



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:28 pm BST

PDB ID : 5ZRE
Title : Tyrosinase from Burkholderia thailandensis (BtTYR) at high pH condition
Authors : Lee, S.; Son, H.-F.; Kim, K.-J.
Deposited on : 2018-04-24
Resolution : 2.50 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

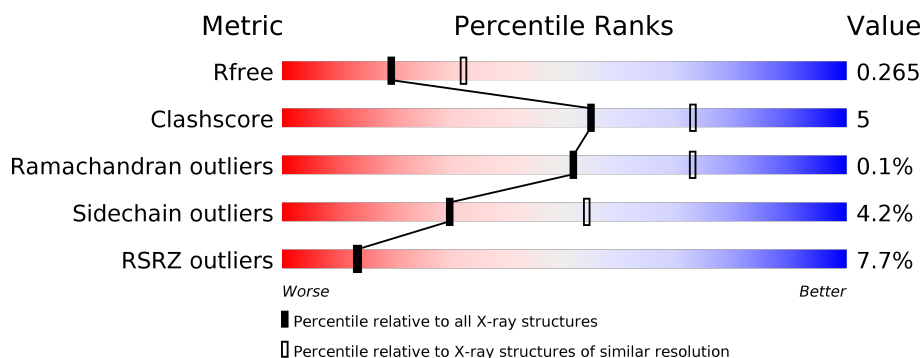
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	549	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	549	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	549	<div> <div>9%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	603	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11214 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	469	Total	C	N	O	S	0	0	0
			3679	2342	638	688	11			
1	B	474	Total	C	N	O	S	0	0	0
			3706	2357	640	698	11			
1	C	472	Total	C	N	O	S	0	0	0
			3694	2351	638	694	11			

There are 45 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
B	540	ALA	-	expression tag	UNP Q2T7K1
B	541	LEU	-	expression tag	UNP Q2T7K1

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

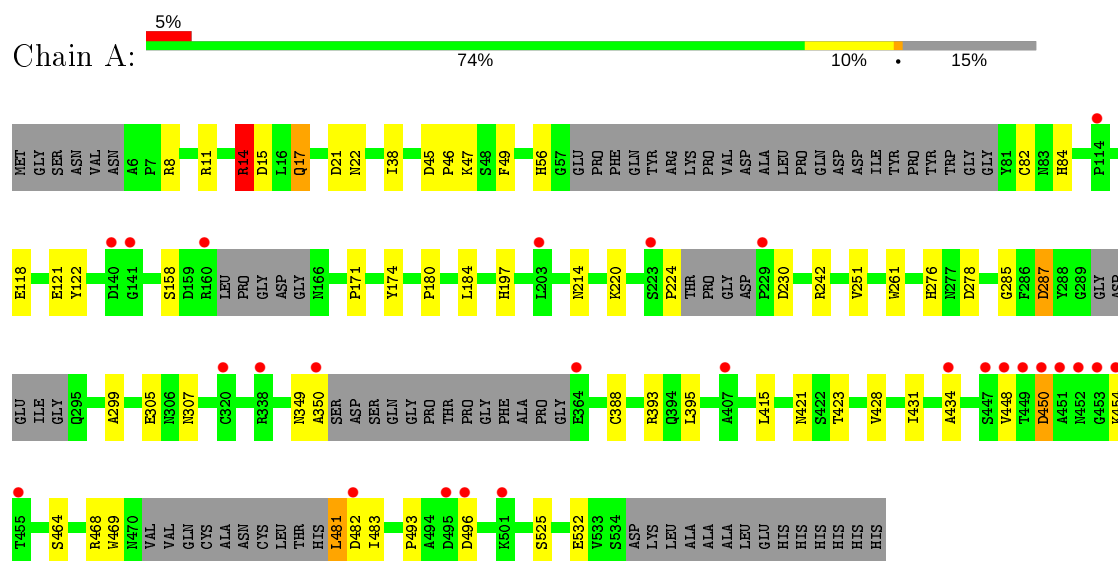
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	45	Total	O	0	0
			45	45		
5	C	24	Total	O	0	0
			24	24		

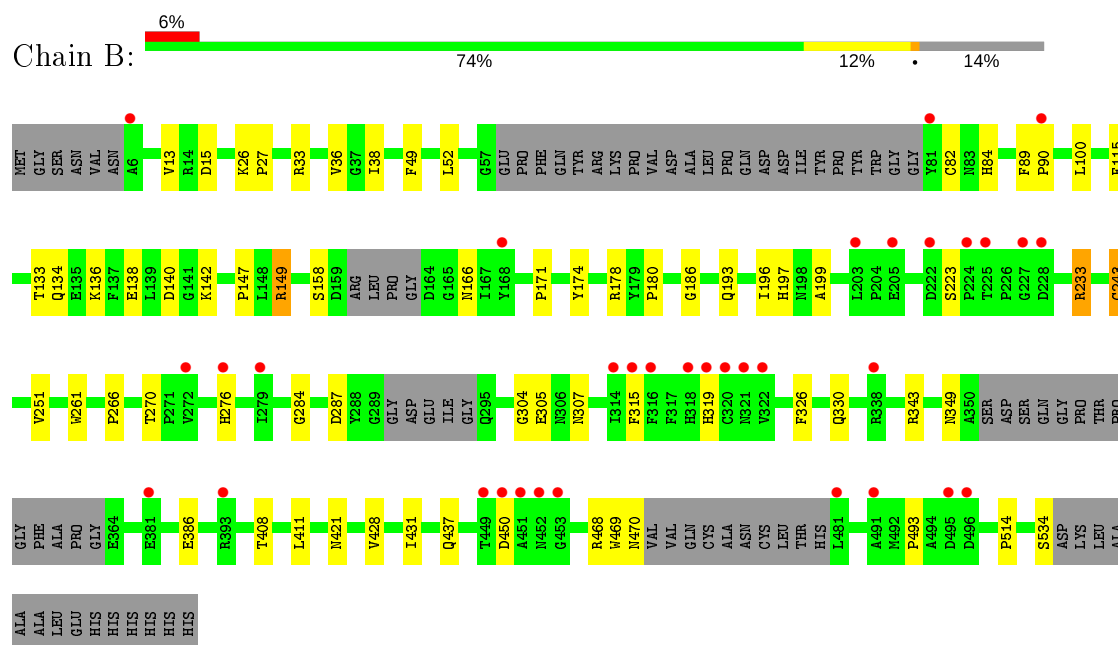
3 Residue-property plots

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.

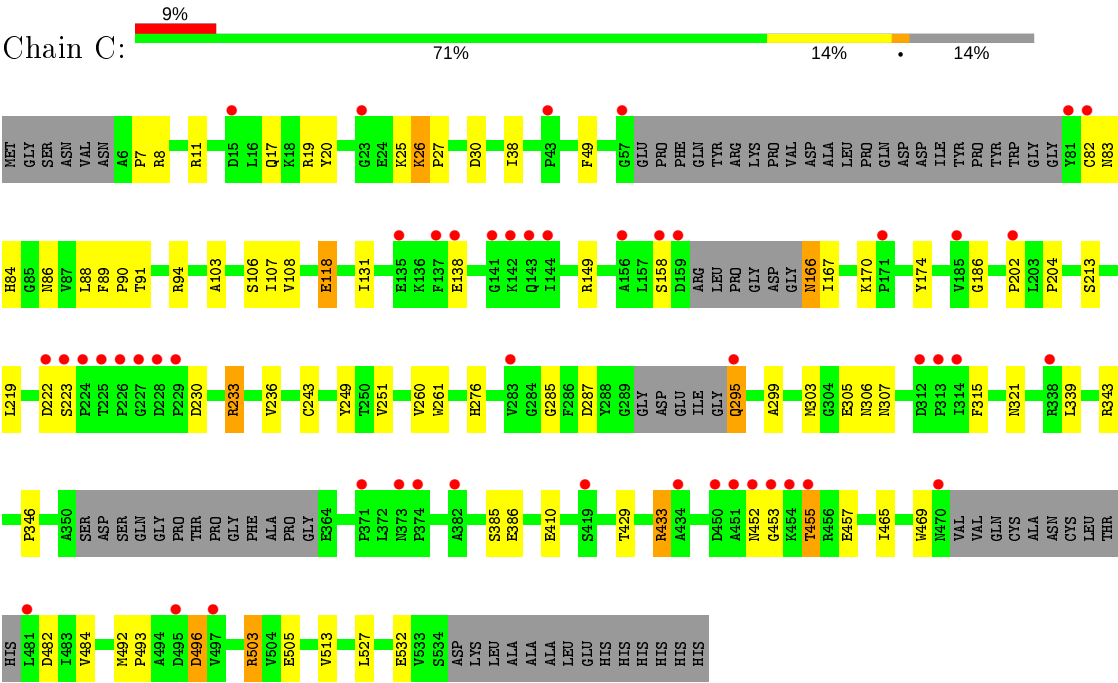
• Molecule 1: Tyrosinase



• Molecule 1: Tyrosinase



● Molecule 1: Tyrosinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.78Å 72.17Å 117.41Å 90.00° 105.29° 90.00°	Depositor
Resolution (Å)	27.85 – 2.50 27.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (27.85-2.50) 95.9 (27.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.199 , 0.263 0.203 , 0.265	Depositor DCC
R_{free} test set	2948 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11214	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, O, CU

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	0.63	0/3775	0.77	0/5126
1	B	0.67	0/3804	0.78	2/5170 (0.0%)
1	C	0.59	0/3792	0.75	0/5154
All	All	0.63	0/11371	0.77	2/15450 (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	3
1	B	0	4
1	C	0	6
All	All	0	13

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	GLN	CB-CA-C	-5.90	98.61	110.40
1	B	178	ARG	NE-CZ-NH2	-5.73	117.44	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain
1	A	14	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	8	ARG	Sidechain
1	B	149	ARG	Sidechain
1	B	233	ARG	Sidechain
1	B	343	ARG	Sidechain
1	B	468	ARG	Sidechain
1	C	149	ARG	Sidechain
1	C	233	ARG	Sidechain
1	C	343	ARG	Sidechain
1	C	433	ARG	Sidechain
1	C	503	ARG	Sidechain
1	C	94	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	3679	0	3599	34	0
1	B	3706	0	3614	33	0
1	C	3694	0	3607	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
4	B	6	0	8	4	0
5	A	51	0	0	2	0
5	B	45	0	0	1	0
5	C	24	0	0	0	0
All	All	11214	0	10828	113	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 5.

All (113) 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:14:ARG:HH11	1:A:17:GLN:HE21	1.20	0.90
1:A:14:ARG:NH1	1:A:17:GLN:HE21	1.76	0.83
1:C:429:THR:HG22	1:C:484:VAL:HG12	1.63	0.79
1:C:307:ASN:HD21	1:C:469:TRP:H	1.34	0.76
1:C:452:ASN:HB2	1:C:453:GLY:HA2	1.68	0.75
1:B:307:ASN:HD21	1:B:469:TRP:H	1.36	0.73
1:A:307:ASN:HD21	1:A:469:TRP:H	1.34	0.73
1:B:133:THR:O	1:B:149:ARG:NH1	2.23	0.70
1:A:14:ARG:NH1	1:A:17:GLN:NE2	2.40	0.69
1:A:82:CYS:SG	1:A:84:HIS:CE1	2.86	0.68
1:C:303:MET:HE3	1:C:315:PHE:HB2	1.78	0.65
1:C:83:ASN:HD22	1:C:88:LEU:HB2	1.62	0.64
2:C:602:CU:CU	3:C:603:O:O	1.49	0.63
1:A:481:LEU:HD12	1:A:481:LEU:N	2.14	0.62
1:C:452:ASN:CB	1:C:453:GLY:HA2	2.29	0.62
1:C:433:ARG:HH11	1:C:433:ARG:HG3	1.64	0.61
1:A:434:ALA:HB2	1:A:481:LEU:HD13	1.83	0.60
1:B:305:GLU:HB3	1:B:307:ASN:HD22	1.67	0.60
1:B:38:ILE:HG23	1:B:49:PHE:HB2	1.84	0.59
1:C:25:LYS:O	1:C:26:LYS:C	2.40	0.58
1:C:219:LEU:HD13	1:C:236:VAL:HB	1.87	0.56
1:C:305:GLU:HB3	1:C:307:ASN:HD22	1.71	0.55
1:A:305:GLU:HB3	1:A:307:ASN:HD22	1.71	0.55
1:C:166:ASN:O	1:C:186:GLY:HA3	2.07	0.55
1:B:33:ARG:NH2	1:B:140:ASP:OD1	2.40	0.54
1:B:138:GLU:HA	1:B:142:LYS:O	2.07	0.54
1:B:180:PRO:O	1:B:197:HIS:HE1	1.91	0.54
1:A:448:VAL:HG11	1:A:496:ASP:HB3	1.91	0.53
1:C:429:THR:HG22	1:C:484:VAL:CG1	2.36	0.53
1:C:107:ILE:HG22	1:C:108:VAL:HG23	1.91	0.52
1:A:421:ASN:HA	1:A:493:PRO:HA	1.90	0.52
1:B:266:PRO:HA	4:B:603:GOL:H12	1.92	0.52
1:C:170:LYS:HD2	1:C:174:TYR:CE2	2.44	0.52
1:B:428:VAL:HG12	1:B:431:ILE:HD11	1.92	0.51
1:C:303:MET:HE1	1:C:315:PHE:HD2	1.76	0.51
1:A:220:LYS:HE2	1:A:230:ASP:HB2	1.93	0.50
1:A:278:ASP:OD1	1:A:464:SER:HB2	2.10	0.50
1:C:202:PRO:O	1:C:204:PRO:HD3	2.11	0.50
1:A:180:PRO:O	1:A:197:HIS:HE1	1.93	0.50
1:A:482:ASP:HB3	5:A:733:HOH:O	2.11	0.50
1:B:166:ASN:O	1:B:186:GLY:HA3	2.12	0.49
1:A:285:GLY:HA3	1:A:299:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:CYS:SG	1:C:84:HIS:HE1	2.36	0.49
1:C:38:ILE:HG23	1:C:49:PHE:HB2	1.94	0.49
1:C:493:PRO:HG2	1:C:496:ASP:HB2	1.95	0.48
1:A:14:ARG:NH2	1:A:122:TYR:CZ	2.81	0.48
1:A:428:VAL:HG12	1:A:431:ILE:HD11	1.95	0.48
1:B:421:ASN:HA	1:B:493:PRO:HA	1.94	0.48
1:A:21:ASP:C	1:A:22:ASN:HD22	2.17	0.48
1:B:437:GLN:NE2	1:B:470:ASN:H	2.12	0.48
1:A:450:ASP:HB2	1:A:454:LYS:O	2.14	0.48
1:B:437:GLN:HE22	1:B:470:ASN:H	1.62	0.48
1:C:20:TYR:CE1	1:C:25:LYS:HD2	2.49	0.48
1:C:167:ILE:HD11	1:C:513:VAL:HG11	1.95	0.48
1:B:408:THR:HG22	1:B:411:LEU:HG	1.95	0.47
1:C:108:VAL:HG12	1:C:108:VAL:O	2.13	0.47
1:B:251:VAL:HG11	1:B:261:TRP:CD2	2.50	0.47
1:A:251:VAL:HG11	1:A:261:TRP:CD2	2.50	0.47
1:C:455:THR:HG22	1:C:455:THR:O	2.15	0.47
1:B:534:SER:HB2	4:B:603:GOL:H2	1.97	0.46
1:C:307:ASN:HD21	1:C:469:TRP:N	2.10	0.46
1:B:136:LYS:HB2	5:B:726:HOH:O	2.16	0.45
1:B:36:VAL:HG23	1:B:147:PRO:HG3	1.98	0.45
1:C:89:PHE:HB3	1:C:90:PRO:HD3	1.98	0.45
1:B:266:PRO:HA	4:B:603:GOL:C1	2.46	0.45
1:B:82:CYS:SG	1:B:84:HIS:HE1	2.40	0.45
1:A:388:CYS:HB2	1:A:395:LEU:HD11	1.98	0.45
1:B:52:LEU:HD13	1:B:100:LEU:CD2	2.47	0.45
1:C:83:ASN:CG	1:C:86:ASN:HD21	2.19	0.45
1:C:465:ILE:N	1:C:465:ILE:HD12	2.33	0.44
1:B:26:LYS:N	1:B:27:PRO:CD	2.81	0.44
1:C:260:VAL:HG21	1:C:346:PRO:HG2	2.00	0.44
1:A:220:LYS:HD3	1:A:224:PRO:HA	2.00	0.43
1:B:196:ILE:O	1:B:199:ALA:HB3	2.19	0.43
1:A:242:ARG:CZ	1:A:415:LEU:HD22	2.48	0.43
1:C:30:ASP:HB3	1:C:108:VAL:HG11	2.01	0.43
1:B:315:PHE:CZ	1:B:319:HIS:CE1	3.06	0.43
1:C:285:GLY:HA3	1:C:299:ALA:O	2.19	0.42
1:B:52:LEU:HD13	1:B:100:LEU:HD23	2.00	0.42
1:A:393:ARG:HD3	5:A:710:HOH:O	2.19	0.42
1:C:452:ASN:CB	1:C:453:GLY:CA	2.97	0.42
1:C:17:GLN:HE22	1:C:131:ILE:H	1.67	0.42
1:B:171:PRO:HD2	1:B:174:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:HG3	1:B:514:PRO:HD3	2.00	0.42
1:C:91:THR:HG21	1:C:385:SER:HB3	2.02	0.42
1:A:278:ASP:OD1	1:A:464:SER:CB	2.68	0.41
1:A:38:ILE:HG23	1:A:49:PHE:HB2	2.02	0.41
1:C:251:VAL:HG11	1:C:261:TRP:CG	2.55	0.41
1:A:22:ASN:N	1:A:22:ASN:HD22	2.16	0.41
1:A:214:ASN:ND2	1:A:287:ASP:HA	2.34	0.41
1:B:13:VAL:HG23	1:B:115:PHE:O	2.20	0.41
1:B:284:GLY:HA3	1:B:304:GLY:N	2.35	0.41
1:B:326:PHE:O	1:B:330:GLN:HG3	2.21	0.41
1:C:452:ASN:HB2	1:C:453:GLY:CA	2.46	0.41
1:C:89:PHE:N	1:C:90:PRO:CD	2.84	0.41
1:C:17:GLN:NE2	1:C:131:ILE:H	2.18	0.41
1:C:26:LYS:HB3	1:C:27:PRO:HD3	2.02	0.41
1:C:295:GLN:HB2	1:C:295:GLN:HE21	1.65	0.41
1:A:45:ASP:OD1	1:A:46:PRO:HD2	2.21	0.41
1:B:89:PHE:HB3	1:B:90:PRO:HD3	2.01	0.41
1:C:249:TYR:HB2	1:C:339:LEU:HD22	2.02	0.41
1:C:38:ILE:HD11	1:C:103:ALA:HB1	2.03	0.41
1:C:251:VAL:HG11	1:C:261:TRP:CD2	2.55	0.41
1:C:457:GLU:OE1	1:C:503:ARG:NH2	2.54	0.40
1:A:38:ILE:HG13	1:A:47:LYS:O	2.21	0.40
1:C:527:LEU:HD23	1:C:527:LEU:HA	1.98	0.40
1:A:349:ASN:HD22	1:A:350:ALA:C	2.25	0.40
1:A:56:HIS:CG	1:A:56:HIS:O	2.73	0.40
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.91	0.40
1:B:534:SER:HB2	4:B:603:GOL:C2	2.52	0.40
1:C:118:GLU:HG3	1:C:321:ASN:ND2	2.37	0.40
1:A:171:PRO:HD2	1:A:174:TYR:HB2	2.03	0.40
1:B:243:CYS:HA	1:B:270:THR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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	455/549 (83%)	437 (96%)	17 (4%)	1 (0%)	47	68
1	B	462/549 (84%)	456 (99%)	6 (1%)	0	100	100
1	C	460/549 (84%)	426 (93%)	33 (7%)	1 (0%)	47	68
All	All	1377/1647 (84%)	1319 (96%)	56 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	PRO
1	A	450	ASP

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	399/462 (86%)	385 (96%)	14 (4%)	36	62
1	B	402/462 (87%)	392 (98%)	10 (2%)	47	73
1	C	401/462 (87%)	374 (93%)	27 (7%)	16	31
All	All	1202/1386 (87%)	1151 (96%)	51 (4%)	30	54

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	15	ASP
1	A	17	GLN
1	A	118	GLU
1	A	121	GLU
1	A	158	SER
1	A	276	HIS
1	A	287	ASP

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Mol	Chain	Res	Type
1	A	423	THR
1	A	468	ARG
1	A	481	LEU
1	A	483	ILE
1	A	525	SER
1	A	532	GLU
1	B	15	ASP
1	B	158	SER
1	B	223	SER
1	B	233	ARG
1	B	243	CYS
1	B	276	HIS
1	B	287	ASP
1	B	349	ASN
1	B	386	GLU
1	B	450	ASP
1	C	8	ARG
1	C	11	ARG
1	C	19	ARG
1	C	26	LYS
1	C	106	SER
1	C	118	GLU
1	C	138	GLU
1	C	158	SER
1	C	166	ASN
1	C	213	SER
1	C	222	ASP
1	C	223	SER
1	C	230	ASP
1	C	233	ARG
1	C	243	CYS
1	C	276	HIS
1	C	287	ASP
1	C	295	GLN
1	C	306	ASN
1	C	386	GLU
1	C	410	GLU
1	C	455	THR
1	C	482	ASP
1	C	492	MET
1	C	496	ASP
1	C	505	GLU

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Mol	Chain	Res	Type
1	C	532	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	22	ASN
1	A	56	HIS
1	A	134	GLN
1	A	197	HIS
1	A	214	ASN
1	A	276	HIS
1	A	306	ASN
1	A	307	ASN
1	A	335	HIS
1	A	349	ASN
1	B	56	HIS
1	B	83	ASN
1	B	197	HIS
1	B	214	ASN
1	B	265	ASN
1	B	276	HIS
1	B	306	ASN
1	B	307	ASN
1	B	373	ASN
1	B	437	GLN
1	C	56	HIS
1	C	83	ASN
1	C	134	GLN
1	C	214	ASN
1	C	276	HIS
1	C	295	GLN
1	C	306	ASN
1	C	307	ASN
1	C	335	HIS
1	C	452	ASN

5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	GOL	B	603	-	5,5,5	0.67	0	5,5,5	1.43	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
4	GOL	B	603	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	GOL	C1-C2-C3-O3
4	B	603	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	GOL	4	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	469/549 (85%)	0.25	26 (5%)	25 26	33, 51, 91, 119	0
1	B	474/549 (86%)	0.27	34 (7%)	15 16	28, 48, 84, 116	0
1	C	472/549 (85%)	0.53	49 (10%)	6 6	33, 61, 94, 153	0
All	All	1415/1647 (85%)	0.35	109 (7%)	13 13	28, 53, 91, 153	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	451	ALA	6.8
1	C	81	TYR	6.8
1	B	452	ASN	6.1
1	C	227	GLY	5.8
1	A	453	GLY	5.8
1	B	450	ASP	5.3
1	C	452	ASN	5.3
1	A	448	VAL	5.1
1	B	225	THR	5.0
1	C	228	ASP	5.0
1	C	223	SER	4.5
1	A	451	ALA	4.4
1	B	453	GLY	4.3
1	A	449	THR	4.1
1	B	81	TYR	4.1
1	C	229	PRO	4.1
1	C	419	SER	4.1
1	B	224	PRO	4.0
1	C	82	CYS	4.0
1	A	495	ASP	3.9
1	C	338	ARG	3.8
1	A	450	ASP	3.8
1	A	364	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	455	THR	3.8
1	A	501	LYS	3.7
1	A	452	ASN	3.7
1	B	318	HIS	3.6
1	C	226	PRO	3.5
1	C	43	PRO	3.5
1	C	57	GLY	3.5
1	C	156	ALA	3.5
1	C	225	THR	3.4
1	C	481	LEU	3.4
1	B	320	CYS	3.4
1	A	320	CYS	3.3
1	C	382	ALA	3.2
1	B	279	ILE	3.2
1	B	227	GLY	3.1
1	C	313	PRO	3.1
1	A	454	LYS	3.1
1	B	496	ASP	3.1
1	C	137	PHE	3.1
1	B	449	THR	3.1
1	C	314	ILE	3.1
1	C	374	PRO	3.0
1	C	222	ASP	3.0
1	C	23	GLY	3.0
1	C	451	ALA	3.0
1	B	319	HIS	2.9
1	C	454	LYS	2.9
1	A	141	GLY	2.9
1	B	228	ASP	2.9
1	C	495	ASP	2.9
1	A	229	PRO	2.8
1	B	495	ASP	2.8
1	C	371	PRO	2.8
1	C	434	ALA	2.8
1	A	407	ALA	2.8
1	B	6	ALA	2.7
1	C	453	GLY	2.7
1	A	338	ARG	2.7
1	C	171	PRO	2.7
1	C	158	SER	2.6
1	C	224	PRO	2.6
1	C	159	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	312	ASP	2.6
1	B	276	HIS	2.6
1	C	470	ASN	2.5
1	C	497	VAL	2.4
1	C	143	GLN	2.4
1	C	455	THR	2.4
1	B	481	LEU	2.4
1	B	222	ASP	2.4
1	C	142	LYS	2.4
1	A	350	ALA	2.4
1	C	138	GLU	2.4
1	B	322	VAL	2.3
1	A	496	ASP	2.3
1	B	338	ARG	2.3
1	C	202	PRO	2.3
1	C	135	GLU	2.3
1	B	272	VAL	2.3
1	B	316	PHE	2.3
1	A	160	ARG	2.2
1	C	185	VAL	2.2
1	A	223	SER	2.2
1	A	434	ALA	2.2
1	B	205	GLU	2.2
1	A	114	PRO	2.2
1	C	373	ASN	2.2
1	A	140	ASP	2.2
1	B	315	PHE	2.2
1	B	90	PRO	2.2
1	A	203	LEU	2.2
1	B	491	ALA	2.2
1	B	381	GLU	2.1
1	B	314	ILE	2.1
1	A	482	ASP	2.1
1	C	15	ASP	2.1
1	C	295	GLN	2.1
1	A	447	SER	2.1
1	B	203	LEU	2.1
1	C	450	ASP	2.1
1	B	321	ASN	2.1
1	B	168	TYR	2.1
1	C	141	GLY	2.1
1	B	393	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	283	VAL	2.0
1	C	144	ILE	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(\AA^2)	Q<0.9
4	GOL	B	603	6/6	0.80	0.17	43,60,63,64	0
2	CU	C	601	1/1	0.99	0.15	54,54,54,54	0
2	CU	B	601	1/1	0.99	0.17	50,50,50,50	0
2	CU	B	602	1/1	0.99	0.12	58,58,58,58	0
2	CU	A	602	1/1	0.99	0.09	62,62,62,62	0
3	O	A	603	1/1	0.99	0.15	22,22,22,22	0
2	CU	C	602	1/1	1.00	0.12	66,66,66,66	0
3	O	C	603	1/1	1.00	0.13	25,25,25,25	0
2	CU	A	601	1/1	1.00	0.15	55,55,55,55	0
3	O	B	604	1/1	1.00	0.17	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.