLN:HG3	1.93	0.50
2:F:337:HIS:CD2	2:F:387:GLU:HA	2.48	0.49
2:F:358:THR:HG22	2:F:403:THR:HG23	1.93	0.49
2:G:241:LEU:HD13	2:G:296:LEU:HD12	1.95	0.49
1:C:89:GLU:HG2	1:C:134:VAL:HB	1.94	0.49
2:G:385:ASN:HD22	2:G:386:LYS:N	2.05	0.49
1:C:126:ASP:O	1:C:129:ARG:HB3	2.12	0.49
2:F:237:LEU:HD12	2:F:264:ALA:HB1	1.95	0.49
2:H:385:ASN:HD22	2:H:386:LYS:N	2.05	0.48
1:A:220:MET:HA	1:A:223:LEU:HD12	1.94	0.48
1:A:103:LEU:HA	1:A:107:LEU:HB2	1.93	0.48
1:D:129:ARG:HD3	1:D:179:PHE:HB2	1.95	0.48
1:B:108:ILE:CD1	1:B:124:LYS:HE2	2.44	0.48
1:B:220:MET:HA	1:B:223:LEU:HD12	1.96	0.48
2:F:328:ASN:HA	2:F:405:ARG:NH2	2.29	0.48
2:F:408:GLU:O	2:F:408:GLU:HG3	2.13	0.48
2:E:319:ARG:HB2	2:E:344:THR:HG22	1.95	0.48
1:B:89:GLU:HG2	1:B:134:VAL:HB	1.95	0.48
2:F:322:ARG:HA	2:F:322:ARG:HE	1.78	0.47
2:G:237:LEU:HD11	2:G:299:GLN:HG3	1.96	0.47
1:D:61:TRP:CE2	1:D:134:VAL:HG12	2.49	0.47
2:G:237:LEU:HD23	2:G:241:LEU:HD22	1.96	0.47
2:H:371:SER:HB3	2:H:380:LYS:HA	1.95	0.47
1:D:121:LEU:CB	1:D:154:ALA:HB2	2.45	0.47
1:B:38:LEU:HD22	1:B:42:GLU:HB3	1.96	0.46
2:G:252:TYR:HE1	2:G:374:SER:HB3	1.79	0.46
1:C:220:MET:HA	1:C:223:LEU:HD12	1.97	0.46
2:E:356:GLN:O	2:E:402:VAL:HB	2.16	0.46
2:E:375:ASN:HB2	2:E:376:TYR:CD2	2.50	0.46
1:A:67:ILE:HA	1:A:70:LYS:HE2	1.98	0.46
1:D:220:MET:HA	1:D:223:LEU:HD12	1.97	0.45
2:H:358:THR:HG22	2:H:403:THR:HB	1.96	0.45
2:H:290:LEU:HD23	2:H:295:LYS:HA	1.98	0.45
2:F:346:LEU:HB2	2:F:380:LYS:HB2	1.99	0.45
1:C:121:LEU:HD22	1:C:153:GLU:HB3	1.99	0.45
1:A:27:ALA:O	1:A:31:VAL:HG23	2.17	0.45
2:F:364:GLY:HA2	2:F:412:LEU:HD11	1.99	0.45
2:E:328:ASN:HA	2:E:405:ARG:NH2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:364:GLY:HA2	2:E:412:LEU:HD11	1.99	0.45
2:F:322:ARG:HG2	2:F:357:GLY:N	2.33	0.44
1:D:129:ARG:HG3	1:D:183:ILE:HG13	1.98	0.44
2:E:327:PHE:HA	2:E:330:VAL:HG23	1.99	0.44
2:F:369:ASP:HA	2:F:382:ILE:HG12	1.99	0.44
2:G:328:ASN:HA	2:G:405:ARG:NH2	2.33	0.44
1:D:89:GLU:HG2	1:D:134:VAL:HB	2.00	0.44
2:F:327:PHE:HA	2:F:330:VAL:HG23	2.00	0.44
2:H:398:ASP:HB2	2:H:402:VAL:H	1.82	0.44
1:C:57:ARG:HB3	1:C:92:LEU:HD12	2.00	0.43
2:F:351:ALA:HA	2:F:359:ILE:CG2	2.45	0.43
1:A:158:SER:HA	1:A:162:MET:HE3	2.01	0.43
2:G:346:LEU:HB2	2:G:380:LYS:HB3	1.99	0.43
2:H:284:LEU:HD13	2:H:340:GLY:HA2	2.00	0.43
2:H:305:PHE:HA	2:H:368:ILE:HD11	2.01	0.43
1:C:27:ALA:O	1:C:31:VAL:HG23	2.19	0.43
2:G:342:LEU:HB3	2:G:384:TYR:HB2	2.00	0.43
1:D:27:ALA:O	1:D:31:VAL:HG23	2.19	0.43
2:E:322:ARG:HD2	2:E:355:GLY:O	2.18	0.43
2:G:318:PHE:HD1	2:G:361:THR:HG22	1.82	0.43
2:H:325:ASP:OD2	2:H:327:PHE:HB2	2.18	0.43
1:A:142:THR:HG22	1:A:146:ASN:HD21	1.83	0.42
1:B:27:ALA:O	1:B:31:VAL:HG23	2.18	0.42
1:A:158:SER:HB2	1:A:169:ARG:HG3	2.01	0.42
2:H:244:ARG:HD2	2:H:293:GLY:HA3	2.01	0.42
1:C:29:LYS:HG3	1:C:102:LEU:HD11	2.02	0.42
1:A:57:ARG:HB3	1:A:92:LEU:HD12	2.01	0.42
1:B:57:ARG:HB3	1:B:92:LEU:HD12	2.01	0.42
2:F:340:GLY:O	2:F:386:LYS:HA	2.19	0.41
2:H:318:PHE:CD1	2:H:361:THR:HG22	2.55	0.41
1:B:36:HIS:CE1	1:C:3:MET:HA	2.55	0.41
1:B:166:HIS:HE1	1:B:168:ILE:HD12	1.85	0.41
2:F:322:ARG:HA	2:F:322:ARG:NE	2.35	0.41
2:G:398:ASP:C	2:G:400:GLN:H	2.28	0.41
2:H:370:VAL:HG23	2:H:381:ALA:HB3	2.03	0.41
2:F:343:SER:HA	2:F:383:LEU:HD23	2.02	0.41
1:A:180:TYR:CD1	1:A:184:LEU:HD12	2.56	0.41
1:B:29:LYS:HG3	1:B:102:LEU:HD11	2.02	0.41
1:D:57:ARG:HB3	1:D:92:LEU:HD12	2.02	0.41
2:E:337:HIS:HD1	2:E:337:HIS:C	2.29	0.41
2:F:356:GLN:HA	2:F:356:GLN:HE21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TYR:CD1	1:B:184:LEU:HD12	2.56	0.41
1:D:29:LYS:HG3	1:D:102:LEU:HD11	2.02	0.40
2:G:327:PHE:HA	2:G:330:VAL:HG23	2.02	0.40
1:B:59:SER:O	1:B:63:VAL:HG23	2.21	0.40
1:C:142:THR:HG22	1:C:146:ASN:HD21	1.86	0.40
1:C:128:PHE:HB3	1:C:147:SER:HB2	2.03	0.40
2:E:376:TYR:CD1	2:E:376:TYR:N	2.90	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	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

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	5	LYS
2	E	256	GLN
2	F	257	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	398	ASP
2	H	288	GLN
2	E	375	ASN
2	F	259	GLY
2	F	310	GLN
2	F	351	ALA
2	G	312	GLU
2	H	287	GLY
1	B	37	GLU
1	B	235	GLN
2	E	255	ARG
2	E	312	GLU
2	H	274	GLY
1	A	73	ARG
2	E	288	GLN
2	F	311	ALA
2	F	420	GLN
2	G	307	LYS
2	G	399	GLU
2	H	259	GLY
2	E	274	GLY
2	E	373	ILE
2	F	274	GLY
2	G	274	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	210/220 (96%)	182 (87%)	28 (13%)	4	18
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	65	SER
1	A	71	THR
1	A	72	GLU
1	A	73	ARG
1	A	75	GLU
1	A	76	LYS
1	A	77	LYS
1	A	82	LYS
1	A	92	LEU
1	A	101	GLU
1	A	113	GLN
1	A	122	LYS
1	A	123	MET
1	A	132	SER
1	A	138	ASP
1	A	156	GLU
1	A	159	LYS
1	A	161	GLU
1	A	162	MET
1	A	185	ASN
1	A	193	LEU
1	A	200	GLU
1	A	210	GLU
1	A	224	ARG
1	A	227	LEU
1	A	231	THR
1	A	237	ASP
1	B	4	ASP
1	B	60	SER
1	B	66	SER
1	B	82	LYS
1	B	92	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	101	GLU
1	B	104	ASP
1	B	113	GLN
1	B	122	LYS
1	B	123	MET
1	B	156	GLU
1	B	159	LYS
1	B	161	GLU
1	B	162	MET
1	B	185	ASN
1	B	210	GLU
1	B	224	ARG
1	B	237	ASP
1	B	238	GLU
1	B	240	GLU
1	C	4	ASP
1	C	65	SER
1	C	69	GLN
1	C	92	LEU
1	C	101	GLU
1	C	104	ASP
1	C	113	GLN
1	C	121	LEU
1	C	122	LYS
1	C	156	GLU
1	C	161	GLU
1	C	162	MET
1	C	185	ASN
1	C	193	LEU
1	C	210	GLU
1	C	224	ARG
1	C	234	ASN
1	C	242	LEU
1	C	243	TYR
1	D	3	MET
1	D	11	LYS
1	D	75	GLU
1	D	78	GLN
1	D	80	MET
1	D	92	LEU
1	D	101	GLU
1	D	122	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	123	MET
1	D	143	THR
1	D	156	GLU
1	D	159	LYS
1	D	161	GLU
1	D	162	MET
1	D	185	ASN
1	D	193	LEU
1	D	210	GLU
1	D	224	ARG
1	D	234	ASN
2	E	237	LEU
2	E	243	LYS
2	E	251	LYS
2	E	253	LEU
2	E	275	ILE
2	E	279	ASP
2	E	282	ARG
2	E	291	ASP
2	E	302	SER
2	E	307	LYS
2	E	312	GLU
2	E	313	GLN
2	E	315	VAL
2	E	317	THR
2	E	321	THR
2	E	330	VAL
2	E	337	HIS
2	E	342	LEU
2	E	360	SER
2	E	373	ILE
2	E	402	VAL
2	E	408	GLU
2	E	423	LEU
2	F	237	LEU
2	F	243	LYS
2	F	244	ARG
2	F	248	ASP
2	F	251	LYS
2	F	253	LEU
2	F	275	ILE
2	F	279	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	288	GLN
2	F	291	ASP
2	F	296	LEU
2	F	302	SER
2	F	307	LYS
2	F	312	GLU
2	F	314	VAL
2	F	317	THR
2	F	321	THR
2	F	322	ARG
2	F	335	VAL
2	F	342	LEU
2	F	350	VAL
2	F	356	GLN
2	F	360	SER
2	F	380	LYS
2	F	402	VAL
2	F	403	THR
2	F	404	ARG
2	F	408	GLU
2	F	414	GLU
2	G	235	LYS
2	G	237	LEU
2	G	241	LEU
2	G	248	ASP
2	G	251	LYS
2	G	256	GLN
2	G	275	ILE
2	G	279	ASP
2	G	282	ARG
2	G	288	GLN
2	G	296	LEU
2	G	306	GLU
2	G	307	LYS
2	G	310	GLN
2	G	313	GLN
2	G	317	THR
2	G	319	ARG
2	G	322	ARG
2	G	356	GLN
2	G	360	SER
2	G	371	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	373	ILE
2	G	375	ASN
2	G	377	LYS
2	G	382	ILE
2	G	383	LEU
2	G	400	GLN
2	G	408	GLU
2	H	237	LEU
2	H	243	LYS
2	H	248	ASP
2	H	251	LYS
2	H	275	ILE
2	H	279	ASP
2	H	282	ARG
2	H	291	ASP
2	H	294	GLN
2	H	296	LEU
2	H	302	SER
2	H	306	GLU
2	H	314	VAL
2	H	317	THR
2	H	322	ARG
2	H	330	VAL
2	H	342	LEU
2	H	360	SER
2	H	374	SER
2	H	398	ASP
2	H	402	VAL
2	H	403	THR
2	H	404	ARG
2	H	408	GLU
2	H	414	GLU
2	H	431	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	B	17	GLN
1	B	78	GLN
1	B	79	GLN
1	B	152	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	234	ASN
1	C	17	GLN
1	C	34	GLN
1	C	36	HIS
1	C	97	ASN
1	C	149	GLN
1	C	152	GLN
1	C	234	ASN
1	D	17	GLN
1	D	152	GLN
2	E	400	GLN
2	F	299	GLN
2	F	385	ASN
2	G	286	GLN
2	G	294	GLN
2	G	328	ASN
2	G	356	GLN
2	G	385	ASN
2	G	420	GLN
2	H	256	GLN
2	H	294	GLN
2	H	385	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](#)

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	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

All (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
2	H	330	VAL	3.6
2	H	256	GLN	3.6
2	G	256	GLN	3.5
1	A	211	GLU	3.5
2	E	376	TYR	3.5
1	C	243	TYR	3.4
1	B	78	GLN	3.4
2	G	255	ARG	3.3
2	H	331	GLU	3.2
1	D	233	GLU	3.1
2	G	260	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	329	ALA	3.1
1	D	83	GLU	3.1
1	D	71	THR	3.0
2	G	309	GLY	3.0
2	F	260	ILE	2.9
2	G	234	ASP	2.9
2	G	257	PRO	2.9
2	G	311	ALA	2.9
2	H	292	ALA	2.9
2	F	415	LEU	2.9
2	F	256	GLN	2.9
1	D	75	GLU	2.8
1	B	104	ASP	2.8
2	F	369	ASP	2.7
2	E	372	GLY	2.7
2	F	372	GLY	2.7
2	H	261	HIS	2.7
2	H	254	GLY	2.7
1	C	185	ASN	2.7
1	B	80	MET	2.6
1	B	113	GLN	2.6
1	D	79	GLN	2.6
1	D	5	LYS	2.6
1	A	221	GLN	2.6
2	F	253	LEU	2.6
2	F	368	ILE	2.6
2	E	259	GLY	2.6
1	B	115	GLU	2.6
2	F	269	LEU	2.5
2	G	308	SER	2.5
2	E	260	ILE	2.5
2	F	373	ILE	2.5
2	E	237	LEU	2.5
1	B	79	GLN	2.5
2	H	400	GLN	2.5
2	F	272	TYR	2.4
2	E	399	GLU	2.4
2	F	430	SER	2.4
1	B	138	ASP	2.4
1	D	55	GLY	2.4
1	C	136	SER	2.4
2	F	381	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	225	ASP	2.3
2	F	279	ASP	2.3
2	F	252	TYR	2.3
1	C	76	LYS	2.3
1	D	3	MET	2.3
2	G	250	GLU	2.3
2	H	424	ASP	2.3
2	E	243	LYS	2.3
1	B	3	MET	2.3
2	E	430	SER	2.3
2	H	255	ARG	2.3
1	C	156	GLU	2.2
1	A	70	LYS	2.2
2	F	380	LYS	2.2
1	C	4	ASP	2.2
1	C	92	LEU	2.2
2	F	243	LYS	2.2
2	E	373	ILE	2.1
1	A	74	ASN	2.1
2	E	257	PRO	2.1
1	D	188	GLU	2.1
2	F	382	ILE	2.1
2	E	234	ASP	2.1
2	G	377	LYS	2.1
2	G	236	ALA	2.1
2	H	366	SER	2.1
1	C	77	LYS	2.1
2	E	296	LEU	2.1
2	G	261	HIS	2.1
1	C	5	LYS	2.0
2	G	374	SER	2.0
1	B	202	ILE	2.0
2	E	288	GLN	2.0
1	C	3	MET	2.0
1	B	239	GLY	2.0
2	G	373	ILE	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 [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.