



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:38 AM UTC

PDB ID : 1Q47 / pdb_00001q47
Title : Structure of the Semaphorin 3A Receptor-Binding Module
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Deposited on : 2003-08-01
Resolution : 2.80 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)	:	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

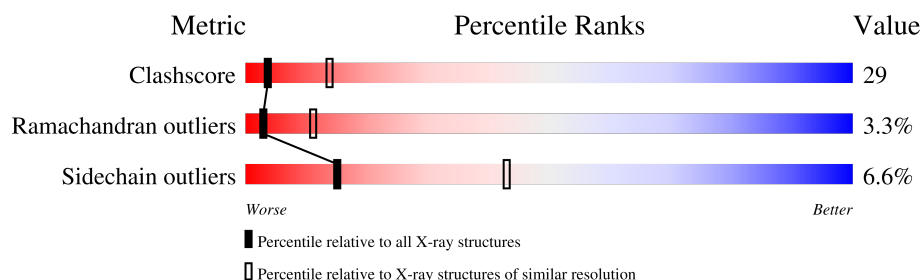
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	495	
1	B	495	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7923 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 Semaphorin 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3883	2474	669	721	19			
1	B	495	Total	C	N	O	S	0	0	0
			3980	2536	684	741	19			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



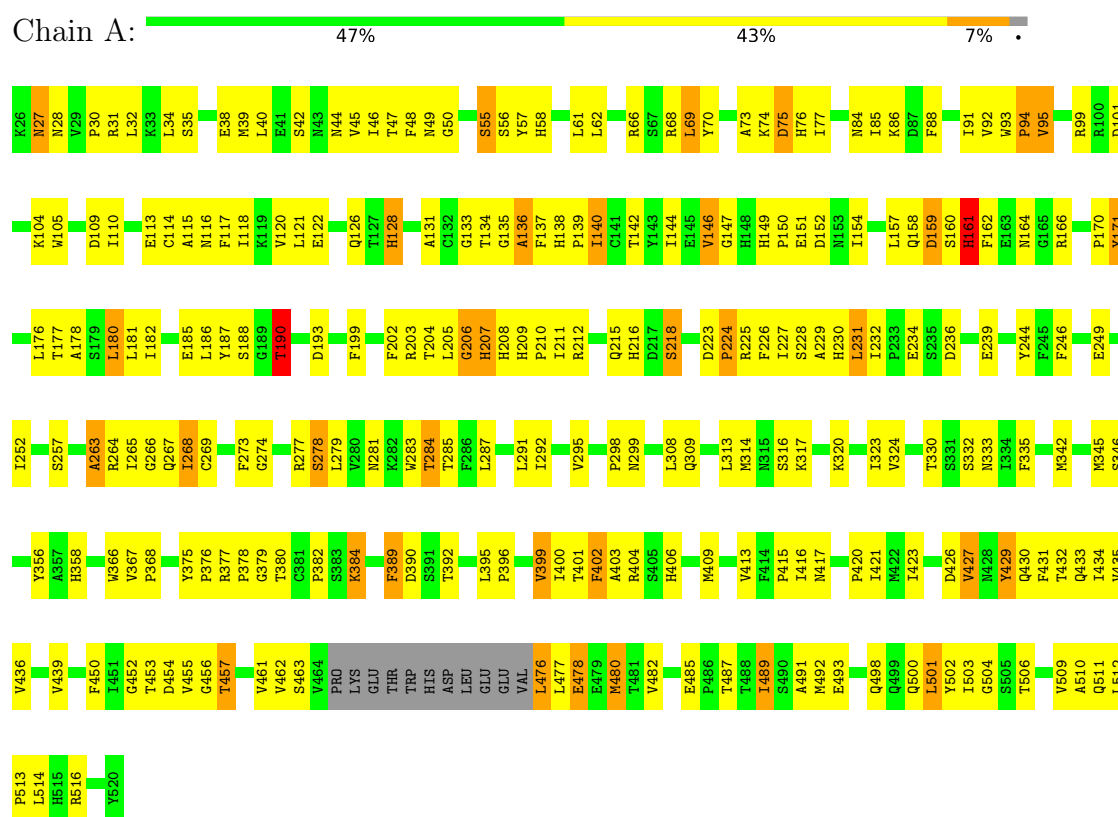
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

3 Residue-property plots

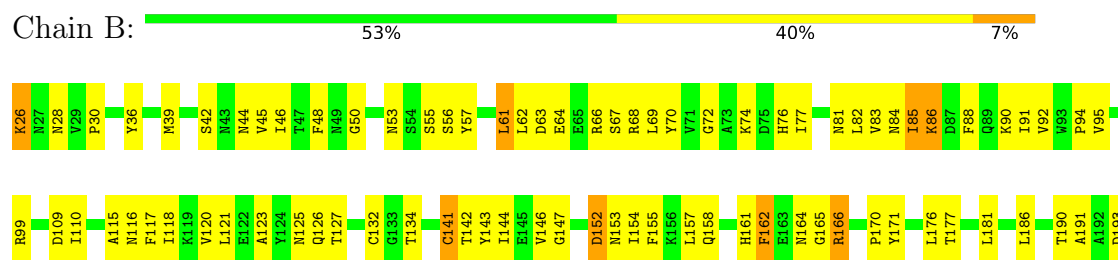
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Semaphorin 3A



• Molecule 1: Semaphorin 3A



F194	M195	D198	F199	F202	R203	H207	H208	H209	P210	I211	R212	T213	F214	Q215	H216	D217	S218	I227	S228	A229	I232	S235	D236	N237	P238	E239	Y244	H256	S257	T261	H262	A263	I268	N271	G274	G275	H276	R277	S278	L279	V280	N281	K282	W283	T284	T285	F286				
L287	R290	L291	I292	C293	S294	P298	N299	H304	F305	D306	E307	L308	L313	I314	K320	V324	Y325	T329	T330	S331	S332	N333	I334	F335	A339	M342	M345	V348	R349	R350	H358	R359	D360	G361	W366	V367	P368	Y369	R372	V373	P374	Y375	P376	G379							
P382	S383	F386	G387	G388	F389	D390	T392	K393	D394	L395	P396	D397	D398	V399	I400	T401	P402	A403	R404	S405	H406	P407	A408	M409	V413	F414	P415	I416	N417	N418	I421	M422	I423	R424	T425	D426	V427	M428	Y429	T432	Q433	I434	V435	V436	D437	A441	E442	D443	G444	V448	M449
F450	T453	D454	V455	T457	V461	K466	E467	T468	W469	H470	D471	L472	L476	M480	T481	V482	F483	R484	I489	S490	A491	M492	E493	L494	S495	T496	K497	Q498	Q499	Q500	L501	Y502	I503	G504	S505	T506	Q511	L512	P513	R516	G517	D518	I519	Y520							

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.79Å 59.73Å 122.72Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.249 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: NAG

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	0/3989	1.04	21/5411 (0.4%)
1	B	0.52	1/4091 (0.0%)	0.94	10/5553 (0.2%)
All	All	0.57	1/8080 (0.0%)	0.99	31/10964 (0.3%)

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	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	MET	SD-CE	5.03	1.92	1.79

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	PHE	N-CA-C	-9.51	98.40	110.19
1	B	263	ALA	N-CA-C	-9.07	97.72	110.50
1	A	126	GLN	N-CA-C	-8.35	103.08	113.18
1	B	402	PHE	N-CA-C	-8.04	100.16	110.53
1	B	498	GLN	N-CA-C	-6.96	105.72	114.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	TYR	Sidechain
1	A	57	TYR	Sidechain
1	B	375	TYR	Sidechain

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	3883	0	3745	236	0
1	B	3980	0	3835	221	0
2	A	30	0	27	3	0
2	B	30	0	27	4	0
All	All	7923	0	7634	452	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 29.

The worst 5 of 452 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:279:LEU:HD21	1:B:404:ARG:HD3	1.41	1.02
1:A:287:LEU:HD22	1:A:409:MET:CE	1.91	0.99
1:A:273:PHE:H	1:A:392:THR:HG21	1.24	0.99
1:B:53:ASN:ND2	2:B:600:NAG:O7	2.01	0.93
1:A:287:LEU:HD22	1:A:409:MET:HE1	1.52	0.89

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	480/495 (97%)	408 (85%)	55 (12%)	17 (4%)	3	10
1	B	493/495 (100%)	410 (83%)	68 (14%)	15 (3%)	3	12
All	All	973/990 (98%)	818 (84%)	123 (13%)	32 (3%)	3	11

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	207	HIS
1	A	257	SER
1	B	153	ASN
1	B	372	ARG

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	428/439 (98%)	400 (94%)	28 (6%)	15	43
1	B	439/439 (100%)	410 (93%)	29 (7%)	15	43
All	All	867/878 (99%)	810 (93%)	57 (7%)	15	43

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	LYS
1	B	482	VAL
1	B	166	ARG
1	B	472	LEU
1	B	417	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	315	ASN
1	B	430	GLN
1	B	358	HIS
1	B	406	HIS
1	B	500	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](#)

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](#)

4 ligands 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	NAG	B	601	-	15,15,15	0.56	0	21,21,21	0.65	0
2	NAG	A	600	-	15,15,15	0.74	0	21,21,21	1.04	1 (4%)
2	NAG	A	601	-	15,15,15	0.65	0	21,21,21	1.31	2 (9%)
2	NAG	B	600	-	15,15,15	0.51	0	21,21,21	0.64	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	NAG	B	601	-	-	6/6/26/26	0/1/1/1
2	NAG	A	600	-	-	4/6/26/26	0/1/1/1
2	NAG	A	601	-	-	3/6/26/26	0/1/1/1
2	NAG	B	600	-	-	3/6/26/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAG	C4-C3-C2	-3.83	104.82	110.40
2	A	601	NAG	O5-C1-C2	2.80	112.33	109.52
2	A	600	NAG	C1-C2-N2	-2.03	108.37	110.73

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NAG	C8-C7-N2-C2
2	A	600	NAG	O7-C7-N2-C2
2	A	601	NAG	C3-C2-N2-C7
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAG	2	0
2	A	601	NAG	3	0
2	B	600	NAG	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.