



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2019 – 10:59 AM EDT

PDB ID : 2Y9X  
Title : Crystal structure of PPO3, a tyrosinase from *Agaricus bisporus*, in deoxy-form that contains additional unknown lectin-like subunit, with inhibitor tropolone  
Authors : Ismaya, W.T.; Rozeboom, H.J.; Weijn, A.; Mes, J.J.; Fusetti, F.; Wichers, H.J.; Dijkstra, B.W.  
Deposited on : 2011-02-17  
Resolution : 2.78 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](mailto: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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

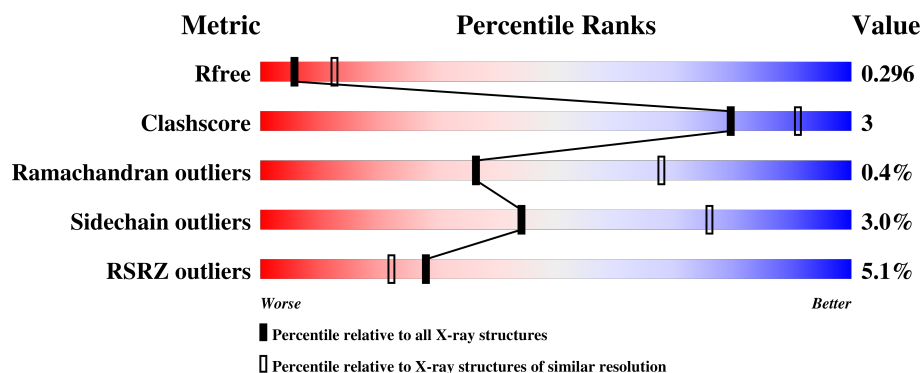
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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))
$R_{free}$	111664	3577 (2.80-2.76)
Clashscore	122126	4033 (2.80-2.76)
Ramachandran outliers	120053	3968 (2.80-2.76)
Sidechain outliers	120020	3970 (2.80-2.76)
RSRZ outliers	108989	3494 (2.80-2.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	391	<div> <div>3%</div> <div>89% 10% .</div> </div>
1	B	391	<div> <div>4%</div> <div>92% 8%</div> </div>
1	C	391	<div> <div>7%</div> <div>87% 13% .</div> </div>
1	D	391	<div> <div>2%</div> <div>90% 10% .</div> </div>
2	E	150	<div> <div>5%</div> <div>77% 13% 9%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	150	<div><div></div><div>5%</div><div>79%</div><div>11%</div><div>9%</div></div>
2	G	150	<div><div></div><div>9%</div><div>80%</div><div>10%</div><div>9%</div></div>
2	H	150	<div><div></div><div>10%</div><div>83%</div><div>7%</div><div>9%</div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17125 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 POLYPHENOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3207	2069	534	592	12			
1	B	391	Total	C	N	O	S	0	0	0
			3207	2069	534	592	12			
1	C	391	Total	C	N	O	S	0	0	0
			3207	2069	534	592	12			
1	D	391	Total	C	N	O	S	0	0	0
			3207	2069	534	592	12			

- Molecule 2 is a protein called LECTIN-LIKE FOLD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	136	Total	C	N	O	S	0	0	0
			1056	666	183	205	2			
2	F	136	Total	C	N	O	S	0	0	0
			1056	666	183	205	2			
2	G	136	Total	C	N	O	S	0	0	0
			1056	666	183	205	2			
2	H	136	Total	C	N	O	S	0	0	0
			1056	666	183	205	2			

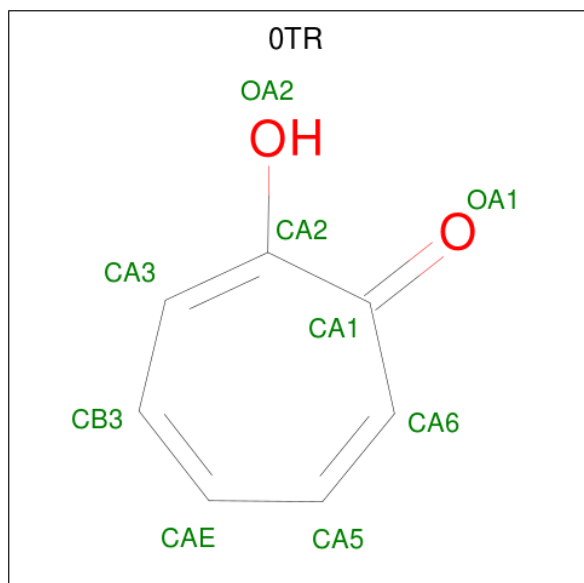
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is HOLMIUM ATOM (three-letter code: HO) (formula: Ho).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ho	0	0
			1	1		
4	A	1	Total	Ho	0	0
			1	1		
4	D	1	Total	Ho	0	0
			1	1		
4	C	1	Total	Ho	0	0
			1	1		

- Molecule 5 is 2-HYDROXYCYCLOHEPTA-2,4,6-TRIEN-1-ONE (three-letter code: OTR) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	C	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		

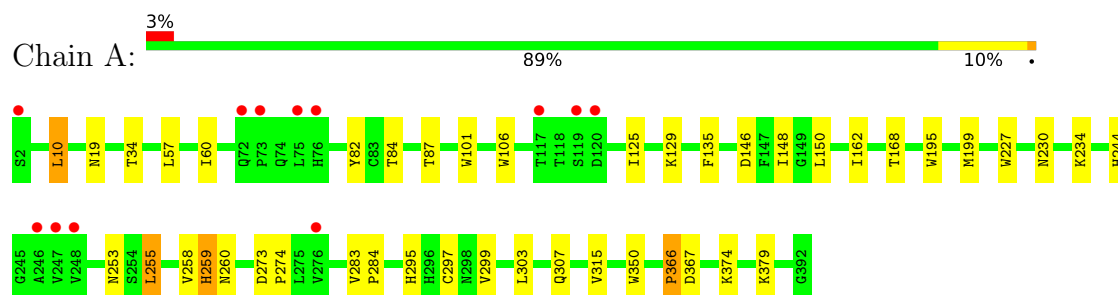
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	O 4	0	0
6	B	6	Total 6	O 6	0	0
6	C	4	Total 4	O 4	0	0
6	D	5	Total 5	O 5	0	0
6	E	1	Total 1	O 1	0	0
6	F	1	Total 1	O 1	0	0
6	G	3	Total 3	O 3	0	0
6	H	1	Total 1	O 1	0	0

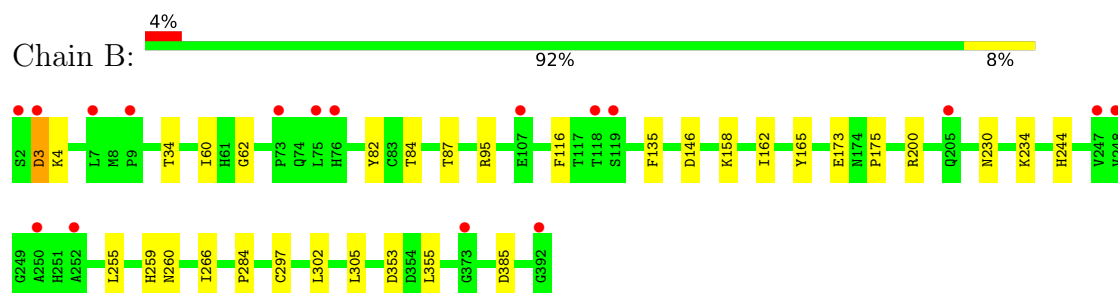
### 3 Residue-property plots

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.

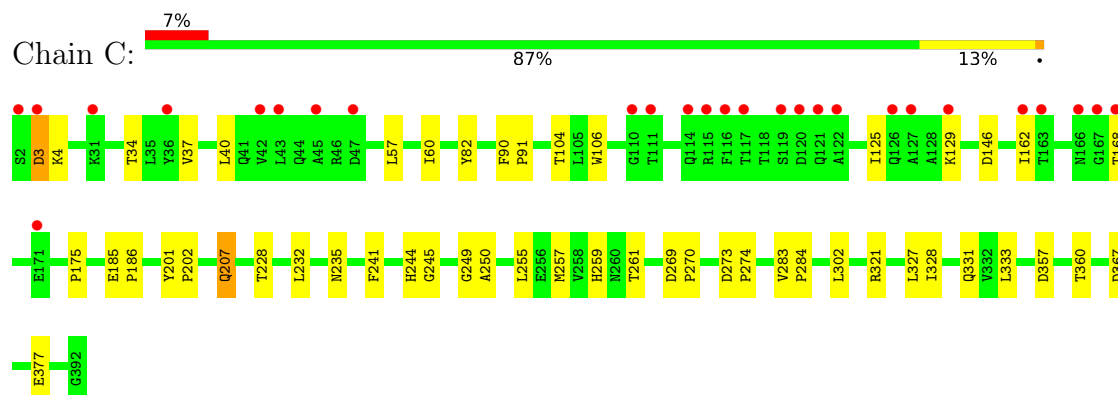
#### • Molecule 1: POLYPHENOL OXIDASE



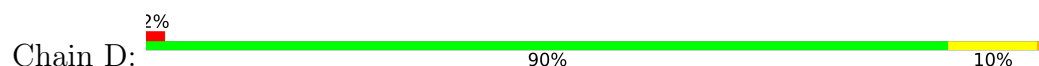
#### • Molecule 1: POLYPHENOL OXIDASE

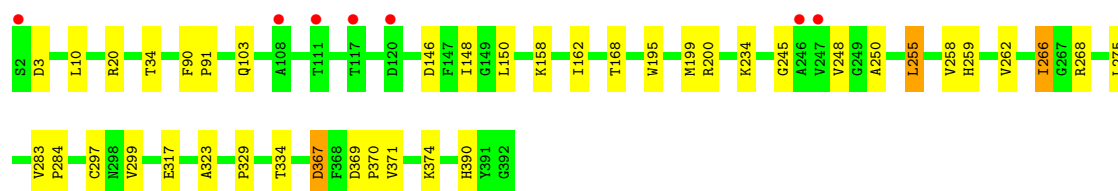


#### • Molecule 1: POLYPHENOL OXIDASE

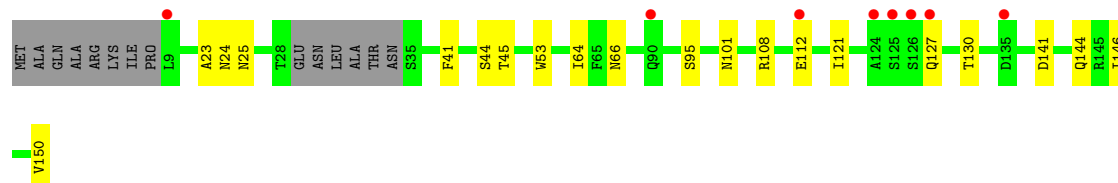
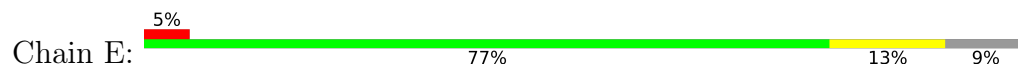


#### • Molecule 1: POLYPHENOL OXIDASE

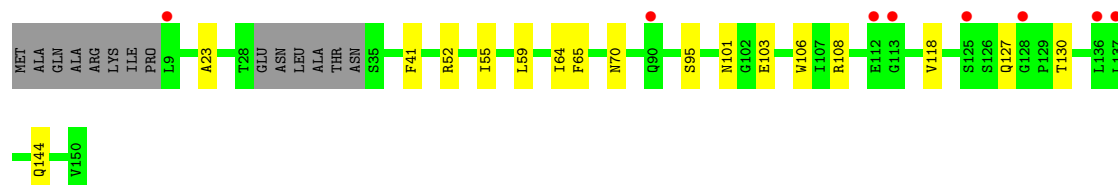
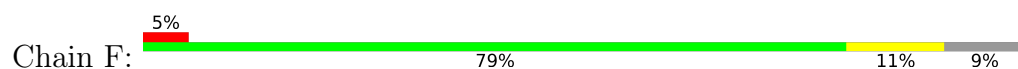




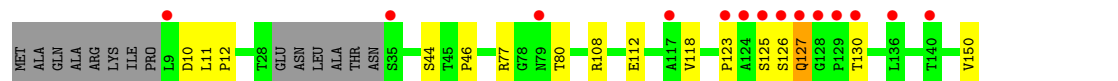
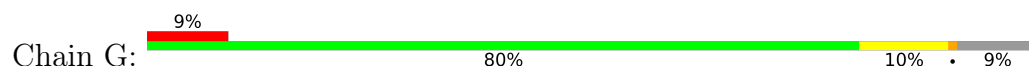
• Molecule 2: LECTIN-LIKE FOLD PROTEIN



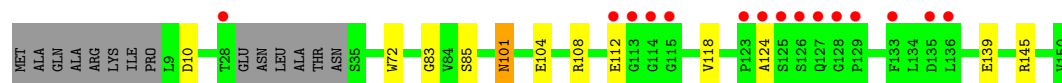
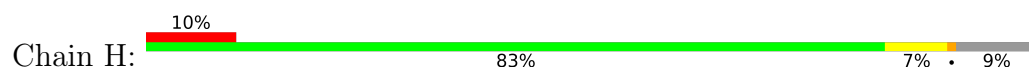
• Molecule 2: LECTIN-LIKE FOLD PROTEIN



• Molecule 2: LECTIN-LIKE FOLD PROTEIN



• Molecule 2: LECTIN-LIKE FOLD PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.84Å 104.82Å 119.36Å 90.00° 110.45° 90.00°	Depositor
Resolution (Å)	58.03 – 2.78 58.03 – 2.78	Depositor EDS
% Data completeness (in resolution range)	89.1 (58.03-2.78) 89.1 (58.03-2.78)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.235 , 0.289 0.242 , 0.296	Depositor DCC
$R_{free}$ test set	2716 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	17125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.35	0/3317	0.48	0/4526
1	B	0.35	0/3317	0.48	0/4526
1	C	0.36	0/3317	0.48	0/4526
1	D	0.36	0/3317	0.48	1/4526 (0.0%)
2	E	0.34	0/1082	0.50	0/1470
2	F	0.35	0/1082	0.49	0/1470
2	G	0.36	0/1082	0.49	0/1470
2	H	0.36	0/1082	0.48	0/1470
All	All	0.36	0/17596	0.48	1/23984 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	LEU	CA-CB-CG	5.53	128.02	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3207	0	3020	20	0
1	B	3207	0	3020	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3207	0	3020	22	0
1	D	3207	0	3020	18	0
2	E	1056	0	1004	9	0
2	F	1056	0	1004	5	0
2	G	1056	0	1004	6	0
2	H	1056	0	1004	9	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	9	0	5	0	0
5	B	9	0	5	0	0
5	C	9	0	5	0	0
5	D	9	0	5	0	0
6	A	4	0	0	0	0
6	B	6	0	0	1	0
6	C	4	0	0	0	0
6	D	5	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
6	H	1	0	0	0	0
All	All	17125	0	16116	100	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 3.

All (100) 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:230:ASN:O	1:B:234:LYS:HB2	1.94	0.68
2:H:101:ASN:HD21	2:H:145:ARG:HH12	1.41	0.67
1:B:353:ASP:OD2	6:B:2005:HOH:O	2.13	0.67
1:C:232:LEU:HD11	1:C:302:LEU:HD22	1.78	0.65
2:F:108:ARG:HG3	2:F:118:VAL:HG12	1.77	0.65
1:C:283:VAL:HB	1:C:284:PRO:HD3	1.80	0.64
1:C:245:GLY:HA3	1:C:250:ALA:HB3	1.79	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:PRO:HD3	2:G:130:THR:HG22	1.80	0.63
1:A:60:ILE:O	1:A:82:TYR:HB2	1.99	0.62
2:E:25:ASN:HB3	2:E:66:ASN:HD22	1.65	0.62
1:D:148:ILE:HG13	1:D:150:LEU:H	1.66	0.59
2:H:101:ASN:HD22	2:H:101:ASN:H	1.49	0.58
2:G:126:SER:O	2:G:127:GLN:HB2	2.03	0.58
1:D:268:ARG:HH11	1:D:275:LEU:HD13	1.69	0.58
1:A:106:TRP:HE1	1:A:129:LYS:HA	1.69	0.58
1:D:10:LEU:HA	1:D:103:GLN:HE22	1.69	0.58
1:D:371:VAL:HG12	1:D:374:LYS:HD2	1.86	0.57
1:A:230:ASN:O	1:A:234:LYS:HB2	2.06	0.56
2:E:95:SER:HB2	2:E:108:ARG:HB3	1.88	0.55
2:H:72:TRP:O	2:H:83:GLY:HA2	2.06	0.55
1:C:249:GLY:HA2	1:C:257:MET:HE3	1.88	0.55
1:C:244:HIS:HB2	1:C:257:MET:HE2	1.90	0.53
1:A:34:THR:HG23	1:A:162:ILE:HB	1.91	0.53
1:C:357:ASP:O	1:C:360:THR:HG22	2.08	0.53
2:H:101:ASN:HD21	2:H:145:ARG:NH1	2.08	0.52
1:D:283:VAL:HB	1:D:284:PRO:HD3	1.92	0.51
1:C:57:LEU:HD11	1:C:104:THR:HG21	1.93	0.50
2:F:55:ILE:HG12	2:F:64:ILE:HG12	1.92	0.50
2:H:101:ASN:HD22	2:H:101:ASN:N	2.08	0.50
1:D:195:TRP:CD2	1:D:199:MET:HG3	2.47	0.49
2:H:108:ARG:HG3	2:H:118:VAL:HG12	1.95	0.49
1:A:303:LEU:O	1:A:307:GLN:HG3	2.13	0.49
1:B:84:THR:OG1	1:B:87:THR:OG1	2.27	0.48
1:D:200:ARG:HD3	1:D:266:ILE:HG23	1.95	0.48
1:A:19:ASN:HB3	1:A:366:PRO:HD3	1.96	0.47
1:C:37:VAL:HG13	1:C:175:PRO:HG3	1.96	0.47
2:E:141:ASP:HB3	2:E:144:GLN:HG3	1.96	0.47
2:E:23:ALA:HB2	2:E:41:PHE:CZ	2.50	0.47
1:A:374:LYS:O	1:A:379:LYS:HE3	2.15	0.47
2:G:108:ARG:HG3	2:G:118:VAL:HG12	1.96	0.46
1:C:328:ILE:O	1:C:331:GLN:HG2	2.15	0.46
1:C:202:PRO:HA	1:C:207:GLN:O	2.15	0.46
1:D:317:GLU:HG2	1:D:334:THR:HG22	1.96	0.46
1:B:62:GLY:HA3	1:B:284:PRO:HA	1.97	0.46
1:A:244:HIS:HD2	1:A:260:ASN:HD21	1.64	0.46
1:B:173:GLU:O	1:B:175:PRO:HD3	2.16	0.46
1:D:245:GLY:HA3	1:D:250:ALA:HB3	1.98	0.46
1:A:57:LEU:HD23	1:A:101:TRP:HA	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:PHE:HB3	1:C:91:PRO:HD3	1.98	0.45
1:B:60:ILE:O	1:B:82:TYR:HB2	2.16	0.45
1:D:323:ALA:HB2	1:D:329:PRO:HB3	1.98	0.45
1:A:195:TRP:CD2	1:A:199:MET:HG3	2.52	0.45
1:D:20:ARG:HD3	1:D:297:CYS:SG	2.57	0.45
1:A:283:VAL:HB	1:A:284:PRO:HD3	1.99	0.44
1:B:116:PHE:CD1	1:B:165:TYR:HA	2.52	0.44
1:D:258:VAL:O	1:D:262:VAL:HG23	2.16	0.44
1:C:3:ASP:HB3	1:C:4:LYS:H	1.66	0.44
1:B:135:PHE:HB3	1:B:297:CYS:SG	2.57	0.44
1:D:34:THR:HG23	1:D:162:ILE:HB	1.98	0.44
2:G:11:LEU:HA	2:G:12:PRO:HD3	1.87	0.44
1:C:269:ASP:OD1	1:C:270:PRO:HD2	2.18	0.44
1:A:135:PHE:HB3	1:A:297:CYS:SG	2.58	0.44
1:D:369:ASP:HB2	1:D:370:PRO:HD3	1.99	0.44
1:A:244:HIS:CD2	1:A:260:ASN:HD21	2.34	0.44
2:E:53:TRP:CE3	2:E:64:ILE:HG22	2.53	0.43
1:D:268:ARG:NH1	1:D:275:LEU:HD13	2.31	0.43
1:B:3:ASP:HB3	1:B:4:LYS:H	1.55	0.43
1:C:321:ARG:HD3	2:E:44:SER:HB2	2.01	0.43
1:D:255:LEU:HD11	1:D:299:VAL:HG13	2.00	0.43
2:H:139:GLU:O	2:H:145:ARG:NH2	2.52	0.43
1:B:34:THR:HG23	1:B:162:ILE:HB	2.01	0.43
1:A:148:ILE:HG13	1:A:150:LEU:H	1.84	0.43
1:A:84:THR:HG1	1:A:87:THR:HG1	1.54	0.43
1:B:302:LEU:HD23	1:B:305:LEU:HD12	2.00	0.43
1:C:34:THR:HG23	1:C:162:ILE:HB	1.99	0.43
1:D:367:ASP:N	1:D:367:ASP:OD1	2.51	0.42
2:F:23:ALA:HB2	2:F:41:PHE:CZ	2.54	0.42
1:A:255:LEU:O	1:A:259:HIS:HB3	2.20	0.42
1:B:95:ARG:HD2	1:B:355:LEU:HD13	2.01	0.42
1:A:295:HIS:O	1:A:299:VAL:HG23	2.19	0.42
1:C:228:THR:HG22	1:C:232:LEU:HD12	2.00	0.42
1:A:273:ASP:HA	1:A:274:PRO:HA	1.90	0.42
1:D:90:PHE:HB3	1:D:91:PRO:HD3	2.01	0.42
1:C:273:ASP:HA	1:C:274:PRO:HA	1.94	0.42
1:C:60:ILE:O	1:C:82:TYR:HB2	2.20	0.42
1:A:227:TRP:CE2	1:A:258:VAL:HG22	2.56	0.41
1:B:244:HIS:CD2	1:B:260:ASN:HD21	2.37	0.41
1:B:200:ARG:HD3	1:B:266:ILE:HG23	2.02	0.41
1:C:235:ASN:HB3	1:C:241:PHE:HB2	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:TRP:HD1	2:F:144:GLN:O	2.04	0.41
2:F:65:PHE:HZ	2:F:70:ASN:HD22	1.68	0.41
1:C:185:GLU:HA	1:C:186:PRO:HD2	1.94	0.41
2:E:121:ILE:HD11	2:E:146:ILE:HD11	2.03	0.40
2:E:44:SER:HA	2:G:150:VAL:OXT	2.22	0.40
1:A:10:LEU:HB3	1:A:350:TRP:NE1	2.36	0.40
2:H:101:ASN:N	2:H:101:ASN:ND2	2.69	0.40
1:C:106:TRP:NE1	1:C:129:LYS:HA	2.36	0.40
1:C:327:LEU:HD13	1:C:333:LEU:HD21	2.04	0.40
2:E:150:VAL:OXT	2:G:44:SER:HA	2.22	0.40
2:H:104:GLU:HB3	2:H:145:ARG:HB3	2.04	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	389/391 (100%)	371 (95%)	16 (4%)	2 (0%)	31	62
1	B	389/391 (100%)	373 (96%)	16 (4%)	0	100	100
1	C	389/391 (100%)	369 (95%)	20 (5%)	0	100	100
1	D	389/391 (100%)	371 (95%)	17 (4%)	1 (0%)	43	74
2	E	132/150 (88%)	122 (92%)	9 (7%)	1 (1%)	21	51
2	F	132/150 (88%)	124 (94%)	8 (6%)	0	100	100
2	G	132/150 (88%)	123 (93%)	6 (4%)	3 (2%)	7	21
2	H	132/150 (88%)	123 (93%)	8 (6%)	1 (1%)	21	51
All	All	2084/2164 (96%)	1976 (95%)	100 (5%)	8 (0%)	36	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	248	VAL
2	G	77	ARG
2	E	112	GLU
2	G	46	PRO
2	G	127	GLN
2	H	124	ALA
1	A	315	VAL
1	A	366	PRO

### 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	342/342 (100%)	334 (98%)	8 (2%)	53	82
1	B	342/342 (100%)	336 (98%)	6 (2%)	62	86
1	C	342/342 (100%)	330 (96%)	12 (4%)	39	71
1	D	342/342 (100%)	333 (97%)	9 (3%)	49	80
2	E	112/123 (91%)	107 (96%)	5 (4%)	30	62
2	F	112/123 (91%)	105 (94%)	7 (6%)	20	47
2	G	112/123 (91%)	108 (96%)	4 (4%)	38	70
2	H	112/123 (91%)	108 (96%)	4 (4%)	38	70
All	All	1816/1860 (98%)	1761 (97%)	55 (3%)	44	76

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	125	ILE
1	A	146	ASP
1	A	168	THR
1	A	253	ASN
1	A	255	LEU
1	A	259	HIS
1	A	367	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	3	ASP
1	B	146	ASP
1	B	158	LYS
1	B	255	LEU
1	B	259	HIS
1	B	385	ASP
1	C	3	ASP
1	C	40	LEU
1	C	125	ILE
1	C	146	ASP
1	C	168	THR
1	C	201	TYR
1	C	207	GLN
1	C	255	LEU
1	C	259	HIS
1	C	261	THR
1	C	367	ASP
1	C	377	GLU
1	D	3	ASP
1	D	146	ASP
1	D	158	LYS
1	D	168	THR
1	D	234	LYS
1	D	259	HIS
1	D	266	ILE
1	D	367	ASP
1	D	390	HIS
2	E	24	ASN
2	E	45	THR
2	E	101	ASN
2	E	127	GLN
2	E	130	THR
2	F	52	ARG
2	F	59	LEU
2	F	95	SER
2	F	101	ASN
2	F	103	GLU
2	F	127	GLN
2	F	130	THR
2	G	10	ASP
2	G	80	THR
2	G	112	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	G	125	SER
2	H	10	ASP
2	H	85	SER
2	H	101	ASN
2	H	112	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	244	HIS
1	A	285	HIS
1	B	205	GLN
1	B	243	ASN
1	B	244	HIS
1	B	285	HIS
1	C	244	HIS
1	D	103	GLN
1	D	196	GLN
1	D	243	ASN
1	D	244	HIS
1	D	285	HIS
1	D	351	GLN
2	E	24	ASN
2	E	143	ASN
2	E	144	GLN
2	F	70	ASN
2	F	101	ASN
2	F	127	GLN
2	F	143	ASN
2	G	18	ASN
2	H	101	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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
5	0TR	A	410	-	8,9,9	1.26	1 (12%)	5,11,11	0.41	0
5	0TR	B	410	-	8,9,9	1.37	2 (25%)	5,11,11	0.26	0
5	0TR	C	410	-	8,9,9	1.27	1 (12%)	5,11,11	0.47	0
5	0TR	D	410	-	8,9,9	1.32	1 (12%)	5,11,11	0.32	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
5	0TR	A	410	-	-	-	0/1/1/1
5	0TR	B	410	-	-	-	0/1/1/1
5	0TR	C	410	-	-	-	0/1/1/1
5	0TR	D	410	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	410	0TR	CB3-CA3	-2.39	1.33	1.38
5	B	410	0TR	CB3-CA3	-2.38	1.33	1.38
5	C	410	0TR	CB3-CA3	-2.22	1.34	1.38
5	A	410	0TR	CB3-CA3	-2.21	1.34	1.38
5	B	410	0TR	OA1-CA1	2.07	1.26	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	391/391 (100%)	0.44	12 (3%)	49	43	38, 49, 62, 74	0
1	B	391/391 (100%)	0.51	17 (4%)	35	29	39, 51, 64, 73	0
1	C	391/391 (100%)	0.64	27 (6%)	17	12	40, 55, 74, 91	0
1	D	391/391 (100%)	0.41	7 (1%)	68	64	38, 52, 68, 80	0
2	E	136/150 (90%)	0.58	8 (5%)	22	17	40, 51, 67, 84	0
2	F	136/150 (90%)	0.63	8 (5%)	22	17	42, 54, 74, 84	0
2	G	136/150 (90%)	0.87	14 (10%)	6	4	40, 54, 74, 88	0
2	H	136/150 (90%)	0.91	15 (11%)	5	3	41, 54, 78, 93	0
All	All	2108/2164 (97%)	0.56	108 (5%)	28	22	38, 52, 68, 93	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	125	SER	6.7
1	C	117	THR	6.0
2	H	125	SER	5.5
2	G	125	SER	5.4
2	F	125	SER	5.2
1	C	121	GLN	4.9
2	H	114	GLY	4.9
2	H	126	SER	4.9
1	A	120	ASP	4.5
2	G	126	SER	4.5
1	B	248	VAL	4.4
1	C	2	SER	4.3
1	A	247	VAL	4.2
2	H	28	THR	4.1
1	D	246	ALA	4.0
1	C	116	PHE	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	115	GLY	3.9
1	C	119	SER	3.8
2	F	9	LEU	3.8
2	H	124	ALA	3.8
1	B	75	LEU	3.7
2	G	128	GLY	3.7
1	A	119	SER	3.7
1	D	2	SER	3.7
1	C	120	ASP	3.5
1	C	45	ALA	3.5
2	H	127	GLN	3.5
1	A	246	ALA	3.4
1	D	120	ASP	3.4
1	B	76	HIS	3.3
1	C	111	THR	3.3
2	H	128	GLY	3.3
1	C	126	GLN	3.2
2	H	136	LEU	3.2
1	C	110	GLY	3.1
2	G	136	LEU	3.1
2	E	127	GLN	3.1
2	G	127	GLN	3.0
1	A	75	LEU	3.0
1	C	122	ALA	3.0
2	H	133	PHE	2.9
2	F	113	GLY	2.9
1	B	373	GLY	2.9
1	C	127	ALA	2.9
2	H	129	PRO	2.9
1	B	73	PRO	2.9
1	A	76	HIS	2.9
1	C	167	GLY	2.9
1	D	117	THR	2.8
2	F	136	LEU	2.8
2	G	124	ALA	2.8
1	C	168	THR	2.8
1	A	248	VAL	2.7
2	G	35	SER	2.7
2	E	9	LEU	2.7
1	C	3	ASP	2.7
1	B	107	GLU	2.7
2	G	117	ALA	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	123	PRO	2.6
1	A	276	VAL	2.6
2	F	90	GLN	2.6
1	B	119	SER	2.6
1	A	117	THR	2.6
1	B	2	SER	2.5
1	B	392	GLY	2.5
1	C	36	TYR	2.4
2	H	135	ASP	2.4
1	D	111	THR	2.4
1	A	2	SER	2.4
2	E	126	SER	2.4
2	E	124	ALA	2.4
2	G	9	LEU	2.4
2	G	140	THR	2.4
2	F	112	GLU	2.4
1	B	247	VAL	2.3
1	B	3	ASP	2.3
1	C	42	VAL	2.3
1	B	252	ALA	2.3
1	C	166	ASN	2.3
2	G	79	ASN	2.3
1	D	247	VAL	2.3
1	A	73	PRO	2.3
1	B	250	ALA	2.3
1	B	7	LEU	2.2
1	B	205	GLN	2.2
1	C	47	ASP	2.2
2	E	112	GLU	2.2
1	C	162	ILE	2.2
2	G	129	PRO	2.2
1	B	9	PRO	2.1
1	D	108	ALA	2.1
1	C	114	GLN	2.1
2	E	135	ASP	2.1
1	C	129	LYS	2.1
2	H	113	GLY	2.1
1	C	171	GLU	2.1
1	A	72	GLN	2.1
2	E	90	GLN	2.1
1	C	115	ARG	2.1
1	B	118	THR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	128	GLY	2.1
1	C	43	LEU	2.0
2	F	137	LEU	2.0
2	G	123	PRO	2.0
2	H	112	GLU	2.0
1	C	163	THR	2.0
2	G	130	THR	2.0
1	C	31	LYS	2.0

## 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	OTR	A	410	9/9	0.81	0.33	82,82,83,83	0
5	OTR	C	410	9/9	0.83	0.42	102,102,102,102	0
5	OTR	B	410	9/9	0.87	0.24	71,71,71,71	0
5	OTR	D	410	9/9	0.93	0.35	73,73,73,74	0
3	CU	B	401	1/1	0.96	0.07	42,42,42,42	0
3	CU	A	400	1/1	0.98	0.08	43,43,43,43	0
3	CU	C	400	1/1	0.98	0.10	42,42,42,42	0
3	CU	D	400	1/1	0.99	0.07	44,44,44,44	0
3	CU	B	400	1/1	0.99	0.08	42,42,42,42	0
3	CU	A	401	1/1	0.99	0.11	40,40,40,40	0
4	HO	C	402	1/1	0.99	0.09	72,72,72,72	0
4	HO	D	402	1/1	0.99	0.07	64,64,64,64	0
4	HO	A	402	1/1	1.00	0.11	63,63,63,63	0
3	CU	C	401	1/1	1.00	0.05	42,42,42,42	0
4	HO	B	402	1/1	1.00	0.09	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CU	D	401	1/1	1.00	0.05	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.