



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4DRT / pdb_00004drt
Title : Three dimensional structure of de novo designed serine hydrolase OSH26, Northeast Structural Genomics Consortium (NESG) target OR89
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Deposited on : 2012-02-17
Resolution : 2.00 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)
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

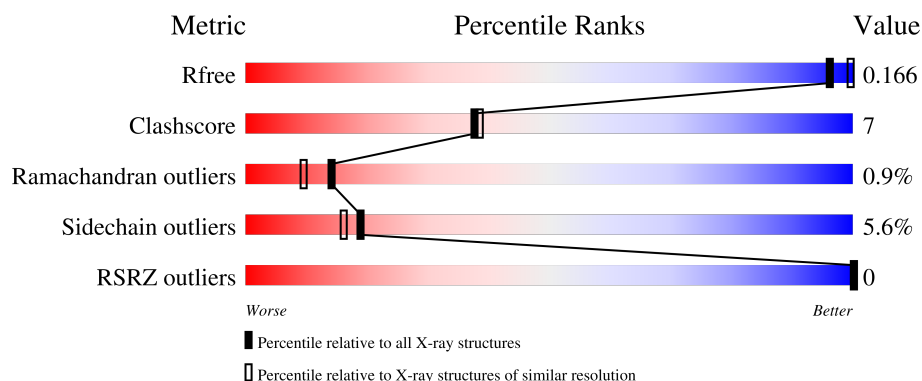
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	361	 79% 16% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3010 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 de novo designed serine hydrolase, OR89.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	Se	0	3	0
			2719	1716	470	520	13			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

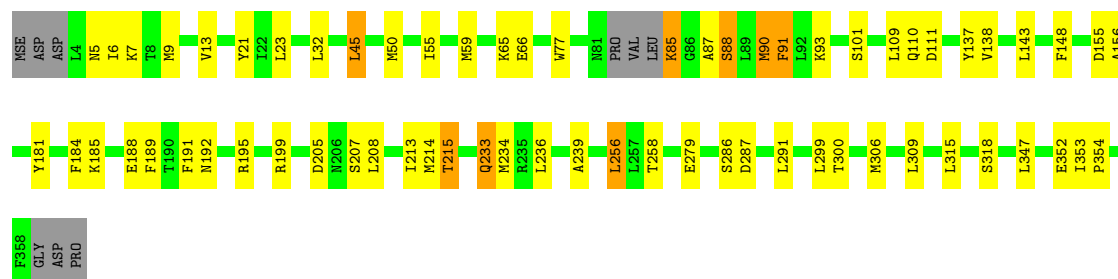
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	289	Total	O	0	0
			289	289		

- Molecule 1: de novo designed serine hydrolase, OR89



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	50.11Å 50.11Å 134.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.54 – 2.00 26.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.54-2.00) 99.7 (26.54-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.72 (at 1.99Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.123 , 0.156 (Not available) , 0.166	Depositor DCC
R_{free} test set	1292 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.097 for -h,-k,l 0.357 for h,-h-k,-l 0.098 for -k,-h,-l	Xtriage
Reported twinning fraction	0.378 for h,-h-k,-l	Depositor
Outliers	0 of 25328 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3010	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: CL, NA

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	0.51	0/2759	0.80	0/3704

There are no bond length outliers.

There are no bond angle outliers.

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	2719	0	2707	38	0
2	A	1	0	0	0	0
3	A	1	0	0	1	0
4	A	289	0	0	2	0
All	All	3010	0	2707	38	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 7.

All (38) 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:137:TYR:OH	3:A:402:CL:CL	2.32	0.83
1:A:77:TRP:HH2	1:A:85:LYS:HB2	1.60	0.67
1:A:234:MSE:HE2	1:A:236:LEU:HD21	1.76	0.66
1:A:77:TRP:CH2	1:A:85:LYS:HB2	2.31	0.65
1:A:181:TYR:HE2	1:A:213:ILE:HG12	1.67	0.59
1:A:155:ASP:N	4:A:601:HOH:O	2.33	0.58
1:A:32:LEU:HD11	1:A:300:THR:HG21	1.87	0.55
1:A:5:ASN:HB3	1:A:7:LYS:H	1.74	0.52
1:A:184:PHE:HE2	1:A:214:MSE:HE3	1.76	0.51
1:A:66:GLU:HB3	1:A:101:SER:HB3	1.94	0.50
1:A:199:ARG:NH1	1:A:215:THR:O	2.44	0.50
1:A:23:LEU:HD22	1:A:256:LEU:HD22	1.93	0.49
1:A:59:MSE:HE1	1:A:66:GLU:HG3	1.92	0.49
1:A:279:GLU:HG3	1:A:315:LEU:HD11	1.93	0.49
1:A:85:LYS:HG3	1:A:91:PHE:CD2	2.48	0.48
1:A:352:GLU:HG2	1:A:354:PRO:HD3	1.95	0.48
1:A:88:SER:C	1:A:90:MSE:H	2.21	0.47
1:A:205:ASP:OD1	1:A:207:SER:OG	2.29	0.47
1:A:55:ILE:O	1:A:59:MSE:HG3	2.16	0.45
1:A:189:PHE:CE2	1:A:191:PHE:HB2	2.52	0.45
1:A:85:LYS:HD2	1:A:93:LYS:HE2	1.99	0.45
1:A:195:ARG:HE	1:A:195:ARG:HB3	1.43	0.45
1:A:91:PHE:CG	1:A:93:LYS:HE3	2.53	0.44
1:A:299:LEU:HD12	1:A:309:LEU:HD21	2.00	0.43
1:A:77:TRP:CE3	1:A:93:LYS:HA	2.54	0.43
1:A:291:LEU:HD13	1:A:347:LEU:HD21	2.01	0.43
1:A:50:MSE:HG2	1:A:148:PHE:CE1	2.54	0.43
1:A:110:GLN:HB3	1:A:111:ASP:H	1.64	0.42
1:A:286:SER:HB2	1:A:353:ILE:HD12	2.00	0.42
1:A:199:ARG:NH2	4:A:749:HOH:O	2.51	0.42
1:A:208:LEU:HD21	1:A:258:THR:HG22	2.01	0.41
1:A:21:TYR:HA	1:A:239:ALA:O	2.21	0.41
1:A:59:MSE:HB3	1:A:59:MSE:HE2	1.75	0.41
1:A:45:LEU:HD23	1:A:199:ARG:NH2	2.36	0.41
1:A:6:ILE:O	1:A:9:MSE:HG2	2.21	0.41
1:A:138:VAL:HG13	1:A:143:LEU:HB2	2.03	0.41
1:A:233:GLN:H	1:A:233:GLN:HG3	1.56	0.40
1:A:91:PHE:HD1	1:A:91:PHE:O	2.04	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	351/361 (97%)	338 (96%)	10 (3%)	3 (1%)	14 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ALA
1	A	156	ALA
1	A	88	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	289/280 (103%)	273 (94%)	16 (6%)	19 17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	45	LEU
1	A	65	LYS
1	A	85	LYS
1	A	90	MSE
1	A	91	PHE
1	A	109	LEU
1	A	185	LYS

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Mol	Chain	Res	Type
1	A	188	GLU
1	A	192	ASN
1	A	215	THR
1	A	233	GLN
1	A	256	LEU
1	A	287	ASP
1	A	306	MSE
1	A	318	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	81	ASN
1	A	139	ASN
1	A	171	GLN
1	A	217	HIS
1	A	233	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	339/361 (93%)	-1.48	0 100 100	13, 27, 58, 100	3 (0%)

There are no RSRZ outliers to report.

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
2	NA	A	401	1/1	0.98	0.05	46,46,46,46	0
3	CL	A	402	1/1	0.99	0.04	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.