



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:34 PM UTC

PDB ID : 5XYA / pdb_00005xya
Title : Crystal structure of a serine protease from Streptococcus species
Authors : Jobichen, C.; Sivaraman, J.
Deposited on : 2017-07-06
Resolution : 3.00 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

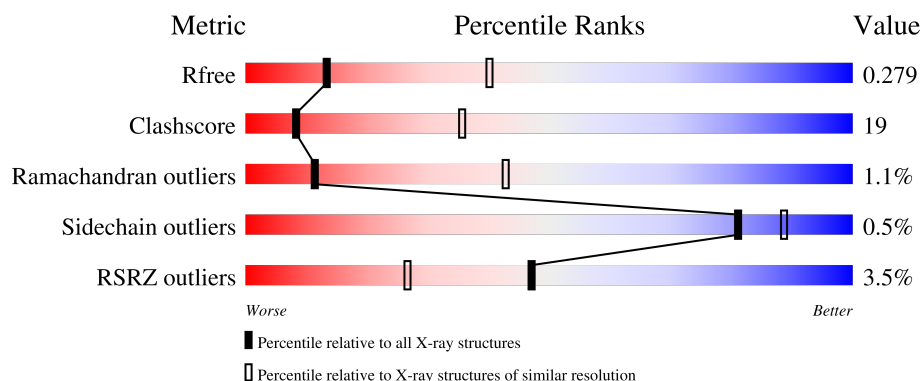
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1530	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1704	-	-	X	-

2 Entry composition [i](#)

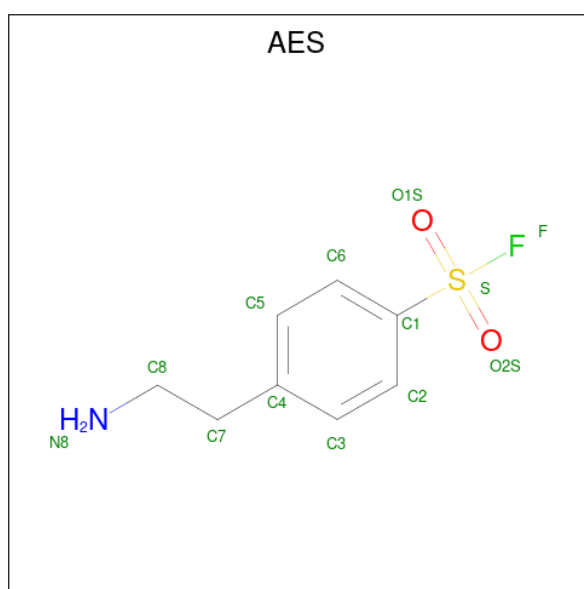
There are 4 unique types of molecules in this entry. The entry contains 10300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chemokine protease C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1358	Total	C	N	O	Se	0	0	0
			10269	6462	1764	2019	24			

- Molecule 2 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (CCD ID: AES) (formula: C₈H₁₀FNO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	8	1	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Ca	0	0
			4	4		

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.

Chain A:

PHE SER ARG LYS LYS SER THR LYS ASP	SER	K1449	V1344	A1236	L1124	T1032
	ASP	Y1450	M1347	G1237	P1125	N1033
	SER	K1348			Q1126	R1034
	LYS	V1452	Y1349	I1241	T1127	P1037
	GLY	V1455	Y1350	E1242	L1128	E1038
	SER	L1455	I1351		G1129	P1039
	THR		P1352	W1246	K1130	L1040
	LYS	L1464	K1353	Y1247	T1131	K1041
	VAL			G1248		D1042
	MSE	F1480	D1356		Y1142	
SER THR LYS LYS ARG ILE VAL GLY LEU LEU VAL LEU GLY THR CYS VAL	SER	V1483	S1357	R1252		L1045
	THR	Y1483	S1358		L1152	A1046
	LYS	Y1359	Y1359	V1256	E1153	G1047
	LYS	K1486	T1360	M1257	M1154	V1048
	ARG	M1487	I1361			
	ILE		S1362	Y1261	D1158	D1051
	VAL	T1496	K1363	V1265	V1162	F1054
	GLY	F1499	R1364	T1266	A1166	Y1055
	LEU	D1500	D1365	Y1267		L1056
	LEU	H1501	G1366	K1277	V1171	P1063
SER THR PRO LYS THR THR THR PRO ALA ALA LYS LEU SER THR GLY GLU LYS MSE GLY LEU LYS LEU ARG ILE VAL GLY LEU VAL LEU GLY LEU THR CYS VAL	SER	L1502	T1368	Q1278	H1172	Y1064
	THR	L1503	L1369	Y1279	S1178	T1065
	PRO	L1521	S1370	T1286	Q1179	V1066
	LYS	E1522	D1371	I1281	L1180	T1067
	THR	Q1523	Y1372	S1282	T1181	I1068
	THR		Y1374		K1182	
	PRO	Y1526		G1293		V1075
	ALA	Y1531	E1377	R1294		S1076
	ALA	G1532	A1380	T1297	F1187	V1077
	LYS	K1533	I1298	I1189	F1188	
SER THR GLY GLU LYS MSE GLY LEU LYS LEU ARG ILE VAL GLY LEU VAL LEU GLY LEU THR CYS VAL	SER	Q1536	V1383	N1299	S1190	N1080
	THR	Y1540	L1388	G1300	P1191	K1081
	GLY	V1544	K1396	V1301	N1192	R1086
	GLU	S1545	D1397	D1302	E1193	
	LYS	L1546	V1400	H1303	D1194	F1092
	MSE	P1547		D1307	K1197	D1097
	GLY	K1548	F1403	S1314		G1102
	LEU	G1549	D1406	E1320	K1203	Y1105
	LYS	Y1550	P1410	F1323	G1204	Y1106
	LEU	I1552		Y1324	M1107	M1107
SER THR GLY LEU VAL LEU GLY LEU THR CYS VAL	SER	E1553	P1415	L1325	Y1210	V1108
	THR		I1415			E1109
	GLY	E1564	Y1416	R1331	L1213	D1110
	LEU	V1565	N1417	K1332	T1214	F1111
	VAL					A1112
	LEU	R1571	R1423	E1337	Y1218	G1113
	GLY	K1574	D1424	G1338		N1114
	LEU	VAL	A1425	K1339	V1115	V1115
	THR	GLY		D1340	H1223	A1116
	CYS	ASP	Y1435	G1341	Q1224	I1117
	VAL	ALA	G1440	I1342	K1225	A1118
				T1343	L1120	

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	190.53Å 190.53Å 248.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.00 19.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.90-3.00) 98.7 (19.90-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.86Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.223 , 0.278 0.227 , 0.279	Depositor DCC
R_{free} test set	1990 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10300	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: SO4, CA, AES

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	0.61	2/10444 (0.0%)	0.88	15/14117 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1300	GLY	C-O	-5.48	1.20	1.24
1	A	580	SER	C-O	-5.36	1.17	1.23

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	VAL	CA-C-N	-7.42	115.39	122.66
1	A	402	VAL	C-N-CA	-7.42	115.39	122.66
1	A	536	PRO	N-CA-CB	7.24	110.85	103.25
1	A	1487	MSE	N-CA-C	7.21	120.38	109.41
1	A	493	PRO	N-CA-CB	6.94	110.63	103.00

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	10269	0	9868	387	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	10	2	0
3	A	15	0	0	2	0
4	A	4	0	0	0	0
All	All	10300	0	9878	387	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 19.

The worst 5 of 387 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:188:TYR:OH	1:A:330:LYS:HE3	1.32	1.25
1:A:401:LEU:O	1:A:581:ASN:ND2	1.82	1.12
1:A:412:THR:HG22	1:A:651:LYS:HD3	1.40	1.04
1:A:910:ASN:ND2	1:A:912:ASP:OD1	1.94	1.00
1:A:188:TYR:OH	1:A:330:LYS:CE	2.13	0.95

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	1350/1530 (88%)	1159 (86%)	176 (13%)	15 (1%)	11	43

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	PRO
1	A	581	ASN
1	A	613	GLN
1	A	582	TRP

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Mol	Chain	Res	Type
1	A	564	VAL

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	1073/1271 (84%)	1068 (100%)	5 (0%)	81 89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	VAL
1	A	612	SER
1	A	614	THR
1	A	923	VAL
1	A	1301	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	785	GLN
1	A	810	ASN
1	A	1478	ASN
1	A	1211	ASN
1	A	1402	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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
3	SO4	A	1702	-	4,4,4	0.72	0	6,6,6	0.52	0
2	AES	A	1701	1	10,12,13	1.05	1 (10%)	14,15,18	1.66	3 (21%)
3	SO4	A	1703	-	4,4,4	0.51	0	6,6,6	0.54	0
3	SO4	A	1704	-	4,4,4	0.62	0	6,6,6	0.81	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
2	AES	A	1701	1	-	3/7/7/9	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	AES	C1-S	2.59	1.84	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	AES	C5-C6-C1	3.55	122.49	119.39
2	A	1701	AES	C2-C1-C6	-3.46	117.72	121.59
2	A	1701	AES	O2S-S-C1	2.22	109.55	104.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1701	AES	C2-C1-S-O2S
2	A	1701	AES	C6-C1-S-O2S
2	A	1701	AES	C4-C7-C8-N8

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1701	AES	2	0
3	A	1704	SO4	2	0

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	1333/1530 (87%)	-0.13	47 (3%)	47 27	6, 39, 88, 117	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	606	ASN	5.4
1	A	206	SER	4.8
1	A	1128	LEU	4.2
1	A	467	ALA	3.9
1	A	175	GLU	3.6

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(Å ²)	Q<0.9
4	CA	A	1708	1/1	0.73	0.34	57,57,57,57	0
2	AES	A	1701	12/13	0.81	0.21	59,81,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1702	5/5	0.82	0.29	28,29,60,83	0
3	SO4	A	1704	5/5	0.91	0.29	35,36,48,81	0
3	SO4	A	1703	5/5	0.93	0.19	37,42,57,73	0
4	CA	A	1706	1/1	0.99	0.05	24,24,24,24	0
4	CA	A	1707	1/1	0.99	0.02	21,21,21,21	0
4	CA	A	1705	1/1	0.99	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.