



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:09 PM GMT

PDB ID : 3X3Z
Title : Copper amine oxidase from *Arthrobacter globiformis*: Aminoresorcinol form produced by anaerobic reduction with ethylamine hydrochloride
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 : 1.51 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

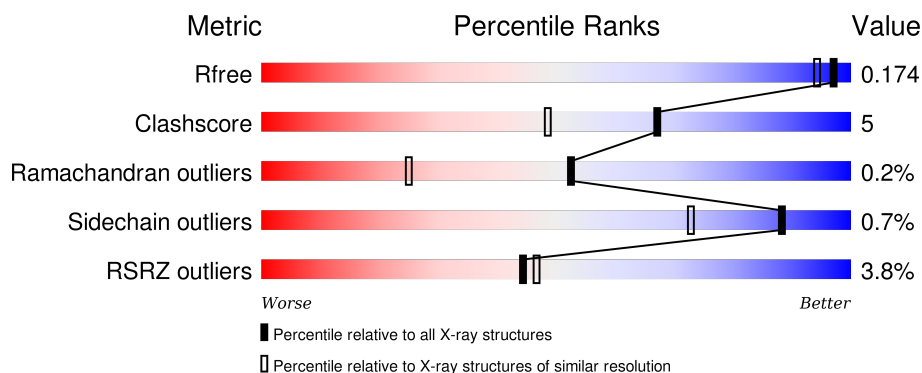
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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	620	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
1	B	620	<div> <div>3%</div> <div>94%</div> <div>6%</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	CL	B	1002	-	-	X	X
6	GOL	A	1005	-	-	-	X
6	GOL	A	1006	-	-	-	X
6	GOL	A	1007	-	-	-	X
6	GOL	A	1008	-	-	-	X
6	GOL	A	1009	-	-	X	X
6	GOL	A	1010	-	-	-	X
6	GOL	B	1006	-	-	-	X
6	GOL	B	1007	-	-	-	X
6	GOL	B	1008	-	-	X	X
6	GOL	B	1009	-	-	-	X
6	GOL	B	1010	-	-	-	X
6	GOL	B	1011	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11549 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
1	A	620	Total	C	N	O	S	0	14	0
			4986	3146	880	948	12			
1	B	620	Total	C	N	O	S	0	11	0
			4966	3131	874	950	11			

- 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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- 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: $C_3H_8O_3$).



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	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
6	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

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		

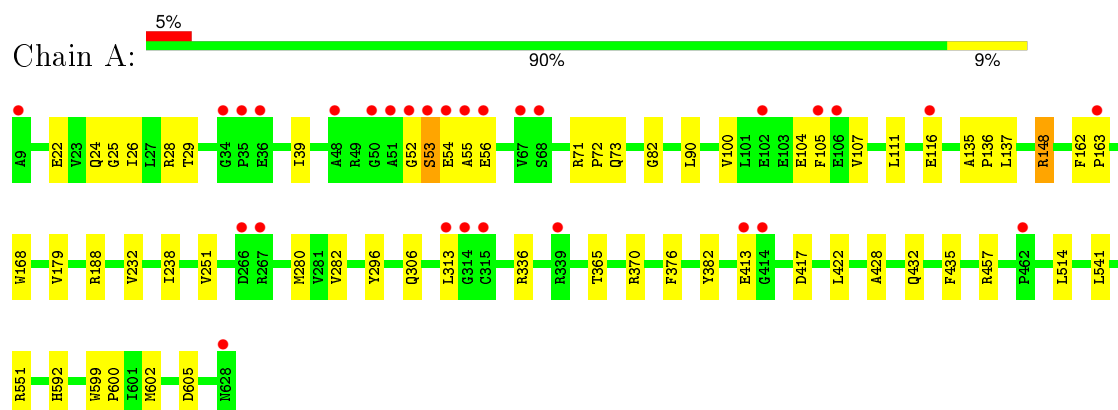
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	711	Total	O	0	0
			711	711		
7	B	800	Total	O	0	0
			800	800		

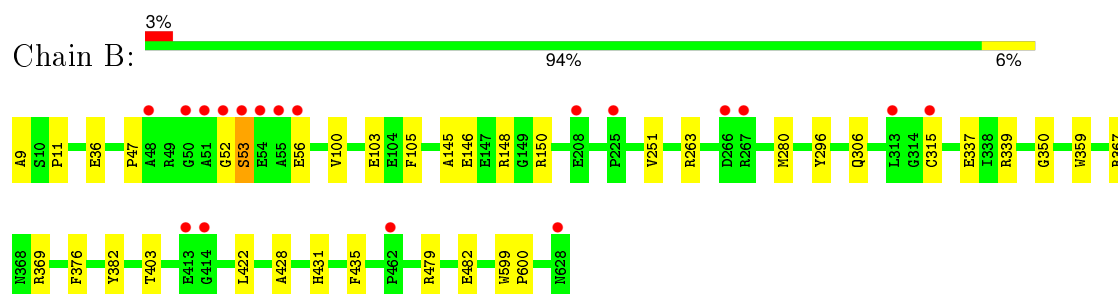
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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	192.55Å 62.73Å 157.65Å 90.00° 117.62° 90.00°	Depositor
Resolution (Å)	22.28 – 1.51 22.28 – 1.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (22.28-1.51) 93.0 (22.28-1.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 1.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.161 , 0.178 0.157 , 0.174	Depositor DCC
R_{free} test set	12205 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 260325 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11549	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 51.98 % 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 5.1918e-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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL, NA, K, TYQ, 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	0.32	0/5093	0.56	0/6930
1	B	0.34	0/5059	0.57	0/6885
All	All	0.33	0/10152	0.56	0/13815

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

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	4986	0	4806	55	0
1	B	4966	0	4766	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	4	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	36	0	48	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	42	0	56	7	0
7	A	711	0	0	18	0
7	B	800	0	0	7	0
All	All	11549	0	9676	94	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 (94) 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:382[A]:TYQ:CZ	3:B:1002:CL:CL	1.99	1.46
1:B:382[A]:TYQ:OH	3:B:1002:CL:CL	0.73	1.09
1:A:100:VAL:HG11	1:A:105:PHE:CE1	1.87	1.08
1:A:336:ARG:NH2	7:A:1618:HOH:O	1.92	1.02
1:A:56:GLU:OE1	7:A:1376:HOH:O	1.81	0.99
1:A:551[A]:ARG:NH2	7:A:1565:HOH:O	1.89	0.94
1:B:56:GLU:HB2	7:B:1564:HOH:O	1.69	0.92
1:B:296:TYR:CD2	1:B:382[B]:TYQ:N5	2.39	0.91
1:A:370:ARG:HH12	6:A:1010:GOL:H11	1.33	0.89
1:A:52:GLY:C	1:A:54:GLU:H	1.76	0.88
1:A:52:GLY:O	1:A:54:GLU:N	2.06	0.86
1:B:9:ALA:HB3	7:B:1667:HOH:O	1.81	0.80
1:B:36[A]:GLU:N	1:B:36[A]:GLU:OE1	2.16	0.75
1:A:168:TRP:HZ2	6:B:1008:GOL:H12	1.52	0.73
1:A:100:VAL:CG1	1:A:105:PHE:CE1	2.69	0.73
1:A:100:VAL:HG11	1:A:105:PHE:CZ	2.25	0.71
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.28	0.69
1:B:36[A]:GLU:HG3	7:B:1889:HOH:O	1.91	0.69
1:A:52:GLY:C	1:A:54:GLU:N	2.48	0.67
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.29	0.67
1:B:422:LEU:HD11	1:B:428:ALA:HB2	1.77	0.65
1:A:73:GLN:OE1	7:A:1471:HOH:O	2.15	0.64
1:A:370:ARG:HH12	6:A:1010:GOL:C1	2.08	0.64
1:A:116:GLU:HG2	7:A:1763:HOH:O	1.97	0.64
1:A:100:VAL:CG1	1:A:105:PHE:CZ	2.80	0.63
1:B:36[A]:GLU:CD	1:B:36[A]:GLU:H	2.01	0.63
1:A:422[A]:LEU:HD11	1:A:428:ALA:HB2	1.80	0.62
1:A:25:GLY:O	1:A:29:THR:HG23	1.99	0.62
1:B:52:GLY:O	1:B:53:SER:HB2	1.97	0.62
1:A:370:ARG:NH1	6:A:1010:GOL:H11	2.10	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382[A]:TYQ:N5	7:B:1896:HOH:O	2.31	0.61
1:B:52:GLY:O	1:B:53:SER:CB	2.48	0.61
1:A:251:VAL:CG2	1:A:306:GLN:HB3	2.32	0.60
1:A:592:HIS:CE1	1:A:602[B]:MET:HE1	2.37	0.60
1:A:251:VAL:HG22	1:A:306:GLN:HB3	1.85	0.57
1:B:146:GLU:O	1:B:150[B]:ARG:HD3	2.04	0.57
1:A:365:THR:HB	1:B:315[A]:CYS:SG	2.45	0.56
1:A:148[A]:ARG:NH2	7:A:1454:HOH:O	2.39	0.55
1:B:369:ARG:HG3	7:B:1514:HOH:O	2.06	0.55
1:A:232:VAL:HG22	1:A:238:ILE:HD12	1.89	0.54
1:B:296:TYR:CE2	1:B:382[B]:TYQ:N5	2.76	0.54
1:B:146:GLU:O	1:B:150[B]:ARG:CD	2.56	0.54
1:A:56:GLU:HG3	7:A:1485:HOH:O	2.08	0.54
1:B:280[B]:MET:HG3	1:B:435:PHE:CD2	2.43	0.53
1:A:24:GLN:O	1:A:28[A]:ARG:HG2	2.08	0.53
1:B:382[A]:TYQ:HD2	1:B:403:THR:O	2.09	0.53
6:A:1009:GOL:H2	7:A:1730:HOH:O	2.09	0.53
1:B:296:TYR:CG	1:B:382[B]:TYQ:N5	2.69	0.53
1:A:313:LEU:HD11	7:A:1650:HOH:O	2.07	0.53
1:A:111:LEU:HD12	1:A:179[B]:VAL:HG11	1.92	0.52
6:A:1009:GOL:H12	7:A:1496:HOH:O	2.09	0.52
1:B:382[A]:TYQ:CE2	3:B:1002:CL:CL	2.86	0.51
6:B:1009:GOL:O1	7:B:1479:HOH:O	2.19	0.51
1:A:72:PRO:HG2	1:A:90:LEU:HB2	1.93	0.51
7:A:1503:HOH:O	6:B:1006:GOL:H11	2.12	0.50
1:A:100:VAL:HG11	1:A:105:PHE:HE1	1.62	0.50
1:A:135:ALA:O	1:A:137[B]:LEU:HD22	2.12	0.50
1:A:39:ILE:O	6:A:1009:GOL:O1	2.18	0.49
1:B:359:TRP:CD2	6:B:1008:GOL:H11	2.48	0.49
1:B:11:PRO:HB2	1:B:47:PRO:HG3	1.94	0.49
6:A:1009:GOL:C1	7:A:1496:HOH:O	2.60	0.48
1:A:104:GLU:O	1:A:107:VAL:HB	2.13	0.48
1:A:71:ARG:NH1	7:A:1318:HOH:O	2.09	0.48
1:B:100:VAL:HG11	1:B:105:PHE:CE1	2.48	0.48
1:A:162:PHE:HB2	1:A:163:PRO:HD2	1.96	0.47
1:A:148[A]:ARG:HD2	7:A:1550:HOH:O	2.14	0.47
1:A:605:ASP:OD2	6:A:1006:GOL:O1	2.24	0.47
1:A:168:TRP:CZ2	6:B:1008:GOL:H12	2.42	0.46
1:B:251:VAL:CG2	1:B:306:GLN:HB3	2.46	0.46
1:B:296:TYR:CE1	1:B:382[B]:TYQ:OH	2.62	0.46
1:A:22:GLU:OE1	7:A:1588:HOH:O	2.21	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HD11	1:A:82:GLY:HA2	1.99	0.45
1:A:105:PHE:HB3	1:A:136:PRO:HG3	1.97	0.45
1:A:280[B]:MET:O	1:A:280[B]:MET:HG3	2.17	0.45
1:A:296:TYR:CD2	1:A:382:TYQ:N5	2.86	0.44
1:A:148[A]:ARG:HD3	7:A:1336:HOH:O	2.16	0.44
1:B:359:TRP:CE3	6:B:1008:GOL:H11	2.52	0.44
1:A:188:ARG:NH1	7:A:1665:HOH:O	2.20	0.44
1:B:280[B]:MET:HG3	1:B:435:PHE:CE2	2.53	0.43
1:B:479:ARG:O	1:B:482[A]:GLU:HG2	2.19	0.43
1:A:457:ARG:NH1	6:B:1006:GOL:H31	2.34	0.43
1:A:54:GLU:O	1:A:55:ALA:HB3	2.19	0.42
1:B:337:GLU:OE2	1:B:339:ARG:NH1	2.48	0.42
1:A:282:VAL:HA	1:A:432:GLN:O	2.19	0.42
1:B:431:HIS:CE1	3:B:1002:CL:CL	3.07	0.42
1:A:105:PHE:HD1	1:A:136:PRO:HB2	1.85	0.41
1:B:103:GLU:HB3	7:B:1390:HOH:O	2.19	0.41
1:A:162:PHE:HB2	1:A:163:PRO:CD	2.50	0.41
1:B:350:GLY:HA2	1:B:367:ARG:NH2	2.35	0.41
1:A:280[A]:MET:HG3	1:A:435:PHE:CE2	2.57	0.40
1:A:514[A]:LEU:HD23	1:A:514[A]:LEU:C	2.42	0.40
1:B:145:ALA:HA	1:B:148[B]:ARG:HD3	2.03	0.40
1:A:592:HIS:CE1	1:A:602[B]:MET:CE	3.04	0.40
1:A:417:ASP:OD1	7:A:1740:HOH:O	2.22	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	631/620 (102%)	610 (97%)	20 (3%)	1 (0%)	52	25
1	B	627/620 (101%)	602 (96%)	24 (4%)	1 (0%)	52	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1258/1240 (102%)	1212 (96%)	44 (4%)	2 (0%)	52	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	B	53	SER

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	527/513 (103%)	521 (99%)	6 (1%)	80	57
1	B	523/513 (102%)	521 (100%)	2 (0%)	93	84
All	All	1050/1026 (102%)	1042 (99%)	8 (1%)	88	69

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	148[A]	ARG
1	A	148[B]	ARG
1	A	376	PHE
1	A	413	GLU
1	A	541	LEU
1	B	263	ARG
1	B	376	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 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	TYQ	A	382	1	12,14,15	1.10	1 (8%)	15,19,21	1.64	3 (20%)
1	TYQ	B	382[A]	1,2	12,14,15	1.21	1 (8%)	15,19,21	1.73	2 (13%)
1	TYQ	B	382[B]	1	12,14,15	1.10	1 (8%)	15,19,21	1.67	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	TYQ	A	382	1	-	0/4/6/8	0/1/1/1
1	TYQ	B	382[A]	1,2	-	0/4/6/8	0/1/1/1
1	TYQ	B	382[B]	1	-	0/4/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[A]	TYQ	CB-CA	-2.93	1.47	1.53
1	B	382[B]	TYQ	CB-CA	-2.43	1.48	1.53
1	A	382	TYQ	CB-CA	-2.11	1.49	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382[B]	TYQ	CE2-CD2-CG	-4.19	118.79	122.44
1	B	382[A]	TYQ	CE2-CD2-CG	-4.07	118.90	122.44
1	A	382	TYQ	CE2-CD2-CG	-4.05	118.91	122.44
1	A	382	TYQ	CB-CG-CD1	-2.56	118.41	121.20
1	A	382	TYQ	CD2-CG-CD1	2.28	120.09	118.16
1	B	382[B]	TYQ	CD2-CG-CD1	2.51	120.30	118.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382[B]	TYQ	OH-CZ-CE2	2.95	121.04	116.36
1	B	382[A]	TYQ	CD2-CG-CD1	3.76	121.36	118.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382	TYQ	1	0
1	B	382[A]	TYQ	5	0
1	B	382[B]	TYQ	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 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	1005	-	5,5,5	0.48	0	5,5,5	0.50	0
6	GOL	A	1006	-	5,5,5	0.26	0	5,5,5	0.60	0
6	GOL	A	1007	-	5,5,5	0.38	0	5,5,5	0.65	0
6	GOL	A	1008	-	5,5,5	0.30	0	5,5,5	0.67	0
6	GOL	A	1009	-	5,5,5	0.36	0	5,5,5	0.20	0
6	GOL	A	1010	-	5,5,5	0.38	0	5,5,5	0.27	0
6	GOL	B	1005	-	5,5,5	0.37	0	5,5,5	0.16	0
6	GOL	B	1006	-	5,5,5	0.48	0	5,5,5	0.34	0
6	GOL	B	1007	-	5,5,5	0.34	0	5,5,5	0.46	0
6	GOL	B	1008	-	5,5,5	0.43	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	1009	-	5,5,5	0.41	0	5,5,5	0.80	0
6	GOL	B	1010	-	5,5,5	0.35	0	5,5,5	0.20	0
6	GOL	B	1011	-	5,5,5	0.36	0	5,5,5	0.47	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	1005	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1006	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1007	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1008	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1009	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1010	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1005	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1006	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1007	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1008	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1009	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1010	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1011	-	-	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.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1006	GOL	1	0
6	A	1009	GOL	4	0
6	A	1010	GOL	3	0
6	B	1006	GOL	2	0
6	B	1008	GOL	4	0
6	B	1009	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	619/620 (99%)	0.07	29 (4%) 35 36	8, 18, 33, 87	0
1	B	619/620 (99%)	-0.10	18 (2%) 55 58	6, 14, 27, 86	0
All	All	1238/1240 (99%)	-0.01	47 (3%) 44 47	6, 16, 31, 87	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	SER	12.2
1	B	51	ALA	11.4
1	A	53	SER	11.1
1	B	52	GLY	10.2
1	A	52	GLY	8.7
1	A	54	GLU	8.4
1	B	54	GLU	8.0
1	A	51	ALA	7.5
1	B	55	ALA	7.4
1	A	105	PHE	6.5
1	A	55	ALA	6.2
1	A	50	GLY	5.9
1	B	50	GLY	5.1
1	A	9	ALA	4.9
1	A	266	ASP	4.8
1	B	266	ASP	4.3
1	B	628	ASN	3.6
1	A	313	LEU	3.6
1	A	48	ALA	3.5
1	B	56	GLU	3.3
1	A	628	ASN	3.2
1	B	315[A]	CYS	3.2
1	A	315[A]	CYS	3.1
1	B	414	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	267	ARG	3.0
1	A	163	PRO	3.0
1	A	314	GLY	2.8
1	A	102	GLU	2.8
1	A	339	ARG	2.7
1	B	313	LEU	2.7
1	A	413	GLU	2.6
1	B	225	PRO	2.5
1	A	106	GLU	2.5
1	B	208	GLU	2.5
1	A	414	GLY	2.4
1	A	67	VAL	2.3
1	A	34	GLY	2.3
1	B	48	ALA	2.3
1	A	462	PRO	2.2
1	A	56	GLU	2.2
1	A	68	SER	2.1
1	A	116	GLU	2.1
1	B	462	PRO	2.0
1	A	36	GLU	2.0
1	B	413	GLU	2.0
1	A	35	PRO	2.0
1	B	267	ARG	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. 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
1	TYQ	A	382	14/15	0.97	0.08	-	11,16,17,17	0
1	TYQ	B	382[B]	14/15	0.93	0.15	-	8,11,15,18	14
1	TYQ	B	382[A]	14/15	0.93	0.15	-	7,15,21,24	14

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
6	GOL	A	1010	6/6	0.78	0.29	30.99	25,33,39,40	0
6	GOL	A	1006	6/6	0.59	0.28	18.48	32,42,42,45	0
6	GOL	A	1008	6/6	0.46	0.22	16.30	32,38,41,44	0
6	GOL	A	1009	6/6	0.16	0.37	15.88	52,59,61,64	0
6	GOL	B	1009	6/6	0.69	0.18	12.70	38,39,41,46	0
6	GOL	B	1011	6/6	0.78	0.22	10.02	29,41,43,45	0
6	GOL	B	1008	6/6	0.82	0.24	8.54	23,36,38,46	0
3	CL	B	1002	1/1	0.97	0.26	8.52	57,57,57,57	1
6	GOL	B	1010	6/6	0.79	0.20	8.35	24,31,31,37	0
6	GOL	A	1007	6/6	0.85	0.15	6.70	30,30,34,34	0
6	GOL	B	1007	6/6	0.77	0.17	6.36	27,31,32,33	0
6	GOL	A	1005	6/6	0.88	0.15	2.30	18,26,31,34	0
6	GOL	B	1006	6/6	0.88	0.16	2.17	18,28,29,31	0
4	NA	A	1003	1/1	1.00	0.14	1.67	13,13,13,13	0
4	NA	B	1003	1/1	1.00	0.11	1.07	9,9,9,9	0
6	GOL	B	1005	6/6	0.98	0.06	-0.62	10,11,11,12	0
3	CL	A	1002	1/1	0.99	0.07	-0.76	14,14,14,14	0
5	K	A	1004	1/1	0.96	0.07	-0.84	28,28,28,28	0
5	K	B	1004	1/1	0.98	0.06	-1.06	17,17,17,17	0
2	CU	A	1001	1/1	1.00	0.03	-	11,11,11,11	0
2	CU	B	1001	1/1	1.00	0.03	-	11,11,11,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.