Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 09:20 AM EST

PDB ID	:	1IU7
Title	:	HOLO FORM OF COPPER-CONTAINING AMINE OXIDASE FROM ARTHROBACTER GLOBIFORMIS
Authors	:	Kishishita, S.; Okajima, T.; Kim, M.; Yamaguchi, H.; Hirota, S.; Suzuki, S.; Kuroda, S.; Tanizawa, K.; Mure, M.
Deposited on	:	2002-02-28
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

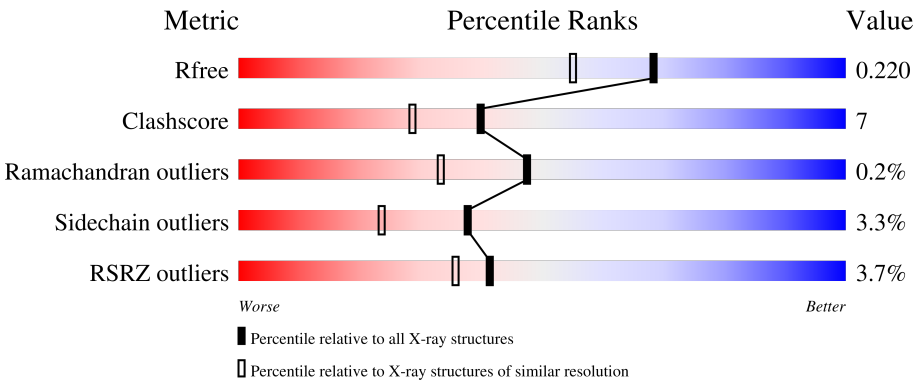
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	638	5% 78% 17% • •
1	B	638	2% 84% 12% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10980 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 AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	620	4868	3074	855	930	9	0	0	0
1	B	620	4868	3074	855	930	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	TPQ	TYR	modified residue	UNP P46881
B	382	TPQ	TYR	modified residue	UNP P46881

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

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

- Molecule 3 is water.

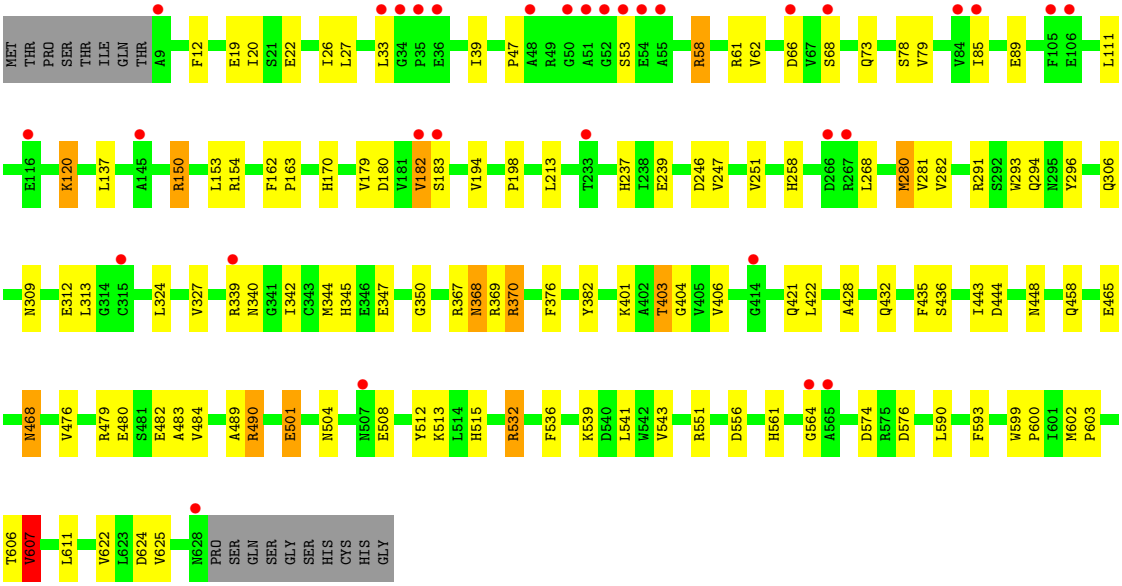
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	561	561	561	0	0
3	B	681	681	681	0	0

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.

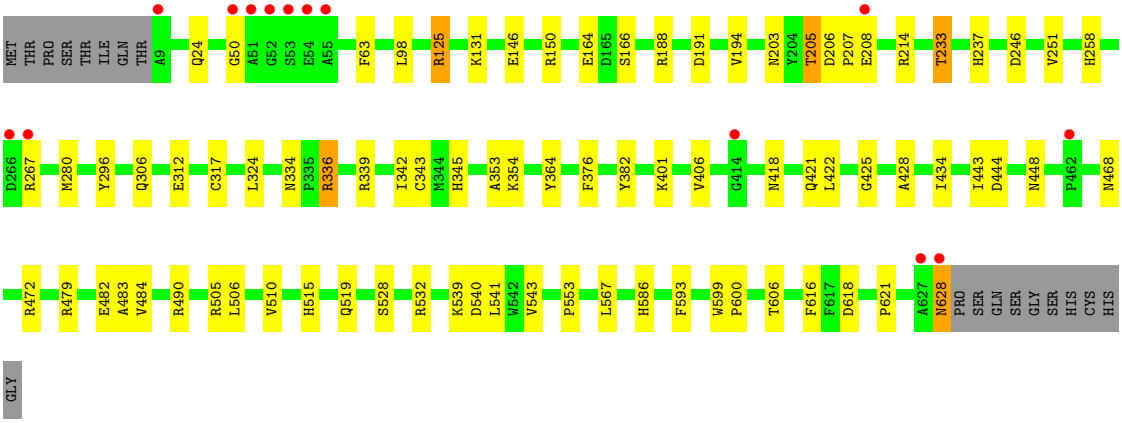
• Molecule 1: AMINE OXIDASE

Chain A: 5% 78% 17%



• Molecule 1: AMINE OXIDASE

Chain B: 2% 84% 12%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.79Å 62.63Å 183.96Å 90.00° 111.74° 90.00°	Depositor
Resolution (Å)	7.00 – 1.80 17.53 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.80) 94.1 (17.53-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	6.34 (at 1.70Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.209 , 0.252 0.182 , 0.220	Depositor DCC
R_{free} test set	8668 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 88.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10980	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8779e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CU, TPQ

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	0.46	0/4975	0.74	3/6774 (0.0%)
1	B	0.48	0/4975	0.74	2/6774 (0.0%)
All	All	0.47	0/9950	0.74	5/13548 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	593	PHE	N-CA-C	-5.86	95.18	111.00
1	B	125	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	607	VAL	CB-CA-C	-5.39	101.16	111.40
1	A	268	LEU	N-CA-C	-5.27	96.76	111.00
1	B	593	PHE	N-CA-C	-5.22	96.91	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	364	TYR	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	4868	0	4686	90	0
1	B	4868	0	4686	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	561	0	0	13	0
3	B	681	0	0	12	0
All	All	10980	0	9372	138	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 7.

All (138) 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:590:LEU:HG	1:A:607:VAL:HG22	1.63	0.81
1:A:458:GLN:HE22	1:B:418:ASN:HD21	1.32	0.78
1:B:532:ARG:HG2	3:B:1458:HOH:O	1.86	0.74
1:A:247:VAL:HG21	1:A:344:MET:CE	2.18	0.74
1:A:20:ILE:HD12	1:A:327:VAL:HG12	1.71	0.72
1:A:294:GLN:HG3	1:A:296:TYR:CZ	2.29	0.68
1:B:166:SER:H	1:B:203:ASN:HD21	1.41	0.68
1:A:403:THR:HG21	1:B:354:LYS:H	1.59	0.67
3:A:1352:HOH:O	1:B:621:PRO:HD2	1.96	0.66
1:A:625:VAL:HB	3:B:1682:HOH:O	1.96	0.65
1:B:479:ARG:HD3	3:B:1588:HOH:O	1.97	0.64
1:A:170:HIS:HD2	1:A:198:PRO:O	1.80	0.64
1:A:490:ARG:HH12	1:B:490:ARG:H	1.47	0.62
1:A:443:ILE:H	1:A:448:ASN:HD21	1.48	0.62
1:A:564:GLY:HA2	3:A:1481:HOH:O	1.99	0.62
1:B:505:ARG:HD3	1:B:618:ASP:HB3	1.83	0.61
1:A:590:LEU:HG	1:A:607:VAL:CG2	2.31	0.61
1:A:622:VAL:O	1:A:625:VAL:HG12	2.01	0.60
1:A:294:GLN:HG3	1:A:296:TYR:OH	2.01	0.60
1:A:406:VAL:HG21	1:A:422:LEU:HD11	1.84	0.59
1:A:162:PHE:HB2	1:A:163:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:HG2	1:A:606:THR:HG22	1.84	0.59
1:A:504:ASN:ND2	1:A:508:GLU:HG3	2.18	0.58
1:B:125:ARG:HG2	1:B:194:VAL:HG23	1.86	0.58
1:A:504:ASN:HD21	1:A:508:GLU:CG	2.17	0.57
1:A:78:SER:HB2	1:A:85:ILE:HD11	1.87	0.57
1:A:137:LEU:HD13	1:A:296:TYR:OH	2.05	0.57
1:A:247:VAL:HG21	1:A:344:MET:HE1	1.87	0.56
1:B:406:VAL:HG21	1:B:422:LEU:HD11	1.89	0.55
1:B:443:ILE:H	1:B:448:ASN:HD21	1.54	0.55
1:A:504:ASN:HD21	1:A:508:GLU:HG3	1.70	0.55
1:B:205:THR:HB	3:B:1174:HOH:O	2.06	0.55
1:B:484:VAL:HG12	1:B:539:LYS:HG3	1.90	0.54
1:A:251:VAL:CG2	1:A:306:GLN:HB3	2.38	0.53
1:A:150:ARG:HH12	1:A:183:SER:HB3	1.74	0.53
1:A:19:GLU:OE2	1:A:58:ARG:HG2	2.09	0.52
1:A:347:GLU:OE1	1:A:370:ARG:HD3	2.10	0.52
1:B:146:GLU:O	1:B:150:ARG:HD3	2.09	0.52
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.44	0.52
1:A:489:ALA:H	1:A:490:ARG:HH21	1.56	0.52
1:B:267:ARG:HG2	1:B:267:ARG:HH11	1.74	0.52
1:A:421:GLN:HG2	1:B:506:LEU:HD13	1.91	0.52
1:A:624:ASP:CG	1:B:214:ARG:HD2	2.31	0.51
1:A:137:LEU:HB3	1:A:296:TYR:CE1	2.46	0.51
1:B:401:LYS:HG2	1:B:606:THR:HG22	1.92	0.50
1:A:350:GLY:HA2	1:A:367:ARG:NH2	2.27	0.50
1:A:403:THR:HG22	1:A:404:GLY:H	1.75	0.50
1:B:125:ARG:NH2	1:B:191:ASP:OD2	2.45	0.50
1:A:551:ARG:HG2	3:A:1520:HOH:O	2.11	0.49
1:A:73:GLN:HG2	1:A:89:GLU:HA	1.93	0.49
1:A:403:THR:HG21	1:B:354:LYS:N	2.27	0.49
1:B:472:ARG:HD3	3:B:1577:HOH:O	2.10	0.49
1:A:484:VAL:HG12	1:A:539:LYS:HG3	1.95	0.49
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.47	0.49
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.78	0.49
1:B:336:ARG:HG3	1:B:336:ARG:HH11	1.77	0.49
1:A:368:ASN:ND2	1:A:369:ARG:H	2.10	0.49
1:A:465:GLU:H	1:A:465:GLU:CD	2.17	0.49
1:A:501:GLU:HB2	3:A:1529:HOH:O	2.14	0.48
1:A:150:ARG:HD3	3:A:1111:HOH:O	2.12	0.48
1:B:125:ARG:HH22	1:B:191:ASP:CG	2.16	0.48
1:A:251:VAL:HG23	1:A:306:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:THR:HG22	1:B:237:HIS:HB3	1.94	0.48
1:A:111:LEU:HD12	1:A:179:VAL:HG11	1.96	0.47
1:A:237:HIS:HD2	1:A:246:ASP:OD1	1.97	0.47
1:A:339:ARG:HH11	1:A:340:ASN:HD22	1.61	0.47
1:A:246:ASP:HB2	1:A:258:HIS:HB2	1.96	0.47
1:A:345:HIS:CD2	3:A:1088:HOH:O	2.68	0.47
1:A:237:HIS:HE1	1:A:239:GLU:OE1	1.98	0.47
1:A:180:ASP:OD1	1:A:182:VAL:HG23	2.15	0.47
1:A:403:THR:HG21	1:B:353:ALA:HA	1.96	0.47
1:A:324:LEU:HB2	1:A:342:ILE:HB	1.97	0.47
1:A:61:ARG:HH22	1:A:556:ASP:CG	2.19	0.47
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.97	0.46
1:A:339:ARG:HD3	3:A:1491:HOH:O	2.15	0.46
1:B:246:ASP:HB2	1:B:258:HIS:HB2	1.96	0.46
1:A:194:VAL:HG13	3:A:1027:HOH:O	2.15	0.46
1:B:528:SER:O	1:B:532:ARG:HD3	2.15	0.46
1:B:540:ASP:O	1:B:586:HIS:HD2	1.99	0.46
1:A:39:ILE:HD12	1:A:62:VAL:HG11	1.98	0.46
1:B:280:MET:HA	1:B:434:ILE:O	2.15	0.46
1:A:468:ASN:HD22	1:A:468:ASN:H	1.64	0.45
1:B:237:HIS:HD2	1:B:246:ASP:OD1	1.99	0.45
1:A:368:ASN:HD22	1:A:369:ARG:H	1.64	0.45
1:A:22:GLU:O	1:A:26:ILE:HG13	2.17	0.45
1:B:586:HIS:HE1	3:B:1014:HOH:O	1.98	0.45
1:A:309:ASN:ND2	1:B:354:LYS:HE3	2.31	0.45
1:A:120:LYS:NZ	1:A:120:LYS:HB2	2.31	0.45
1:A:483:ALA:HB1	1:A:543:VAL:HB	1.99	0.45
1:A:294:GLN:HE21	1:A:296:TYR:HE2	1.65	0.44
1:B:131:LYS:HA	1:B:131:LYS:HD3	1.77	0.44
1:B:510:VAL:HB	1:B:616:PHE:HA	2.00	0.44
1:A:12:PHE:CE1	1:A:47:PRO:HD2	2.53	0.44
1:B:317:CYS:SG	1:B:343:CYS:CB	3.06	0.44
1:A:479:ARG:NH1	1:A:576:ASP:HB2	2.33	0.43
1:B:483:ALA:HB1	1:B:543:VAL:HB	1.99	0.43
1:B:484:VAL:CG1	1:B:539:LYS:HG3	2.47	0.43
1:A:479:ARG:O	1:A:482:GLU:HG2	2.18	0.43
1:B:63:PHE:HB3	1:B:98:LEU:HD13	1.99	0.43
1:A:370:ARG:O	1:A:370:ARG:HG2	2.18	0.43
1:A:282:VAL:HA	1:A:432:GLN:O	2.19	0.43
1:B:324:LEU:HB2	1:B:342:ILE:HB	2.00	0.43
1:B:131:LYS:HG3	3:B:1590:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:HIS:HB3	3:A:1037:HOH:O	2.18	0.43
1:B:24:GLN:HE22	1:B:334:ASN:ND2	2.16	0.43
1:A:515:HIS:HE1	3:A:1043:HOH:O	2.01	0.43
1:A:532:ARG:HG2	1:A:532:ARG:HH11	1.84	0.43
1:A:476:VAL:HG12	3:A:1206:HOH:O	2.19	0.42
1:A:280:MET:HG3	1:A:435:PHE:CD2	2.54	0.42
1:B:146:GLU:OE1	1:B:188:ARG:NH1	2.52	0.42
1:B:421:GLN:HE21	1:B:425:GLY:H	1.66	0.42
1:B:553:PRO:HA	1:B:567:LEU:HG	2.01	0.42
1:A:22:GLU:HG2	1:A:79:VAL:HG13	2.01	0.42
1:A:27:LEU:HB3	1:A:33:LEU:HB2	2.00	0.42
1:B:532:ARG:NH1	3:B:1458:HOH:O	2.52	0.42
1:A:137:LEU:HD22	1:A:296:TYR:CZ	2.55	0.42
1:A:436:SER:HB2	1:A:536:PHE:CE2	2.54	0.42
1:B:233:THR:HB	3:B:1128:HOH:O	2.19	0.41
1:A:513:LYS:O	1:A:611:LEU:HA	2.20	0.41
1:A:20:ILE:CD1	1:A:327:VAL:HG12	2.45	0.41
1:B:490:ARG:HD3	3:B:1609:HOH:O	2.20	0.41
1:B:515:HIS:HE1	3:B:1080:HOH:O	2.03	0.41
1:A:66:ASP:OD1	1:A:68:SER:HB2	2.20	0.41
1:A:443:ILE:H	1:A:448:ASN:ND2	2.17	0.41
1:B:479:ARG:O	1:B:482:GLU:HG2	2.20	0.41
1:B:206:ASP:HA	1:B:207:PRO:HD2	1.94	0.41
1:B:251:VAL:HG22	1:B:306:GLN:HB2	2.02	0.41
1:B:345:HIS:HE1	3:B:1298:HOH:O	2.02	0.41
1:A:345:HIS:HD2	3:A:1088:HOH:O	2.04	0.41
1:B:628:ASN:HD22	1:B:628:ASN:HA	1.74	0.41
1:A:291:ARG:HG2	1:A:294:GLN:OE1	2.21	0.41
1:A:603:PRO:HG2	3:A:1352:HOH:O	2.20	0.41
1:B:422:LEU:HD11	1:B:428:ALA:HB2	2.03	0.41
1:A:590:LEU:CG	1:A:607:VAL:HG22	2.43	0.40
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.96	0.40
1:A:602:MET:HA	1:A:603:PRO:HD3	1.93	0.40
1:A:154:ARG:HD2	1:A:293:TRP:CD2	2.56	0.40
1:A:480:GLU:HB2	1:A:574:ASP:HA	2.03	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	617/638 (97%)	587 (95%)	29 (5%)	1 (0%)	47	33
1	B	617/638 (97%)	588 (95%)	28 (4%)	1 (0%)	47	33
All	All	1234/1276 (97%)	1175 (95%)	57 (5%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	B	50	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	513/529 (97%)	492 (96%)	21 (4%)	30	16
1	B	513/529 (97%)	500 (98%)	13 (2%)	47	34
All	All	1026/1058 (97%)	992 (97%)	34 (3%)	38	23

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	120	LYS
1	A	150	ARG
1	A	182	VAL

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Mol	Chain	Res	Type
1	A	213	LEU
1	A	280	MET
1	A	281	VAL
1	A	312	GLU
1	A	313	LEU
1	A	368	ASN
1	A	370	ARG
1	A	376	PHE
1	A	403	THR
1	A	444	ASP
1	A	468	ASN
1	A	490	ARG
1	A	501	GLU
1	A	512	TYR
1	A	532	ARG
1	A	541	LEU
1	A	607	VAL
1	B	164	GLU
1	B	205	THR
1	B	208	GLU
1	B	233	THR
1	B	296	TYR
1	B	312	GLU
1	B	336	ARG
1	B	376	PHE
1	B	444	ASP
1	B	468	ASN
1	B	519	GLN
1	B	541	LEU
1	B	628	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	237	HIS
1	A	273	ASN
1	A	309	ASN
1	A	334	ASN
1	A	340	ASN
1	A	345	HIS
1	A	368	ASN

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Mol	Chain	Res	Type
1	A	421	GLN
1	A	448	ASN
1	A	458	GLN
1	A	468	ASN
1	A	515	HIS
1	A	628	ASN
1	B	203	ASN
1	B	224	GLN
1	B	237	HIS
1	B	273	ASN
1	B	334	ASN
1	B	345	HIS
1	B	421	GLN
1	B	448	ASN
1	B	468	ASN
1	B	507	ASN
1	B	515	HIS
1	B	519	GLN
1	B	561	HIS
1	B	586	HIS
1	B	628	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPQ	B	382	1	13,14,15	2.37	5 (38%)	15,19,21	1.38	2 (13%)
1	TPQ	A	382	1	13,14,15	2.44	7 (53%)	15,19,21	1.89	3 (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
1	TPQ	B	382	1	-	2/5/22/24	0/1/1/1
1	TPQ	A	382	1	-	1/5/22/24	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	TPQ	O2-C2	4.39	1.36	1.24
1	B	382	TPQ	O5-C5	4.12	1.35	1.24
1	B	382	TPQ	O2-C2	4.11	1.35	1.24
1	B	382	TPQ	C3-C4	3.60	1.41	1.35
1	A	382	TPQ	C3-C4	3.54	1.41	1.35
1	A	382	TPQ	O5-C5	3.48	1.33	1.24
1	B	382	TPQ	C1-C2	-2.99	1.44	1.49
1	A	382	TPQ	C1-C2	-2.79	1.44	1.49
1	B	382	TPQ	C6-C1	2.68	1.41	1.34
1	A	382	TPQ	CB-CA	2.45	1.59	1.53
1	A	382	TPQ	C6-C1	2.22	1.40	1.34
1	A	382	TPQ	C6-C5	-2.08	1.39	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	382	TPQ	CB-CA-C	-4.89	102.30	111.47
1	A	382	TPQ	CA-CB-C1	3.48	120.16	113.51
1	B	382	TPQ	CB-CA-C	-3.23	105.41	111.47
1	B	382	TPQ	O2-C2-C3	-2.75	115.49	121.78
1	A	382	TPQ	O2-C2-C3	-2.69	115.61	121.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382	TPQ	O-C-CA-CB
1	B	382	TPQ	O-C-CA-CB
1	B	382	TPQ	N-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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	619/638 (97%)	0.04	32 (5%)	27	22	5, 18, 42, 91	0
1	B	619/638 (97%)	-0.29	14 (2%)	60	56	4, 14, 28, 88	0
All	All	1238/1276 (97%)	-0.13	46 (3%)	41	36	4, 16, 39, 91	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	ALA	19.0
1	A	51	ALA	14.8
1	B	53	SER	11.8
1	A	52	GLY	11.6
1	B	52	GLY	11.0
1	A	53	SER	9.3
1	A	54	GLU	8.2
1	A	628	ASN	7.8
1	B	54	GLU	7.7
1	A	9	ALA	7.3
1	A	50	GLY	7.2
1	A	55	ALA	7.0
1	A	266	ASP	6.3
1	B	50	GLY	6.0
1	B	9	ALA	4.7
1	A	68	SER	4.6
1	A	183	SER	4.4
1	B	266	ASP	4.2
1	B	55	ALA	4.2
1	B	628	ASN	4.2
1	A	564	GLY	3.7
1	B	208	GLU	3.6
1	A	33	LEU	3.4
1	A	565	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	3.2
1	B	627	ALA	3.0
1	B	414	GLY	2.6
1	B	267	ARG	2.5
1	A	315	CYS	2.5
1	A	36	GLU	2.5
1	B	462	PRO	2.4
1	A	85	ILE	2.4
1	A	182	VAL	2.4
1	A	267	ARG	2.4
1	A	105	PHE	2.4
1	A	35	PRO	2.3
1	A	414	GLY	2.2
1	A	48	ALA	2.2
1	A	145	ALA	2.1
1	A	106	GLU	2.1
1	A	233	THR	2.1
1	A	66	ASP	2.1
1	A	84	VAL	2.1
1	A	339	ARG	2.1
1	A	116	GLU	2.0
1	A	507	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPQ	A	382	14/15	0.88	0.15	10,26,32,39	0
1	TPQ	B	382	14/15	0.89	0.14	9,24,32,35	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	CU	A	1001	1/1	1.00	0.04	14,14,14,14	0
2	CU	B	1002	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.