



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:22 PM UTC

PDB ID : 5ZRE / pdb_00005zre
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

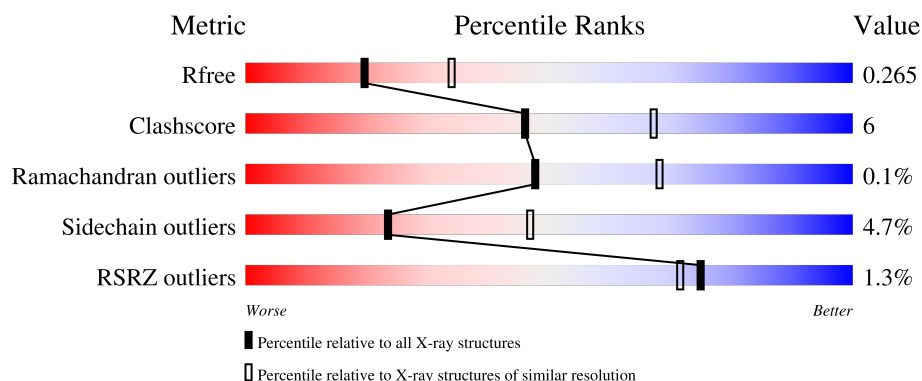
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	0% 73% 12% • 15%
1	B	549	0% 72% 13% • 14%
1	C	549	2% 68% 16% • 14%

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 (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

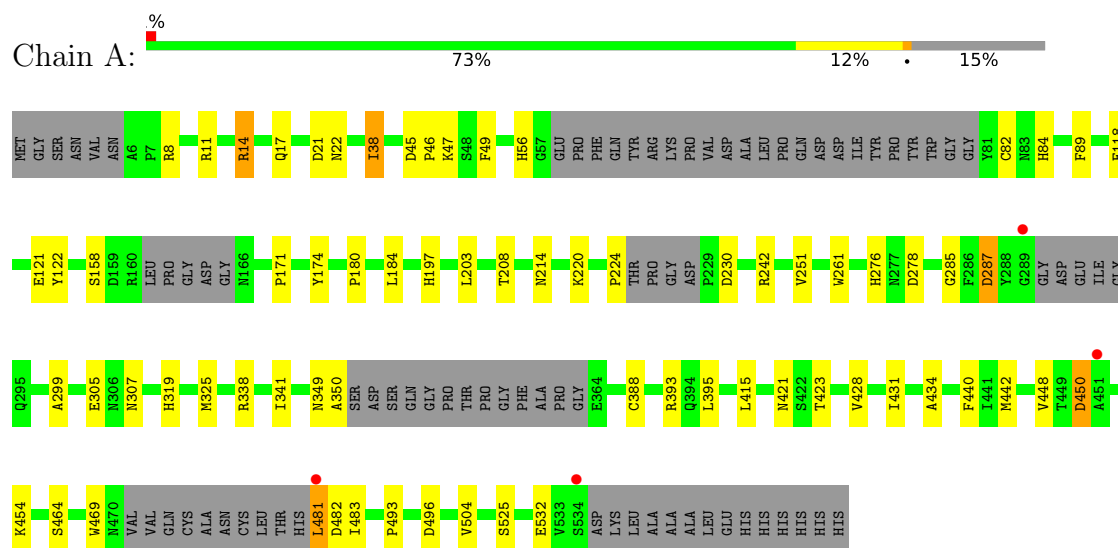
- Molecule 5 is water.

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		

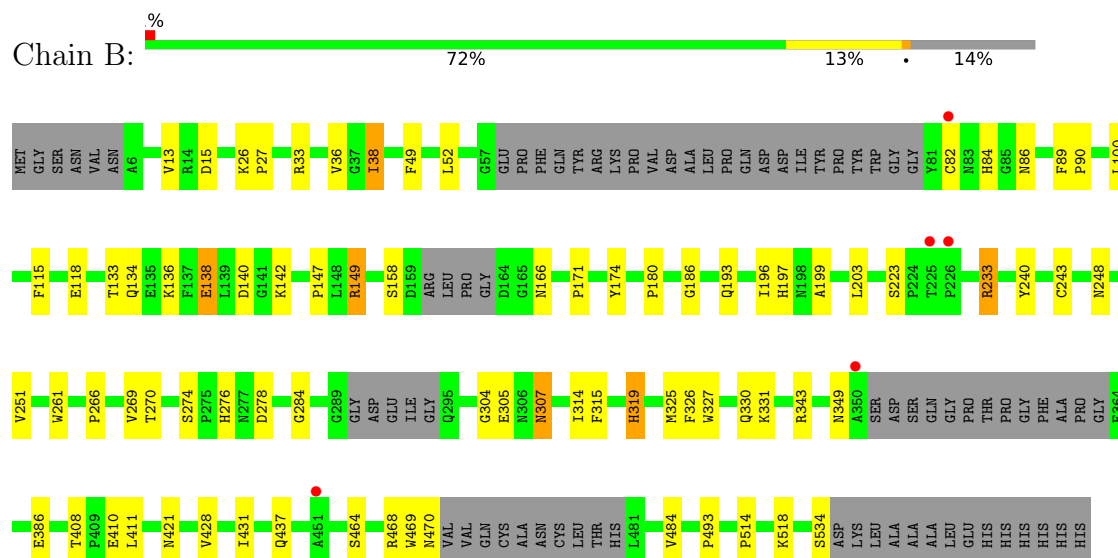
3 Residue-property plots [i](#)

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

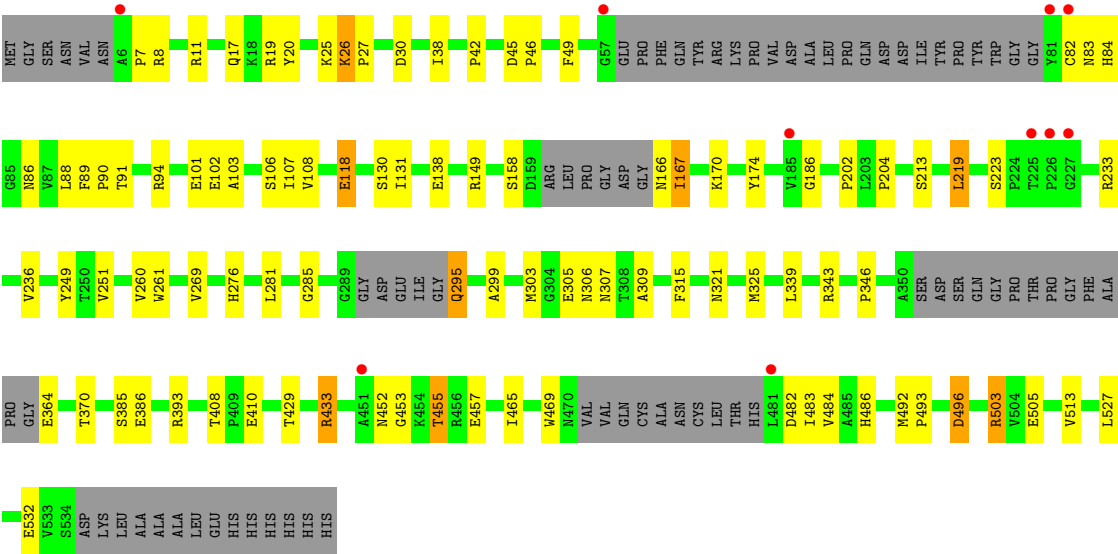


• Molecule 1: Tyrosinase



• Molecule 1: Tyrosinase





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 27.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (27.85-2.50) 95.8 (27.85-2.50)	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 (4.77%)	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)	0.33 , 54.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: O, GOL, 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	0.95	2/3775 (0.1%)	1.06	1/5126 (0.0%)
1	B	1.01	2/3804 (0.1%)	1.08	5/5170 (0.1%)
1	C	0.91	2/3792 (0.1%)	1.07	4/5154 (0.1%)
All	All	0.96	6/11371 (0.1%)	1.07	10/15450 (0.1%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	486	HIS	C-O	-6.46	1.16	1.24
1	C	408	THR	N-CA	6.46	1.51	1.45
1	B	248	ASN	N-CA	5.73	1.52	1.46
1	A	319	HIS	CE1-NE2	5.58	1.38	1.32
1	A	89	PHE	C-O	-5.33	1.19	1.24
1	B	307	ASN	C-O	-5.23	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	PRO	CA-C-N	11.88	131.60	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	PRO	C-N-CA	11.88	131.60	119.24
1	B	274	SER	CA-C-N	-7.61	111.88	119.56
1	B	274	SER	C-N-CA	-7.61	111.88	119.56
1	B	134	GLN	CB-CA-C	-6.15	98.61	109.62
1	A	208	THR	CA-CB-OG1	-5.70	101.05	109.60
1	B	319	HIS	CA-CB-CG	-5.33	108.47	113.80
1	C	370	THR	CA-C-N	5.09	125.25	119.90
1	C	370	THR	C-N-CA	5.09	125.25	119.90
1	B	138	GLU	CB-CG-CD	5.04	121.16	112.60

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
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 [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	3679	0	3599	36	0
1	B	3706	0	3614	40	0
1	C	3694	0	3607	51	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	128	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.

All (128) 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:C:303:MET:HE1	1:C:315:PHE:HD2	1.52	0.74
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:325:MET:HA	1:B:325:MET:HE2	1.71	0.72
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: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:25:LYS:O	1:C:26:LYS:C	2.40	0.62
1:C:452:ASN:CB	1:C:453:GLY:HA2	2.29	0.62
1:C:325:MET:HA	1:C:325:MET:HE2	1.81	0.62
1:C:433:ARG:HH11	1:C:433:ARG:HG3	1.64	0.61
1:C:303:MET:HE1	1:C:315:PHE:CD2	2.34	0.61
1:A:434:ALA:HB2	1:A:481:LEU:HD13	1.83	0.60
1:B:327:TRP:CD1	1:B:331:LYS:HZ3	2.19	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:303:MET:HE2	1:C:309:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MET:HE2	1:A:325:MET:HA	1.87	0.57
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:A:21:ASP:C	1:A:22:ASN:HD22	2.17	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: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:B:278:ASP:OD1	1:B:464:SER:OG	2.28	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:C:83:ASN:CG	1:C:86:ASN:HD21	2.19	0.49
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
1:C:82:CYS:SG	1:C:84:HIS:HE1	2.36	0.49
1:C:303:MET:HE3	1:C:309:ALA:O	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:THR:O	1:C:455:THR:HG22	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:36:VAL:HG23	1:B:147:PRO:HG3	1.98	0.45
1:B:136:LYS:HB2	5:B:726:HOH:O	2.16	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:A:349:ASN:HD22	1:A:350:ALA:C	2.25	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:465:ILE:HD12	1:C:465:ILE:N	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:86:ASN:OD1	1:B:86:ASN:C	2.61	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:C:303:MET:HE2	1:C:303:MET:HA	2.01	0.42
1:B:314:ILE:O	1:B:315:PHE:C	2.60	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
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:C:45:ASP:O	1:C:46:PRO:C	2.61	0.41
1:A:38:ILE:HG23	1:A:49:PHE:HB2	2.02	0.41
1:A:278:ASP:OD1	1:A:464:SER:CB	2.68	0.41
1:C:251:VAL:HG11	1:C:261:TRP:CG	2.55	0.41
1:A:22:ASN:HD22	1:A:22:ASN:N	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:118:GLU:OE2	1:B:240:TYR:OH	2.32	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:B:327:TRP:CD1	1:B:331:LYS:NZ	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PHE:N	1:C:90:PRO:CD	2.84	0.41
1:C:452:ASN:HB2	1:C:453:GLY:CA	2.46	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:HE21	1:C:295:GLN:HB2	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:38:ILE:HD11	1:C:103:ALA:HB1	2.03	0.41
1:C:249:TYR:HB2	1:C:339:LEU:HD22	2.02	0.41
1:C:251:VAL:HG11	1:C:261:TRP:CD2	2.55	0.41
1:A:440:PHE:HE2	1:A:442:MET:HE2	1.86	0.41
1:C:101:GLU:O	1:C:102:GLU:C	2.62	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:56:HIS:O	1:A:56:HIS:CG	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

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	455/549 (83%)	437 (96%)	17 (4%)	1 (0%)	43	63
1	B	462/549 (84%)	456 (99%)	6 (1%)	0	100	100
1	C	460/549 (84%)	426 (93%)	33 (7%)	1 (0%)	43	63
All	All	1377/1647 (84%)	1319 (96%)	56 (4%)	2 (0%)	48	68

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%)	384 (96%)	15 (4%)	29	56
1	B	402/462 (87%)	389 (97%)	13 (3%)	34	62
1	C	401/462 (87%)	372 (93%)	29 (7%)	13	28
All	All	1202/1386 (87%)	1145 (95%)	57 (5%)	23	47

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	118	GLU
1	A	121	GLU
1	A	158	SER
1	A	203	LEU
1	A	276	HIS
1	A	287	ASP
1	A	338	ARG
1	A	341	ILE
1	A	423	THR
1	A	481	LEU
1	A	483	ILE
1	A	504	VAL
1	A	525	SER
1	A	532	GLU
1	B	15	ASP
1	B	38	ILE
1	B	158	SER
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	223	SER
1	B	233	ARG
1	B	269	VAL
1	B	276	HIS
1	B	349	ASN
1	B	386	GLU
1	B	410	GLU
1	B	484	VAL
1	B	518	LYS
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	130	SER
1	C	138	GLU
1	C	158	SER
1	C	167	ILE
1	C	213	SER
1	C	219	LEU
1	C	223	SER
1	C	269	VAL
1	C	276	HIS
1	C	281	LEU
1	C	295	GLN
1	C	306	ASN
1	C	364	GLU
1	C	386	GLU
1	C	393	ARG
1	C	410	GLU
1	C	455	THR
1	C	482	ASP
1	C	483	ILE
1	C	492	MET
1	C	496	ASP
1	C	505	GLU
1	C	532	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	22	ASN
1	A	93	HIS
1	A	134	GLN
1	A	166	ASN
1	A	197	HIS
1	A	214	ASN
1	A	276	HIS
1	A	307	ASN
1	A	319	HIS
1	A	335	HIS
1	A	349	ASN
1	B	17	GLN
1	B	39	GLN
1	B	56	HIS
1	B	126	HIS
1	B	143	GLN
1	B	197	HIS
1	B	265	ASN
1	B	276	HIS
1	B	277	ASN
1	B	306	ASN
1	B	307	ASN
1	B	319	HIS
1	B	373	ASN
1	B	437	GLN
1	C	22	ASN
1	C	56	HIS
1	C	83	ASN
1	C	134	GLN
1	C	214	ASN
1	C	234	ASN
1	C	265	ASN
1	C	276	HIS
1	C	295	GLN
1	C	300	ASN
1	C	306	ASN
1	C	307	ASN
1	C	335	HIS
1	C	390	ASN
1	C	394	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.70	0	5,5,5	1.51	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
4	GOL	B	603	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	GOL	O3-C3-C2	2.07	119.67	110.38

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%)	-0.09	4 (0%) 81 78	33, 51, 91, 119	0
1	B	474/549 (86%)	-0.17	5 (1%) 78 75	28, 48, 84, 116	0
1	C	472/549 (85%)	0.20	10 (2%) 63 59	33, 61, 94, 153	0
All	All	1415/1647 (85%)	-0.02	19 (1%) 75 71	28, 53, 91, 153	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	ALA	3.8
1	C	451	ALA	3.6
1	C	57	GLY	3.5
1	B	226	PRO	2.9
1	C	6	ALA	2.8
1	C	225	THR	2.6
1	A	289	GLY	2.6
1	B	451	ALA	2.5
1	C	185	VAL	2.4
1	C	81	TYR	2.4
1	C	481	LEU	2.4
1	B	225	THR	2.4
1	C	82	CYS	2.3
1	A	481	LEU	2.2
1	A	451	ALA	2.1
1	C	227	GLY	2.1
1	C	226	PRO	2.1
1	A	534	SER	2.1
1	B	82	CYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	GOL	B	603	6/6	0.86	0.15	43,60,63,64	0
3	O	A	603	1/1	0.98	0.06	22,22,22,22	0
2	CU	B	602	1/1	0.99	0.04	58,58,58,58	0
2	CU	C	602	1/1	0.99	0.02	66,66,66,66	0
2	CU	A	601	1/1	0.99	0.02	55,55,55,55	0
3	O	C	603	1/1	0.99	0.03	25,25,25,25	0
2	CU	A	602	1/1	0.99	0.03	62,62,62,62	0
3	O	B	604	1/1	1.00	0.02	16,16,16,16	0
2	CU	B	601	1/1	1.00	0.02	50,50,50,50	0
2	CU	C	601	1/1	1.00	0.02	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.