wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 04:59 PM JST

PDB ID	:	5ZRD
Title	:	Tyrosinase from Burkholderia thailandensis (BtTYR) at low pH condition
Authors	:	Lee, S.; Son, H.-F.; Kim, K.-J.
Deposited on	:	2018-04-24
Resolution	:	2.30 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:

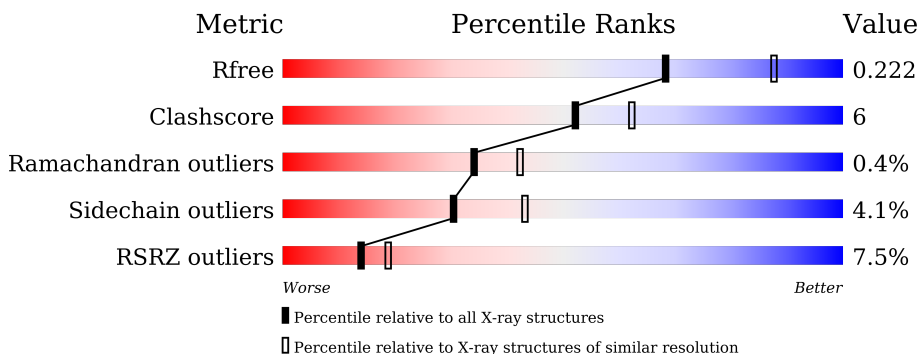|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	Percentile Ranks	Value
Rfree		0.222
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		4.1%
RSRZ outliers		7.5%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	549	9% 85% 12% ··
1	B	549	10% 84% 11% ··
1	C	549	5% 83% 12% ··
1	D	549	5% 84% 11% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	C	601	-	X	-	-
3	GOL	A	602	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17209 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total 4163	C 2646	N 717	O 787	S 13	0	0	0
1	B	531	Total 4140	C 2631	N 713	O 783	S 13	0	0	0
1	C	529	Total 4123	C 2621	N 710	O 779	S 13	0	0	0
1	D	528	Total 4118	C 2618	N 709	O 778	S 13	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q2T7K1
A	1	GLY	-	expression tag	UNP Q2T7K1
A	536	LYS	-	expression tag	UNP Q2T7K1
A	537	LEU	-	expression tag	UNP Q2T7K1
A	538	ALA	-	expression tag	UNP Q2T7K1
A	539	ALA	-	expression tag	UNP Q2T7K1
A	540	ALA	-	expression tag	UNP Q2T7K1
A	541	LEU	-	expression tag	UNP Q2T7K1
A	542	GLU	-	expression tag	UNP Q2T7K1
A	543	HIS	-	expression tag	UNP Q2T7K1
A	544	HIS	-	expression tag	UNP Q2T7K1
A	545	HIS	-	expression tag	UNP Q2T7K1
A	546	HIS	-	expression tag	UNP Q2T7K1
A	547	HIS	-	expression tag	UNP Q2T7K1
A	548	HIS	-	expression tag	UNP Q2T7K1
B	0	MET	-	expression tag	UNP Q2T7K1
B	1	GLY	-	expression tag	UNP Q2T7K1
B	536	LYS	-	expression tag	UNP Q2T7K1
B	537	LEU	-	expression tag	UNP Q2T7K1
B	538	ALA	-	expression tag	UNP Q2T7K1
B	539	ALA	-	expression tag	UNP Q2T7K1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	540	ALA	-	expression tag	UNP Q2T7K1
B	541	LEU	-	expression tag	UNP Q2T7K1
B	542	GLU	-	expression tag	UNP Q2T7K1
B	543	HIS	-	expression tag	UNP Q2T7K1
B	544	HIS	-	expression tag	UNP Q2T7K1
B	545	HIS	-	expression tag	UNP Q2T7K1
B	546	HIS	-	expression tag	UNP Q2T7K1
B	547	HIS	-	expression tag	UNP Q2T7K1
B	548	HIS	-	expression tag	UNP Q2T7K1
C	0	MET	-	expression tag	UNP Q2T7K1
C	1	GLY	-	expression tag	UNP Q2T7K1
C	536	LYS	-	expression tag	UNP Q2T7K1
C	537	LEU	-	expression tag	UNP Q2T7K1
C	538	ALA	-	expression tag	UNP Q2T7K1
C	539	ALA	-	expression tag	UNP Q2T7K1
C	540	ALA	-	expression tag	UNP Q2T7K1
C	541	LEU	-	expression tag	UNP Q2T7K1
C	542	GLU	-	expression tag	UNP Q2T7K1
C	543	HIS	-	expression tag	UNP Q2T7K1
C	544	HIS	-	expression tag	UNP Q2T7K1
C	545	HIS	-	expression tag	UNP Q2T7K1
C	546	HIS	-	expression tag	UNP Q2T7K1
C	547	HIS	-	expression tag	UNP Q2T7K1
C	548	HIS	-	expression tag	UNP Q2T7K1
D	0	MET	-	expression tag	UNP Q2T7K1
D	1	GLY	-	expression tag	UNP Q2T7K1
D	536	LYS	-	expression tag	UNP Q2T7K1
D	537	LEU	-	expression tag	UNP Q2T7K1
D	538	ALA	-	expression tag	UNP Q2T7K1
D	539	ALA	-	expression tag	UNP Q2T7K1
D	540	ALA	-	expression tag	UNP Q2T7K1
D	541	LEU	-	expression tag	UNP Q2T7K1
D	542	GLU	-	expression tag	UNP Q2T7K1
D	543	HIS	-	expression tag	UNP Q2T7K1
D	544	HIS	-	expression tag	UNP Q2T7K1
D	545	HIS	-	expression tag	UNP Q2T7K1
D	546	HIS	-	expression tag	UNP Q2T7K1
D	547	HIS	-	expression tag	UNP Q2T7K1
D	548	HIS	-	expression tag	UNP Q2T7K1

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

CIT
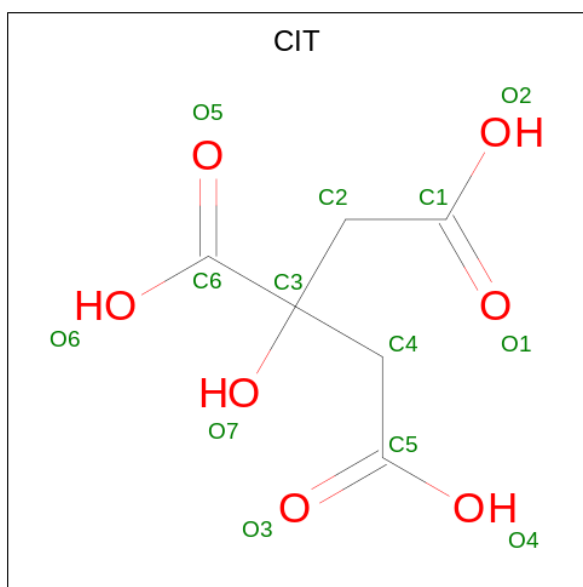
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 6	O 7	0	0
2	B	1	Total 13	C 6	O 7	0	0
2	C	1	Total 13	C 6	O 7	0	0
2	D	1	Total 13	C 6	O 7	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
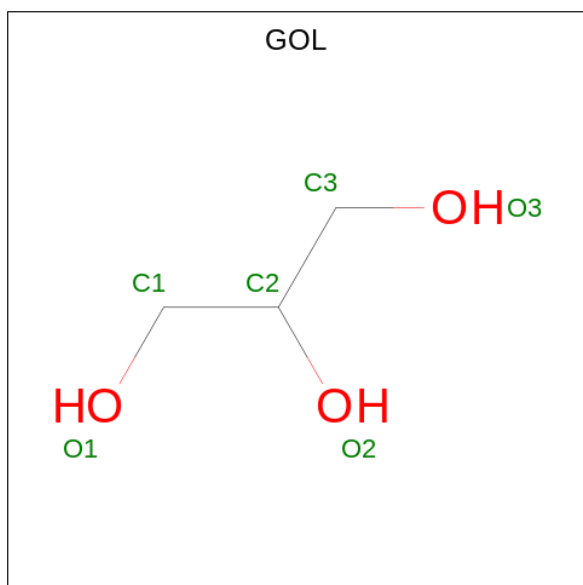
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cu 2	0	0
4	B	2	Total 2	Cu 2	0	0
4	C	2	Total 2	Cu 2	0	0
4	D	2	Total 2	Cu 2	0	0

- Molecule 5 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	1	Total 1	O 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	160	Total 160	O 160	0	0
6	B	139	Total 139	O 139	0	0
6	C	102	Total 102	O 102	0	0
6	D	116	Total 116	O 116	0	0

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.
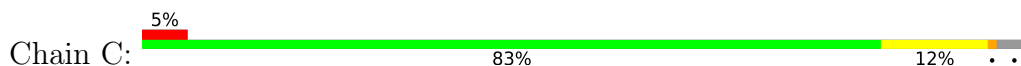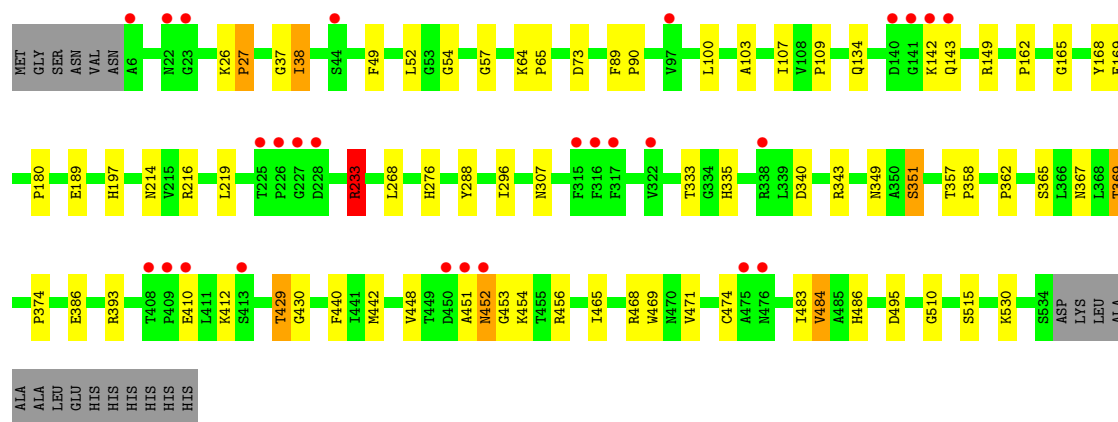
- Molecule 1: Tyrosinase
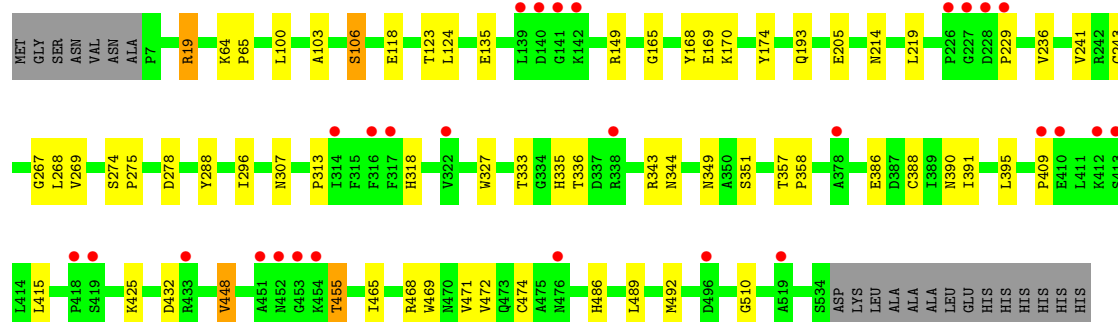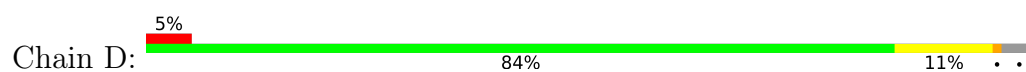

- Molecule 1: Tyrosinase

- Molecule 1: Tyrosinase

• Molecule 1: Tyrosinase

Chain D:
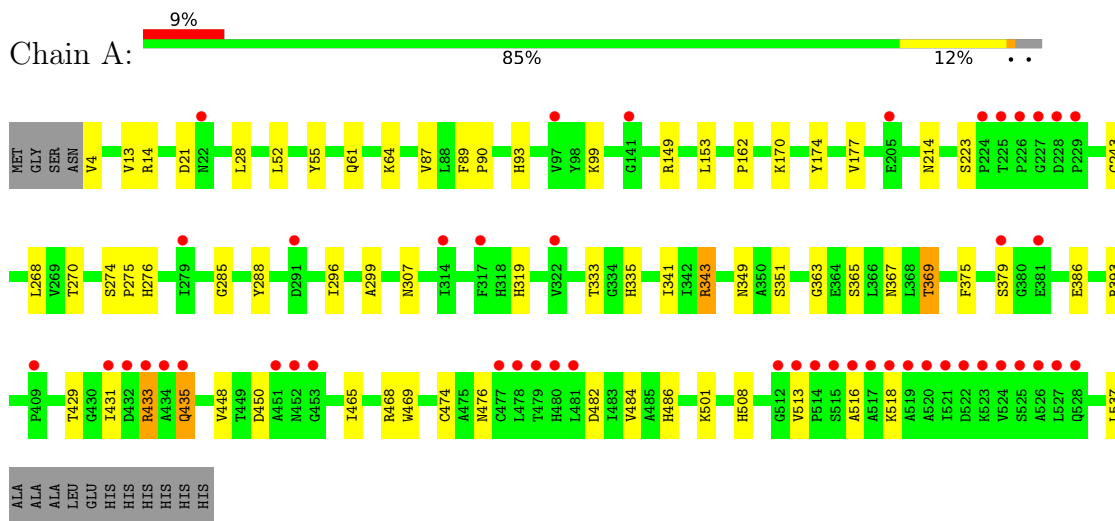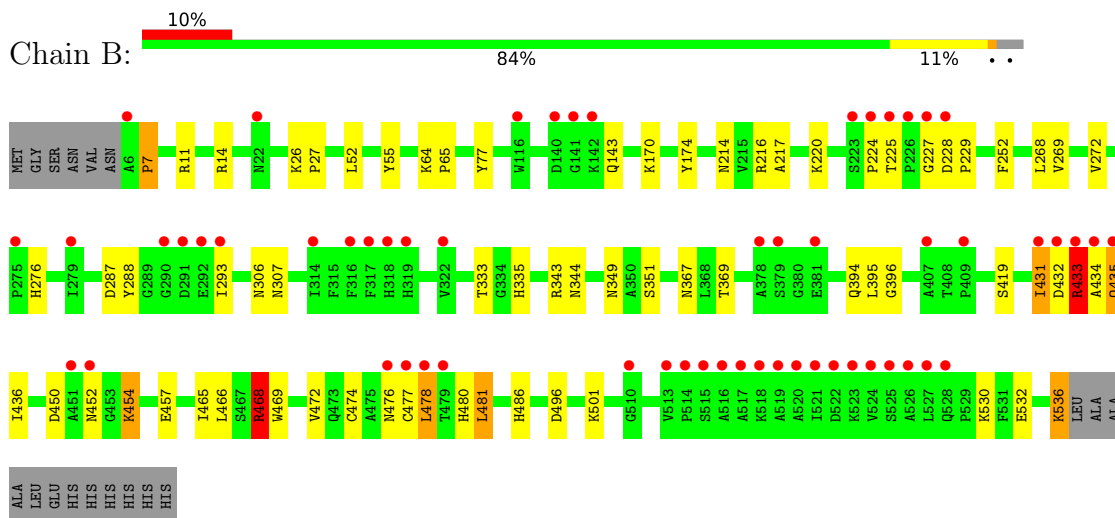
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.91Å 142.91Å 256.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.88 – 2.30 28.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.88-2.30) 97.9 (28.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.27 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.180 , 0.221 0.187 , 0.222	Depositor DCC
R_{free} test set	6679 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17209	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 24.69 % 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 3.6570e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

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: GOL, CIT, CU, O

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	0.64	0/4282	0.80	1/5834 (0.0%)
1	B	0.63	0/4259	0.81	3/5802 (0.1%)
1	C	0.59	0/4242	0.79	2/5780 (0.0%)
1	D	0.61	0/4237	0.77	0/5772
All	All	0.62	0/17020	0.79	6/23188 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	3
1	D	0	1
All	All	0	10

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	468	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	C	73	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	496	ASP	CB-CG-OD1	5.58	123.33	118.30
1	B	468	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	21	ASP	CB-CG-OD1	5.22	123.00	118.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	393	ARG	Sidechain
1	B	11	ARG	Sidechain
1	B	216	ARG	Sidechain
1	B	433	ARG	Sidechain

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	4163	0	4043	49	0
1	B	4140	0	4017	46	0
1	C	4123	0	3998	46	0
1	D	4118	0	3994	43	0
2	A	13	0	5	2	0
2	B	13	0	5	1	0
2	C	13	0	5	4	0
2	D	13	0	5	4	0
3	A	24	0	32	11	0
3	B	24	0	32	3	0
3	C	12	0	16	3	0
3	D	24	0	32	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	160	0	0	2	0
6	B	139	0	0	2	0
6	C	102	0	0	2	0
6	D	116	0	0	1	0
All	All	17209	0	16184	182	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 6.

The worst 5 of 182 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:468:ARG:HH12	3:A:602:GOL:C3	1.73	1.01
1:A:468:ARG:HH12	3:A:602:GOL:H32	1.26	0.98
1:C:486:HIS:HD2	2:C:601:CIT:O1	1.48	0.96
2:C:601:CIT:O3	2:C:601:CIT:H22	1.61	0.96
1:C:486:HIS:CD2	2:C:601:CIT:O1	2.28	0.85

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	532/549 (97%)	510 (96%)	21 (4%)	1 (0%)	47	58
1	B	529/549 (96%)	503 (95%)	21 (4%)	5 (1%)	17	20
1	C	527/549 (96%)	506 (96%)	18 (3%)	3 (1%)	25	31
1	D	526/549 (96%)	506 (96%)	20 (4%)	0	100	100
All	All	2114/2196 (96%)	2025 (96%)	80 (4%)	9 (0%)	34	42

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	433	ARG
1	B	477	CYS
1	B	431	ILE
1	C	452	ASN
1	C	134	GLN

5.3.2 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	451/462 (98%)	434 (96%)	17 (4%)	33	47
1	B	448/462 (97%)	430 (96%)	18 (4%)	31	44
1	C	446/462 (96%)	421 (94%)	25 (6%)	21	29
1	D	446/462 (96%)	432 (97%)	14 (3%)	40	55
All	All	1791/1848 (97%)	1717 (96%)	74 (4%)	30	43

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	474	CYS
1	D	455	THR
1	C	495	ASP
1	D	243	CYS
1	B	419	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	307	ASN
1	D	56	HIS
1	C	319	HIS
1	C	373	ASN
1	D	248	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 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	GOL	D	605	-	5,5,5	0.86	0	5,5,5	0.55	0
2	CIT	C	601	-	12,12,12	1.52	2 (16%)	17,17,17	3.20	10 (58%)
2	CIT	B	601	-	12,12,12	1.62	4 (33%)	17,17,17	2.84	5 (29%)
3	GOL	B	604	-	5,5,5	0.15	0	5,5,5	0.70	0
2	CIT	D	601	-	12,12,12	1.96	2 (16%)	17,17,17	3.22	7 (41%)
3	GOL	D	603	-	5,5,5	0.29	0	5,5,5	0.70	0
3	GOL	B	605	-	5,5,5	0.53	0	5,5,5	0.50	0
3	GOL	A	603	-	5,5,5	0.28	0	5,5,5	1.00	0
3	GOL	D	604	-	5,5,5	0.49	0	5,5,5	0.43	0
3	GOL	D	602	-	5,5,5	0.71	0	5,5,5	0.86	0
2	CIT	A	601	-	12,12,12	1.35	1 (8%)	17,17,17	3.36	8 (47%)
3	GOL	C	602	-	5,5,5	0.50	0	5,5,5	0.59	0
3	GOL	B	603	-	5,5,5	0.30	0	5,5,5	0.65	0
3	GOL	A	604	-	5,5,5	0.38	0	5,5,5	0.55	0
3	GOL	B	602	-	5,5,5	0.62	0	5,5,5	0.87	0
3	GOL	A	605	-	5,5,5	0.59	0	5,5,5	1.12	1 (20%)
3	GOL	C	603	-	5,5,5	0.69	0	5,5,5	0.65	0
3	GOL	A	602	-	5,5,5	0.41	0	5,5,5	1.38	1 (20%)

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	GOL	D	605	-	-	2/4/4/4	-
2	CIT	C	601	-	-	7/16/16/16	-
2	CIT	B	601	-	-	7/16/16/16	-
3	GOL	B	604	-	-	0/4/4/4	-
2	CIT	D	601	-	-	8/16/16/16	-
3	GOL	D	603	-	-	0/4/4/4	-
3	GOL	B	605	-	-	2/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	D	604	-	-	2/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
2	CIT	A	601	-	-	8/16/16/16	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
3	GOL	B	602	-	-	4/4/4/4	-
3	GOL	A	605	-	-	4/4/4/4	-
3	GOL	C	603	-	-	2/4/4/4	-
3	GOL	A	602	-	-	3/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	CIT	C3-C6	4.90	1.58	1.53
2	B	601	CIT	C3-C6	3.50	1.57	1.53
2	C	601	CIT	C3-C6	3.42	1.57	1.53
2	D	601	CIT	C2-C3	-3.01	1.50	1.53
2	B	601	CIT	C2-C3	-2.74	1.50	1.53

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	CIT	O6-C6-C3	9.14	128.93	113.05
2	B	601	CIT	O6-C6-C3	8.71	128.19	113.05
2	A	601	CIT	O7-C3-C4	-7.88	90.96	109.40
2	A	601	CIT	C4-C3-C6	6.99	125.12	110.11
2	C	601	CIT	O6-C6-C3	6.74	124.75	113.05

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CIT	C1-C2-C3-O7
2	A	601	CIT	C1-C2-C3-C4
2	A	601	CIT	O7-C3-C6-O5
2	A	601	CIT	O7-C3-C6-O6
2	A	601	CIT	C4-C3-C6-O5

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	605	GOL	1	0
2	C	601	CIT	4	0
2	B	601	CIT	1	0
2	D	601	CIT	4	0
2	A	601	CIT	2	0
3	C	602	GOL	3	0
3	B	602	GOL	3	0
3	A	605	GOL	2	0
3	A	602	GOL	9	0

5.7 Other polymers ⓘ

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	534/549 (97%)	0.22	48 (8%)	9	12	25, 39, 108, 170	0
1	B	531/549 (96%)	0.21	57 (10%)	6	8	26, 42, 111, 159	0
1	C	529/549 (96%)	0.09	27 (5%)	28	35	30, 47, 83, 136	0
1	D	528/549 (96%)	0.08	28 (5%)	26	33	27, 46, 80, 114	0
All	All	2122/2196 (96%)	0.15	160 (7%)	14	19	25, 43, 91, 170	0

The worst 5 of 160 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	ILE	15.6
1	B	526	ALA	8.9
1	A	512	GLY	8.7
1	A	520	ALA	8.0
1	B	516	ALA	7.9

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
3	GOL	A	604	6/6	0.78	0.23	69,77,80,81	0
3	GOL	D	605	6/6	0.79	0.25	57,65,70,71	0
3	GOL	C	602	6/6	0.83	0.14	69,72,77,86	0
3	GOL	D	604	6/6	0.87	0.28	57,69,75,75	0
3	GOL	A	605	6/6	0.87	0.43	59,66,69,74	0
3	GOL	B	604	6/6	0.88	0.13	64,67,78,80	0
3	GOL	A	603	6/6	0.89	0.20	52,69,77,79	0
3	GOL	C	603	6/6	0.89	0.20	54,69,72,73	0
3	GOL	D	603	6/6	0.92	0.17	55,63,67,69	0
3	GOL	B	602	6/6	0.92	0.09	54,61,64,64	0
3	GOL	D	602	6/6	0.92	0.16	50,58,62,67	0
3	GOL	B	603	6/6	0.93	0.14	58,63,64,72	0
2	CIT	B	601	13/13	0.93	0.16	34,55,67,70	0
3	GOL	B	605	6/6	0.93	0.19	53,62,68,74	0
2	CIT	D	601	13/13	0.94	0.14	47,55,60,60	0
2	CIT	C	601	13/13	0.94	0.15	50,56,63,64	0
2	CIT	A	601	13/13	0.95	0.12	33,51,60,61	0
5	O	B	608	1/1	0.95	0.24	25,25,25,25	0
3	GOL	A	602	6/6	0.96	0.10	47,50,52,52	0
5	O	A	608	1/1	0.98	0.18	25,25,25,25	0
4	CU	B	606	1/1	0.98	0.13	47,47,47,47	0
5	O	C	606	1/1	0.98	0.25	28,28,28,28	0
5	O	D	608	1/1	0.98	0.23	34,34,34,34	0
4	CU	B	607	1/1	0.99	0.12	36,36,36,36	0
4	CU	C	604	1/1	0.99	0.14	54,54,54,54	0
4	CU	A	607	1/1	0.99	0.10	45,45,45,45	0
4	CU	A	606	1/1	1.00	0.11	33,33,33,33	0
4	CU	C	605	1/1	1.00	0.13	42,42,42,42	0
4	CU	D	606	1/1	1.00	0.14	40,40,40,40	0
4	CU	D	607	1/1	1.00	0.15	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.