



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:08 PM GMT

PDB ID : 3T0U
Title : Hansenula polymorpha copper amine oxidase-1 in complex with Cu(I)
Authors : Klema, V.J.; Wilmot, C.M.
Deposited on : 2011-07-20
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

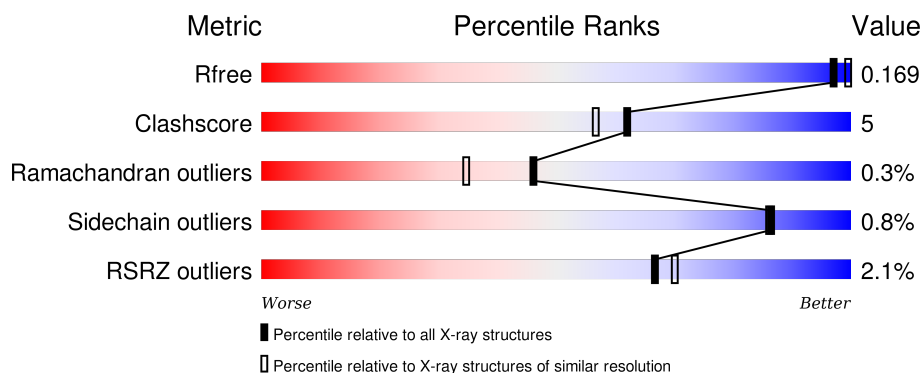
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	692	<div> <div>89%</div> <div>6% 5%</div> </div>
1	B	692	<div> <div>3%</div> <div>88%</div> <div>8% . .</div> </div>
1	C	692	<div> <div>2%</div> <div>87%</div> <div>8% .</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
3	GOL	A	802	-	-	-	X
3	GOL	A	803	-	-	-	X
3	GOL	A	805	-	-	-	X
3	GOL	A	806	-	-	-	X
3	GOL	B	803	-	-	-	X
3	GOL	B	806	-	-	-	X
3	GOL	B	807	-	-	-	X
3	GOL	C	802	-	-	-	X
3	GOL	C	803	-	-	-	X
3	GOL	C	804	-	-	-	X
3	GOL	C	806	-	-	-	X
3	GOL	C	808	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18801 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 Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	657	Total	C	N	O	S	0	15	0
			5276	3366	902	981	27			
1	B	668	Total	C	N	O	S	0	16	0
			5350	3409	913	999	29			
1	C	665	Total	C	N	O	S	0	16	0
			5317	3391	907	991	28			

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



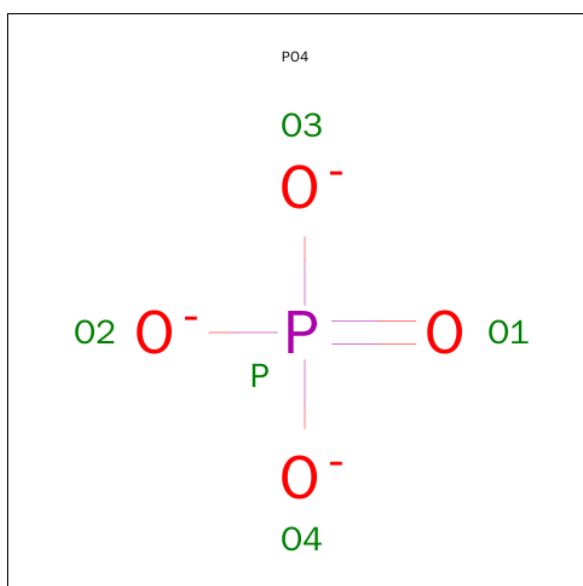
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

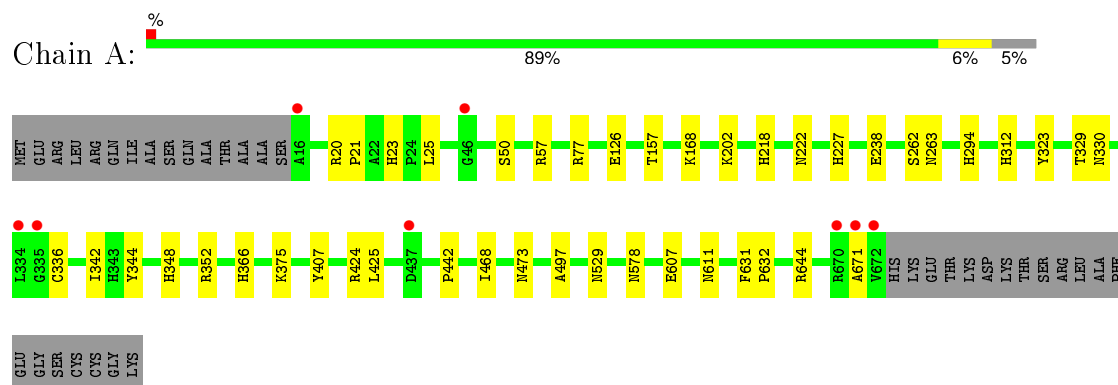
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	914	Total	O	0	0
			914	914		
5	B	915	Total	O	0	0
			915	915		
5	C	907	Total	O	0	0
			907	907		

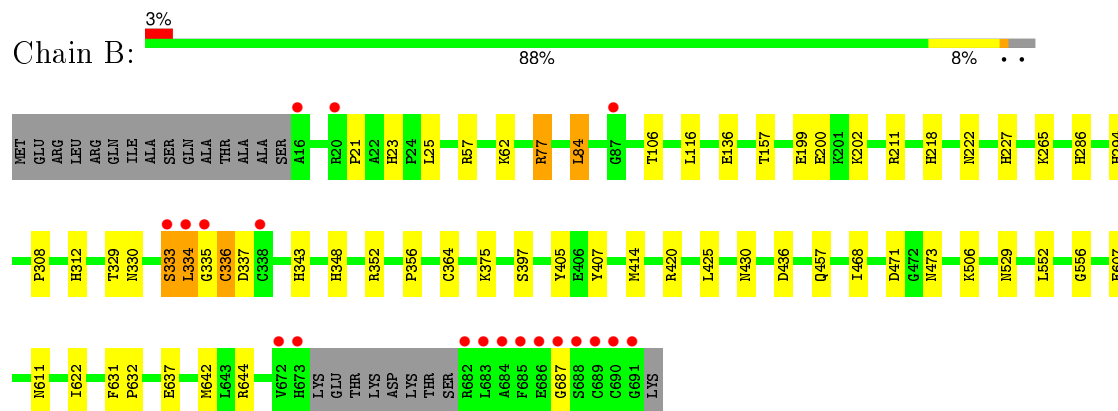
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

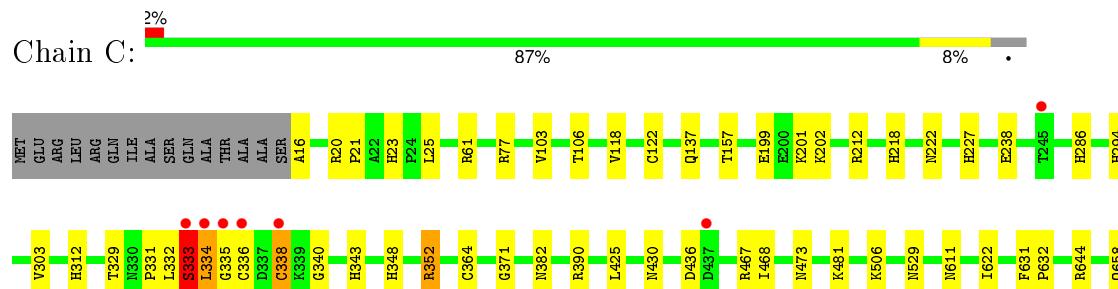
- Molecule 1: Peroxisomal primary amine oxidase

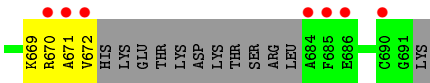


- Molecule 1: Peroxisomal primary amine oxidase



- Molecule 1: Peroxisomal primary amine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.45Å 153.67Å 223.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 1.90 49.14 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.14-1.90) 99.9 (49.14-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.125 , 0.168 0.127 , 0.169	Depositor DCC
R_{free} test set	9388 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 187019 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18801	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, CU1

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	0.68	0/5472	0.66	0/7446
1	B	0.69	0/5550	0.65	1/7549 (0.0%)
1	C	0.67	0/5516	0.66	1/7504 (0.0%)
All	All	0.68	0/16538	0.66	2/22499 (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	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	352	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	333	SER	Peptide

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	5276	0	5160	49	0
1	B	5350	0	5210	71	0
1	C	5317	0	5201	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	30	0	40	1	0
3	B	36	0	48	4	0
3	C	48	0	64	3	0
4	B	5	0	0	0	0
5	A	914	0	0	20	5
5	B	915	0	0	29	2
5	C	907	0	0	30	4
All	All	18801	0	15723	169	7

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 (169) 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:157:THR:CG2	5:A:1786:HOH:O	1.78	1.28
1:A:607:GLU:HG2	5:A:1562:HOH:O	1.35	1.21
1:A:578[B]:ASN:ND2	5:A:1802:HOH:O	1.88	1.05
1:B:157:THR:HG22	5:B:1482:HOH:O	1.57	1.04
1:C:16:ALA:HB1	5:C:1291:HOH:O	1.64	0.96
1:A:644:ARG:NH2	1:B:637[B]:GLU:OE2	2.02	0.92
1:C:23:HIS:HD2	1:C:25:LEU:H	1.15	0.92
1:B:157:THR:CG2	5:B:1482:HOH:O	2.16	0.90
1:B:23:HIS:HD2	1:B:25:LEU:H	1.18	0.90
1:A:57:ARG:NH1	5:A:1803:HOH:O	1.84	0.90
1:C:468:ILE:H	1:C:473:ASN:HD21	1.17	0.89
1:A:23:HIS:HD2	1:A:25:LEU:H	1.16	0.87
1:C:16:ALA:HA	5:C:1427:HOH:O	1.75	0.86
1:C:506[A]:LYS:HE2	5:C:1517:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ILE:H	1:B:473:ASN:HD21	1.28	0.82
1:B:414[B]:MET:SD	1:B:420:ARG:NH1	2.52	0.82
1:A:157:THR:HG22	5:A:1786:HOH:O	1.55	0.82
1:C:670:ARG:C	1:C:672:VAL:H	1.86	0.79
1:C:382[B]:ASN:OD1	5:C:1711:HOH:O	2.01	0.78
1:A:348:HIS:HD2	5:A:1360:HOH:O	1.65	0.77
1:B:336:CYS:HB3	5:B:1792:HOH:O	1.85	0.76
1:B:529:ASN:HD21	1:B:611:ASN:HD21	1.31	0.76
1:A:238:GLU:HG3	5:A:1799:HOH:O	1.85	0.75
1:B:607[A]:GLU:OE1	5:B:1806:HOH:O	2.04	0.75
1:A:529:ASN:HD21	1:A:611:ASN:HD21	1.31	0.74
1:A:50:SER:HB2	1:A:352[A]:ARG:CG	2.19	0.73
1:A:468:ILE:H	1:A:473:ASN:HD21	1.34	0.73
1:C:529:ASN:HD21	1:C:611:ASN:HD21	1.37	0.72
1:A:50:SER:HB2	1:A:352[A]:ARG:HG3	1.73	0.71
1:B:343:HIS:HD2	5:B:1276:HOH:O	1.74	0.70
1:C:157:THR:HG22	5:C:1572:HOH:O	1.91	0.70
1:C:338:CYS:HG	1:C:364:CYS:CB	2.05	0.70
1:C:137:GLN:HE22	1:C:212:ARG:HH12	1.38	0.69
1:B:57:ARG:NH1	5:B:1372:HOH:O	2.07	0.68
1:A:126:GLU:HB2	1:B:687:GLY:HA3	1.76	0.67
1:C:333:SER:HB3	5:C:1389:HOH:O	1.93	0.67
1:B:506[A]:LYS:HE2	5:B:1249:HOH:O	1.95	0.67
1:C:286:HIS:HD2	5:C:1748:HOH:O	1.78	0.66
1:C:332:LEU:HD13	5:C:1286:HOH:O	1.96	0.66
1:B:556:GLY:O	5:B:1392:HOH:O	2.13	0.66
1:A:578[B]:ASN:ND2	5:A:1798:HOH:O	2.08	0.65
1:B:333:SER:O	1:B:334:LEU:HG	1.96	0.65
1:A:23:HIS:CD2	1:A:25:LEU:H	2.08	0.65
1:C:218:HIS:HE1	5:C:1526:HOH:O	1.79	0.64
1:C:436:ASP:O	5:C:1592:HOH:O	2.14	0.64
1:C:294:HIS:HD2	5:C:946:HOH:O	1.80	0.64
1:C:118[A]:VAL:HG22	5:C:1077:HOH:O	1.99	0.63
1:B:57:ARG:NH2	5:B:1279:HOH:O	2.30	0.62
1:B:335:GLY:HA3	1:B:337:ASP:N	2.14	0.62
1:A:336:CYS:SG	5:B:1779:HOH:O	2.47	0.62
1:B:348:HIS:HD2	5:B:1480:HOH:O	1.83	0.61
1:B:218:HIS:HE1	5:B:1255:HOH:O	1.84	0.60
1:C:20:ARG:NH2	5:C:1677:HOH:O	2.22	0.60
1:B:199:GLU:HG3	5:B:953:HOH:O	2.01	0.60
1:A:157:THR:HG22	1:A:323:TYR:OH	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:HIS:HE1	5:A:1523:HOH:O	1.85	0.59
1:B:335:GLY:HA3	1:B:337:ASP:H	1.67	0.59
1:C:436:ASP:H	3:C:808:GOL:H11	1.67	0.59
1:C:340:GLY:HA3	5:C:1641:HOH:O	2.02	0.59
1:C:157:THR:CG2	5:C:1572:HOH:O	2.49	0.59
1:C:343:HIS:HD2	5:C:1463:HOH:O	1.86	0.59
1:C:201:LYS:HD3	5:C:1800:HOH:O	2.03	0.58
1:C:122[B]:CYS:SG	5:C:1418:HOH:O	2.47	0.58
1:C:23:HIS:CD2	1:C:25:LEU:H	2.07	0.58
1:C:670:ARG:C	1:C:672:VAL:N	2.56	0.58
1:B:116:LEU:HD12	1:B:157:THR:HB	1.85	0.57
1:B:200[B]:GLU:CD	1:B:202:LYS:NZ	2.58	0.57
1:C:468:ILE:N	1:C:473:ASN:HD21	1.96	0.57
1:A:342:ILE:HD11	1:A:344:TYR:CE2	2.40	0.57
1:A:644:ARG:CZ	1:B:637[B]:GLU:OE2	2.53	0.56
1:C:348:HIS:HD2	5:C:1243:HOH:O	1.87	0.56
1:A:424:ARG:NE	5:A:1458:HOH:O	2.38	0.56
1:B:506[A]:LYS:HD3	5:B:1304:HOH:O	2.06	0.56
1:A:407:TYR:CD2	1:A:425[B]:LEU:CD2	2.89	0.56
1:C:430:ASN:ND2	5:C:1799:HOH:O	2.10	0.56
1:B:333:SER:O	1:B:334:LEU:CB	2.54	0.55
1:B:294:HIS:HD2	5:B:913:HOH:O	1.89	0.55
1:B:23:HIS:CD2	1:B:25:LEU:H	2.11	0.55
1:C:371:GLY:HA2	1:C:390:ARG:NH2	2.22	0.55
1:B:106:THR:CG2	1:B:106:THR:O	2.55	0.55
1:A:157:THR:HG21	5:A:1786:HOH:O	1.68	0.54
1:B:106:THR:HG23	1:B:106:THR:O	2.07	0.54
1:B:352[B]:ARG:HG2	5:B:1629:HOH:O	2.07	0.54
1:A:126:GLU:HB2	1:B:687:GLY:CA	2.37	0.54
1:B:436:ASP:O	5:B:1391:HOH:O	2.19	0.53
1:B:506[A]:LYS:HE3	5:B:1443:HOH:O	2.09	0.53
1:A:424:ARG:CG	5:A:1458:HOH:O	2.56	0.53
1:B:436:ASP:H	3:B:806:GOL:H32	1.73	0.52
1:A:20:ARG:HH11	1:A:20:ARG:HG3	1.73	0.52
1:C:631:PHE:CG	1:C:632:PRO:HA	2.44	0.52
1:B:62:LYS:HE3	5:B:1352:HOH:O	2.09	0.52
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.40	0.52
1:A:375:LYS:NZ	1:B:330:ASN:HD22	2.08	0.52
1:C:669:LYS:O	1:C:672:VAL:HA	2.11	0.51
1:B:457:GLN:HE22	1:B:552:LEU:H	1.58	0.51
1:C:336:CYS:HB3	5:C:1389:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:SER:O	1:B:334:LEU:CG	2.59	0.51
1:A:342:ILE:HG22	1:A:366:HIS:HB3	1.92	0.51
1:B:506[B]:LYS:HE2	5:B:1329:HOH:O	2.11	0.50
1:A:442:PRO:HG3	3:B:807:GOL:H31	1.94	0.50
1:A:330:ASN:HD22	1:B:375:LYS:NZ	2.09	0.50
1:B:84:LEU:HD23	1:B:84:LEU:N	2.26	0.50
1:B:222:ASN:HB3	1:B:227:HIS:CG	2.48	0.49
1:C:468:ILE:H	1:C:473:ASN:ND2	1.96	0.49
1:C:137:GLN:HE21	1:C:212:ARG:HH22	1.59	0.49
1:C:312:HIS:HD2	5:C:1054:HOH:O	1.96	0.49
1:B:364[A]:CYS:SG	1:B:397:SER:OG	2.71	0.48
1:B:200[B]:GLU:CD	1:B:202:LYS:HZ2	2.14	0.48
1:C:16:ALA:CB	5:C:1291:HOH:O	2.40	0.48
1:C:338:CYS:HG	1:C:364:CYS:HB2	1.75	0.48
1:A:468:ILE:H	1:A:473:ASN:ND2	2.07	0.48
1:B:471:ASP:OD1	5:B:1501:HOH:O	2.20	0.48
1:B:644:ARG:NH1	5:B:1533:HOH:O	2.47	0.48
1:A:424:ARG:HG2	5:A:1458:HOH:O	2.13	0.47
1:B:631:PHE:CG	1:B:632:PRO:HA	2.49	0.47
1:B:116:LEU:CD1	1:B:157:THR:HB	2.45	0.47
1:C:506[B]:LYS:HD2	5:C:1670:HOH:O	2.14	0.47
1:C:669:LYS:HE2	5:C:1755:HOH:O	2.14	0.47
1:B:468:ILE:H	1:B:473:ASN:ND2	2.04	0.47
1:B:405:TYR:CD1	1:B:425[A]:LEU:HD11	2.49	0.47
1:C:201:LYS:NZ	5:C:1521:HOH:O	2.47	0.47
1:A:631:PHE:CG	1:A:632:PRO:HA	2.49	0.47
1:C:425[B]:LEU:HD12	1:C:622:ILE:HD11	1.97	0.47
1:A:294:HIS:HD2	5:A:1787:HOH:O	1.97	0.47
3:B:805:GOL:H31	5:B:1315:HOH:O	2.15	0.47
1:B:211:ARG:NH2	5:B:1803:HOH:O	2.47	0.47
1:B:430:ASN:ND2	5:B:1802:HOH:O	2.23	0.46
1:A:50:SER:HB2	1:A:352[A]:ARG:HG2	1.94	0.46
1:B:312:HIS:HD2	5:B:1009:HOH:O	1.97	0.46
1:C:23:HIS:HE1	3:C:806:GOL:O1	1.98	0.46
1:B:468:ILE:N	1:B:473:ASN:HD21	2.05	0.46
1:C:658:GLN:NE2	5:C:1790:HOH:O	2.12	0.46
1:B:407:TYR:CD2	1:B:425[B]:LEU:CD2	2.98	0.46
1:A:312:HIS:HD2	5:A:973:HOH:O	1.98	0.46
1:C:303:VAL:HG23	5:C:1261:HOH:O	2.15	0.45
1:A:342:ILE:CD1	1:A:344:TYR:CE2	3.00	0.45
1:A:168:LYS:HE2	5:A:1570:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:CD2	1:B:84:LEU:N	2.79	0.45
5:A:1405:HOH:O	1:B:642:MET:CE	2.65	0.45
5:A:1419:HOH:O	1:B:286:HIS:HD2	2.00	0.44
1:B:407:TYR:CE2	1:B:425[B]:LEU:HD22	2.53	0.44
1:A:23:HIS:HE1	3:A:802:GOL:O1	2.00	0.44
1:A:375:LYS:NZ	1:B:337:ASP:OD1	2.51	0.44
1:B:265:LYS:NZ	5:B:1634:HOH:O	2.51	0.44
1:C:331:PRO:HD2	5:C:1315:HOH:O	2.17	0.44
1:C:670:ARG:O	1:C:672:VAL:N	2.49	0.43
1:C:61:ARG:NH2	1:C:467:ARG:HG3	2.33	0.43
1:B:506[B]:LYS:HD2	5:B:1330:HOH:O	2.19	0.43
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.48	0.43
1:A:330:ASN:HD22	1:B:375:LYS:HZ3	1.66	0.43
1:B:425[B]:LEU:HD12	1:B:622:ILE:HD11	2.01	0.43
1:A:497:ALA:HB2	1:B:308:PRO:HB3	2.00	0.42
1:B:200[B]:GLU:OE1	1:B:202:LYS:NZ	2.49	0.42
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.49	0.42
1:A:407:TYR:CD2	1:A:425[B]:LEU:HD22	2.55	0.41
1:B:136:GLU:HG3	5:B:1278:HOH:O	2.19	0.41
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.55	0.41
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.55	0.41
1:C:199:GLU:OE1	1:C:352:ARG:NH2	2.48	0.41
1:C:103:VAL:HG11	1:C:106[B]:THR:CG2	2.50	0.41
1:C:333:SER:HA	1:C:334:LEU:C	2.41	0.41
1:B:23:HIS:HE1	3:B:803:GOL:O3	2.03	0.41
1:A:238:GLU:CD	5:A:1799:HOH:O	2.58	0.40
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.56	0.40
3:C:803:GOL:H12	5:C:1783:HOH:O	2.20	0.40
1:C:506[B]:LYS:HD3	1:C:506[B]:LYS:HA	1.88	0.40
1:A:238:GLU:CG	5:A:1799:HOH:O	2.55	0.40
1:A:262:SER:O	1:A:263:ASN:HB2	2.21	0.40
1:C:338:CYS:CB	1:C:364:CYS:SG	3.10	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1570:HOH:O	5:A:1570:HOH:O[3_555]	1.65	0.55
5:B:1468:HOH:O	5:C:1725:HOH:O[3_555]	1.91	0.29
5:A:1777:HOH:O	5:B:1481:HOH:O[3_555]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1359:HOH:O	5:C:1765:HOH:O[3_555]	2.01	0.19
5:A:1352:HOH:O	5:C:901:HOH:O[5_455]	2.06	0.14
5:A:1348:HOH:O	5:C:1585:HOH:O[5_555]	2.15	0.05
5:A:931:HOH:O	5:A:1433:HOH:O[4_565]	2.16	0.04

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	670/692 (97%)	646 (96%)	23 (3%)	1 (0%)	56	46
1	B	680/692 (98%)	659 (97%)	19 (3%)	2 (0%)	46	35
1	C	677/692 (98%)	653 (96%)	21 (3%)	3 (0%)	39	27
All	All	2027/2076 (98%)	1958 (97%)	63 (3%)	6 (0%)	46	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	SER
1	B	334	LEU
1	C	333	SER
1	C	671	ALA
1	A	671	ALA
1	C	335	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/594 (98%)	578 (100%)	2 (0%)	94	95
1	B	588/594 (99%)	584 (99%)	4 (1%)	88	88
1	C	586/594 (99%)	579 (99%)	7 (1%)	78	76
All	All	1754/1782 (98%)	1741 (99%)	13 (1%)	86	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LYS
1	A	329	THR
1	B	84	LEU
1	B	329	THR
1	B	336	CYS
1	B	356	PRO
1	C	202	LYS
1	C	238	GLU
1	C	329	THR
1	C	334	LEU
1	C	338	CYS
1	C	481	LYS
1	C	644	ARG

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

Mol	Chain	Res	Type
1	A	23	HIS
1	A	218	HIS
1	A	286	HIS
1	A	294	HIS
1	A	312	HIS
1	A	330	ASN
1	A	343	HIS
1	A	348	HIS
1	A	361	ASN
1	A	450	ASN
1	A	473	ASN
1	A	529	ASN
1	B	23	HIS
1	B	66	GLN
1	B	70	GLN
1	B	218	HIS

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Mol	Chain	Res	Type
1	B	286	HIS
1	B	294	HIS
1	B	312	HIS
1	B	330	ASN
1	B	343	HIS
1	B	348	HIS
1	B	450	ASN
1	B	457	GLN
1	B	473	ASN
1	B	529	ASN
1	B	547	GLN
1	C	23	HIS
1	C	70	GLN
1	C	137	GLN
1	C	218	HIS
1	C	286	HIS
1	C	288	ASN
1	C	294	HIS
1	C	312	HIS
1	C	330	ASN
1	C	343	HIS
1	C	348	HIS
1	C	361	ASN
1	C	450	ASN
1	C	473	ASN
1	C	529	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	802	-	5,5,5	0.25	0	5,5,5	0.61	0
3	GOL	A	803	-	5,5,5	0.36	0	5,5,5	0.39	0
3	GOL	A	804	-	5,5,5	0.47	0	5,5,5	0.33	0
3	GOL	A	805	-	5,5,5	0.26	0	5,5,5	0.80	0
3	GOL	A	806	-	5,5,5	0.42	0	5,5,5	0.33	0
3	GOL	B	802	-	5,5,5	0.28	0	5,5,5	0.49	0
3	GOL	B	803	-	5,5,5	0.37	0	5,5,5	0.68	0
4	PO4	B	804	-	4,4,4	0.37	0	6,6,6	0.25	0
3	GOL	B	805	-	5,5,5	0.45	0	5,5,5	0.29	0
3	GOL	B	806	-	5,5,5	0.42	0	5,5,5	0.29	0
3	GOL	B	807	-	5,5,5	0.39	0	5,5,5	0.64	0
3	GOL	B	808	-	5,5,5	0.40	0	5,5,5	0.49	0
3	GOL	C	802	-	5,5,5	0.45	0	5,5,5	0.62	0
3	GOL	C	803	-	5,5,5	0.41	0	5,5,5	0.41	0
3	GOL	C	804	-	5,5,5	0.27	0	5,5,5	0.75	0
3	GOL	C	805	-	5,5,5	0.44	0	5,5,5	0.40	0
3	GOL	C	806	-	5,5,5	0.30	0	5,5,5	0.61	0
3	GOL	C	807	-	5,5,5	0.34	0	5,5,5	0.64	0
3	GOL	C	808	-	5,5,5	0.40	0	5,5,5	0.47	0
3	GOL	C	809	-	5,5,5	0.33	0	5,5,5	0.24	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
3	GOL	A	802	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
3	GOL	A	805	-	-	0/4/4/4	0/0/0/0
3	GOL	A	806	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	802	-	-	0/4/4/4	0/0/0/0
3	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	PO4	B	804	-	-	0/0/0/0	0/0/0/0
3	GOL	B	805	-	-	0/4/4/4	0/0/0/0
3	GOL	B	806	-	-	0/4/4/4	0/0/0/0
3	GOL	B	807	-	-	0/4/4/4	0/0/0/0
3	GOL	B	808	-	-	0/4/4/4	0/0/0/0
3	GOL	C	802	-	-	0/4/4/4	0/0/0/0
3	GOL	C	803	-	-	0/4/4/4	0/0/0/0
3	GOL	C	804	-	-	0/4/4/4	0/0/0/0
3	GOL	C	805	-	-	0/4/4/4	0/0/0/0
3	GOL	C	806	-	-	0/4/4/4	0/0/0/0
3	GOL	C	807	-	-	0/4/4/4	0/0/0/0
3	GOL	C	808	-	-	0/4/4/4	0/0/0/0
3	GOL	C	809	-	-	0/4/4/4	0/0/0/0

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.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	GOL	1	0
3	B	803	GOL	1	0
3	B	805	GOL	1	0
3	B	806	GOL	1	0
3	B	807	GOL	1	0
3	C	803	GOL	1	0
3	C	806	GOL	1	0
3	C	808	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	657/692 (94%)	-0.45	8 (1%) 81 83	4, 11, 25, 55	0
1	B	668/692 (96%)	-0.37	19 (2%) 56 60	5, 11, 28, 68	0
1	C	665/692 (96%)	-0.48	14 (2%) 67 70	4, 10, 27, 63	0
All	All	1990/2076 (95%)	-0.43	41 (2%) 67 70	4, 10, 27, 68	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	683	LEU	7.8
1	B	333	SER	6.9
1	C	672	VAL	6.9
1	B	673	HIS	6.9
1	B	682	ARG	6.7
1	B	334	LEU	6.2
1	A	672	VAL	5.9
1	B	685	PHE	5.5
1	B	684	ALA	4.7
1	C	334	LEU	4.6
1	B	689	CYS	4.5
1	C	684	ALA	4.2
1	B	16	ALA	4.0
1	C	335	GLY	4.0
1	B	672	VAL	3.8
1	A	335	GLY	3.8
1	B	690	CYS	3.5
1	B	686	GLU	3.4
1	B	338[A]	CYS	3.2
1	B	687	GLY	2.8
1	C	336	CYS	2.8
1	A	437	ASP	2.7
1	A	16	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	688	SER	2.6
1	A	334	LEU	2.6
1	A	671	ALA	2.6
1	C	671	ALA	2.5
1	A	670	ARG	2.4
1	C	245	THR	2.4
1	C	333	SER	2.4
1	B	691	GLY	2.4
1	A	46	GLY	2.4
1	B	335	GLY	2.3
1	C	338	CYS	2.3
1	B	87	GLY	2.3
1	C	686	GLU	2.2
1	C	437	ASP	2.2
1	C	690	CYS	2.2
1	B	20	ARG	2.1
1	C	670	ARG	2.1
1	C	685	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	C	802	6/6	0.92	0.15	16.83	32,39,40,41	0
3	GOL	A	803	6/6	0.86	0.20	9.44	36,41,45,51	0
3	GOL	C	803	6/6	0.89	0.18	6.43	47,53,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	807	6/6	0.88	0.15	4.49	36,43,46,46	0
3	GOL	A	802	6/6	0.95	0.18	4.38	20,25,28,29	0
3	GOL	A	805	6/6	0.89	0.21	3.99	29,34,36,37	0
3	GOL	C	806	6/6	0.95	0.11	3.84	17,25,31,37	0
3	GOL	A	806	6/6	0.95	0.13	3.74	15,21,22,23	0
3	GOL	B	803	6/6	0.97	0.12	3.37	21,25,27,30	0
3	GOL	B	806	6/6	0.87	0.15	2.86	28,37,38,39	0
3	GOL	C	808	6/6	0.74	0.18	2.66	37,39,41,43	0
3	GOL	C	804	6/6	0.91	0.15	2.23	31,36,39,44	0
3	GOL	C	809	6/6	0.92	0.15	1.88	35,37,40,44	0
3	GOL	B	808	6/6	0.96	0.10	1.55	12,16,21,22	0
3	GOL	B	802	6/6	0.97	0.08	0.87	13,22,25,30	0
3	GOL	C	805	6/6	0.98	0.09	0.75	14,16,20,22	0
2	CU1	C	801	1/1	1.00	0.06	-1.54	9,9,9,9	0
2	CU1	B	801	1/1	1.00	0.05	-2.80	9,9,9,9	0
2	CU1	A	801	1/1	1.00	0.06	-3.12	9,9,9,9	0
3	GOL	B	805	6/6	0.82	0.22	-	54,58,59,61	0
4	PO4	B	804	5/5	0.89	0.22	-	33,49,52,52	0
3	GOL	C	807	6/6	0.80	0.17	-	28,36,42,45	0
3	GOL	A	804	6/6	0.78	0.28	-	61,64,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.