



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:23 PM UTC

PDB ID : 8P7A / pdb_00008p7a
Title : Crystal structure of the ORD domain of human ORP8
Authors : Eisenreichova, A.; Klima, M.; Boura, E.
Deposited on : 2023-05-30
Resolution : 2.56 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
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

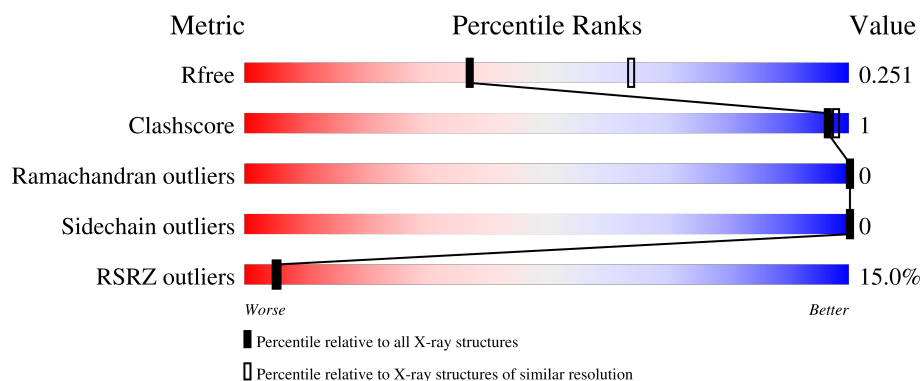
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	381	14% 89% 8%
1	B	381	14% 88% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5605 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.

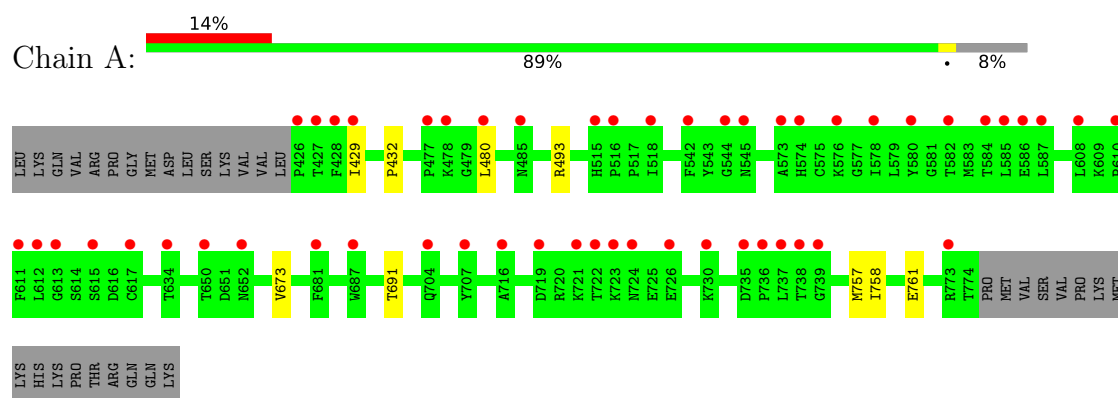
- Molecule 1 is a protein called Oxysterol-binding protein-related protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	1	0
			2835	1823	476	526	10			
1	B	345	Total	C	N	O	S	0	0	0
			2770	1776	463	521	10			

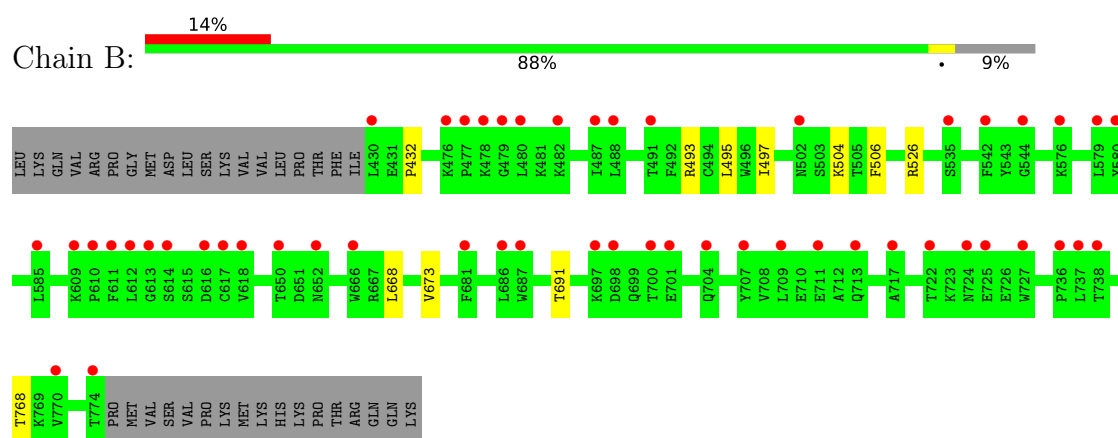
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Oxysterol-binding protein-related protein 8



- Molecule 1: Oxysterol-binding protein-related protein 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.61Å 190.24Å 58.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 2.56 47.56 – 2.56	Depositor EDS
% Data completeness (in resolution range)	52.8 (47.56-2.56) 52.9 (47.56-2.56)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.251 0.219 , 0.251	Depositor DCC
R_{free} test set	1016 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5605	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.39% 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](#)

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	0.22	0/2913	0.36	0/3948
1	B	0.18	0/2846	0.35	0/3866
All	All	0.20	0/5759	0.36	0/7814

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	2835	0	2734	5	0
1	B	2770	0	2621	6	0
All	All	5605	0	5355	11	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 1.

All (11) 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:493:ARG:NH2	1:B:673:VAL:HG11	2.21	0.55
1:A:493:ARG:HD2	1:A:761:GLU:CD	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HD11	1:B:504:LYS:HD3	1.91	0.53
1:B:432:PRO:HB2	1:B:691:THR:HG23	1.91	0.53
1:B:495:LEU:HD12	1:B:506:PHE:CE2	2.49	0.48
1:B:526:ARG:NH1	1:B:768:THR:HG21	2.29	0.48
1:A:757:MET:C	1:A:758:ILE:HD12	2.39	0.47
1:A:432:PRO:HB2	1:A:691:THR:HG23	1.98	0.46
1:B:497:ILE:O	1:B:668:LEU:HD22	2.15	0.46
1:A:429:ILE:HG22	1:A:480:LEU:HA	1.98	0.44
1:A:493:ARG:HE	1:A:673:VAL:HG21	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	348/381 (91%)	345 (99%)	3 (1%)	0	100	100
1	B	343/381 (90%)	340 (99%)	3 (1%)	0	100	100
All	All	691/762 (91%)	685 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	302/342 (88%)	302 (100%)	0	100	100
1	B	291/342 (85%)	291 (100%)	0	100	100
All	All	593/684 (87%)	593 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	HIS
1	A	502	ASN
1	A	671	HIS
1	A	713	GLN
1	A	715	GLN
1	A	767	GLN
1	B	514	HIS
1	B	515	HIS
1	B	592	ASN
1	B	767	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](#)

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	349/381 (91%)	0.76	52 (14%) 5 5	5, 30, 70, 98	1 (0%)
1	B	345/381 (90%)	0.87	52 (15%) 5 5	8, 33, 73, 97	0
All	All	694/762 (91%)	0.81	104 (14%) 5 5	5, 32, 72, 98	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	611	PHE	6.9
1	A	428	PHE	6.1
1	A	427	THR	5.9
1	B	478	LYS	4.8
1	A	480	LEU	4.5
1	A	477	PRO	4.4
1	B	480	LEU	4.2
1	B	487	ILE	4.1
1	A	611	PHE	4.1
1	A	426	PRO	4.1
1	A	737	LEU	4.0
1	B	477	PRO	3.8
1	B	709	LEU	3.7
1	A	610	PRO	3.6
1	B	613	GLY	3.6
1	B	612	LEU	3.5
1	A	429	ILE	3.5
1	B	610	PRO	3.5
1	B	738	THR	3.4
1	A	544	GLY	3.4
1	A	478	LYS	3.3
1	A	650	THR	3.3
1	B	700	THR	3.3
1	A	585	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	687	TRP	3.1
1	A	707	TYR	3.1
1	A	724	ASN	3.1
1	A	617	CYS	3.0
1	B	491	THR	3.0
1	A	542	PHE	3.0
1	B	722	THR	3.0
1	A	736	PRO	3.0
1	B	701	GLU	2.9
1	B	616	ASP	2.9
1	B	617	CYS	2.8
1	B	681	PHE	2.8
1	A	613	GLY	2.8
1	A	612	LEU	2.8
1	B	482	LYS	2.8
1	A	578	ILE	2.7
1	B	727	TRP	2.7
1	A	582	THR	2.7
1	A	722	THR	2.7
1	B	737	LEU	2.7
1	B	736	PRO	2.7
1	A	587	LEU	2.7
1	B	585	LEU	2.7
1	B	609	LYS	2.7
1	A	545	ASN	2.7
1	B	652	ASN	2.7
1	B	697	LYS	2.7
1	B	725	GLU	2.6
1	B	479	GLY	2.6
1	B	430	LEU	2.6
1	B	614	SER	2.6
1	B	717	ALA	2.5
1	B	713	GLN	2.5
1	B	724	ASN	2.5
1	B	666	TRP	2.5
1	A	730	LYS	2.5
1	A	716	ALA	2.5
1	A	634	THR	2.5
1	A	738	THR	2.5
1	A	723	LYS	2.4
1	A	739	GLY	2.4
1	B	687	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	584	THR	2.4
1	B	711	GLU	2.4
1	B	542	PHE	2.4
1	A	735	ASP	2.4
1	A	573	ALA	2.4
1	A	586	GLU	2.4
1	A	615	SER	2.3
1	B	476	LYS	2.3
1	B	698	ASP	2.3
1	B	580	TYR	2.3
1	A	576	LYS	2.2
1	B	488	LEU	2.2
1	B	576	LYS	2.2
1	A	726	GLU	2.2
1	A	580	TYR	2.2
1	A	721	LYS	2.2
1	B	618	VAL	2.2
1	B	704	GLN	2.2
1	A	652	ASN	2.2
1	B	650	THR	2.2
1	B	535	SER	2.2
1	A	516	PRO	2.1
1	A	681	PHE	2.1
1	A	515	HIS	2.1
1	A	608	LEU	2.1
1	B	579	LEU	2.1
1	A	518	ILE	2.1
1	A	485	ASN	2.1
1	B	502	ASN	2.1
1	B	707	TYR	2.1
1	A	574	HIS	2.1
1	A	773	ARG	2.0
1	B	686	LEU	2.0
1	B	774	THR	2.0
1	A	719	ASP	2.0
1	A	704	GLN	2.0
1	B	770	VAL	2.0
1	B	544	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.