



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:30 am BST

PDB ID : 5ZMY
Title : Crystal structure of a cis-epoxysuccinate hydrolase producing D(-)-tartaric acids
Authors : Dong, S.; Liu, X.; Wang, X.; Feng, Y.
Deposited on : 2018-04-06
Resolution : 1.87 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

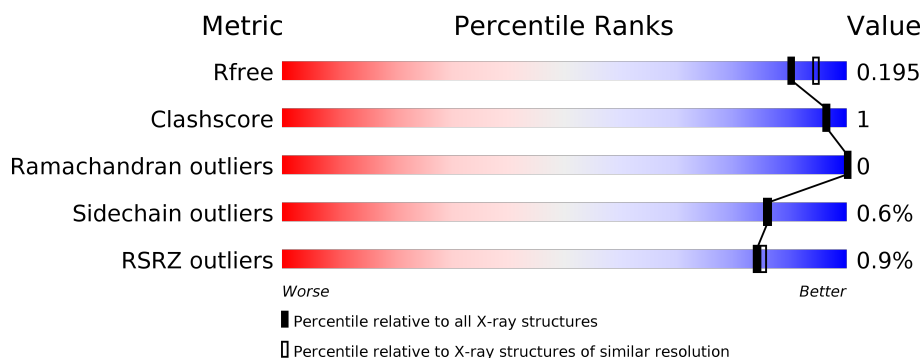
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 on 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	314	<div> <div>86%</div> <div>11%</div> </div>
1	B	314	<div> <div>85%</div> <div>11%</div> </div>
1	C	314	<div> <div>86%</div> <div>11%</div> </div>
1	D	314	<div> <div>%</div> <div>87%</div> <div>11%</div> </div>
1	E	314	<div> <div>3%</div> <div>86%</div> <div>11%</div> </div>
1	F	314	<div> <div>86%</div> <div>11%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	314	<div><div></div><div>86%</div><div></div><div>•</div><div>11%</div></div>
1	H	314	<div>%<div><div></div><div>85%</div><div></div><div>•</div><div>11%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37865 atoms, of which 17499 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 Cis-epoxysuccinate hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	280	Total	C	H	N	O	S	0	5	0
			4412	1400	2188	401	414	9			
1	B	279	Total	C	H	N	O	S	0	6	0
			4429	1404	2201	405	409	10			
1	C	280	Total	C	H	N	O	S	0	4	0
			4421	1400	2197	405	410	9			
1	D	278	Total	C	H	N	O	S	0	5	0
			4391	1391	2180	402	408	10			
1	E	278	Total	C	H	N	O	S	0	3	0
			4354	1382	2160	396	407	9			
1	F	279	Total	C	H	N	O	S	0	5	0
			4388	1393	2176	397	411	11			
1	G	280	Total	C	H	N	O	S	0	3	0
			4376	1388	2173	398	407	10			
1	H	279	Total	C	H	N	O	S	0	5	0
			4411	1396	2192	405	409	9			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP F1LJ99
A	2	GLY	-	expression tag	UNP F1LJ99
A	3	SER	-	expression tag	UNP F1LJ99
A	4	SER	-	expression tag	UNP F1LJ99
A	5	HIS	-	expression tag	UNP F1LJ99
A	6	HIS	-	expression tag	UNP F1LJ99
A	7	HIS	-	expression tag	UNP F1LJ99
A	8	HIS	-	expression tag	UNP F1LJ99
A	9	HIS	-	expression tag	UNP F1LJ99
A	10	HIS	-	expression tag	UNP F1LJ99
A	11	SER	-	expression tag	UNP F1LJ99
A	12	SER	-	expression tag	UNP F1LJ99
A	13	GLY	-	expression tag	UNP F1LJ99

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	-	expression tag	UNP F1LJ99
A	15	VAL	-	expression tag	UNP F1LJ99
A	16	PRO	-	expression tag	UNP F1LJ99
A	17	ARG	-	expression tag	UNP F1LJ99
A	18	GLY	-	expression tag	UNP F1LJ99
A	19	SER	-	expression tag	UNP F1LJ99
A	20	HIS	-	expression tag	UNP F1LJ99
A	135	ALA	ASP	engineered mutation	UNP F1LJ99
B	1	MET	-	expression tag	UNP F1LJ99
B	2	GLY	-	expression tag	UNP F1LJ99
B	3	SER	-	expression tag	UNP F1LJ99
B	4	SER	-	expression tag	UNP F1LJ99
B	5	HIS	-	expression tag	UNP F1LJ99
B	6	HIS	-	expression tag	UNP F1LJ99
B	7	HIS	-	expression tag	UNP F1LJ99
B	8	HIS	-	expression tag	UNP F1LJ99
B	9	HIS	-	expression tag	UNP F1LJ99
B	10	HIS	-	expression tag	UNP F1LJ99
B	11	SER	-	expression tag	UNP F1LJ99
B	12	SER	-	expression tag	UNP F1LJ99
B	13	GLY	-	expression tag	UNP F1LJ99
B	14	LEU	-	expression tag	UNP F1LJ99
B	15	VAL	-	expression tag	UNP F1LJ99
B	16	PRO	-	expression tag	UNP F1LJ99
B	17	ARG	-	expression tag	UNP F1LJ99
B	18	GLY	-	expression tag	UNP F1LJ99
B	19	SER	-	expression tag	UNP F1LJ99
B	20	HIS	-	expression tag	UNP F1LJ99
B	135	ALA	ASP	engineered mutation	UNP F1LJ99
C	1	MET	-	expression tag	UNP F1LJ99
C	2	GLY	-	expression tag	UNP F1LJ99
C	3	SER	-	expression tag	UNP F1LJ99
C	4	SER	-	expression tag	UNP F1LJ99
C	5	HIS	-	expression tag	UNP F1LJ99
C	6	HIS	-	expression tag	UNP F1LJ99
C	7	HIS	-	expression tag	UNP F1LJ99
C	8	HIS	-	expression tag	UNP F1LJ99
C	9	HIS	-	expression tag	UNP F1LJ99
C	10	HIS	-	expression tag	UNP F1LJ99
C	11	SER	-	expression tag	UNP F1LJ99
C	12	SER	-	expression tag	UNP F1LJ99
C	13	GLY	-	expression tag	UNP F1LJ99

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	14	LEU	-	expression tag	UNP F1LJ99
C	15	VAL	-	expression tag	UNP F1LJ99
C	16	PRO	-	expression tag	UNP F1LJ99
C	17	ARG	-	expression tag	UNP F1LJ99
C	18	GLY	-	expression tag	UNP F1LJ99
C	19	SER	-	expression tag	UNP F1LJ99
C	20	HIS	-	expression tag	UNP F1LJ99
C	135	ALA	ASP	engineered mutation	UNP F1LJ99
D	1	MET	-	expression tag	UNP F1LJ99
D	2	GLY	-	expression tag	UNP F1LJ99
D	3	SER	-	expression tag	UNP F1LJ99
D	4	SER	-	expression tag	UNP F1LJ99
D	5	HIS	-	expression tag	UNP F1LJ99
D	6	HIS	-	expression tag	UNP F1LJ99
D	7	HIS	-	expression tag	UNP F1LJ99
D	8	HIS	-	expression tag	UNP F1LJ99
D	9	HIS	-	expression tag	UNP F1LJ99
D	10	HIS	-	expression tag	UNP F1LJ99
D	11	SER	-	expression tag	UNP F1LJ99
D	12	SER	-	expression tag	UNP F1LJ99
D	13	GLY	-	expression tag	UNP F1LJ99
D	14	LEU	-	expression tag	UNP F1LJ99
D	15	VAL	-	expression tag	UNP F1LJ99
D	16	PRO	-	expression tag	UNP F1LJ99
D	17	ARG	-	expression tag	UNP F1LJ99
D	18	GLY	-	expression tag	UNP F1LJ99
D	19	SER	-	expression tag	UNP F1LJ99
D	20	HIS	-	expression tag	UNP F1LJ99
D	135	ALA	ASP	engineered mutation	UNP F1LJ99
E	1	MET	-	expression tag	UNP F1LJ99
E	2	GLY	-	expression tag	UNP F1LJ99
E	3	SER	-	expression tag	UNP F1LJ99
E	4	SER	-	expression tag	UNP F1LJ99
E	5	HIS	-	expression tag	UNP F1LJ99
E	6	HIS	-	expression tag	UNP F1LJ99
E	7	HIS	-	expression tag	UNP F1LJ99
E	8	HIS	-	expression tag	UNP F1LJ99
E	9	HIS	-	expression tag	UNP F1LJ99
E	10	HIS	-	expression tag	UNP F1LJ99
E	11	SER	-	expression tag	UNP F1LJ99
E	12	SER	-	expression tag	UNP F1LJ99
E	13	GLY	-	expression tag	UNP F1LJ99

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	14	LEU	-	expression tag	UNP F1LJ99
E	15	VAL	-	expression tag	UNP F1LJ99
E	16	PRO	-	expression tag	UNP F1LJ99
E	17	ARG	-	expression tag	UNP F1LJ99
E	18	GLY	-	expression tag	UNP F1LJ99
E	19	SER	-	expression tag	UNP F1LJ99
E	20	HIS	-	expression tag	UNP F1LJ99
E	135	ALA	ASP	engineered mutation	UNP F1LJ99
F	1	MET	-	expression tag	UNP F1LJ99
F	2	GLY	-	expression tag	UNP F1LJ99
F	3	SER	-	expression tag	UNP F1LJ99
F	4	SER	-	expression tag	UNP F1LJ99
F	5	HIS	-	expression tag	UNP F1LJ99
F	6	HIS	-	expression tag	UNP F1LJ99
F	7	HIS	-	expression tag	UNP F1LJ99
F	8	HIS	-	expression tag	UNP F1LJ99
F	9	HIS	-	expression tag	UNP F1LJ99
F	10	HIS	-	expression tag	UNP F1LJ99
F	11	SER	-	expression tag	UNP F1LJ99
F	12	SER	-	expression tag	UNP F1LJ99
F	13	GLY	-	expression tag	UNP F1LJ99
F	14	LEU	-	expression tag	UNP F1LJ99
F	15	VAL	-	expression tag	UNP F1LJ99
F	16	PRO	-	expression tag	UNP F1LJ99
F	17	ARG	-	expression tag	UNP F1LJ99
F	18	GLY	-	expression tag	UNP F1LJ99
F	19	SER	-	expression tag	UNP F1LJ99
F	20	HIS	-	expression tag	UNP F1LJ99
F	135	ALA	ASP	engineered mutation	UNP F1LJ99
G	1	MET	-	expression tag	UNP F1LJ99
G	2	GLY	-	expression tag	UNP F1LJ99
G	3	SER	-	expression tag	UNP F1LJ99
G	4	SER	-	expression tag	UNP F1LJ99
G	5	HIS	-	expression tag	UNP F1LJ99
G	6	HIS	-	expression tag	UNP F1LJ99
G	7	HIS	-	expression tag	UNP F1LJ99
G	8	HIS	-	expression tag	UNP F1LJ99
G	9	HIS	-	expression tag	UNP F1LJ99
G	10	HIS	-	expression tag	UNP F1LJ99
G	11	SER	-	expression tag	UNP F1LJ99
G	12	SER	-	expression tag	UNP F1LJ99
G	13	GLY	-	expression tag	UNP F1LJ99

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	14	LEU	-	expression tag	UNP F1LJ99
G	15	VAL	-	expression tag	UNP F1LJ99
G	16	PRO	-	expression tag	UNP F1LJ99
G	17	ARG	-	expression tag	UNP F1LJ99
G	18	GLY	-	expression tag	UNP F1LJ99
G	19	SER	-	expression tag	UNP F1LJ99
G	20	HIS	-	expression tag	UNP F1LJ99
G	135	ALA	ASP	engineered mutation	UNP F1LJ99
H	1	MET	-	expression tag	UNP F1LJ99
H	2	GLY	-	expression tag	UNP F1LJ99
H	3	SER	-	expression tag	UNP F1LJ99
H	4	SER	-	expression tag	UNP F1LJ99
H	5	HIS	-	expression tag	UNP F1LJ99
H	6	HIS	-	expression tag	UNP F1LJ99
H	7	HIS	-	expression tag	UNP F1LJ99
H	8	HIS	-	expression tag	UNP F1LJ99
H	9	HIS	-	expression tag	UNP F1LJ99
H	10	HIS	-	expression tag	UNP F1LJ99
H	11	SER	-	expression tag	UNP F1LJ99
H	12	SER	-	expression tag	UNP F1LJ99
H	13	GLY	-	expression tag	UNP F1LJ99
H	14	LEU	-	expression tag	UNP F1LJ99
H	15	VAL	-	expression tag	UNP F1LJ99
H	16	PRO	-	expression tag	UNP F1LJ99
H	17	ARG	-	expression tag	UNP F1LJ99
H	18	GLY	-	expression tag	UNP F1LJ99
H	19	SER	-	expression tag	UNP F1LJ99
H	20	HIS	-	expression tag	UNP F1LJ99
H	135	ALA	ASP	engineered mutation	UNP F1LJ99

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

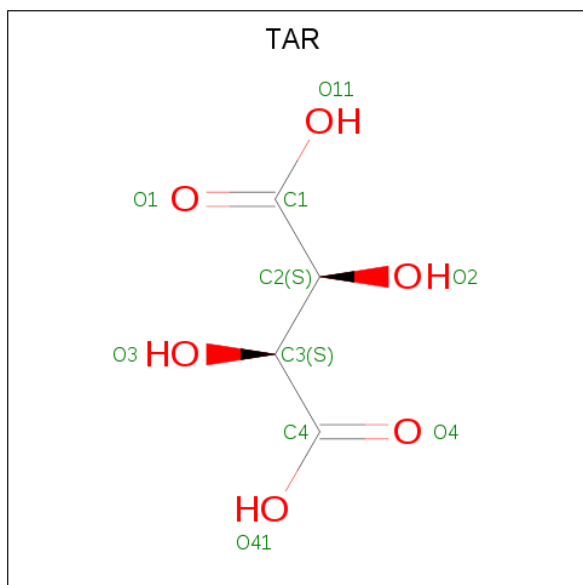
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	4	4	6		
3	B	1	Total	C	H	O	0	0
			14	4	4	6		
3	C	1	Total	C	H	O	0	0
			14	4	4	6		
3	D	1	Total	C	H	O	0	0
			14	4	4	6		
3	E	1	Total	C	H	O	0	0
			14	4	4	6		
3	F	1	Total	C	H	O	0	0
			14	4	4	6		
3	G	1	Total	C	H	O	0	0
			14	4	4	6		
3	H	1	Total	C	H	O	0	0
			14	4	4	6		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	344	Total O 344 344	0	0
4	B	371	Total O 371 371	0	0
4	C	345	Total O 345 345	0	0
4	D	337	Total O 337 337	0	0
4	E	274	Total O 274 274	0	0
4	F	287	Total O 287 287	0	0
4	G	320	Total O 320 320	0	0
4	H	285	Total O 285 285	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

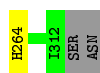
- Molecule 1: Cis-epoxysuccinate hydrolase

Chain A: 




- Molecule 1: Cis-epoxysuccinate hydrolase

Chain B: 




- Molecule 1: Cis-epoxysuccinate hydrolase

Chain C: 




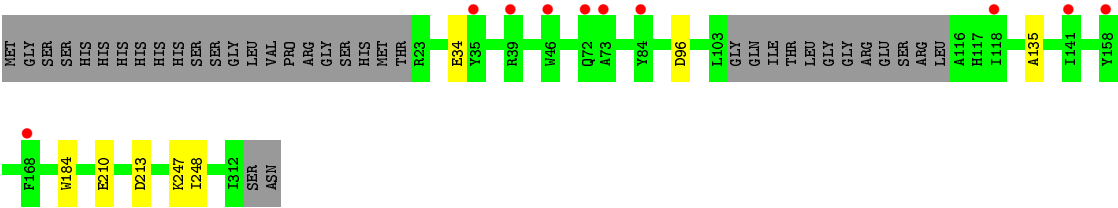
- Molecule 1: Cis-epoxysuccinate hydrolase

Chain D: 

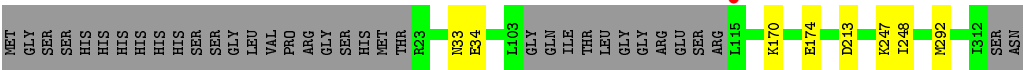
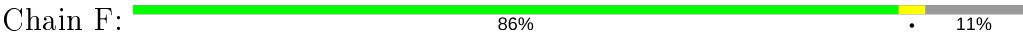


- Molecule 1: Cis-epoxysuccinate hydrolase

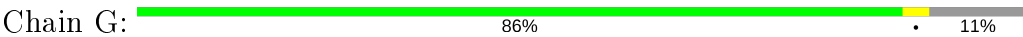
Chain E: 



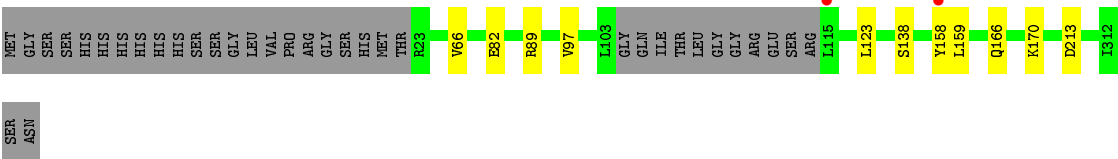
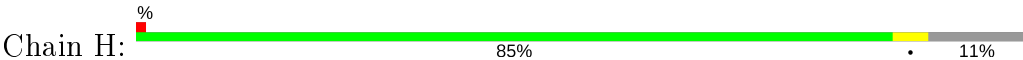
● Molecule 1: Cis-epoxysuccinate hydrolase



● Molecule 1: Cis-epoxysuccinate hydrolase



● Molecule 1: Cis-epoxysuccinate hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.16Å 158.35Å 134.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 1.87 134.09 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.11-1.87) 94.8 (134.09-1.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.168 , 0.195 0.168 , 0.195	Depositor DCC
R_{free} test set	1996 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.109 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37865	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 56.94 % 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 2.5444e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TAR

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	0.66	0/2275	0.71	2/3090 (0.1%)
1	B	0.64	0/2280	0.69	0/3097
1	C	0.60	0/2275	0.70	0/3089
1	D	0.60	0/2262	0.70	1/3072 (0.0%)
1	E	0.52	0/2245	0.61	0/3050
1	F	0.57	0/2263	0.66	0/3075
1	G	0.62	0/2254	0.66	0/3062
1	H	0.55	0/2270	0.64	0/3083
All	All	0.60	0/18124	0.67	3/24618 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	71	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	71	ARG	NE-CZ-NH1	5.72	123.16	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	2224	2188	2182	4	0
1	B	2228	2201	2194	6	0
1	C	2224	2197	2192	5	0
1	D	2211	2180	2174	2	0
1	E	2194	2160	2156	6	0
1	F	2212	2176	2170	4	0
1	G	2203	2173	2169	6	0
1	H	2219	2192	2186	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	10	4	2	0	0
3	B	10	4	2	0	0
3	C	10	4	3	0	0
3	D	10	4	2	0	0
3	E	10	4	3	2	0
3	F	10	4	2	0	0
3	G	10	4	2	1	0
3	H	10	4	2	0	0
4	A	344	0	0	0	1
4	B	371	0	0	1	0
4	C	345	0	0	2	0
4	D	337	0	0	0	0
4	E	274	0	0	1	0
4	F	287	0	0	0	0
4	G	320	0	0	0	0
4	H	285	0	0	0	0
All	All	20366	17499	17441	35	1

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 (35) 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:80:ASP:OD1	4:B:501:HOH:O	2.16	0.60
1:B:66:VAL:HG23	1:B:97:VAL:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:VAL:HG23	1:G:97:VAL:HG21	1.87	0.56
1:A:66:VAL:HG23	1:A:97:VAL:HG21	1.89	0.55
1:E:34:GLU:OE1	3:E:401:TAR:O3	2.17	0.55
1:G:34:GLU:OE1	3:G:401:TAR:O3	2.27	0.53
1:C:66:VAL:HG23	1:C:97:VAL:HG21	1.90	0.51
1:F:292[B]:MET:SD	1:G:292[B]:MET:SD	3.12	0.48
1:B:82:GLU:OE2	1:B:89:ARG:NH2	2.46	0.47
1:F:170:LYS:O	1:F:174:GLU:HG3	2.15	0.46
1:F:33:ASN:O	1:F:34:GLU:C	2.55	0.45
1:H:66:VAL:HG23	1:H:97:VAL:HG21	1.99	0.45
1:B:243:THR:HB	1:B:264:HIS:HB2	1.99	0.44
1:G:88:ILE:HG12	1:G:99:VAL:HG11	1.99	0.44
1:E:135:ALA:HB1	1:E:184:TRP:CZ3	2.53	0.44
1:A:82:GLU:OE2	1:A:89:ARG:NH2	2.51	0.43
1:F:247:LYS:HA	1:F:248:ILE:HA	1.87	0.42
1:E:210:GLU:OE1	3:E:401:TAR:O4	2.38	0.42
1:E:247:LYS:HA	1:E:248:ILE:HA	1.86	0.42
1:C:36:MET:SD	1:C:37:PRO:HD2	2.60	0.42
1:C:88:ILE:HG12	1:C:99:VAL:HG11	2.02	0.41
1:G:33:ASN:O	1:G:34:GLU:C	2.58	0.41
1:G:157:VAL:HG21	1:H:159:LEU:HD21	2.02	0.41
1:H:82:GLU:OE2	1:H:89:ARG:NH2	2.53	0.41
1:B:123:LEU:HD11	1:H:123:LEU:HB3	2.02	0.41
1:C:149:LYS:NZ	4:C:519:HOH:O	2.53	0.41
1:E:135:ALA:HB1	1:E:184:TRP:HZ3	1.86	0.41
1:B:183:ALA:HB2	1:B:207:LEU:HD11	2.01	0.41
1:A:292[B]:MET:SD	1:D:292[B]:MET:SD	3.18	0.41
1:D:243:THR:HB	1:D:264:HIS:HB2	2.01	0.41
1:A:247:LYS:HA	1:A:248:ILE:HA	1.90	0.40
1:C:57:GLN:NE2	4:C:505:HOH:O	2.31	0.40
1:E:96:ASP:OD2	4:E:501:HOH:O	2.22	0.40
1:H:166:GLN:O	1:H:170:LYS:HG3	2.21	0.40
1:H:138:SER:HA	1:H:158:TYR:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:783:HOH:O	4:A:833:HOH:O[2_455]	2.13	0.07

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	281/314 (90%)	277 (99%)	4 (1%)	0	100	100
1	B	281/314 (90%)	277 (99%)	4 (1%)	0	100	100
1	C	280/314 (89%)	275 (98%)	5 (2%)	0	100	100
1	D	279/314 (89%)	275 (99%)	4 (1%)	0	100	100
1	E	277/314 (88%)	272 (98%)	5 (2%)	0	100	100
1	F	280/314 (89%)	277 (99%)	3 (1%)	0	100	100
1	G	279/314 (89%)	274 (98%)	5 (2%)	0	100	100
1	H	280/314 (89%)	275 (98%)	5 (2%)	0	100	100
All	All	2237/2512 (89%)	2202 (98%)	35 (2%)	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	230/254 (91%)	229 (100%)	1 (0%)	91	90
1	B	231/254 (91%)	230 (100%)	1 (0%)	91	90
1	C	230/254 (91%)	228 (99%)	2 (1%)	78	76
1	D	229/254 (90%)	227 (99%)	2 (1%)	78	76
1	E	227/254 (89%)	226 (100%)	1 (0%)	91	90
1	F	230/254 (91%)	229 (100%)	1 (0%)	91	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	228/254 (90%)	227 (100%)	1 (0%)	91	90
1	H	230/254 (91%)	229 (100%)	1 (0%)	91	90
All	All	1835/2032 (90%)	1825 (100%)	10 (0%)	86	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	ASP
1	B	213	ASP
1	C	173	ARG
1	C	213	ASP
1	D	158	TYR
1	D	213	ASP
1	E	213	ASP
1	F	213	ASP
1	G	213	ASP
1	H	213	ASP

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
3	TAR	H	401	2	3,9,9	0.99	0	6,12,12	2.41	2 (33%)
3	TAR	D	401	2	3,9,9	0.53	0	6,12,12	2.92	4 (66%)
3	TAR	B	401	2	3,9,9	0.42	0	6,12,12	2.47	2 (33%)
3	TAR	F	401	2	3,9,9	0.54	0	6,12,12	2.11	2 (33%)
3	TAR	G	401	2	3,9,9	0.76	0	6,12,12	2.60	3 (50%)
3	TAR	E	401	2	3,9,9	0.60	0	6,12,12	1.99	1 (16%)
3	TAR	C	401	2	3,9,9	1.01	0	6,12,12	3.14	3 (50%)
3	TAR	A	401	2	3,9,9	0.86	0	6,12,12	1.57	1 (16%)

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
3	TAR	H	401	2	-	0/4/12/12	-
3	TAR	D	401	2	-	0/4/12/12	-
3	TAR	B	401	2	-	0/4/12/12	-
3	TAR	F	401	2	-	0/4/12/12	-
3	TAR	G	401	2	-	0/4/12/12	-
3	TAR	E	401	2	-	0/4/12/12	-
3	TAR	C	401	2	-	0/4/12/12	-
3	TAR	A	401	2	-	0/4/12/12	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	TAR	C4-C3-C2	-5.93	100.35	113.11
3	G	401	TAR	C4-C3-C2	-4.64	103.13	113.11
3	E	401	TAR	C4-C3-C2	-4.45	103.54	113.11
3	B	401	TAR	C4-C3-C2	-4.26	103.94	113.11
3	F	401	TAR	C1-C2-C3	-4.17	104.13	113.11
3	D	401	TAR	C4-C3-C2	-4.05	104.40	113.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	TAR	C1-C2-C3	-3.88	104.75	113.11
3	B	401	TAR	C1-C2-C3	-3.76	105.01	113.11
3	H	401	TAR	C4-C3-C2	-3.67	105.20	113.11
3	D	401	TAR	C1-C2-C3	-3.53	105.52	113.11
3	A	401	TAR	C1-C2-C3	-3.19	106.25	113.11
3	C	401	TAR	C1-C2-C3	-3.13	106.38	113.11
3	D	401	TAR	O2-C2-C3	-3.09	98.59	108.90
3	G	401	TAR	C1-C2-C3	-3.02	106.61	113.11
3	D	401	TAR	O2-C2-C1	2.84	117.95	111.10
3	C	401	TAR	O3-C3-C4	2.68	117.56	111.10
3	F	401	TAR	C4-C3-C2	-2.55	107.62	113.11
3	G	401	TAR	O2-C2-C3	-2.38	100.95	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	TAR	1	0
3	E	401	TAR	2	0

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 ⓘ

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	280/314 (89%)	-0.13	1 (0%) 92 93	11, 17, 32, 39	0
1	B	279/314 (88%)	-0.14	1 (0%) 92 93	11, 17, 29, 41	0
1	C	280/314 (89%)	-0.15	0 100 100	12, 19, 34, 41	0
1	D	278/314 (88%)	-0.09	3 (1%) 80 82	11, 19, 35, 43	0
1	E	278/314 (88%)	0.08	10 (3%) 42 44	17, 28, 47, 70	0
1	F	279/314 (88%)	-0.03	1 (0%) 92 93	14, 22, 39, 51	0
1	G	280/314 (89%)	-0.16	1 (0%) 92 93	13, 19, 33, 42	0
1	H	279/314 (88%)	-0.08	2 (0%) 87 88	14, 24, 35, 44	0
All	All	2233/2512 (88%)	-0.09	19 (0%) 84 85	11, 21, 38, 70	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	84	TYR	4.3
1	E	39	ARG	3.8
1	A	115	LEU	3.5
1	F	115	LEU	3.2
1	D	184	TRP	2.6
1	B	158	TYR	2.6
1	E	141	ILE	2.6
1	D	115	LEU	2.5
1	E	158	TYR	2.4
1	E	46	TRP	2.3
1	D	168	PHE	2.3
1	H	158	TYR	2.2
1	E	118	ILE	2.2
1	E	72	GLN	2.2
1	E	168	PHE	2.2
1	G	115	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	115	LEU	2.1
1	E	73	ALA	2.0
1	E	35	TYR	2.0

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 carbohydrates 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
3	TAR	E	401	10/10	0.87	0.18	28,31,38,38	0
3	TAR	D	401	10/10	0.90	0.16	24,32,35,37	0
2	ZN	E	400	1/1	0.93	0.09	21,21,21,21	1
3	TAR	H	401	10/10	0.93	0.12	23,30,36,37	0
3	TAR	F	401	10/10	0.93	0.12	22,26,32,33	0
3	TAR	C	401	10/10	0.94	0.12	20,26,32,32	0
3	TAR	G	401	10/10	0.96	0.14	20,26,32,32	0
3	TAR	A	401	10/10	0.96	0.14	18,21,24,25	0
3	TAR	B	401	10/10	0.97	0.09	18,22,25,26	0
2	ZN	A	400	1/1	0.99	0.09	15,15,15,15	1
2	ZN	G	400	1/1	0.99	0.11	13,13,13,13	1
2	ZN	B	400	1/1	0.99	0.09	15,15,15,15	1
2	ZN	H	400	1/1	0.99	0.09	13,13,13,13	1
2	ZN	F	400	1/1	0.99	0.12	17,17,17,17	1
2	ZN	C	400	1/1	0.99	0.12	14,14,14,14	1
2	ZN	D	400	1/1	1.00	0.07	17,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.