



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:42 AM UTC

PDB ID : 2SEM / pdb_00002sem
Title : SEM5 SH3 DOMAIN COMPLEXED WITH PEPTOID INHIBITOR
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Deposited on : 1998-11-02
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

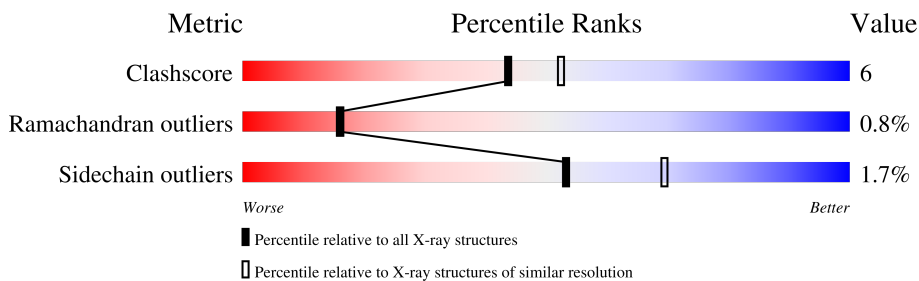
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	60	
1	B	60	
2	C	9	
2	D	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1171 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 PROTEIN (SEX MUSCLE ABNORMAL PROTEIN 5).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	58	Total 481	C 308	N 82	O 90	S 1	0	0	0
1	B	59	Total 487	C 310	N 84	O 92	S 1	0	0	0

- Molecule 2 is a protein called PROTEIN (SH3 PEPTOID INHIBITOR).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	8	Total 56	C 38	N 10	O 8	0	0	0
2	D	9	Total 68	C 44	N 14	O 10	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total 34	O 34	0	0
3	B	35	Total 35	O 35	0	0
3	C	4	Total 4	O 4	0	0
3	D	6	Total 6	O 6	0	0

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. 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: PROTEIN (SEX MUSCLE ABNORMAL PROTEIN 5)

Chain A: 



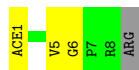
- Molecule 1: PROTEIN (SEX MUSCLE ABNORMAL PROTEIN 5)

Chain B: 



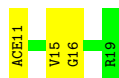
- Molecule 2: PROTEIN (SH3 PEPTOID INHIBITOR)

Chain C: 



- Molecule 2: PROTEIN (SH3 PEPTOID INHIBITOR)

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	33.20Å 59.90Å 33.60Å 90.00° 102.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.0 (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.206 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1171	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: ACE, IPG

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	0.37	0/495	0.92	3/672 (0.4%)
1	B	0.36	0/501	0.93	3/679 (0.4%)
2	C	1.34	1/49 (2.0%)	0.86	0/67
2	D	1.15	1/61 (1.6%)	0.85	0/81
All	All	0.52	2/1106 (0.2%)	0.92	6/1499 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	ACE	C-N	-8.94	1.34	1.43
2	D	11	ACE	C-N	-8.40	1.35	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ASN	CA-C-N	6.13	126.08	119.76
1	A	166	ASN	C-N-CA	6.13	126.08	119.76
1	B	312	ASN	N-CA-C	5.76	117.56	111.28
1	B	266	ASN	CA-C-N	5.41	125.42	119.90
1	B	266	ASN	C-N-CA	5.41	125.42	119.90
1	A	184	ILE	N-CA-C	-5.08	107.85	112.12

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	481	0	448	8	0
1	B	487	0	453	3	0
2	C	56	0	62	1	0
2	D	68	0	75	1	0
3	A	34	0	0	0	0
3	B	35	0	0	0	0
3	C	4	0	0	0	0
3	D	6	0	0	0	0
All	All	1171	0	1038	13	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 (13) 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:262:LEU:O	1:B:277:ARG:HG3	2.06	0.56
1:A:162:LEU:HD21	1:A:209:CYS:SG	2.49	0.53
1:A:209:CYS:HB2	1:A:210:PRO:HD2	1.91	0.53
1:A:162:LEU:HD23	1:A:208:VAL:HA	1.91	0.53
1:A:167:PRO:HG2	1:A:174:ALA:HB2	1.97	0.47
1:B:262:LEU:HD21	1:B:309:CYS:SG	2.56	0.45
1:A:192:TRP:O	1:A:202:ILE:HA	2.18	0.44
2:D:15:VAL:HA	2:D:16:IPG:HCN	1.87	0.44
2:C:5:VAL:HA	2:C:6:IPG:HCN	1.85	0.43
1:A:162:LEU:O	1:A:177:ARG:HG3	2.19	0.42
1:B:296:LEU:HD23	1:B:299:ARG:NH2	2.35	0.42
1:A:188:ASP:HA	1:A:189:PRO:HD3	1.91	0.40
1:A:197:ASN:HB3	1:A:198:ASN:H	1.62	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	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
1	B	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	4
2	C	5/9 (56%)	5 (100%)	0	0	100	100
2	D	6/9 (67%)	6 (100%)	0	0	100	100
All	All	124/138 (90%)	118 (95%)	5 (4%)	1 (1%)	16	16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	LYS

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	52/54 (96%)	51 (98%)	1 (2%)	50	66
1	B	53/54 (98%)	52 (98%)	1 (2%)	50	66
2	C	6/7 (86%)	6 (100%)	0	100	100
2	D	7/7 (100%)	7 (100%)	0	100	100
All	All	118/122 (97%)	116 (98%)	2 (2%)	53	69

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	B	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	166	ASN
1	A	168	GLN
1	A	212	ASN
1	B	260	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	IPG	D	16	2	5,6,7	0.63	0	4,6,8	0.76	0
2	IPG	C	6	2	5,6,7	0.64	0	4,6,8	0.77	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	IPG	D	16	2	-	1/3/4/5	-
2	IPG	C	6	2	-	0/3/4/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	16	IPG	C-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	16	IPG	1	0
2	C	6	IPG	1	0

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

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.