wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 09:48 AM EDT

PDB ID	:	1Q47
Title	:	Structure of the Semaphorin 3A Receptor-Binding Module
Authors	:	Antipenko, A.; Himanen, J.-P.; van Leyen, K.; Nardi-Dei, V.; Lesniak, J.; Barton, W.A.; Rajashankar, K.R.; Lu, M.; Hoemme, C.; Puschel, A.; Nikolov, D.
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 (i) 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 (i)) were used in the production of this report:

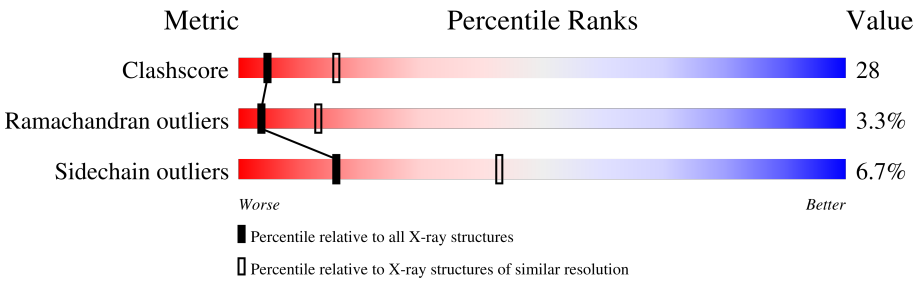
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	495	49% 43% 5% •
1	B	495	55% 40% 5%

2 Entry composition (i)

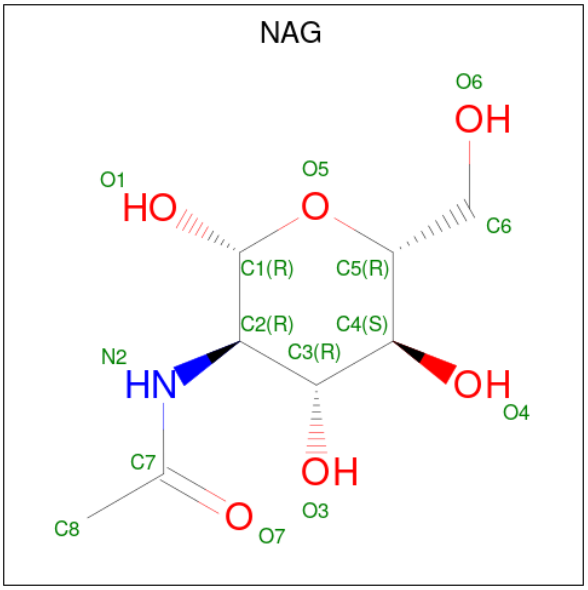
There are 2 unique types of molecules in this entry. The entry contains 7923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	484	3883	2474	669	721	19	0	0	0
1	B	495	3980	2536	684	741	19	0	0	0

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



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

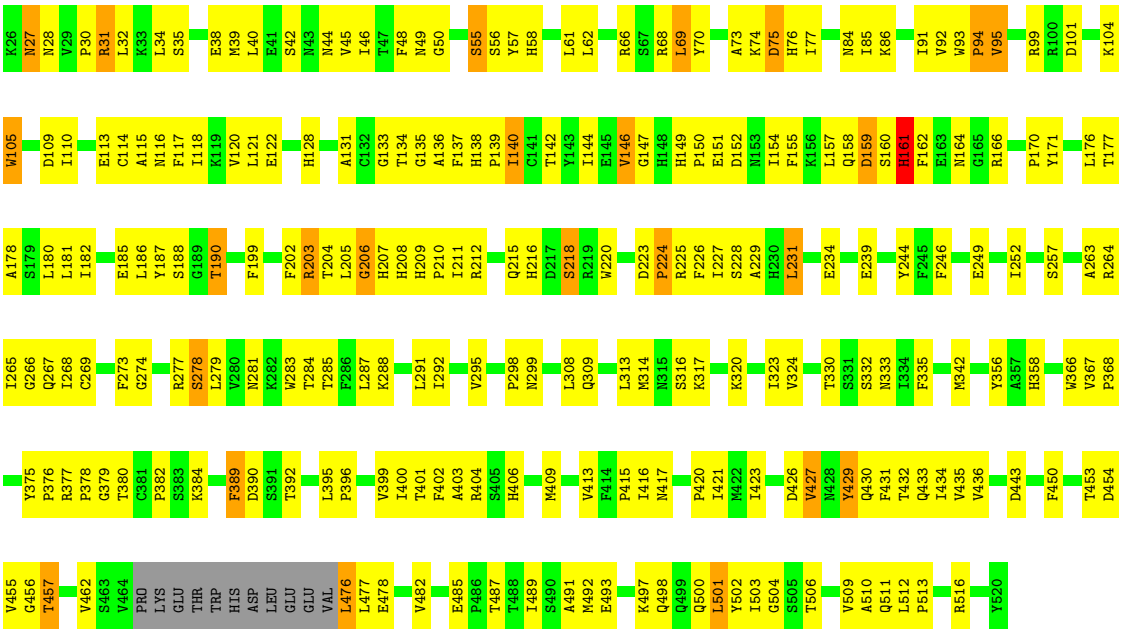
3 Residue-property plots (i)

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.

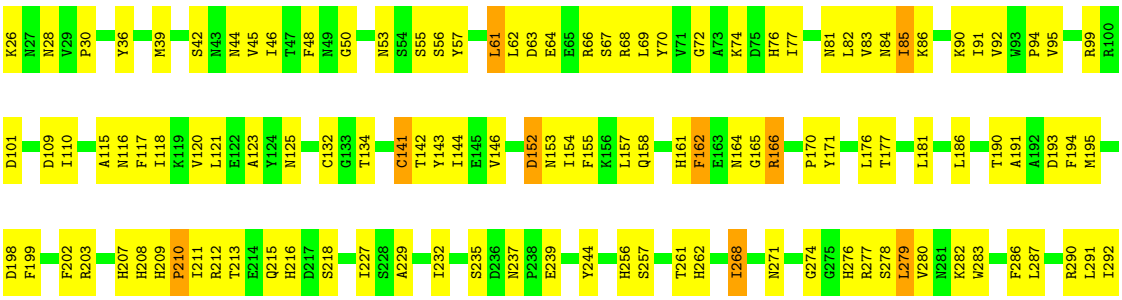
• Molecule 1: Semaphorin 3A

Chain A: 49% 43% 5% •



• Molecule 1: Semaphorin 3A

Chain B: 55% 40% 5%



C293 S294 P298 N299 D302 T303 H304 F305 D306 E307 L308 L313 M314 K320 V324 T329 T330 S331 S332 N333 I334 F335 A339 M342 M345 S346 D347 V348 R349 R350 H358 R359 D360 G361 W366 V367 P368 Y369 R372 V373 P374 Y375 P376 G379 P382 S383
F386 G387 G388 F389 D390 S391 T392 K393 D394 L395 P396 D397 D398 V399 I400 T401 F402 A403 R404 S405 H406 P407 A408 M409 V413 F414 P415 I416 N417 N418 I421 M422 T425 D426 V427 N428 Y429 T432 Q433 I434 V435 V436 D437 A441 E442 D443 G444 V448 M449 F450 T453 D454
V455 G456 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 C517 D518 I519 Y520

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	0.53	0/3989	0.72	0/5411
1	B	0.48	0/4091	0.65	0/5553
All	All	0.50	0/8080	0.69	0/10964

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

There are no bond length outliers.

There are no bond angle outliers.

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	226	0
1	B	3980	0	3835	213	0
2	A	30	0	27	3	0
2	B	30	0	27	4	0
All	All	7923	0	7634	434	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 28.

The worst 5 of 434 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	1.55	0.88

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 12
1	B	493/495 (100%)	410 (83%)	68 (14%)	15 (3%)	4 15
All	All	973/990 (98%)	818 (84%)	123 (13%)	32 (3%)	4 13

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 (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	428/439 (98%)	397 (93%)	31 (7%)	14 38
1	B	439/439 (100%)	412 (94%)	27 (6%)	18 47
All	All	867/878 (99%)	809 (93%)	58 (7%)	16 43

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	487	THR
1	B	469	TRP
1	B	121	LEU
1	B	436	VAL
1	B	389	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	433	GLN
1	B	445	GLN
1	B	511	GLN
1	B	27	ASN
1	A	511	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 monosaccharides 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	600	-	15,15,15	0.51	0	21,21,21	0.63	0
2	NAG	B	601	-	15,15,15	0.56	0	21,21,21	0.64	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	1.30	2 (9%)

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	600	-	-	3/6/26/26	0/1/1/1
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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	NAG	C4-C3-C2	-3.77	104.82	110.34
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	600	NAG	2	0
2	B	601	NAG	2	0
2	A	601	NAG	3	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.