



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:54 AM UTC

PDB ID : 1SGT / pdb_00001sgt
Title : REFINED CRYSTAL STRUCTURE OF STREPTOMYCES GRISEUS
TRYPSIN AT 1.7 ANGSTROMS RESOLUTION
Authors : Read, R.J.; James, M.N.G.
Deposited on : 1988-04-13
Resolution : 1.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

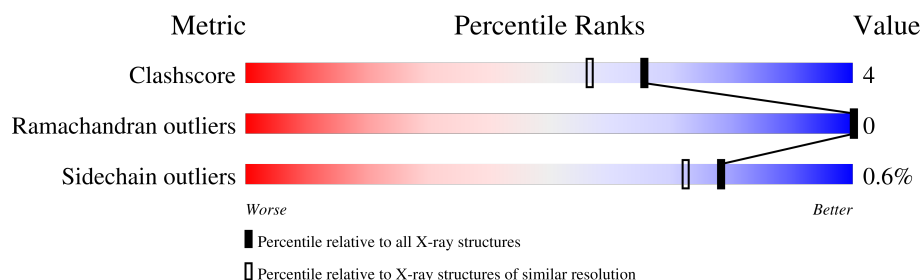
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	223	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1813 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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1620	1009	284	318	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	SER	conflict	UNP P00775
A	79	ALA	SER	conflict	UNP P00775

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

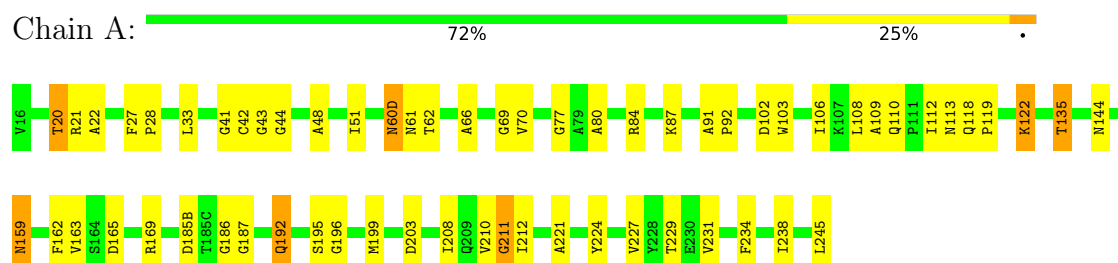
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	192	Total	O	0	0
			192	192		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: TRYPSIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	72.29Å 50.98Å 120.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70	Depositor
% Data completeness (in resolution range)	80.6 (8.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1813	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.51	9/1652 (0.5%)	2.17	67/2247 (3.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	GLY	N-CA	8.22	1.52	1.44
1	A	27	PHE	CA-CB	5.97	1.60	1.53
1	A	162	PHE	CA-C	5.84	1.60	1.52
1	A	44	GLY	CA-C	5.76	1.57	1.51
1	A	211	GLY	N-CA	5.74	1.50	1.45
1	A	163	VAL	N-CA	5.52	1.52	1.46
1	A	186	GLY	CA-C	5.30	1.59	1.52
1	A	192	GLN	CA-C	5.20	1.59	1.52
1	A	108	LEU	CA-C	5.09	1.59	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH1	12.62	134.12	121.50
1	A	224	TYR	O-C-N	11.88	132.13	121.32
1	A	21	ARG	NE-CZ-NH1	11.45	132.95	121.50
1	A	21	ARG	NE-CZ-NH2	-9.38	110.76	119.20
1	A	60(D)	ASN	CA-CB-CG	-8.26	104.34	112.60
1	A	192	GLN	O-C-N	8.04	132.71	123.06
1	A	42	CYS	CA-C-N	-7.93	114.13	122.30
1	A	42	CYS	C-N-CA	-7.93	114.13	122.30
1	A	169	ARG	NE-CZ-NH2	-7.90	112.09	119.20
1	A	165	ASP	O-C-N	7.80	130.39	122.12
1	A	118	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	A	77	GLY	N-CA-C	-7.58	104.98	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ILE	CA-C-O	-7.45	112.57	120.39
1	A	159	ASN	CA-CB-CG	-7.39	105.21	112.60
1	A	43	GLY	N-CA-C	-7.20	101.20	112.58
1	A	112	ILE	N-CA-C	-7.17	97.52	107.99
1	A	169	ARG	CD-NE-CZ	7.07	134.29	124.40
1	A	70	VAL	O-C-N	6.80	130.75	123.00
1	A	87	LYS	O-C-N	6.75	130.94	123.25
1	A	234	PHE	O-C-N	6.74	130.39	122.24
1	A	122	LYS	CA-C-O	-6.66	113.71	121.16
1	A	195	SER	CA-C-O	-6.60	114.31	121.44
1	A	42	CYS	O-C-N	6.57	131.69	123.15
1	A	102	ASP	O-C-N	6.47	131.03	122.56
1	A	187	GLY	O-C-N	6.43	131.06	122.70
1	A	227	VAL	O-C-N	6.33	129.83	123.18
1	A	122	LYS	N-CA-CB	-6.14	100.95	109.97
1	A	106	ILE	CA-C-O	-6.09	114.05	120.39
1	A	51	ILE	O-C-N	6.06	129.27	123.03
1	A	61	ASN	O-C-N	6.05	130.63	122.59
1	A	221	ALA	N-CA-CB	-6.04	103.04	112.41
1	A	159	ASN	O-C-N	6.04	130.88	123.21
1	A	208	ILE	O-C-N	5.98	129.69	123.05
1	A	162	PHE	O-C-N	5.86	130.08	122.87
1	A	224	TYR	CA-C-O	-5.86	113.35	120.74
1	A	102	ASP	CA-C-O	-5.67	115.55	122.64
1	A	122	LYS	O-C-N	5.64	129.77	122.89
1	A	210	VAL	CA-C-N	-5.62	115.52	121.48
1	A	210	VAL	C-N-CA	-5.62	115.52	121.48
1	A	87	LYS	CA-C-N	-5.61	115.15	122.94
1	A	87	LYS	C-N-CA	-5.61	115.15	122.94
1	A	135	THR	O-C-N	5.59	129.59	123.27
1	A	199	MET	N-CA-C	-5.59	99.41	108.52
1	A	48	ALA	N-CA-C	-5.57	100.84	109.14
1	A	41	GLY	O-C-N	-5.53	115.51	122.70
1	A	106	ILE	O-C-N	5.53	129.06	123.20
1	A	159	ASN	N-CA-CB	5.52	119.57	110.69
1	A	103	TRP	CA-C-O	5.50	127.15	120.99
1	A	42	CYS	CA-C-O	-5.47	115.04	121.44
1	A	210	VAL	CA-C-O	-5.44	114.11	118.90
1	A	20	THR	CA-CB-OG1	-5.43	101.46	109.60
1	A	231	VAL	CA-C-O	-5.42	115.31	120.95
1	A	195	SER	O-C-N	5.39	129.72	122.82
1	A	80	ALA	CA-C-O	-5.35	115.30	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASN	OD1-CG-ND2	5.30	127.90	122.60
1	A	135	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	185(B)	ASP	N-CA-C	5.29	116.85	111.14
1	A	66	ALA	CA-C-O	-5.28	114.63	120.38
1	A	33	LEU	CB-CA-C	5.27	118.34	109.48
1	A	113	ASN	N-CA-CB	-5.27	102.64	110.60
1	A	238	ILE	O-C-N	5.25	127.36	121.90
1	A	69	GLY	N-CA-C	5.25	122.34	115.36
1	A	159	ASN	CA-C-O	-5.24	115.16	120.71
1	A	196	GLY	CA-C-O	-5.22	114.03	119.20
1	A	22	ALA	N-CA-C	-5.15	102.86	110.48
1	A	144	ASN	CB-CA-C	5.08	119.15	110.56
1	A	238	ILE	CB-CG1-CD1	-5.06	103.17	113.80

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	1620	0	1565	12	0
2	A	1	0	0	0	0
3	A	192	0	0	3	0
All	All	1813	0	1565	12	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 4.

All (12) 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:122:LYS:NZ	1:A:203:ASP:OD2	2.15	0.80
1:A:62:THR:O	1:A:84:ARG:NH1	2.24	0.70
1:A:110:GLN:NE2	3:A:288:HOH:O	2.32	0.62
1:A:60(D):ASN:HB3	3:A:380:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:HA2	1:A:229:THR:O	2.12	0.49
1:A:20:THR:HG22	3:A:376:HOH:O	2.12	0.48
1:A:28:PRO:HB2	1:A:119:PRO:HD2	1.97	0.46
1:A:109:ALA:C	1:A:110:GLN:HG3	2.42	0.43
1:A:91:ALA:HA	1:A:92:PRO:HD3	1.85	0.42
1:A:192:GLN:O	1:A:192:GLN:HG3	2.21	0.41
1:A:203:ASP:OD1	1:A:203:ASP:C	2.63	0.40
1:A:135:THR:CG2	1:A:159:ASN:HB3	2.51	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	221/223 (99%)	217 (98%)	4 (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	163/163 (100%)	162 (99%)	1 (1%)	78	72

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

Mol	Chain	Res	Type
1	A	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	132	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.