



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:57 PM UTC

PDB ID : 1BT1 / pdb_00001bt1
Title : CATECHOL OXIDASE FROM IPOMOEA BATATAS (SWEET POTATOES) IN THE NATIVE CU(II)-CU(II) STATE
Authors : Klabunde, T.; Eicken, C.; Sacchettini, J.C.; Krebs, B.
Deposited on : 1998-09-02
Resolution : 2.70 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

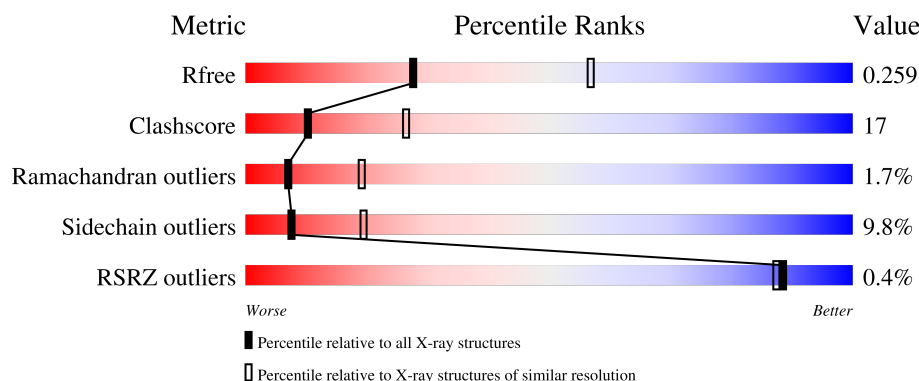
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	345	 60% 29% 8% . .
1	B	345	 60% 29% 7% . .

2 Entry composition [i](#)

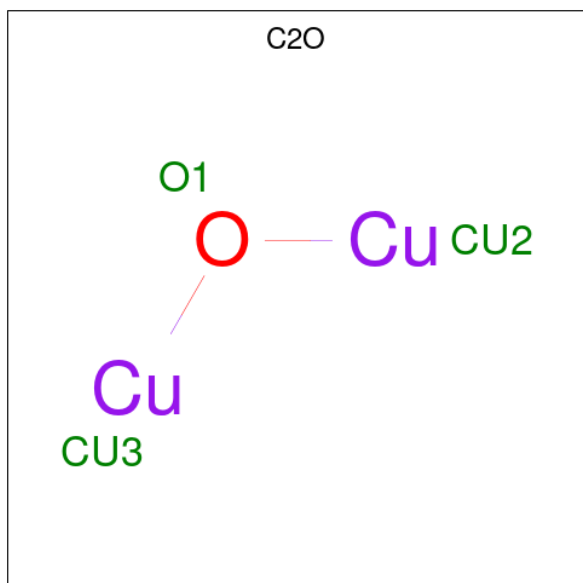
There are 3 unique types of molecules in this entry. The entry contains 5506 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CATECHOL OXIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2666	1703	452	496	15			
1	B	336	Total	C	N	O	S	0	0	0
			2666	1703	452	496	15			

- Molecule 2 is CU-O-CU LINKAGE (CCD ID: C2O) (formula: Cu_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Cu	O	0	0
			3	2	1		
2	B	1	Total	Cu	O	0	0
			3	2	1		

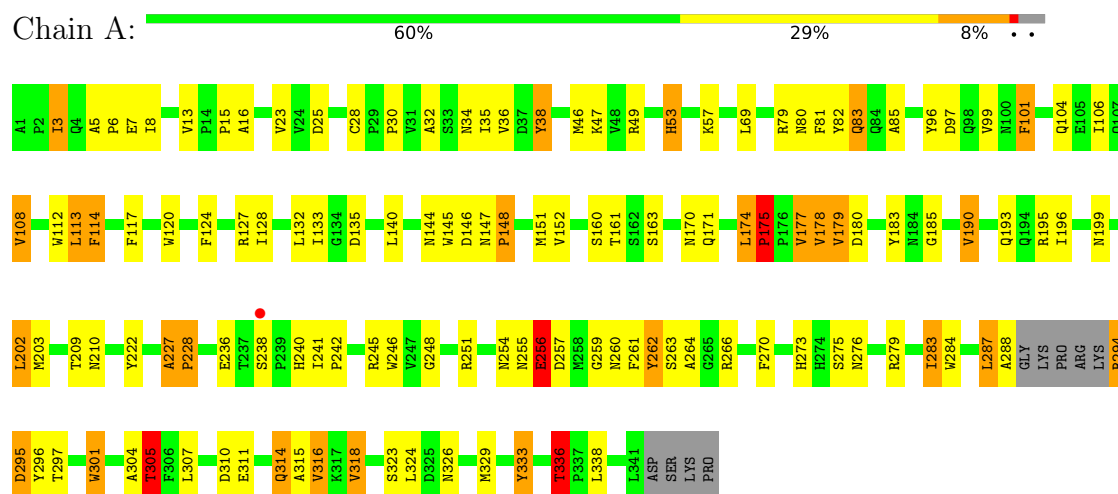
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	85	Total 85	O 85	0	0

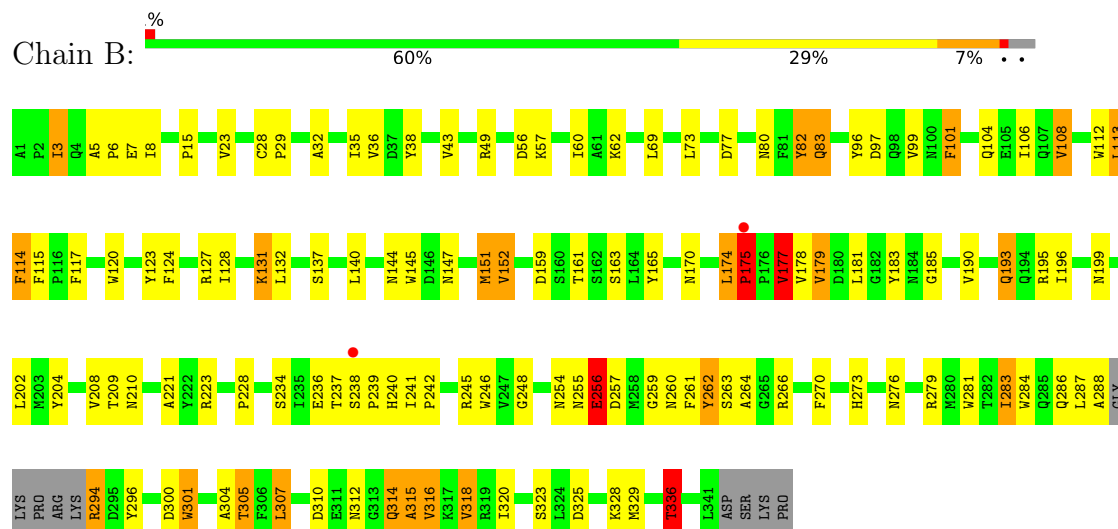
3 Residue-property plots [i](#)

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: PROTEIN (CATECHOL OXIDASE)



• Molecule 1: PROTEIN (CATECHOL OXIDASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.82Å 164.75Å 52.16Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70 8.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	84.2 (8.00-2.70) 80.9 (8.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.35 (at 2.40Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.168 , 0.256 0.176 , 0.259	Depositor DCC
R_{free} test set	1135 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.8	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	5506	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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: C2O

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	0.92	2/2750 (0.1%)	1.28	30/3758 (0.8%)
1	B	0.94	2/2750 (0.1%)	1.28	30/3758 (0.8%)
All	All	0.93	4/5500 (0.1%)	1.28	60/7516 (0.8%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	MET	SD-CE	-7.41	1.61	1.79
1	A	177	VAL	CA-CB	5.84	1.60	1.54
1	B	43	VAL	CA-CB	5.35	1.59	1.53
1	A	256	GLU	CA-C	-5.07	1.46	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	PRO	N-CA-C	12.50	125.95	110.70
1	B	175	PRO	CA-C-N	-11.77	105.13	119.84
1	B	175	PRO	C-N-CA	-11.77	105.13	119.84
1	B	238	SER	CA-C-N	-11.74	105.16	119.84
1	B	238	SER	C-N-CA	-11.74	105.16	119.84
1	B	175	PRO	N-CA-C	11.12	124.27	110.70
1	B	174	LEU	CA-C-N	11.04	131.75	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	LEU	C-N-CA	11.04	131.75	120.38
1	A	238	SER	CA-C-N	-10.80	106.34	119.84
1	A	238	SER	C-N-CA	-10.80	106.34	119.84
1	A	175	PRO	CA-C-N	-9.91	107.45	119.84
1	A	175	PRO	C-N-CA	-9.91	107.45	119.84
1	B	240	HIS	N-CA-C	9.86	122.03	111.28
1	A	174	LEU	CA-C-N	9.69	130.36	120.38
1	A	174	LEU	C-N-CA	9.69	130.36	120.38
1	A	240	HIS	N-CA-C	9.65	121.39	111.07
1	B	256	GLU	N-CA-C	8.83	129.61	110.80
1	A	99	VAL	N-CA-C	8.22	118.99	110.36
1	A	256	GLU	N-CA-C	7.63	127.06	110.80
1	B	99	VAL	N-CA-C	7.21	118.84	110.62
1	B	301	TRP	N-CA-C	-6.86	101.07	111.56
1	B	163	SER	N-CA-C	-6.61	104.70	112.89
1	A	261	PHE	N-CA-C	6.59	119.29	111.71
1	A	256	GLU	CA-C-N	-6.18	109.74	121.54
1	A	256	GLU	C-N-CA	-6.18	109.74	121.54
1	B	256	GLU	CA-C-N	-6.16	109.77	121.54
1	B	256	GLU	C-N-CA	-6.16	109.77	121.54
1	A	301	TRP	N-CA-C	-6.15	102.16	111.56
1	A	3	ILE	N-CA-C	-6.13	99.55	108.87
1	A	16	ALA	N-CA-C	6.11	118.72	111.33
1	A	161	THR	N-CA-C	-6.02	105.66	114.39
1	B	315	ALA	N-CA-C	-5.94	101.05	109.96
1	A	163	SER	N-CA-C	-5.92	105.32	112.54
1	A	46	MET	N-CA-C	5.91	118.40	108.23
1	A	238	SER	N-CA-C	5.85	122.74	109.81
1	A	336	THR	CA-C-N	5.62	126.87	119.84
1	A	336	THR	C-N-CA	5.62	126.87	119.84
1	B	28	CYS	N-CA-C	5.53	116.79	109.93
1	B	237	THR	N-CA-C	5.51	117.15	111.03
1	B	238	SER	N-CA-C	5.47	121.91	109.81
1	B	261	PHE	N-CA-C	5.44	117.21	111.28
1	A	38	TYR	N-CA-C	5.43	117.55	109.25
1	B	29	PRO	N-CA-C	-5.36	104.16	110.70
1	B	3	ILE	N-CA-C	-5.35	100.74	108.87
1	A	160	SER	N-CA-C	5.34	120.73	113.37
1	B	152	VAL	N-CA-C	-5.28	101.30	108.06
1	B	83	GLN	N-CA-C	-5.26	105.55	111.28
1	B	336	THR	CA-C-N	5.22	126.36	119.84
1	B	336	THR	C-N-CA	5.22	126.36	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	THR	N-CA-C	-5.22	105.65	113.89
1	B	82	TYR	N-CA-C	5.21	117.03	111.36
1	A	305	THR	N-CA-C	5.20	117.09	109.24
1	A	297	THR	N-CA-C	-5.20	106.96	113.72
1	B	97	ASP	N-CA-C	-5.20	101.41	109.72
1	A	97	ASP	N-CA-C	-5.14	101.49	109.72
1	A	275	SER	N-CA-C	-5.13	105.77	111.36
1	A	227	ALA	N-CA-C	-5.11	102.85	110.20
1	B	177	VAL	N-CA-C	5.08	115.65	109.30
1	A	83	GLN	N-CA-C	-5.04	105.79	111.28
1	B	234	SER	N-CA-C	5.00	116.55	111.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	TYR	Sidechain
1	A	82	TYR	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	2666	0	2525	88	0
1	B	2666	0	2525	90	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	83	0	0	6	0
3	B	85	0	0	3	0
All	All	5506	0	5050	178	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 17.

All (178) 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:5:ALA:H	1:A:305:THR:HG22	1.35	0.88
1:B:5:ALA:H	1:B:305:THR:HG22	1.46	0.80
1:A:5:ALA:N	1:A:305:THR:HG22	2.01	0.76
1:B:145:TRP:HE1	1:B:273:HIS:HD2	1.33	0.76
1:B:283:ILE:O	1:B:286:GLN:HG2	1.87	0.74
1:B:193:GLN:HG2	3:B:502:HOH:O	1.85	0.74
1:A:145:TRP:HE1	1:A:273:HIS:HD2	1.36	0.73
1:A:151:MET:HE1	1:A:196:ILE:HA	1.71	0.72
1:A:151:MET:HE3	1:A:199:ASN:HD22	1.57	0.70
1:B:5:ALA:N	1:B:305:THR:HG22	2.06	0.70
1:B:151:MET:HE3	1:B:199:ASN:HD22	1.58	0.68
1:A:147:ASN:O	1:A:151:MET:HG3	1.93	0.68
1:B:260:ASN:ND2	1:B:262:TYR:H	1.91	0.68
1:B:264:ALA:HB1	1:B:270:PHE:HD2	1.57	0.67
1:B:35:ILE:HD13	1:B:307:LEU:HD11	1.74	0.67
1:B:151:MET:HE1	1:B:196:ILE:HA	1.77	0.67
1:A:23:VAL:HG22	1:A:262:TYR:OH	1.97	0.65
1:B:264:ALA:HB1	1:B:270:PHE:CD2	2.31	0.65
1:B:38:TYR:HD1	1:B:316:VAL:HG21	1.63	0.63
1:A:174:LEU:HB3	1:A:175:PRO:HD2	1.80	0.63
1:B:179:VAL:HA	1:B:246:TRP:CZ2	2.34	0.62
1:B:36:VAL:HG22	1:B:314:GLN:HE21	1.64	0.62
1:B:23:VAL:HG22	1:B:262:TYR:OH	2.00	0.61
1:A:255:ASN:HB3	1:A:259:GLY:HA3	1.83	0.60
1:B:62:LYS:HB3	3:B:522:HOH:O	2.02	0.60
1:B:101:PHE:CD1	1:B:101:PHE:N	2.69	0.60
1:A:287:LEU:O	1:A:288:ALA:HB2	2.02	0.59
1:A:53:HIS:HD2	3:A:515:HOH:O	1.84	0.59
1:A:101:PHE:N	1:A:101:PHE:CD1	2.70	0.59
1:A:108:VAL:HG11	1:A:117:PHE:CD2	2.37	0.59
1:B:145:TRP:HE1	1:B:273:HIS:CD2	2.18	0.59
1:A:104:GLN:HA	1:A:104:GLN:OE1	2.01	0.59
1:A:124:PHE:O	1:A:128:ILE:HG13	2.03	0.59
1:B:325:ASP:O	1:B:329:MET:HG3	2.02	0.58
1:A:264:ALA:HB1	1:A:270:PHE:HD2	1.67	0.58
1:B:174:LEU:HB3	1:B:175:PRO:HD2	1.84	0.58
1:B:5:ALA:HB2	1:B:305:THR:CG2	2.34	0.58
1:B:260:ASN:HD22	1:B:262:TYR:H	1.52	0.58
1:A:179:VAL:HA	1:A:246:TRP:CZ2	2.39	0.58
1:B:131:LYS:NZ	1:B:312:ASN:ND2	2.52	0.57
1:B:287:LEU:O	1:B:288:ALA:HB3	2.05	0.57
1:A:8:ILE:HD12	1:A:307:LEU:HD21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:TRP:HE3	1:A:296:TYR:CE2	2.22	0.57
1:B:147:ASN:O	1:B:151:MET:HG3	2.05	0.57
1:B:80:ASN:HD22	1:B:83:GLN:H	1.52	0.56
1:A:80:ASN:HD22	1:A:83:GLN:H	1.53	0.56
1:A:113:LEU:HD22	1:A:222:TYR:HD2	1.70	0.56
1:A:260:ASN:ND2	1:A:262:TYR:HD2	2.04	0.56
1:B:15:PRO:HD3	3:B:547:HOH:O	2.06	0.56
1:A:85:ALA:HB3	3:A:528:HOH:O	2.06	0.56
1:B:284:TRP:O	1:B:294:ARG:NH1	2.40	0.55
1:B:77:ASP:O	1:B:83:GLN:HG3	2.07	0.55
1:A:144:ASN:OD1	1:A:336:THR:HG21	2.07	0.55
1:A:145:TRP:NE1	1:A:273:HIS:HD2	2.04	0.55
1:A:264:ALA:HB1	1:A:270:PHE:CD2	2.42	0.55
1:B:325:ASP:HB3	1:B:328:LYS:HB2	1.88	0.55
1:A:35:ILE:HD13	1:A:307:LEU:HD11	1.88	0.54
1:B:73:LEU:HD11	1:B:132:LEU:HD11	1.87	0.54
1:A:170:ASN:HB2	1:A:248:GLY:O	2.06	0.54
1:A:251:ARG:NH2	3:A:577:HOH:O	2.39	0.54
1:B:8:ILE:HD12	1:B:307:LEU:HD21	1.90	0.54
1:B:108:VAL:HG11	1:B:117:PHE:CD2	2.43	0.54
1:B:80:ASN:ND2	1:B:82:TYR:H	2.06	0.54
1:A:47:LYS:NZ	3:A:574:HOH:O	2.39	0.53
1:A:301:TRP:CH2	1:A:324:LEU:HD11	2.42	0.53
1:B:131:LYS:NZ	1:B:312:ASN:HD22	2.06	0.53
1:B:145:TRP:NE1	1:B:273:HIS:HD2	2.05	0.53
1:B:38:TYR:CD1	1:B:316:VAL:HG21	2.43	0.53
1:A:151:MET:C	1:A:179:VAL:HG12	2.34	0.52
1:B:151:MET:C	1:B:179:VAL:HG12	2.36	0.51
1:A:260:ASN:ND2	1:A:262:TYR:H	2.08	0.51
1:B:178:VAL:HG23	1:B:195:ARG:HG2	1.91	0.51
1:A:5:ALA:HB2	1:A:305:THR:CG2	2.41	0.51
1:B:151:MET:CE	1:B:199:ASN:HD22	2.21	0.51
1:B:170:ASN:HB2	1:B:248:GLY:O	2.10	0.51
1:A:254:ASN:HB2	1:A:256:GLU:OE1	2.11	0.50
1:B:114:PHE:CE1	1:B:236:GLU:HG3	2.47	0.50
1:B:223:ARG:NH1	1:B:300:ASP:OD2	2.44	0.50
1:B:3:ILE:HG13	1:B:304:ALA:HB1	1.93	0.50
1:A:3:ILE:HG12	1:A:113:LEU:HD21	1.93	0.49
1:A:120:TRP:CE2	1:A:318:VAL:HG13	2.47	0.49
1:A:6:PRO:HB2	1:A:96:TYR:CD1	2.48	0.49
1:A:146:ASP:HB3	1:A:203:MET:HE2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD22	1:A:222:TYR:CD2	2.47	0.49
1:A:8:ILE:HD13	1:A:32:ALA:H	1.76	0.49
1:A:279:ARG:O	1:A:283:ILE:HD12	2.13	0.48
1:A:284:TRP:CZ3	1:A:294:ARG:HG3	2.48	0.48
1:B:3:ILE:HG12	1:B:113:LEU:HD21	1.94	0.48
1:B:123:TYR:O	1:B:127:ARG:HG3	2.13	0.48
1:B:144:ASN:OD1	1:B:336:THR:HG21	2.14	0.48
1:B:296:TYR:HB2	1:B:301:TRP:CE3	2.49	0.48
1:A:3:ILE:C	1:A:3:ILE:HD12	2.39	0.47
1:A:34:ASN:HB2	3:A:569:HOH:O	2.13	0.47
1:B:260:ASN:ND2	1:B:262:TYR:HD2	2.12	0.47
1:B:276:ASN:ND2	1:B:279:ARG:HE	2.12	0.47
1:B:255:ASN:HB3	1:B:259:GLY:HA3	1.95	0.47
1:A:151:MET:CE	1:A:199:ASN:HD22	2.26	0.47
1:A:209:THR:HG22	1:A:210:ASN:ND2	2.30	0.47
1:B:112:TRP:HE3	1:B:296:TYR:CE2	2.32	0.47
1:B:152:VAL:HG13	1:B:175:PRO:O	2.14	0.47
1:A:148:PRO:HA	1:A:151:MET:SD	2.55	0.47
1:A:336:THR:O	1:A:338:LEU:HD22	2.15	0.47
1:A:202:LEU:C	1:A:202:LEU:HD13	2.40	0.47
1:A:256:GLU:O	1:A:263:SER:OG	2.25	0.46
1:A:260:ASN:HD22	1:A:262:TYR:H	1.64	0.46
1:B:80:ASN:ND2	1:B:82:TYR:N	2.64	0.46
1:A:152:VAL:HG13	1:A:175:PRO:O	2.16	0.46
1:A:146:ASP:CB	1:A:203:MET:HE2	2.45	0.46
1:B:159:ASP:O	1:B:165:TYR:HB2	2.15	0.46
1:B:8:ILE:HD13	1:B:32:ALA:H	1.81	0.45
1:A:13:VAL:CG2	1:A:28:CYS:SG	3.04	0.45
1:A:80:ASN:O	1:A:81:PHE:C	2.58	0.45
1:A:295:ASP:HB3	1:A:301:TRP:CH2	2.51	0.45
1:B:49:ARG:HB3	1:B:140:LEU:O	2.16	0.45
1:A:145:TRP:HE1	1:A:273:HIS:CD2	2.24	0.45
1:A:180:ASP:HB2	1:A:195:ARG:HD2	1.97	0.45
1:B:35:ILE:HD13	1:B:307:LEU:CD1	2.43	0.45
1:B:241:ILE:O	1:B:245:ARG:HG2	2.17	0.45
1:A:6:PRO:HB3	1:A:106:ILE:HD12	1.99	0.45
1:A:190:VAL:HG22	1:A:195:ARG:HE	1.81	0.45
1:B:209:THR:HG22	1:B:210:ASN:ND2	2.32	0.45
1:B:120:TRP:NE1	1:B:323:SER:HB3	2.32	0.45
1:B:183:TYR:CZ	1:B:185:GLY:HA2	2.52	0.45
1:A:3:ILE:HG13	1:A:304:ALA:HB1	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:TRP:CE2	1:B:318:VAL:HG13	2.52	0.44
1:B:179:VAL:HA	1:B:246:TRP:CE2	2.52	0.44
1:A:128:ILE:O	1:A:132:LEU:HG	2.18	0.44
1:A:296:TYR:HB2	1:A:301:TRP:CE3	2.52	0.44
1:B:264:ALA:CB	1:B:270:PHE:CD2	3.00	0.44
1:A:178:VAL:HG23	1:A:195:ARG:HG2	2.00	0.44
1:A:263:SER:O	1:A:266:ARG:HG3	2.17	0.44
1:A:124:PHE:CD1	1:A:310:ASP:HA	2.53	0.43
1:B:287:LEU:O	1:B:288:ALA:CB	2.65	0.43
1:A:120:TRP:NE1	1:A:323:SER:HB3	2.34	0.43
1:A:127:ARG:HH11	1:A:311:GLU:CD	2.27	0.43
1:B:104:GLN:HA	1:B:104:GLN:OE1	2.17	0.43
1:B:174:LEU:O	1:B:177:VAL:HG13	2.18	0.43
1:A:112:TRP:CD1	1:A:113:LEU:HD13	2.54	0.43
1:A:114:PHE:CE1	1:A:236:GLU:HG3	2.53	0.43
1:B:124:PHE:O	1:B:128:ILE:HG13	2.17	0.43
1:B:131:LYS:HZ1	1:B:312:ASN:ND2	2.15	0.43
1:B:254:ASN:HB2	1:B:256:GLU:OE1	2.19	0.43
1:B:256:GLU:O	1:B:263:SER:OG	2.29	0.43
1:B:56:ASP:O	1:B:60:ILE:HG13	2.19	0.43
1:B:284:TRP:CZ3	1:B:294:ARG:HG2	2.54	0.43
1:A:38:TYR:CD1	1:A:316:VAL:HG21	2.53	0.42
1:A:79:ARG:NH1	1:A:311:GLU:O	2.51	0.42
1:B:5:ALA:HB2	1:B:305:THR:HG22	2.00	0.42
1:A:49:ARG:HB3	1:A:140:LEU:O	2.20	0.42
1:B:131:LYS:HZ2	1:B:312:ASN:HD22	1.66	0.42
1:B:6:PRO:HB3	1:B:106:ILE:HD12	2.00	0.42
1:A:36:VAL:HG22	1:A:314:GLN:HE21	1.84	0.42
1:A:32:ALA:CB	1:A:315:ALA:HB2	2.49	0.42
1:B:204:TYR:CE1	1:B:208:VAL:HG21	2.54	0.42
1:B:260:ASN:HD22	1:B:262:TYR:N	2.17	0.42
1:A:49:ARG:HD2	1:A:333:TYR:CE1	2.54	0.42
1:A:133:ILE:HG13	1:A:135:ASP:H	1.85	0.42
1:A:152:VAL:CG1	1:A:175:PRO:O	2.68	0.42
1:A:53:HIS:CD2	3:A:515:HOH:O	2.65	0.42
1:B:152:VAL:CG1	1:B:175:PRO:O	2.67	0.42
1:B:32:ALA:CB	1:B:315:ALA:HB2	2.50	0.42
1:A:227:ALA:HB1	1:A:228:PRO:HD2	2.02	0.42
1:A:241:ILE:O	1:A:245:ARG:HG2	2.20	0.42
1:A:179:VAL:HA	1:A:246:TRP:CE2	2.55	0.41
1:B:223:ARG:NH1	1:B:300:ASP:HB2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ALA:HB3	1:B:320:ILE:HD12	2.02	0.41
1:B:38:TYR:HD1	1:B:316:VAL:CG2	2.33	0.41
1:A:326:ASN:O	1:A:329:MET:N	2.52	0.41
1:B:124:PHE:CD1	1:B:310:ASP:HA	2.55	0.41
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.79	0.41
1:B:263:SER:O	1:B:266:ARG:HG3	2.21	0.41
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.94	0.41
1:A:276:ASN:ND2	1:A:279:ARG:HE	2.19	0.40
1:B:6:PRO:HB2	1:B:96:TYR:CD1	2.56	0.40
1:A:151:MET:O	1:A:179:VAL:HG12	2.21	0.40
1:B:112:TRP:CD2	1:B:221:ALA:HA	2.56	0.40
1:B:115:PHE:HB3	1:B:281:TRP:CE3	2.56	0.40
1:A:183:TYR:CZ	1:A:185:GLY:HA2	2.57	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	332/345 (96%)	303 (91%)	23 (7%)	6 (2%)	6	18
1	B	332/345 (96%)	311 (94%)	16 (5%)	5 (2%)	8	22
All	All	664/690 (96%)	614 (92%)	39 (6%)	11 (2%)	7	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PRO
1	A	256	GLU
1	B	175	PRO
1	B	256	GLU
1	A	114	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	257	ASP
1	B	257	ASP
1	B	114	PHE
1	A	53	HIS
1	A	171	GLN
1	B	239	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	285/293 (97%)	255 (90%)	30 (10%)	6	17
1	B	285/293 (97%)	259 (91%)	26 (9%)	9	22
All	All	570/586 (97%)	514 (90%)	56 (10%)	7	19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	15	PRO
1	A	25	ASP
1	A	30	PRO
1	A	57	LYS
1	A	69	LEU
1	A	101	PHE
1	A	108	VAL
1	A	113	LEU
1	A	148	PRO
1	A	175	PRO
1	A	177	VAL
1	A	178	VAL
1	A	179	VAL
1	A	190	VAL
1	A	193	GLN
1	A	202	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	228	PRO
1	A	242	PRO
1	A	256	GLU
1	A	262	TYR
1	A	283	ILE
1	A	287	LEU
1	A	294	ARG
1	A	295	ASP
1	A	305	THR
1	A	314	GLN
1	A	316	VAL
1	A	318	VAL
1	A	336	THR
1	B	7	GLU
1	B	57	LYS
1	B	69	LEU
1	B	101	PHE
1	B	108	VAL
1	B	113	LEU
1	B	131	LYS
1	B	137	SER
1	B	175	PRO
1	B	177	VAL
1	B	179	VAL
1	B	190	VAL
1	B	193	GLN
1	B	202	LEU
1	B	228	PRO
1	B	242	PRO
1	B	256	GLU
1	B	262	TYR
1	B	283	ILE
1	B	294	ARG
1	B	305	THR
1	B	307	LEU
1	B	314	GLN
1	B	316	VAL
1	B	318	VAL
1	B	336	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	53	HIS
1	A	80	ASN
1	A	158	ASN
1	A	194	GLN
1	A	210	ASN
1	A	255	ASN
1	A	260	ASN
1	A	273	HIS
1	A	276	ASN
1	B	34	ASN
1	B	53	HIS
1	B	80	ASN
1	B	158	ASN
1	B	194	GLN
1	B	210	ASN
1	B	260	ASN
1	B	273	HIS
1	B	276	ASN
1	B	312	ASN
1	B	314	GLN
1	B	326	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	C2O	A	500	1	0,2,2	-	-	-		
2	C2O	B	500	1	0,2,2	-	-	-		

There are no bond length outliers.

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	336/345 (97%)	-0.76	1 (0%) 90 89	3, 11, 28, 41	0
1	B	336/345 (97%)	-0.76	2 (0%) 85 85	3, 12, 28, 41	0
All	All	672/690 (97%)	-0.76	3 (0%) 88 87	3, 11, 28, 41	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	SER	2.7
1	B	175	PRO	2.5
1	A	238	SER	2.2

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(Å ²)	Q<0.9
2	C2O	B	500	3/3	0.99	0.03	11,11,16,16	0
2	C2O	A	500	3/3	1.00	0.01	10,10,12,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.