



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:30 PM BST

PDB ID : 3X42
Title : Crystal structure of copper amine oxidase from *Arthrobacter globiformis* in the presence of sodium bromide
Authors : Okajima, T.; Nakanishi, S.; Murakawa, T.; Kataoka, M.; Hayashi, H.; Hamaguchi, A.; Nakai, T.; Kawano, Y.; Yamaguchi, H.; Tanizawa, K.
Deposited on : 2015-03-10
Resolution : 1.88 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

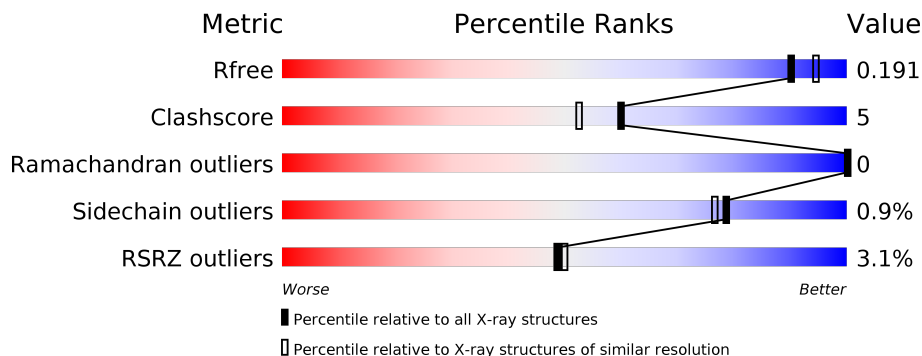
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	621	 2% 93% 7%
1	B	621	 4% 90% 10%

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	BR	A	703	-	-	X	-
3	BR	B	703	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11083 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	621	4893	3088	861	934	10	0	2	0
1	B	621	4904	3094	865	935	10	0	3	0

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

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Br	0	0
			4	4		
3	A	4	Total	Br	0	0
			4	4		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	A	1	Total K 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

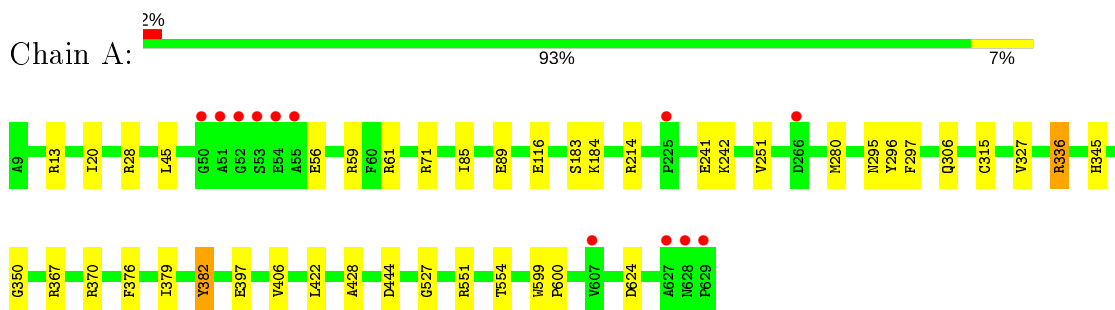
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	660	Total	O	0	0
			660	660		
7	B	534	Total	O	0	0
			534	534		

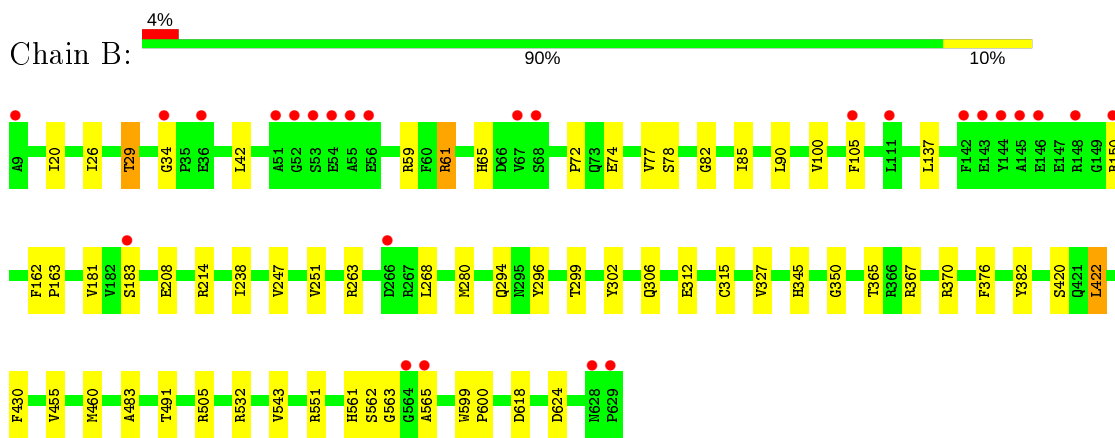
3 Residue-property plots [i](#)

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: Phenylethylamine oxidase



- Molecule 1: Phenylethylamine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.68Å 63.51Å 158.10Å 90.00° 117.55° 90.00°	Depositor
Resolution (Å)	24.74 – 1.88 46.72 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.8 (24.74-1.88) 90.0 (46.72-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.42 (at 1.88Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.158 , 0.190 0.159 , 0.191	Depositor DCC
R_{free} test set	6862 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtrriage
Anisotropy	0.691	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11083	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.98 % 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 1.0377e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BR, NA, K, TPQ, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/5001	0.54	0/6808
1	B	0.33	0/5012	0.52	0/6822
All	All	0.35	0/10013	0.53	0/13630

There are no bond length outliers.

There are no bond angle outliers.

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	4893	0	4708	41	0
1	B	4904	0	4721	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	3	0
3	B	4	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	42	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	36	0	48	4	0
7	A	660	0	0	9	0
7	B	534	0	0	6	0
All	All	11083	0	9533	90	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 5.

All (90) 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:315[A]:CYS:SG	7:B:1252:HOH:O	2.34	0.85
1:A:13:ARG:NH2	1:A:56:GLU:OE2	2.09	0.84
1:B:100:VAL:HG11	1:B:105:PHE:CE1	2.11	0.84
1:B:137:LEU:HD13	1:B:296:TYR:OH	1.78	0.83
1:B:561:HIS:ND1	1:B:562:SER:O	2.14	0.81
1:B:315[B]:CYS:HB2	7:B:1252:HOH:O	1.84	0.78
1:A:527:GLY:HA3	1:B:460:MET:HE3	1.66	0.76
1:B:59:ARG:CZ	1:B:85:ILE:HD13	2.20	0.71
1:B:312:GLU:HB2	1:B:315[A]:CYS:SG	2.32	0.69
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.29	0.68
6:B:708:GOL:O1	7:B:902:HOH:O	2.04	0.67
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.30	0.67
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.76	0.66
1:B:181:VAL:O	7:B:1257:HOH:O	2.13	0.66
1:B:238:ILE:HD13	1:B:247:VAL:HG23	1.77	0.66
1:B:65:HIS:HD2	7:B:969:HOH:O	1.79	0.65
1:A:336:ARG:HH11	1:A:336:ARG:CG	2.09	0.65
1:A:370:ARG:HH11	6:A:709:GOL:H2	1.62	0.64
1:B:162:PHE:HB2	1:B:163:PRO:HD2	1.80	0.64
1:B:370:ARG:HH22	6:B:711:GOL:H32	1.62	0.64
1:B:551:ARG:HD3	6:B:709:GOL:H32	1.81	0.62
1:B:251:VAL:CG2	1:B:306:GLN:HB3	2.30	0.61
1:A:71:ARG:NH2	7:A:1435:HOH:O	2.23	0.61
1:A:59:ARG:CZ	1:A:85:ILE:HD13	2.32	0.59
1:B:455:VAL:HG13	1:B:491:THR:O	2.04	0.58
1:A:370:ARG:NH1	6:A:709:GOL:H2	2.20	0.56
1:B:561:HIS:CE1	1:B:565:ALA:HB2	2.42	0.55
1:B:238:ILE:N	1:B:238:ILE:HD12	2.20	0.55
1:A:89:GLU:OE2	7:A:1435:HOH:O	2.18	0.54
1:A:527:GLY:CA	1:B:460:MET:HE3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:HIS:HE1	3:A:703:BR:BR	2.46	0.54
1:A:551[B]:ARG:NH2	7:A:1279:HOH:O	2.40	0.54
1:B:162:PHE:HB2	1:B:163:PRO:CD	2.39	0.52
1:A:336:ARG:NH1	1:A:336:ARG:CG	2.70	0.51
1:A:551[B]:ARG:HH21	1:A:551[B]:ARG:HG2	1.73	0.51
1:A:251:VAL:CG2	1:A:306:GLN:HB3	2.41	0.51
1:B:532:ARG:HB3	1:B:563:GLY:HA3	1.91	0.51
1:A:295:ASN:O	7:A:1187:HOH:O	2.19	0.51
1:B:26:ILE:HD11	1:B:82:GLY:HA2	1.94	0.50
1:B:345:HIS:HE1	3:B:703:BR:BR	2.49	0.50
1:B:422:LEU:HD13	1:B:599:TRP:HB2	1.93	0.50
1:B:150:ARG:HH22	1:B:183:SER:HB3	1.77	0.49
1:B:280:MET:HG2	1:B:299:THR:OG1	2.12	0.49
1:A:315[B]:CYS:SG	1:B:365:THR:HB	2.53	0.49
3:A:704:BR:BR	7:A:1271:HOH:O	2.75	0.49
1:B:65:HIS:HE1	7:B:1303:HOH:O	1.95	0.49
1:A:370:ARG:HH22	6:A:712:GOL:H32	1.77	0.48
1:A:397:GLU:OE2	6:A:712:GOL:O1	2.16	0.48
1:B:34:GLY:HA3	3:B:704:BR:BR	2.69	0.48
1:B:350:GLY:HA2	1:B:367:ARG:NH2	2.29	0.47
1:A:336:ARG:HG3	1:A:336:ARG:HH11	1.77	0.47
1:B:61:ARG:NH2	1:B:74:GLU:OE2	2.40	0.47
1:A:527:GLY:HA3	1:B:460:MET:CE	2.40	0.47
1:A:116:GLU:HG3	7:A:1159:HOH:O	2.13	0.47
1:A:20:ILE:HD12	1:A:327:VAL:HG12	1.97	0.46
1:B:137:LEU:HD13	1:B:296:TYR:HH	1.77	0.46
1:A:551[B]:ARG:HG2	1:A:551[B]:ARG:NH2	2.30	0.46
1:B:105:PHE:HZ	1:B:302:TYR:HD1	1.63	0.46
1:B:42:LEU:C	1:B:42:LEU:HD23	2.35	0.46
1:B:105:PHE:HZ	1:B:302:TYR:CD1	2.33	0.46
1:B:72:PRO:HG2	1:B:90:LEU:HB2	1.97	0.45
1:A:183:SER:O	1:A:184:LYS:HB2	2.16	0.45
1:A:624:ASP:O	1:B:214:ARG:HG2	2.17	0.45
1:A:345:HIS:CE1	3:A:703:BR:BR	3.25	0.45
1:B:483:ALA:HB1	1:B:543:VAL:HB	1.99	0.44
1:A:554:THR:O	6:A:708:GOL:H12	2.18	0.44
1:B:251:VAL:HG23	1:B:306:GLN:HB3	1.99	0.44
1:A:241:GLU:O	1:A:242:LYS:HB2	2.18	0.44
1:B:263[A]:ARG:HG2	1:B:268:LEU:HD13	2.00	0.43
1:A:336:ARG:NH2	7:A:1391:HOH:O	2.47	0.42
1:B:26:ILE:O	1:B:29:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ARG:HD3	1:B:618:ASP:HB3	2.00	0.42
1:A:214:ARG:HG3	1:B:624:ASP:O	2.20	0.42
1:B:561:HIS:CE1	1:B:562:SER:O	2.72	0.42
1:A:350:GLY:HA2	1:A:367:ARG:NH2	2.35	0.42
1:A:379:ILE:O	1:A:382:TPQ:H6	2.20	0.42
1:B:26:ILE:HG21	1:B:77:VAL:HG13	2.00	0.42
1:B:294:GLN:HG3	1:B:296:TYR:CZ	2.55	0.42
1:B:551:ARG:CD	6:B:709:GOL:H32	2.49	0.41
1:A:45:LEU:HD21	1:A:61:ARG:HB2	2.01	0.41
1:A:551[B]:ARG:NH2	7:A:1387:HOH:O	2.52	0.41
1:B:78:SER:HB2	1:B:85:ILE:HD11	2.02	0.41
1:A:28:ARG:NH1	7:A:1204:HOH:O	2.34	0.41
1:B:345:HIS:CE1	3:B:703:BR:BR	3.27	0.41
1:A:280:MET:O	1:A:297:PHE:HA	2.20	0.41
1:A:406:VAL:HG21	1:A:422:LEU:HD11	2.03	0.41
1:B:20:ILE:HD12	1:B:327:VAL:HG12	2.03	0.41
1:B:420:SER:OG	1:B:430:PHE:HE1	2.03	0.40
1:A:336:ARG:NH1	1:A:336:ARG:HG2	2.36	0.40
1:A:527:GLY:CA	1:B:460:MET:CE	2.98	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	620/621 (100%)	599 (97%)	21 (3%)	0	100	100
1	B	621/621 (100%)	598 (96%)	23 (4%)	0	100	100
All	All	1241/1242 (100%)	1197 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	516/514 (100%)	512 (99%)	4 (1%)	81	80
1	B	517/514 (101%)	512 (99%)	5 (1%)	76	73
All	All	1033/1028 (100%)	1024 (99%)	9 (1%)	78	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	TYR
1	A	336	ARG
1	A	376	PHE
1	A	444	ASP
1	B	29	THR
1	B	61	ARG
1	B	208	GLU
1	B	376	PHE
1	B	422	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	HIS

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	A	382	1	13,14,15	1.51	3 (23%)	15,19,21	1.20	1 (6%)
1	TPQ	B	382	1	13,14,15	1.45	3 (23%)	15,19,21	1.56	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	A	382	1	-	1/5/22/24	0/1/1/1
1	TPQ	B	382	1	-	1/5/22/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	TPQ	C3-C4	2.43	1.39	1.35
1	B	382	TPQ	C3-C4	2.28	1.39	1.35
1	B	382	TPQ	O4-C4	2.16	1.39	1.34
1	A	382	TPQ	C6-C5	2.16	1.50	1.44
1	B	382	TPQ	C3-C2	2.13	1.50	1.44
1	A	382	TPQ	C3-C2	2.03	1.50	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	TPQ	CB-CA-C	-4.35	103.30	111.47
1	A	382	TPQ	CB-CA-C	-3.33	105.22	111.47
1	B	382	TPQ	C6-C5-C4	2.09	120.57	117.03
1	B	382	TPQ	C6-C1-C2	2.03	120.20	118.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382	TPQ	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	$\# Z > 2$
6	GOL	A	713	-	5,5,5	0.33	0	5,5,5	0.23	0
6	GOL	B	711	-	5,5,5	0.43	0	5,5,5	0.20	0
6	GOL	B	712	-	5,5,5	0.37	0	5,5,5	0.38	0
6	GOL	A	708	-	5,5,5	0.36	0	5,5,5	0.96	0
6	GOL	B	708	-	5,5,5	0.30	0	5,5,5	0.55	0
6	GOL	A	712	-	5,5,5	0.43	0	5,5,5	0.13	0
6	GOL	A	711	-	5,5,5	0.38	0	5,5,5	0.60	0
6	GOL	B	713	-	5,5,5	0.35	0	5,5,5	0.33	0
6	GOL	A	709	-	5,5,5	0.35	0	5,5,5	0.35	0
6	GOL	B	710	-	5,5,5	0.39	0	5,5,5	0.24	0
6	GOL	A	710	-	5,5,5	0.33	0	5,5,5	0.20	0
6	GOL	A	714	-	5,5,5	0.35	0	5,5,5	0.45	0
6	GOL	B	709	-	5,5,5	0.38	0	5,5,5	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
6	GOL	A	713	-	-	2/4/4/4	-
6	GOL	B	711	-	-	4/4/4/4	-
6	GOL	B	712	-	-	2/4/4/4	-
6	GOL	A	708	-	-	3/4/4/4	-
6	GOL	B	708	-	-	0/4/4/4	-
6	GOL	A	712	-	-	4/4/4/4	-
6	GOL	A	711	-	-	4/4/4/4	-
6	GOL	B	713	-	-	2/4/4/4	-
6	GOL	A	709	-	-	3/4/4/4	-
6	GOL	B	710	-	-	2/4/4/4	-
6	GOL	A	710	-	-	0/4/4/4	-
6	GOL	A	714	-	-	2/4/4/4	-
6	GOL	B	709	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	713	GOL	O1-C1-C2-C3
6	B	711	GOL	O1-C1-C2-C3
6	B	712	GOL	O1-C1-C2-C3
6	A	714	GOL	O1-C1-C2-C3
6	B	710	GOL	O1-C1-C2-C3
6	B	709	GOL	O1-C1-C2-C3
6	A	712	GOL	O1-C1-C2-C3
6	A	712	GOL	C1-C2-C3-O3
6	A	711	GOL	O1-C1-C2-C3
6	A	708	GOL	O1-C1-C2-C3
6	A	709	GOL	O1-C1-C2-C3
6	A	713	GOL	O1-C1-C2-O2
6	B	711	GOL	O1-C1-C2-O2
6	A	711	GOL	O2-C2-C3-O3
6	A	711	GOL	C1-C2-C3-O3
6	A	708	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	710	GOL	O1-C1-C2-O2
6	B	709	GOL	O1-C1-C2-O2
6	A	712	GOL	O1-C1-C2-O2
6	A	711	GOL	O1-C1-C2-O2
6	A	709	GOL	O1-C1-C2-O2
6	B	712	GOL	O1-C1-C2-O2
6	A	714	GOL	O1-C1-C2-O2
6	A	712	GOL	O2-C2-C3-O3
6	A	708	GOL	O1-C1-C2-O2
6	B	711	GOL	O2-C2-C3-O3
6	B	713	GOL	O1-C1-C2-O2
6	B	709	GOL	O2-C2-C3-O3
6	B	711	GOL	C1-C2-C3-O3
6	B	709	GOL	C1-C2-C3-O3
6	B	713	GOL	O1-C1-C2-C3
6	A	709	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	711	GOL	1	0
6	A	708	GOL	1	0
6	B	708	GOL	1	0
6	A	712	GOL	2	0
6	A	709	GOL	2	0
6	B	709	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	620/621 (99%)	-0.33	12 (1%) 66 68	10, 18, 34, 100	0
1	B	620/621 (99%)	-0.07	26 (4%) 36 37	12, 24, 45, 88	0
All	All	1240/1242 (99%)	-0.20	38 (3%) 49 50	10, 20, 41, 100	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	SER	9.7
1	A	53	SER	7.5
1	B	52	GLY	7.4
1	B	55	ALA	6.4
1	A	52	GLY	5.9
1	B	629	PRO	5.8
1	A	629	PRO	5.3
1	B	266	ASP	5.2
1	B	51	ALA	4.8
1	A	628	ASN	4.8
1	B	54	GLU	4.5
1	A	51	ALA	4.5
1	A	55	ALA	4.3
1	A	54	GLU	3.9
1	B	148	ARG	3.6
1	B	144	TYR	3.6
1	B	628	ASN	3.2
1	A	627	ALA	3.0
1	B	105	PHE	3.0
1	B	143	GLU	2.9
1	B	111	LEU	2.9
1	B	68	SER	2.8
1	B	142	PHE	2.8
1	A	266	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	67	VAL	2.8
1	B	145	ALA	2.7
1	B	9	ALA	2.7
1	B	565	ALA	2.6
1	B	564	GLY	2.6
1	A	225	PRO	2.6
1	B	183	SER	2.4
1	B	34	GLY	2.4
1	B	56	GLU	2.3
1	B	150	ARG	2.3
1	A	50	GLY	2.2
1	B	146	GLU	2.1
1	A	607	VAL	2.1
1	B	36	GLU	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	B	382	14/15	0.94	0.12	17,27,49,59	0
1	TPQ	A	382	14/15	0.95	0.12	12,18,27,27	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
6	GOL	B	712	6/6	0.50	0.24	56,60,66,67	0
6	GOL	A	709	6/6	0.63	0.36	50,54,55,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	710	6/6	0.64	0.27	46,48,51,55	0
6	GOL	B	709	6/6	0.70	0.25	59,64,64,67	0
6	GOL	A	710	6/6	0.71	0.31	38,42,46,46	0
6	GOL	B	708	6/6	0.74	0.29	41,46,50,54	0
6	GOL	B	713	6/6	0.75	0.37	39,53,56,57	0
6	GOL	A	711	6/6	0.77	0.22	42,46,52,54	0
6	GOL	A	713	6/6	0.84	0.38	48,51,53,58	0
6	GOL	A	714	6/6	0.84	0.36	35,47,48,55	0
6	GOL	A	712	6/6	0.86	0.32	35,44,44,49	0
6	GOL	B	711	6/6	0.88	0.23	31,42,43,44	0
3	BR	B	702	1/1	0.90	0.20	112,112,112,112	0
3	BR	B	704	1/1	0.92	0.23	85,85,85,85	0
6	GOL	A	708	6/6	0.96	0.12	15,17,21,25	0
3	BR	B	705	1/1	0.96	0.12	104,104,104,104	0
5	K	B	707	1/1	0.97	0.07	42,42,42,42	0
3	BR	A	704	1/1	0.97	0.14	76,76,76,76	0
3	BR	A	705	1/1	0.98	0.18	56,56,56,56	0
3	BR	B	703	1/1	0.98	0.11	53,53,53,53	0
4	NA	B	706	1/1	0.99	0.09	16,16,16,16	0
3	BR	A	702	1/1	0.99	0.08	36,36,36,36	0
5	K	A	707	1/1	0.99	0.05	21,21,21,21	0
4	NA	A	706	1/1	0.99	0.08	11,11,11,11	0
2	CU	B	701	1/1	1.00	0.08	17,17,17,17	0
3	BR	A	703	1/1	1.00	0.12	48,48,48,48	0
2	CU	A	701	1/1	1.00	0.06	14,14,14,14	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.