



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID : 1OLZ
Title : THE LIGAND-BINDING FACE OF THE SEMAPHORINS REVEALED BY
THE HIGH RESOLUTION CRYSTAL STRUCTURE OF SEMA4D
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Deposited on : 2003-08-19
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

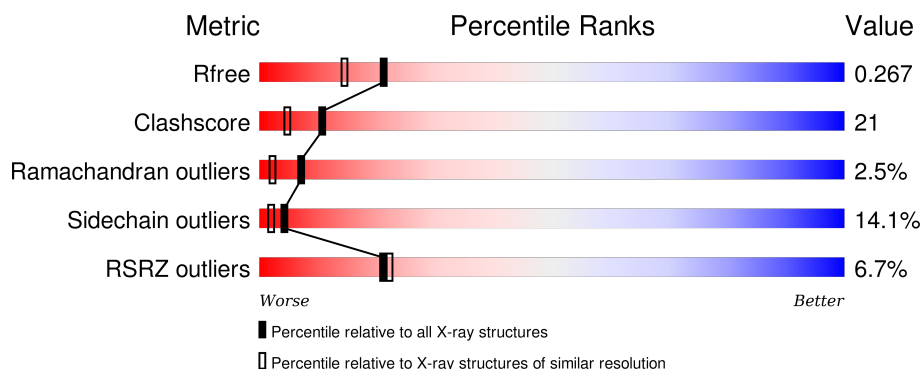
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	663	 5% 57% 28% 8% • 6%
1	B	663	 7% 60% 26% 8% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10669 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 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	0	1
			4914	3128	850	913	23			
1	B	622	Total	C	N	O	S	0	0	1
			4914	3128	850	913	23			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	398	Total	O	0	0
			398	398		
2	B	443	Total	O	0	0
			443	443		

LEU	L573	R464	R345	V224
SER	K574	N471	F346	F225
VAL	A575	S472	D351	R226
VAL	E576	G473	S352	I229
GLN	S577	V474	E353	P230
THR	P578	V475	A354	R231
GLU	K579	L479	R355	R234
GLY	T580	L479	A356	R234
SER	G581	K484	A357	Q240
ARG	L582	E489	N358	R257
ILE	M583	R495	T369	R257
ALA	G584	P503	L370	Q240
THR	R585	P504	F372	R262
LYS	K586	L511	D380	P263
VAL	N587	H512	D386	D264
LEU	L588	Q513	D387	S265
VAL	L589	G596	N388	L272
ALA	I590	M525	R389	L278
ALA	I590	S526	P390	R279
SER	F591	G527	R391	S280
THR	N592	C532	L392	P281
THR	N593	P533	I393	G282
LYS	L593	D534	K394	L283
HIS	S594	K335	K395	V285
HIS	E595	S336	D396	L291
HIS	G596	R337	V397	N297
HIS	D597	G538	N398	N297
HIS	S598	F541	Y399	L301
HIS	S599	Q542	V403	L301
HIS	G599	H543	Q408	N308
	Y601	F544	F409	L309
	L604	F545	L410	K320
	E607	T550	V414	Y321
R608	V617	A551	M418	M322
V609	V618	E552	F419	Q323
K610	A619	C555	E434	S324
N611	K620	S556	H435	T325
K612	H621	Q557	F446	T326
T613	V622	F446	Q447	V327
	L623	A562	D448	E328
	E624	R563	Q453	Q329
	V625	V564	K459	S330
	K626	F565	S458	H331
	V627	K567	K460	K332
	V628	Q569	K461	K336
PRO	PRO	Q569	G462	P342
LYS	LYS	N570	G571	K343
PRO	PRO	V572	N463	P344
VAL	VAL			
VAL	VAL			
ALA	ALA			
PRO	PRO			
THR	THR			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.32Å 76.76Å 89.41Å 77.41° 73.35° 63.57°	Depositor
Resolution (Å)	20.00 – 2.00 19.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-2.00) 93.6 (19.51-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.270 0.206 , 0.267	Depositor DCC
R_{free} test set	5440 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 107916 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10669	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/5034	0.64	1/6825 (0.0%)
1	B	0.39	0/5034	0.68	2/6825 (0.0%)
All	All	0.39	0/10068	0.66	3/13650 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	SER	C-N-CD	-7.49	104.11	120.60
1	B	199	SER	C-N-CA	6.12	147.71	122.00
1	A	457	LEU	CA-CB-CG	5.20	127.25	115.30

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	4914	0	4841	223	0
1	B	4914	0	4841	198	0
2	A	398	0	0	24	0
2	B	443	0	0	39	0
All	All	10669	0	9682	414	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 21.

The worst 5 of 414 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:495:ARG:HG3	1:A:495:ARG:HH11	1.06	1.12
1:A:608:ARG:HD2	1:A:608:ARG:H	1.13	1.12
1:B:200:PRO:HD3	1:B:205:GLY:HA2	1.35	1.08
1:B:343:LYS:HB3	1:B:344:PRO:HD3	1.33	1.07
1:B:199:SER:HB3	1:B:200:PRO:C	1.82	1.00

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	618/663 (93%)	565 (91%)	35 (6%)	18 (3%)	6	2
1	B	618/663 (93%)	567 (92%)	38 (6%)	13 (2%)	9	3
All	All	1236/1326 (93%)	1132 (92%)	73 (6%)	31 (2%)	7	2

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	A	511	LEU
1	A	516	SER
1	A	610	LYS
1	B	199	SER

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	545/582 (94%)	471 (86%)	74 (14%)	5	2
1	B	545/582 (94%)	465 (85%)	80 (15%)	4	2
All	All	1090/1164 (94%)	936 (86%)	154 (14%)	4	2

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	606	GLU
1	B	82	SER
1	B	592	ASN
1	A	608	ARG
1	B	38	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	308	ASN
1	B	338	ASN
1	B	463	ASN
1	B	13	HIS
1	B	471	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 carbohydrates 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 [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	622/663 (93%)	0.03	36 (5%) 26 28	13, 36, 81, 100	0
1	B	622/663 (93%)	-0.02	47 (7%) 17 18	8, 29, 85, 100	0
All	All	1244/1326 (93%)	0.00	83 (6%) 21 22	8, 33, 84, 100	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	8.6
1	A	327	VAL	8.3
1	B	577	SER	8.0
1	A	628	VAL	7.9
1	A	199	SER	7.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.