



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2021 – 12:10 PM JST

PDB ID : 7DMO
Title : Crystal structures of two pericyclases catalyzing [4+2] cycloadditions
Authors : Wang, Z.D.; Chi, C.B.; Ma, M.
Deposited on : 2020-12-04
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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

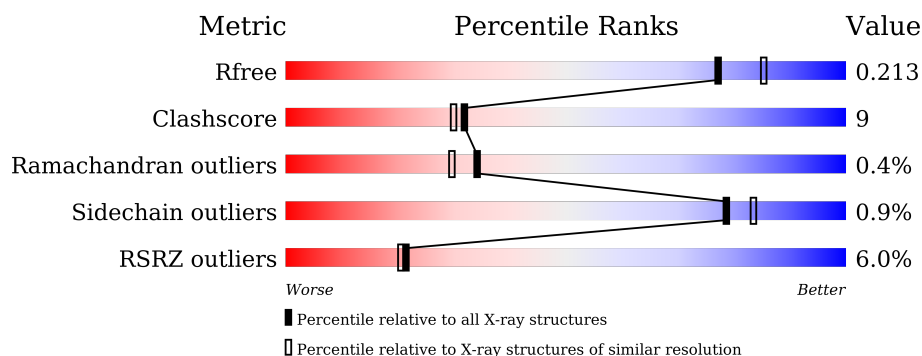
1 Overall quality at a glance ⓘ

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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	389	<div> <div>7%</div> <div>87%</div> <div>7%</div> <div>..</div> </div>
1	B	389	<div> <div>4%</div> <div>83%</div> <div>12%</div> <div>..</div> </div>
1	C	389	<div> <div>7%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	D	389	<div> <div>6%</div> <div>85%</div> <div>10%</div> <div>..</div> </div>
1	E	389	<div> <div>5%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	F	389	<div> <div>6%</div> <div>88%</div> <div>7%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18922 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 Diels-Alderase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2835	1798	475	554	8			
1	B	375	Total	C	N	O	S	0	0	0
			2843	1802	476	557	8			
1	C	375	Total	C	N	O	S	0	0	0
			2844	1804	477	555	8			
1	D	374	Total	C	N	O	S	0	0	0
			2835	1798	475	554	8			
1	E	375	Total	C	N	O	S	0	0	0
			2844	1804	477	555	8			
1	F	374	Total	C	N	O	S	0	0	0
			2838	1801	476	553	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2Z5XAU0
A	2	SER	-	expression tag	UNP A0A2Z5XAU0
A	3	HIS	-	expression tag	UNP A0A2Z5XAU0
B	1	GLY	-	expression tag	UNP A0A2Z5XAU0
B	2	SER	-	expression tag	UNP A0A2Z5XAU0
B	3	HIS	-	expression tag	UNP A0A2Z5XAU0
C	1	GLY	-	expression tag	UNP A0A2Z5XAU0
C	2	SER	-	expression tag	UNP A0A2Z5XAU0
C	3	HIS	-	expression tag	UNP A0A2Z5XAU0
D	1	GLY	-	expression tag	UNP A0A2Z5XAU0
D	2	SER	-	expression tag	UNP A0A2Z5XAU0
D	3	HIS	-	expression tag	UNP A0A2Z5XAU0
E	1	GLY	-	expression tag	UNP A0A2Z5XAU0
E	2	SER	-	expression tag	UNP A0A2Z5XAU0
E	3	HIS	-	expression tag	UNP A0A2Z5XAU0
F	1	GLY	-	expression tag	UNP A0A2Z5XAU0
F	2	SER	-	expression tag	UNP A0A2Z5XAU0

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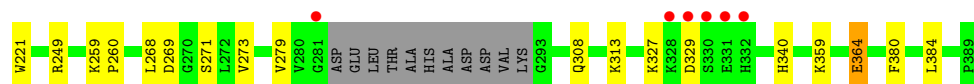
Chain	Residue	Modelled	Actual	Comment	Reference
F	3	HIS	-	expression tag	UNP A0A2Z5XAU0

- Molecule 2 is water.

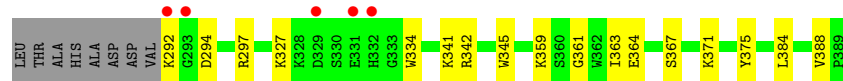
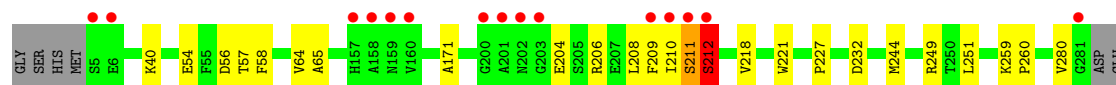
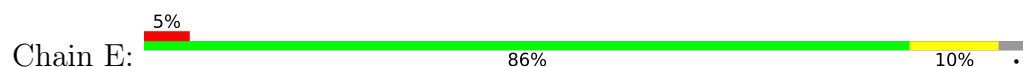
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	304	Total 304	O 304	0	0
2	B	308	Total 308	O 308	0	0
2	C	325	Total 325	O 325	0	0
2	D	317	Total 317	O 317	0	0
2	E	324	Total 324	O 324	0	0
2	F	305	Total 305	O 305	0	0

- Molecule 1: Diels-Alderase

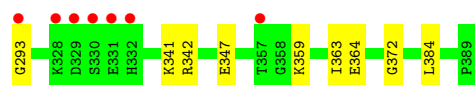
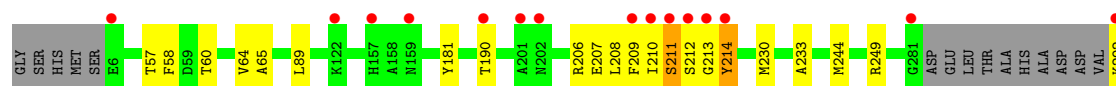
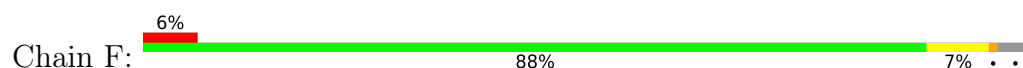




● Molecule 1: Diels-Alderase



● Molecule 1: Diels-Alderase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.20Å 150.53Å 100.05Å 90.00° 96.94° 90.00°	Depositor
Resolution (Å)	13.43 – 2.00 13.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (13.43-2.00) 93.5 (13.43-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 1.99Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.173 , 0.210 0.181 , 0.213	Depositor DCC
R_{free} test set	1853 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18922	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2655e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

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	0.52	1/2916 (0.0%)	0.68	0/3972
1	B	0.53	0/2924	0.69	2/3983 (0.1%)
1	C	0.53	0/2925	0.68	2/3983 (0.1%)
1	D	0.57	2/2916 (0.1%)	0.69	1/3972 (0.0%)
1	E	0.55	1/2925 (0.0%)	0.69	0/3983
1	F	0.54	2/2919 (0.1%)	0.67	0/3975
All	All	0.54	6/17525 (0.0%)	0.68	5/23868 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	364	GLU	CD-OE2	-5.58	1.19	1.25
1	F	207	GLU	CG-CD	-5.35	1.44	1.51
1	E	364	GLU	CD-OE2	-5.18	1.20	1.25
1	A	209	PHE	CB-CG	-5.13	1.42	1.51
1	D	209	PHE	CB-CG	-5.09	1.42	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	297	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	D	181	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	B	120	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	297	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2683	58	0
1	B	2843	0	2687	52	0
1	C	2844	0	2696	77	0
1	D	2835	0	2683	70	0
1	E	2844	0	2696	40	0
1	F	2838	0	2691	73	0
2	A	304	0	0	0	0
2	B	308	0	0	0	0
2	C	325	0	0	0	0
2	D	317	0	0	0	0
2	E	324	0	0	0	0
2	F	305	0	0	0	0
All	All	18922	0	16136	294	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 9.

The worst 5 of 294 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:F:57:THR:CG2	1:F:190:THR:HG21	1.57	1.33
1:D:210:ILE:O	1:D:212:SER:N	1.61	1.33
1:A:271:SER:HB2	1:C:210:ILE:CD1	1.57	1.31
1:A:271:SER:CB	1:C:210:ILE:HD12	1.60	1.28
1:C:271:SER:HB2	1:F:210:ILE:CD1	1.63	1.28

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	370/389 (95%)	357 (96%)	12 (3%)	1 (0%)	41	37
1	B	371/389 (95%)	356 (96%)	14 (4%)	1 (0%)	41	37
1	C	371/389 (95%)	355 (96%)	15 (4%)	1 (0%)	41	37
1	D	370/389 (95%)	353 (95%)	15 (4%)	2 (0%)	29	23
1	E	371/389 (95%)	359 (97%)	10 (3%)	2 (0%)	29	23
1	F	370/389 (95%)	355 (96%)	13 (4%)	2 (0%)	29	23
All	All	2223/2334 (95%)	2135 (96%)	79 (4%)	9 (0%)	34	30

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	SER
1	C	211	SER
1	D	211	SER
1	E	211	SER
1	E	212	SER

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	301/313 (96%)	294 (98%)	7 (2%)	50	53
1	B	302/313 (96%)	298 (99%)	4 (1%)	69	74
1	C	302/313 (96%)	301 (100%)	1 (0%)	92	95
1	D	301/313 (96%)	300 (100%)	1 (0%)	92	95
1	E	302/313 (96%)	300 (99%)	2 (1%)	84	88
1	F	301/313 (96%)	299 (99%)	2 (1%)	84	88
All	All	1809/1878 (96%)	1792 (99%)	17 (1%)	78	83

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	244	MET
1	F	244	MET
1	B	204	GLU
1	B	206	ARG
1	B	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	374/389 (96%)	0.02	26 (6%)	16 15	15, 23, 43, 67	0
1	B	375/389 (96%)	-0.04	17 (4%)	33 32	14, 22, 42, 81	0
1	C	375/389 (96%)	-0.07	27 (7%)	15 14	13, 21, 42, 74	0
1	D	374/389 (96%)	-0.06	23 (6%)	21 20	13, 20, 42, 80	0
1	E	375/389 (96%)	-0.02	20 (5%)	26 25	14, 21, 44, 79	0
1	F	374/389 (96%)	0.02	22 (5%)	22 21	14, 23, 43, 83	0
All	All	2247/2334 (96%)	-0.03	135 (6%)	21 20	13, 22, 43, 83	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	SER	13.8
1	B	211	SER	11.3
1	E	211	SER	10.8
1	E	202	ASN	10.0
1	C	211	SER	9.8

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 monosaccharides 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.