



wwPDB X-ray Structure Validation Summary Report i

Sep 13, 2023 – 04:08 PM EDT

PDB ID : 4QRO

Title : CRYSTAL STRUCTURE of DIHYDROXYBENZOIC ACID DECARBOXYLASE BPRO_2061 (TARGET EFI-500288) FROM POLAROMONAS SP. JS666 WITH BOUND MANGANESE AND AN INHIBITOR, 2-NITRORESORCINOL

Authors : Patkovsky, Y.; Vladimirova, A.; Toro, R.; Bhosle, R.; Gerlt, J.A.; Raushel, M.; Almo, S.C.

Deposited on : 2014-07-01

Resolution : 1.65 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 i 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](#) i) were used in the production of this report:

MolProbitiy : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriaige (Phenix) : 1.13

EDS : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

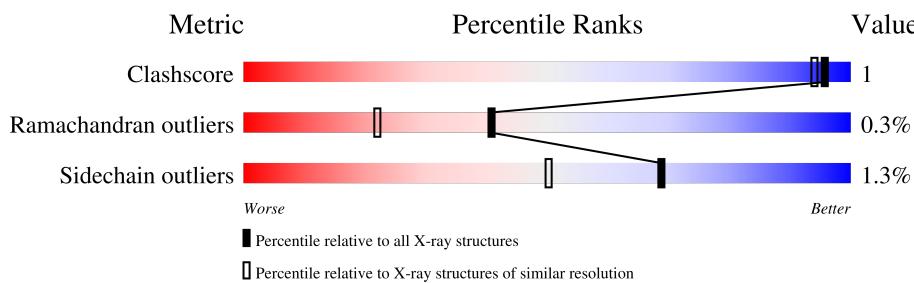
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

2 Entry composition [\(i\)](#)

There are 7 unique types of molecules in this entry. The entry contains 23784 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 Gamma-resorcylate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total 2729	C 1745	N 481	O 493	S 10	0	6	0
1	B	324	Total 2655	C 1699	N 465	O 481	S 10	0	5	0
1	C	325	Total 2648	C 1692	N 463	O 483	S 10	0	3	0
1	D	323	Total 2628	C 1681	N 459	O 479	S 9	0	2	0
1	E	324	Total 2645	C 1691	N 461	O 484	S 9	0	5	0
1	F	324	Total 2660	C 1700	N 468	O 482	S 10	0	5	0
1	G	327	Total 2702	C 1732	N 469	O 491	S 10	0	7	0
1	H	324	Total 2671	C 1707	N 469	O 485	S 10	0	8	0

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	-	expression tag	UNP Q12BV1
A	328	GLU	-	expression tag	UNP Q12BV1
A	329	ASN	-	expression tag	UNP Q12BV1
A	330	LEU	-	expression tag	UNP Q12BV1
A	331	TYR	-	expression tag	UNP Q12BV1
A	332	PHE	-	expression tag	UNP Q12BV1
A	333	GLN	-	expression tag	UNP Q12BV1
A	334	SER	-	expression tag	UNP Q12BV1
A	335	HIS	-	expression tag	UNP Q12BV1
A	336	HIS	-	expression tag	UNP Q12BV1
A	337	HIS	-	expression tag	UNP Q12BV1
A	338	HIS	-	expression tag	UNP Q12BV1
A	339	HIS	-	expression tag	UNP Q12BV1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	HIS	-	expression tag	UNP Q12BV1
A	341	TRP	-	expression tag	UNP Q12BV1
A	342	SER	-	expression tag	UNP Q12BV1
A	343	HIS	-	expression tag	UNP Q12BV1
A	344	PRO	-	expression tag	UNP Q12BV1
A	345	GLN	-	expression tag	UNP Q12BV1
A	346	PHE	-	expression tag	UNP Q12BV1
A	347	GLU	-	expression tag	UNP Q12BV1
A	348	LYS	-	expression tag	UNP Q12BV1
B	327	ALA	-	expression tag	UNP Q12BV1
B	328	GLU	-	expression tag	UNP Q12BV1
B	329	ASN	-	expression tag	UNP Q12BV1
B	330	LEU	-	expression tag	UNP Q12BV1
B	331	TYR	-	expression tag	UNP Q12BV1
B	332	PHE	-	expression tag	UNP Q12BV1
B	333	GLN	-	expression tag	UNP Q12BV1
B	334	SER	-	expression tag	UNP Q12BV1
B	335	HIS	-	expression tag	UNP Q12BV1
B	336	HIS	-	expression tag	UNP Q12BV1
B	337	HIS	-	expression tag	UNP Q12BV1
B	338	HIS	-	expression tag	UNP Q12BV1
B	339	HIS	-	expression tag	UNP Q12BV1
B	340	HIS	-	expression tag	UNP Q12BV1
B	341	TRP	-	expression tag	UNP Q12BV1
B	342	SER	-	expression tag	UNP Q12BV1
B	343	HIS	-	expression tag	UNP Q12BV1
B	344	PRO	-	expression tag	UNP Q12BV1
B	345	GLN	-	expression tag	UNP Q12BV1
B	346	PHE	-	expression tag	UNP Q12BV1
B	347	GLU	-	expression tag	UNP Q12BV1
B	348	LYS	-	expression tag	UNP Q12BV1
C	327	ALA	-	expression tag	UNP Q12BV1
C	328	GLU	-	expression tag	UNP Q12BV1
C	329	ASN	-	expression tag	UNP Q12BV1
C	330	LEU	-	expression tag	UNP Q12BV1
C	331	TYR	-	expression tag	UNP Q12BV1
C	332	PHE	-	expression tag	UNP Q12BV1
C	333	GLN	-	expression tag	UNP Q12BV1
C	334	SER	-	expression tag	UNP Q12BV1
C	335	HIS	-	expression tag	UNP Q12BV1
C	336	HIS	-	expression tag	UNP Q12BV1
C	337	HIS	-	expression tag	UNP Q12BV1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	338	HIS	-	expression tag	UNP Q12BV1
C	339	HIS	-	expression tag	UNP Q12BV1
C	340	HIS	-	expression tag	UNP Q12BV1
C	341	TRP	-	expression tag	UNP Q12BV1
C	342	SER	-	expression tag	UNP Q12BV1
C	343	HIS	-	expression tag	UNP Q12BV1
C	344	PRO	-	expression tag	UNP Q12BV1
C	345	GLN	-	expression tag	UNP Q12BV1
C	346	PHE	-	expression tag	UNP Q12BV1
C	347	GLU	-	expression tag	UNP Q12BV1
C	348	LYS	-	expression tag	UNP Q12BV1
D	327	ALA	-	expression tag	UNP Q12BV1
D	328	GLU	-	expression tag	UNP Q12BV1
D	329	ASN	-	expression tag	UNP Q12BV1
D	330	LEU	-	expression tag	UNP Q12BV1
D	331	TYR	-	expression tag	UNP Q12BV1
D	332	PHE	-	expression tag	UNP Q12BV1
D	333	GLN	-	expression tag	UNP Q12BV1
D	334	SER	-	expression tag	UNP Q12BV1
D	335	HIS	-	expression tag	UNP Q12BV1
D	336	HIS	-	expression tag	UNP Q12BV1
D	337	HIS	-	expression tag	UNP Q12BV1
D	338	HIS	-	expression tag	UNP Q12BV1
D	339	HIS	-	expression tag	UNP Q12BV1
D	340	HIS	-	expression tag	UNP Q12BV1
D	341	TRP	-	expression tag	UNP Q12BV1
D	342	SER	-	expression tag	UNP Q12BV1
D	343	HIS	-	expression tag	UNP Q12BV1
D	344	PRO	-	expression tag	UNP Q12BV1
D	345	GLN	-	expression tag	UNP Q12BV1
D	346	PHE	-	expression tag	UNP Q12BV1
D	347	GLU	-	expression tag	UNP Q12BV1
D	348	LYS	-	expression tag	UNP Q12BV1
E	327	ALA	-	expression tag	UNP Q12BV1
E	328	GLU	-	expression tag	UNP Q12BV1
E	329	ASN	-	expression tag	UNP Q12BV1
E	330	LEU	-	expression tag	UNP Q12BV1
E	331	TYR	-	expression tag	UNP Q12BV1
E	332	PHE	-	expression tag	UNP Q12BV1
E	333	GLN	-	expression tag	UNP Q12BV1
E	334	SER	-	expression tag	UNP Q12BV1
E	335	HIS	-	expression tag	UNP Q12BV1

Continued on next page...

Continued from previous page...

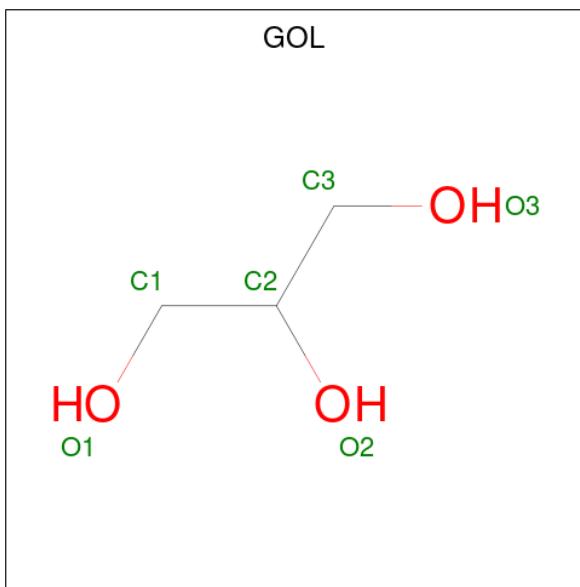
Chain	Residue	Modelled	Actual	Comment	Reference
E	336	HIS	-	expression tag	UNP Q12BV1
E	337	HIS	-	expression tag	UNP Q12BV1
E	338	HIS	-	expression tag	UNP Q12BV1
E	339	HIS	-	expression tag	UNP Q12BV1
E	340	HIS	-	expression tag	UNP Q12BV1
E	341	TRP	-	expression tag	UNP Q12BV1
E	342	SER	-	expression tag	UNP Q12BV1
E	343	HIS	-	expression tag	UNP Q12BV1
E	344	PRO	-	expression tag	UNP Q12BV1
E	345	GLN	-	expression tag	UNP Q12BV1
E	346	PHE	-	expression tag	UNP Q12BV1
E	347	GLU	-	expression tag	UNP Q12BV1
E	348	LYS	-	expression tag	UNP Q12BV1
F	327	ALA	-	expression tag	UNP Q12BV1
F	328	GLU	-	expression tag	UNP Q12BV1
F	329	ASN	-	expression tag	UNP Q12BV1
F	330	LEU	-	expression tag	UNP Q12BV1
F	331	TYR	-	expression tag	UNP Q12BV1
F	332	PHE	-	expression tag	UNP Q12BV1
F	333	GLN	-	expression tag	UNP Q12BV1
F	334	SER	-	expression tag	UNP Q12BV1
F	335	HIS	-	expression tag	UNP Q12BV1
F	336	HIS	-	expression tag	UNP Q12BV1
F	337	HIS	-	expression tag	UNP Q12BV1
F	338	HIS	-	expression tag	UNP Q12BV1
F	339	HIS	-	expression tag	UNP Q12BV1
F	340	HIS	-	expression tag	UNP Q12BV1
F	341	TRP	-	expression tag	UNP Q12BV1
F	342	SER	-	expression tag	UNP Q12BV1
F	343	HIS	-	expression tag	UNP Q12BV1
F	344	PRO	-	expression tag	UNP Q12BV1
F	345	GLN	-	expression tag	UNP Q12BV1
F	346	PHE	-	expression tag	UNP Q12BV1
F	347	GLU	-	expression tag	UNP Q12BV1
F	348	LYS	-	expression tag	UNP Q12BV1
G	327	ALA	-	expression tag	UNP Q12BV1
G	328	GLU	-	expression tag	UNP Q12BV1
G	329	ASN	-	expression tag	UNP Q12BV1
G	330	LEU	-	expression tag	UNP Q12BV1
G	331	TYR	-	expression tag	UNP Q12BV1
G	332	PHE	-	expression tag	UNP Q12BV1
G	333	GLN	-	expression tag	UNP Q12BV1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	334	SER	-	expression tag	UNP Q12BV1
G	335	HIS	-	expression tag	UNP Q12BV1
G	336	HIS	-	expression tag	UNP Q12BV1
G	337	HIS	-	expression tag	UNP Q12BV1
G	338	HIS	-	expression tag	UNP Q12BV1
G	339	HIS	-	expression tag	UNP Q12BV1
G	340	HIS	-	expression tag	UNP Q12BV1
G	341	TRP	-	expression tag	UNP Q12BV1
G	342	SER	-	expression tag	UNP Q12BV1
G	343	HIS	-	expression tag	UNP Q12BV1
G	344	PRO	-	expression tag	UNP Q12BV1
G	345	GLN	-	expression tag	UNP Q12BV1
G	346	PHE	-	expression tag	UNP Q12BV1
G	347	GLU	-	expression tag	UNP Q12BV1
G	348	LYS	-	expression tag	UNP Q12BV1
H	327	ALA	-	expression tag	UNP Q12BV1
H	328	GLU	-	expression tag	UNP Q12BV1
H	329	ASN	-	expression tag	UNP Q12BV1
H	330	LEU	-	expression tag	UNP Q12BV1
H	331	TYR	-	expression tag	UNP Q12BV1
H	332	PHE	-	expression tag	UNP Q12BV1
H	333	GLN	-	expression tag	UNP Q12BV1
H	334	SER	-	expression tag	UNP Q12BV1
H	335	HIS	-	expression tag	UNP Q12BV1
H	336	HIS	-	expression tag	UNP Q12BV1
H	337	HIS	-	expression tag	UNP Q12BV1
H	338	HIS	-	expression tag	UNP Q12BV1
H	339	HIS	-	expression tag	UNP Q12BV1
H	340	HIS	-	expression tag	UNP Q12BV1
H	341	TRP	-	expression tag	UNP Q12BV1
H	342	SER	-	expression tag	UNP Q12BV1
H	343	HIS	-	expression tag	UNP Q12BV1
H	344	PRO	-	expression tag	UNP Q12BV1
H	345	GLN	-	expression tag	UNP Q12BV1
H	346	PHE	-	expression tag	UNP Q12BV1
H	347	GLU	-	expression tag	UNP Q12BV1
H	348	LYS	-	expression tag	UNP Q12BV1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 12 6 6	0	1
2	B	1	Total C O 12 6 6	0	1
2	C	1	Total C O 6 3 3	0	0
2	F	1	Total C O 12 6 6	0	1
2	H	1	Total C O 12 6 6	0	1

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

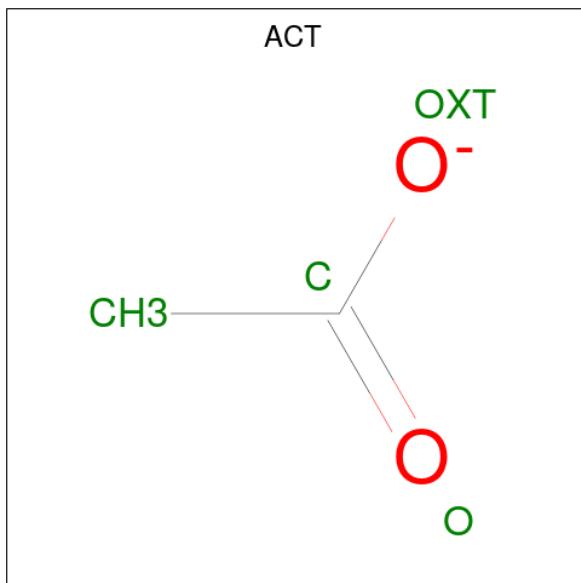
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mn 1 1	0	0
3	H	1	Total Mn 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



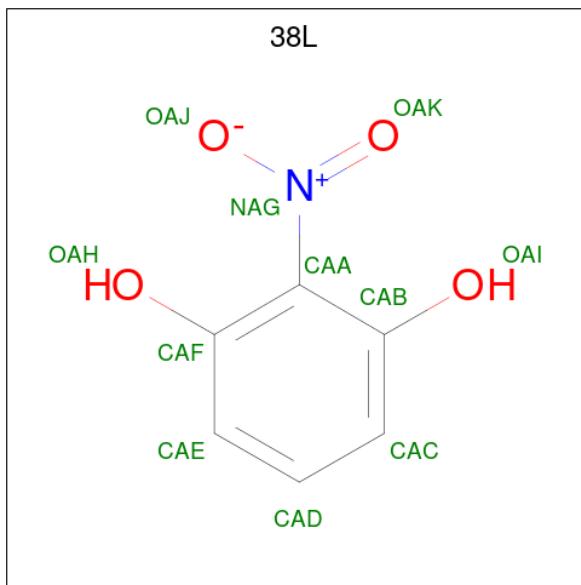
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

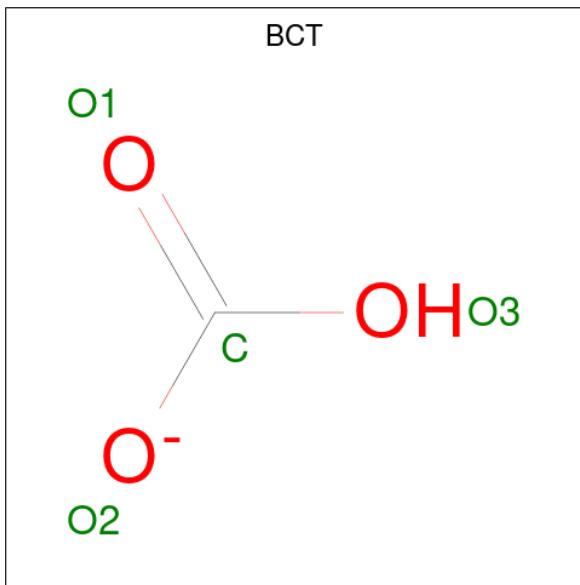
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is 2-nitrobenzene-1,3-diol (three-letter code: 38L) (formula: C₆H₅NO₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 11 6 1 4	0	0
5	B	1	Total C N O 11 6 1 4	0	0
5	C	1	Total C N O 11 6 1 4	0	0
5	D	1	Total C N O 11 6 1 4	0	0
5	E	1	Total C N O 11 6 1 4	0	0
5	F	1	Total C N O 11 6 1 4	0	0
5	G	1	Total C N O 11 6 1 4	0	0
5	H	1	Total C N O 11 6 1 4	0	0

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 4 1 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	287	Total O 288 288	0	1
7	B	245	Total O 245 245	0	0
7	C	273	Total O 273 273	0	0
7	D	240	Total O 240 240	0	0
7	E	312	Total O 312 312	0	0
7	F	290	Total O 290 290	0	0
7	G	310	Total O 310 310	0	0
7	H	284	Total O 284 284	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.96 Å 151.06 Å 143.83 Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	50.00 – 1.65	Depositor
% Data completeness (in resolution range)	99.8 (50.00-1.65)	Depositor
R _{merge}	0.10	Depositor
R _{sym}	0.10	Depositor
$< I/\sigma(I) >$ ¹	1.95 (at 1.65 Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R _{free}	0.189, 0.223	Depositor
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.807	Xtriage
L-test for twinning ²	$< L > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
Total number of atoms	23784	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 41.54 % 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 2.3262e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality i

4.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GOL, ACT, BCT, 38L

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	0.56	0/2813	0.70	4/3819 (0.1%)
1	B	0.54	0/2740	0.65	0/3720
1	C	0.55	0/2721	0.69	0/3696
1	D	0.58	2/2704 (0.1%)	0.69	0/3674
1	E	0.74	0/2727	0.75	2/3705 (0.1%)
1	F	0.69	1/2742 (0.0%)	0.73	1/3723 (0.0%)
1	G	0.73	0/2788	0.80	5/3783 (0.1%)
1	H	0.70	0/2759	0.72	0/3746
All	All	0.64	3/21994 (0.0%)	0.72	12/29866 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	148	TRP	CB-CG	5.93	1.60	1.50
1	D	45[A]	ARG	N-CA	5.14	1.56	1.46
1	D	45[B]	ARG	N-CA	5.14	1.56	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	ARG	NE-CZ-NH2	8.92	124.76	120.30
1	A	174	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	G	45	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	133	ASP	CB-CG-OD1	5.53	123.28	118.30
1	F	247	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2729	0	2654	9	0
1	B	2655	0	2592	5	0
1	C	2648	0	2567	1	0
1	D	2628	0	2548	1	0
1	E	2645	0	2565	4	0
1	F	2660	0	2591	7	0
1	G	2702	0	2630	8	0
1	H	2671	0	2603	8	0
2	A	18	0	24	4	0
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	F	12	0	16	1	0
2	H	12	0	16	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	4	0	3	1	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
4	E	8	0	6	0	0
4	F	4	0	3	0	0
4	G	4	0	3	0	0
4	H	8	0	6	0	0
5	A	11	0	3	0	0
5	B	11	0	4	0	0
5	C	11	0	3	0	0
5	D	11	0	3	0	0
5	E	11	0	3	0	0
5	F	11	0	3	0	0
5	G	11	0	3	0	0
5	H	11	0	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	4	0	0	0	0
7	A	288	0	0	5	0
7	B	245	0	0	1	0
7	C	273	0	0	1	0
7	D	240	0	0	0	0
7	E	312	0	0	1	0
7	F	290	0	0	2	0
7	G	310	0	0	2	0
7	H	284	0	0	2	0
All	All	23784	0	20888	46	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.

The worst 5 of 46 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)
4:A:404:ACT:H1	7:A:783:HOH:O	1.80	0.79
2:F:401[A]:GOL:H32	1:G:267:THR:OG1	1.84	0.78
1:H:267:THR:OG1	2:H:401[A]:GOL:H32	1.83	0.78
1:A:41:ASP:OD1	1:A:45[A]:ARG:NH1	2.20	0.74
1:H:146:GLN:HE21	1:H:146:GLN:H	1.36	0.73

There are no symmetry-related clashes.

4.3 Torsion angles [\(i\)](#)

4.3.1 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	336/348 (97%)	328 (98%)	7 (2%)	1 (0%)	41 22
1	B	327/348 (94%)	317 (97%)	9 (3%)	1 (0%)	41 22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	326/348 (94%)	317 (97%)	8 (2%)	1 (0%)	41 22
1	D	323/348 (93%)	314 (97%)	8 (2%)	1 (0%)	41 22
1	E	327/348 (94%)	318 (97%)	8 (2%)	1 (0%)	41 22
1	F	327/348 (94%)	319 (98%)	8 (2%)	0	100 100
1	G	330/348 (95%)	321 (97%)	8 (2%)	1 (0%)	41 22
1	H	330/348 (95%)	322 (98%)	7 (2%)	1 (0%)	41 22
All	All	2626/2784 (94%)	2556 (97%)	63 (2%)	7 (0%)	41 22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	187	TRP
1	A	187	TRP
1	B	187	TRP
1	C	187	TRP
1	E	187	TRP

4.3.2 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	281/294 (96%)	278 (99%)	3 (1%)	73 57
1	B	276/294 (94%)	272 (99%)	4 (1%)	67 46
1	C	273/294 (93%)	269 (98%)	4 (2%)	65 44
1	D	272/294 (92%)	269 (99%)	3 (1%)	73 57
1	E	274/294 (93%)	270 (98%)	4 (2%)	65 44
1	F	276/294 (94%)	272 (99%)	4 (1%)	67 46
1	G	281/294 (96%)	277 (99%)	4 (1%)	67 46
1	H	277/294 (94%)	273 (99%)	4 (1%)	67 46
All	All	2210/2352 (94%)	2180 (99%)	30 (1%)	69 46

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	7	LEU
1	H	146	GLN
1	E	307	GLU
1	H	233	ARG
1	G	307[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	132	GLN
1	H	254	ASN
1	D	254	ASN
1	E	2	ASN
1	E	134	ASN

4.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [\(i\)](#)

Of 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 for Mogul analysis.

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
4	ACT	G	402	-	3,3,3	0.93	0	3,3,3	1.26	0
4	ACT	B	403	-	3,3,3	0.96	0	3,3,3	0.28	0
4	ACT	E	403	-	3,3,3	0.90	0	3,3,3	1.34	0
2	GOL	A	402[A]	-	5,5,5	0.47	0	5,5,5	0.30	0
2	GOL	H	401[A]	-	5,5,5	0.46	0	5,5,5	0.46	0
5	38L	H	405	3	10,11,11	1.02	1 (10%)	11,15,15	1.01	1 (9%)
4	ACT	F	403	-	3,3,3	0.82	0	3,3,3	1.09	0
2	GOL	B	401[A]	-	5,5,5	0.31	0	5,5,5	0.37	0
6	BCT	G	404	-	2,3,3	0.57	0	2,3,3	0.61	0
5	38L	F	404	3	10,11,11	1.22	2 (20%)	11,15,15	0.94	1 (9%)
4	ACT	C	404	-	3,3,3	0.73	0	3,3,3	0.61	0
4	ACT	D	402	-	3,3,3	0.87	0	3,3,3	0.30	0
5	38L	B	404	3	10,11,11	1.16	1 (10%)	11,15,15	0.87	0
2	GOL	A	402[B]	-	5,5,5	0.28	0	5,5,5	0.65	0
2	GOL	H	401[B]	-	5,5,5	0.38	0	5,5,5	0.89	0
4	ACT	H	403	-	3,3,3	0.95	0	3,3,3	0.56	0
5	38L	A	405	3	10,11,11	0.88	1 (10%)	11,15,15	1.22	2 (18%)
4	ACT	E	402	-	3,3,3	0.80	0	3,3,3	1.04	0
2	GOL	B	401[B]	-	5,5,5	0.43	0	5,5,5	0.34	0
2	GOL	F	401[A]	-	5,5,5	0.47	0	5,5,5	0.86	0
5	38L	D	403	3	10,11,11	0.94	1 (10%)	11,15,15	1.32	1 (9%)
4	ACT	A	404	-	3,3,3	0.73	0	3,3,3	1.04	0
5	38L	E	404	3	10,11,11	1.13	1 (10%)	11,15,15	1.21	2 (18%)
5	38L	C	405	3	10,11,11	0.61	0	11,15,15	1.21	2 (18%)
5	38L	G	403	3	10,11,11	1.59	1 (10%)	11,15,15	1.03	2 (18%)
2	GOL	A	401	-	5,5,5	0.27	0	5,5,5	0.41	0
4	ACT	H	404	-	3,3,3	0.73	0	3,3,3	0.90	0
2	GOL	F	401[B]	-	5,5,5	0.24	0	5,5,5	0.38	0
4	ACT	C	403	-	3,3,3	0.85	0	3,3,3	0.50	0
2	GOL	C	401	-	5,5,5	0.31	0	5,5,5	0.21	0

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
2	GOL	H	401[A]	-	-	4/4/4/4	-
5	38L	C	405	3	-	0/2/4/4	0/1/1/1
5	38L	G	403	3	-	0/2/4/4	0/1/1/1
5	38L	H	405	3	-	0/2/4/4	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	38L	E	404	3	-	0/2/4/4	0/1/1/1
5	38L	A	405	3	-	0/2/4/4	0/1/1/1
2	GOL	B	401[A]	-	-	4/4/4/4	-
2	GOL	B	401[B]	-	-	4/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	F	401[A]	-	-	4/4/4/4	-
5	38L	D	403	3	-	0/2/4/4	0/1/1/1
2	GOL	F	401[B]	-	-	4/4/4/4	-
5	38L	F	404	3	-	0/2/4/4	0/1/1/1
5	38L	B	404	3	-	0/2/4/4	0/1/1/1
2	GOL	A	402[B]	-	-	3/4/4/4	-
2	GOL	H	401[B]	-	-	2/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
2	GOL	A	402[A]	-	-	4/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	403	38L	CAA-NAG	-4.00	1.38	1.45
5	B	404	38L	CAA-NAG	-2.84	1.40	1.45
5	E	404	38L	CAA-NAG	-2.72	1.40	1.45
5	D	403	38L	CAA-NAG	-2.56	1.41	1.45
5	F	404	38L	CAA-NAG	-2.45	1.41	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	403	38L	CAC-CAB-CAA	2.65	120.47	118.30
5	C	405	38L	CAE-CAF-CAA	2.64	120.46	118.30
5	A	405	38L	CAE-CAF-CAA	2.59	120.42	118.30
5	A	405	38L	CAC-CAB-CAA	2.44	120.30	118.30
5	E	404	38L	CAE-CAF-CAA	2.39	120.26	118.30

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402[A]	GOL	O1-C1-C2-C3
2	A	402[B]	GOL	O1-C1-C2-C3
2	B	401[A]	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	401[A]	GOL	C1-C2-C3-O3
2	B	401[B]	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402[A]	GOL	3	0
2	H	401[A]	GOL	1	0
2	A	402[B]	GOL	1	0
2	H	401[B]	GOL	2	0
2	F	401[A]	GOL	1	0
4	A	404	ACT	1	0

4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data [\(i\)](#)

5.1 Protein, DNA and RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [\(i\)](#)

EDS failed to run properly - this section is therefore empty.