



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9IRJ / pdb_00009irj
Title : X-ray structure of PSmOrange3 (trigonal form)
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Deposited on : 2024-07-16
Resolution : 2.80 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

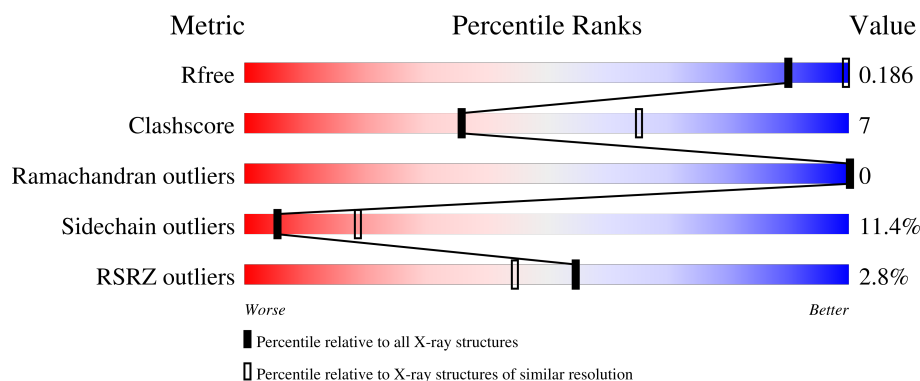
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	233	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1755 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 mOrange.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1737	1113	290	326	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	HIS	ARG	conflict	UNP D0VWW2
A	21	THR	SER	conflict	UNP D0VWW2
A	29	VAL	ILE	conflict	UNP D0VWW2
A	32	LYS	GLU	conflict	UNP D0VWW2
A	36	HIS	ARG	conflict	UNP D0VWW2
A	44	VAL	ALA	conflict	UNP D0VWW2
A	64	LEU	GLN	conflict	UNP D0VWW2
A	65	VAL	PHE	conflict	UNP D0VWW2
A	229	CRO	GLY	chromophore	UNP D0VWW2
A	229	CRO	TYR	chromophore	UNP D0VWW2
A	229	CRO	GLY	chromophore	UNP D0VWW2
A	330	TYR	PHE	conflict	UNP D0VWW2
A	355	MET	LEU	conflict	UNP D0VWW2
A	392	VAL	ILE	conflict	UNP D0VWW2
A	393	ARG	LYS	conflict	UNP D0VWW2
A	408	ALA	VAL	conflict	UNP D0VWW2
A	417	SER	PRO	conflict	UNP D0VWW2
A	419	LEU	GLN	conflict	UNP D0VWW2
A	439	PHE	TYR	conflict	UNP D0VWW2
A	448	SER	ALA	conflict	UNP D0VWW2
A	450	ALA	GLY	conflict	UNP D0VWW2
A	457	LYS	MET	conflict	UNP D0VWW2

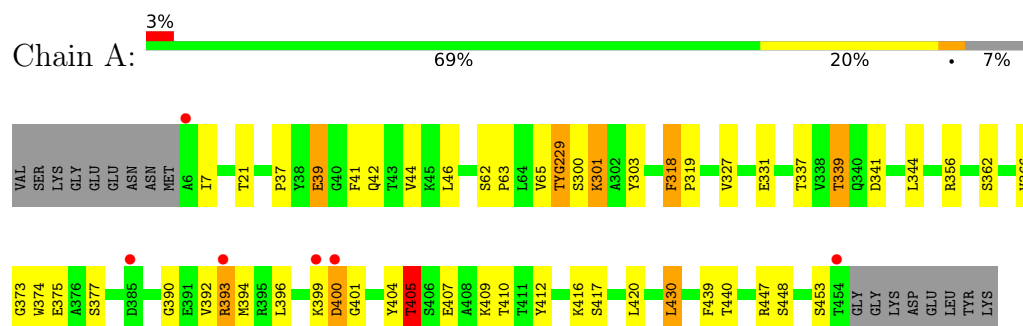
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		

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 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: mOrange



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.16Å 137.16Å 55.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.59 – 2.80 68.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.6 (68.59-2.80) 93.6 (68.59-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.210 0.185 , 0.186	Depositor DCC
R_{free} test set	651 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1755	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: CRO

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	1.01	0/1758	1.50	14/2365 (0.6%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	THR	CA-CB-OG1	-12.72	90.52	109.60
1	A	21	THR	CA-CB-OG1	-8.07	97.49	109.60
1	A	337	THR	CA-CB-OG1	-6.58	99.72	109.60
1	A	405	THR	CA-CB-OG1	-6.51	99.84	109.60
1	A	356	ARG	CA-C-N	6.22	126.47	122.18
1	A	356	ARG	C-N-CA	6.22	126.47	122.18
1	A	327	VAL	CA-C-O	-5.83	114.38	120.27
1	A	390	GLY	CA-C-O	-5.68	116.63	121.57
1	A	440	THR	N-CA-C	-5.64	106.44	113.38
1	A	404	TYR	CB-CA-C	5.51	118.74	109.48
1	A	439	PHE	CB-CA-C	-5.44	104.17	111.89
1	A	373	GLY	CA-C-O	-5.31	117.69	122.57
1	A	301	LYS	N-CA-C	-5.24	106.74	113.23
1	A	318	PHE	CA-CB-CG	-5.02	108.78	113.80

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	1737	0	1700	25	0
2	A	18	0	0	1	0
All	All	1755	0	1700	25	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 (25) 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:42:GLN:HE22	1:A:300:SER:HB3	1.43	0.80
1:A:393:ARG:HH21	1:A:393:ARG:HB2	1.53	0.73
1:A:39:GLU:HB3	1:A:41:PHE:CD1	2.37	0.58
1:A:229:CRO:HD1	1:A:229:CRO:N2	2.19	0.57
1:A:331:GLU:OE1	1:A:405:THR:HB	2.05	0.57
1:A:229:CRO:CE2	1:A:394:MET:HE3	2.36	0.55
1:A:400:ASP:CG	1:A:401:GLY:N	2.65	0.54
1:A:229:CRO:HE1	1:A:430:LEU:HB2	1.91	0.52
1:A:368:GLN:O	1:A:370:LYS:HE3	2.09	0.52
1:A:393:ARG:NH2	1:A:407:GLU:OE1	2.41	0.52
1:A:65:VAL:O	1:A:65:VAL:HG12	2.11	0.50
1:A:375:GLU:HA	1:A:375:GLU:OE1	2.12	0.49
1:A:318:PHE:HB3	1:A:319:PRO:HA	1.94	0.49
1:A:62:SER:N	1:A:63:PRO:CD	2.76	0.49
1:A:41:PHE:CE2	1:A:447:ARG:HG2	2.48	0.48
1:A:37:PRO:HA	1:A:303:TYR:HA	1.97	0.45
1:A:229:CRO:HE2	1:A:394:MET:HE3	1.98	0.44
1:A:410:THR:HG21	1:A:412:TYR:CZ	2.53	0.44
1:A:370:LYS:HA	1:A:370:LYS:HE2	1.99	0.44
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.86	0.44
1:A:393:ARG:HB2	1:A:393:ARG:NH2	2.29	0.43
1:A:366:VAL:HB	2:A:514:HOH:O	2.19	0.41
1:A:374:TRP:CZ3	1:A:396:LEU:HG	2.56	0.41
1:A:41:PHE:CD2	1:A:447:ARG:HG2	2.56	0.41
1:A:331:GLU:OE1	1:A:405:THR:N	2.53	0.41

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	211/233 (91%)	199 (94%)	12 (6%)	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	184/198 (93%)	163 (89%)	21 (11%)	5	19

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	39	GLU
1	A	44	VAL
1	A	46	LEU
1	A	301	LYS
1	A	339	THR
1	A	341	ASP
1	A	344	LEU
1	A	362	SER
1	A	377	SER
1	A	392	VAL
1	A	393	ARG
1	A	399	LYS

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Mol	Chain	Res	Type
1	A	400	ASP
1	A	405	THR
1	A	409	LYS
1	A	416	LYS
1	A	417	SER
1	A	430	LEU
1	A	448	SER
1	A	453	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	345	GLN
1	A	368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CRO	A	229	1	22,23,24	2.99	5 (22%)	30,32,34	3.80	12 (40%)

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
1	CRO	A	229	1	-	7/12/31/32	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	CRO	CB2-CA2	10.65	1.45	1.35
1	A	229	CRO	CA2-C2	-5.14	1.43	1.48
1	A	229	CRO	C1-N2	3.71	1.37	1.32
1	A	229	CRO	C2-N3	-3.62	1.31	1.40
1	A	229	CRO	O2-C2	3.52	1.30	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	CRO	O2-C2-CA2	-12.96	122.75	131.02
1	A	229	CRO	CG2-CB2-CA2	-7.31	121.18	129.87
1	A	229	CRO	C2-N3-C1	-6.85	104.90	108.07
1	A	229	CRO	CA2-C2-N3	6.59	109.03	103.50
1	A	229	CRO	C3-CA3-N3	4.84	123.44	112.43
1	A	229	CRO	OG1-CB1-CG1	-4.79	95.37	109.68
1	A	229	CRO	O3-C3-CA3	-3.28	110.70	125.47
1	A	229	CRO	C1-CA1-N1	-2.92	104.56	109.78
1	A	229	CRO	OG1-CB1-CA1	2.92	115.22	109.00
1	A	229	CRO	CA3-N3-C2	-2.59	117.99	123.67
1	A	229	CRO	CA2-N2-C1	-2.42	103.91	105.80
1	A	229	CRO	CD1-CE1-CZ	2.35	122.36	119.88

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	229	CRO	C1-CA1-CB1-CG1
1	A	229	CRO	C3-CA3-N3-C1
1	A	229	CRO	C3-CA3-N3-C2
1	A	229	CRO	N1-CA1-CB1-CG1
1	A	229	CRO	C1-CA1-CB1-OG1
1	A	229	CRO	N2-C1-CA1-CB1
1	A	229	CRO	N3-C1-CA1-CB1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	229	CRO	4	0

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 [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	215/233 (92%)	-0.20	6 (2%) 55 45	38, 55, 87, 115	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.0
1	A	454	THR	4.9
1	A	393	ARG	3.6
1	A	385	ASP	3.2
1	A	399	LYS	3.0
1	A	400	ASP	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CRO	A	229	22/23	0.96	0.11	57,77,92,98	0

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.