



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:25 PM UTC

PDB ID : 4KFF / pdb_00004kff
Title : Crystal structure of Hansenula polymorpha copper amine oxidase-1 reduced by methylamine at pH 8.5
Authors : Johnson, B.J.; Yukl, E.T.; Klema, V.J.; Wilmot, C.M.
Deposited on : 2013-04-26
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

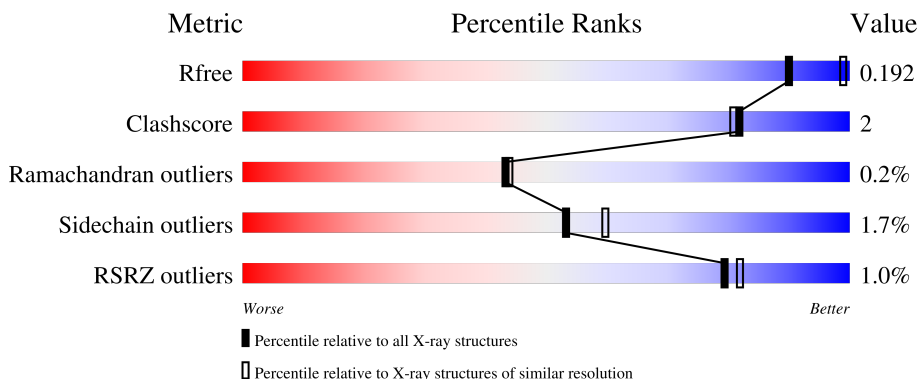
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	692	% 88% 7% 5%
1	B	692	% 86% 8% 5%
1	C	692	% 88% 6% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16993 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	2	0
			5217	3321	896	977	23			
1	B	657	Total	C	N	O	S	0	3	0
			5223	3325	896	979	23			
1	C	656	Total	C	N	O	S	0	5	0
			5223	3324	897	977	25			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is GLYCEROL (CCD ID: 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	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	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	426	Total 426	O 426	0	0
4	B	399	Total 399	O 399	0	0
4	C	418	Total 418	O 418	0	0

- Molecule 1: Peroxisomal primary amine oxidase



GLU
GLY
SER
CYS
CYS
GLY
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.02Å 153.32Å 223.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.56 – 2.15 38.56 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.56-2.15) 100.0 (38.56-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.142 , 0.185 0.152 , 0.192	Depositor DCC
R_{free} test set	6494 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16993	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	1.24	5/5344 (0.1%)	1.11	6/7274 (0.1%)
1	B	1.26	11/5353 (0.2%)	1.11	12/7286 (0.2%)
1	C	1.25	8/5359 (0.1%)	1.11	11/7294 (0.2%)
All	All	1.25	24/16056 (0.1%)	1.11	29/21854 (0.1%)

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	3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	PRO	C-O	-7.23	1.18	1.24
1	C	208	ILE	C-O	-7.20	1.17	1.23
1	A	573	VAL	C-O	-7.06	1.17	1.24
1	B	333	SER	N-CA	6.95	1.55	1.46
1	B	217	LYS	C-O	-6.83	1.14	1.24
1	A	551	LEU	C-O	-6.52	1.16	1.24
1	A	120	ASP	C-O	-6.49	1.16	1.24
1	C	75	PRO	CA-C	-6.48	1.48	1.51
1	B	510	ASP	C-O	-6.42	1.16	1.24
1	C	357	ILE	C-O	-5.83	1.18	1.24
1	C	536	GLY	C-O	-5.78	1.16	1.24
1	B	215	VAL	N-CA	-5.66	1.39	1.46
1	C	555	GLU	CA-C	-5.54	1.45	1.52
1	B	504	THR	C-O	-5.50	1.17	1.23
1	B	441	GLY	N-CA	5.39	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	VAL	CA-C	-5.24	1.46	1.52
1	B	246	GLN	N-CA	-5.23	1.41	1.46
1	B	458	HIS	C-O	5.17	1.29	1.24
1	C	204	ILE	C-O	-5.15	1.18	1.24
1	B	662	ALA	C-O	-5.15	1.18	1.23
1	C	508	VAL	C-O	5.12	1.30	1.24
1	A	210	ASN	C-O	-5.08	1.18	1.24
1	B	135	ILE	C-O	-5.07	1.18	1.24
1	A	101	LEU	CA-C	-5.06	1.46	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	THR	CB-CA-C	-9.58	92.47	109.62
1	B	157	THR	CB-CA-C	-9.39	92.82	109.62
1	C	157	THR	CB-CA-C	-8.95	93.59	109.62
1	B	157	THR	N-CA-CB	8.60	122.68	110.04
1	A	157	THR	N-CA-CB	8.25	122.16	110.04
1	B	224	TYR	CA-C-N	7.31	126.85	119.24
1	B	224	TYR	C-N-CA	7.31	126.85	119.24
1	C	549	PRO	CA-C-N	-6.99	112.58	119.78
1	C	549	PRO	C-N-CA	-6.99	112.58	119.78
1	C	179	SER	CB-CA-C	-6.92	99.30	110.79
1	C	157	THR	N-CA-CB	6.86	120.12	110.04
1	C	441	GLY	N-CA-C	-6.57	98.94	112.34
1	B	549	PRO	CA-C-N	-6.50	113.09	119.78
1	B	549	PRO	C-N-CA	-6.50	113.09	119.78
1	B	441	GLY	N-CA-C	-6.03	100.04	112.34
1	C	330	ASN	CB-CA-C	-5.76	100.80	109.26
1	B	563	ALA	CA-C-N	5.72	125.58	119.28
1	B	563	ALA	C-N-CA	5.72	125.58	119.28
1	A	98	LEU	N-CA-C	5.58	118.13	111.71
1	C	75	PRO	O-C-N	5.57	123.87	121.31
1	C	563	ALA	CA-C-N	5.50	125.33	119.28
1	C	563	ALA	C-N-CA	5.50	125.33	119.28
1	A	537	LYS	CA-C-N	-5.36	115.80	119.66
1	A	537	LYS	C-N-CA	-5.36	115.80	119.66
1	A	340	GLY	N-CA-C	-5.33	105.22	112.52
1	C	280	ASP	N-CA-C	-5.21	104.23	111.52
1	B	179	SER	N-CA-C	-5.16	105.84	111.82
1	B	397	SER	CB-CA-C	-5.09	99.78	109.66
1	B	170	LEU	N-CA-C	5.08	117.53	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	333	SER	Peptide
1	B	335	GLY	Peptide
1	B	671	ALA	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	5217	0	5050	28	0
1	B	5223	0	5056	26	0
1	C	5223	0	5058	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	42	0	56	0	0
3	B	18	0	24	2	0
3	C	24	0	32	2	0
4	A	426	0	0	3	0
4	B	399	0	0	2	0
4	C	418	0	0	2	0
All	All	16993	0	15276	76	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 2.

All (76) 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:280:ASP:OD2	3:B:803:GOL:H12	1.69	0.92
1:C:23:HIS:HD2	1:C:25:LEU:H	1.25	0.83
1:B:23:HIS:HD2	1:B:25:LEU:H	1.24	0.82
1:A:23:HIS:HD2	1:A:25:LEU:H	1.28	0.81
1:A:157:THR:HB	1:A:159:GLY:H	1.51	0.75
1:A:405[B]:TYY:N5	4:A:957:HOH:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLU:HG3	4:C:1195:HOH:O	1.90	0.70
1:C:179:SER:HB2	1:C:183:ASP:OD2	1.96	0.65
1:B:157:THR:HB	1:B:159:GLY:H	1.64	0.62
1:A:631:PHE:CG	1:A:632:PRO:HA	2.34	0.61
1:C:157:THR:HB	1:C:159:GLY:H	1.66	0.61
1:C:663:MET:HE3	1:C:668:ALA:HB2	1.83	0.60
1:A:402:ALA:O	1:A:405[B]:TYY:HD2	2.03	0.59
1:B:333:SER:HA	1:B:334:LEU:C	2.29	0.57
1:B:280:ASP:OD2	3:B:803:GOL:C1	2.48	0.57
1:C:663:MET:HE3	1:C:668:ALA:CB	2.35	0.57
1:A:157:THR:HB	1:A:159:GLY:N	2.20	0.55
1:B:405[A]:TYY:N5	1:B:634:MET:HE2	2.21	0.54
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.43	0.54
1:B:631:PHE:CG	1:B:632:PRO:HA	2.43	0.54
1:A:344:TYR:HB3	1:A:361:ASN:HD22	1.73	0.54
1:B:642:MET:HE3	1:B:644:ARG:HD2	1.90	0.53
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.39	0.53
1:A:334:LEU:HD21	4:A:1256:HOH:O	2.09	0.53
1:B:157:THR:HB	1:B:159:GLY:N	2.24	0.52
1:B:62:LYS:HE3	4:B:1271:HOH:O	2.09	0.52
1:C:631:PHE:CG	1:C:632:PRO:HA	2.45	0.52
1:B:414:MET:HE3	1:B:418:ALA:HB3	1.92	0.51
1:A:404:ASN:HD21	1:A:405[B]:TYY:CZ	2.24	0.51
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.46	0.50
1:B:670:ARG:O	1:B:672:VAL:N	2.44	0.50
1:A:414:MET:HE3	1:A:418:ALA:HB3	1.93	0.49
1:B:402:ALA:O	1:B:405[B]:TYY:HD2	2.13	0.48
1:C:199:GLU:CG	4:C:1195:HOH:O	2.55	0.48
1:A:404:ASN:HD21	1:A:405[B]:TYY:CE1	2.27	0.48
1:B:23:HIS:CD2	1:B:25:LEU:H	2.15	0.48
1:B:301:MET:HG3	1:B:320:ILE:HD12	1.96	0.47
1:A:303:VAL:HG23	4:A:1065:HOH:O	2.14	0.46
1:B:342:ILE:HG22	1:B:366:HIS:HB3	1.98	0.45
1:C:404:ASN:HD21	1:C:405[B]:TYY:CZ	2.28	0.45
1:A:645:PRO:O	1:A:646:ARG:HD2	2.17	0.45
1:B:514:ASN:OD1	1:B:568:HIS:HA	2.16	0.44
1:C:634:MET:HG2	1:C:635:PRO:O	2.17	0.44
1:B:34:LYS:NZ	1:B:355:ASP:OD1	2.43	0.44
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.33	0.44
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.53	0.44
1:A:157:THR:HG21	1:A:588:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLU:HA	1:C:238:GLU:OE2	2.16	0.44
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.53	0.44
1:A:123:SER:HB2	1:A:201:LYS:HE3	2.00	0.43
1:B:670:ARG:C	1:B:672:VAL:H	2.24	0.43
1:C:84:LEU:HD12	1:C:84:LEU:N	2.33	0.43
1:A:514:ASN:OD1	1:A:568:HIS:HA	2.18	0.43
1:A:405[A]:TYY:HD2	1:A:426:THR:O	2.18	0.43
1:B:375:LYS:HE2	4:B:1278:HOH:O	2.19	0.43
1:B:404:ASN:HD21	1:B:405[B]:TYY:CZ	2.31	0.43
1:C:68:LYS:HE3	3:C:703:GOL:H32	2.01	0.43
1:A:20:ARG:HE	1:A:20:ARG:HB3	1.75	0.42
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.54	0.42
1:B:641:LEU:HD12	1:B:641:LEU:C	2.45	0.42
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.50	0.42
1:A:472:GLY:C	1:A:473:ASN:HD22	2.27	0.42
1:C:461:SER:HB2	1:C:565:TRP:CE3	2.55	0.42
1:B:319:ASP:HB3	1:B:328:MET:HE1	2.02	0.42
1:C:405[A]:TYY:HD2	1:C:426:THR:O	2.19	0.41
1:A:414:MET:HE1	1:A:642:MET:HE2	2.02	0.41
1:C:334:LEU:HD23	1:C:335:GLY:H	1.86	0.41
1:A:342:ILE:HG21	1:A:344:TYR:CZ	2.56	0.41
1:C:50:SER:HB2	1:C:352:ARG:CD	2.51	0.41
1:C:319:ASP:HB3	1:C:328:MET:HE1	2.03	0.41
1:A:84:LEU:N	1:A:84:LEU:HD12	2.36	0.40
1:A:186:TYR:CD2	1:A:428:ILE:HG21	2.55	0.40
1:C:310:PHE:CE1	3:C:704:GOL:H31	2.57	0.40
1:A:222:ASN:HB3	1:A:227:HIS:ND1	2.37	0.40
1:C:333:SER:HB2	1:C:336[B]:CYS:SG	2.62	0.40
1:A:634:MET:HG2	1:A:635:PRO:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	655/692 (95%)	631 (96%)	24 (4%)	0	100	100
1	B	656/692 (95%)	630 (96%)	23 (4%)	3 (0%)	24	20
1	C	657/692 (95%)	632 (96%)	25 (4%)	0	100	100
All	All	1968/2076 (95%)	1893 (96%)	72 (4%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	SER
1	B	671	ALA
1	B	335	GLY

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	566/593 (95%)	558 (99%)	8 (1%)	59	66
1	B	567/593 (96%)	554 (98%)	13 (2%)	44	49
1	C	568/593 (96%)	561 (99%)	7 (1%)	63	70
All	All	1701/1779 (96%)	1673 (98%)	28 (2%)	53	61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	THR
1	A	211	ARG
1	A	265	LYS
1	A	329	THR
1	A	334	LEU
1	A	338	CYS
1	A	506	LYS
1	A	509	LYS
1	B	48	LYS
1	B	157	THR

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Mol	Chain	Res	Type
1	B	200	GLU
1	B	201	LYS
1	B	230	GLU
1	B	238	GLU
1	B	329	THR
1	B	333	SER
1	B	334	LEU
1	B	342	ILE
1	B	357	ILE
1	B	637	GLU
1	B	672	VAL
1	C	157	THR
1	C	179	SER
1	C	202	LYS
1	C	329	THR
1	C	334	LEU
1	C	357	ILE
1	C	531	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	70	GLN
1	A	113	GLN
1	A	243	ASN
1	A	263	ASN
1	A	286	HIS
1	A	361	ASN
1	A	529	ASN
1	A	611	ASN
1	B	23	HIS
1	B	66	GLN
1	B	113	GLN
1	B	257	ASN
1	B	263	ASN
1	B	382	ASN
1	B	578	ASN
1	C	23	HIS
1	C	263	ASN
1	C	361	ASN
1	C	578	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	TYY	C	405[A]	-	13,14,15	2.15	2 (15%)	10,19,21	1.67	3 (30%)
1	TYY	B	405[A]	-	13,14,15	2.15	1 (7%)	10,19,21	0.95	0
1	TYY	A	405[A]	-	13,14,15	1.87	3 (23%)	10,19,21	0.84	0
1	TYY	C	405[B]	-	13,14,15	2.08	4 (30%)	10,19,21	1.93	2 (20%)
1	TYY	A	405[B]	-	13,14,15	2.07	4 (30%)	10,19,21	1.96	4 (40%)
1	TYY	B	405[B]	-	13,14,15	1.90	4 (30%)	10,19,21	1.82	2 (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	TYY	C	405[A]	-	-	4/5/22/24	0/1/1/1
1	TYY	B	405[A]	-	-	4/5/22/24	0/1/1/1
1	TYY	A	405[A]	-	-	4/5/22/24	0/1/1/1
1	TYY	C	405[B]	-	-	3/5/22/24	0/1/1/1
1	TYY	A	405[B]	-	-	2/5/22/24	0/1/1/1
1	TYY	B	405[B]	-	-	2/5/22/24	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405[A]	TYY	CE2-N5	6.92	1.39	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405[A]	TYY	CE2-N5	5.75	1.37	1.28
1	A	405[B]	TYY	CD2-CE2	-4.94	1.33	1.43
1	B	405[B]	TYY	CD2-CE2	-4.63	1.34	1.43
1	A	405[A]	TYY	CE2-N5	4.39	1.35	1.28
1	C	405[B]	TYY	CD2-CE2	-4.21	1.35	1.43
1	C	405[B]	TYY	CE2-N5	3.73	1.34	1.28
1	A	405[B]	TYY	CE2-N5	3.13	1.33	1.28
1	A	405[B]	TYY	CZ-CE2	3.00	1.50	1.45
1	A	405[A]	TYY	CD2-CE2	-2.83	1.37	1.43
1	C	405[B]	TYY	CZ-CE2	2.81	1.50	1.45
1	A	405[A]	TYY	CD2-CG	2.67	1.41	1.34
1	B	405[B]	TYY	CE2-N5	2.61	1.32	1.28
1	C	405[A]	TYY	CD2-CG	2.57	1.41	1.34
1	A	405[B]	TYY	CE1-CD1	-2.52	1.38	1.44
1	B	405[B]	TYY	CZ-CE2	2.32	1.49	1.45
1	C	405[B]	TYY	CE1-CZ	2.10	1.39	1.36
1	B	405[B]	TYY	CE1-CD1	-2.02	1.39	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	405[B]	TYY	CD2-CG-CD1	4.84	122.10	118.66
1	A	405[B]	TYY	CD2-CG-CD1	4.31	121.73	118.66
1	B	405[B]	TYY	CB-CG-CD1	3.41	124.52	118.56
1	C	405[A]	TYY	CB-CG-CD1	-3.23	112.91	118.56
1	B	405[B]	TYY	OH-CZ-CE2	2.95	123.16	117.57
1	A	405[B]	TYY	OH-CZ-CE2	2.92	123.10	117.57
1	C	405[B]	TYY	CB-CG-CD1	2.51	122.94	118.56
1	C	405[A]	TYY	OH-CZ-CE1	-2.21	115.53	121.60
1	C	405[A]	TYY	OH-CZ-CE2	2.15	121.64	117.57
1	A	405[B]	TYY	CB-CG-CD1	2.14	122.30	118.56
1	A	405[B]	TYY	OH-CZ-CE1	-2.11	115.81	121.60

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	405[A]	TYY	C-CA-CB-CG
1	A	405[A]	TYY	CA-CB-CG-CD1
1	A	405[B]	TYY	N-CA-CB-CG
1	B	405[A]	TYY	C-CA-CB-CG
1	B	405[A]	TYY	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	B	405[B]	TYT	N-CA-CB-CG
1	C	405[A]	TYT	C-CA-CB-CG
1	C	405[A]	TYT	CA-CB-CG-CD1
1	C	405[B]	TYT	N-CA-CB-CG
1	C	405[B]	TYT	C-CA-CB-CG
1	A	405[A]	TYT	CA-CB-CG-CD2
1	B	405[A]	TYT	CA-CB-CG-CD2
1	C	405[A]	TYT	CA-CB-CG-CD2
1	A	405[A]	TYT	N-CA-CB-CG
1	A	405[B]	TYT	C-CA-CB-CG
1	B	405[A]	TYT	N-CA-CB-CG
1	B	405[B]	TYT	C-CA-CB-CG
1	C	405[A]	TYT	N-CA-CB-CG
1	C	405[B]	TYT	CA-CB-CG-CD1

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	405[A]	TYT	1	0
1	B	405[A]	TYT	1	0
1	A	405[A]	TYT	1	0
1	C	405[B]	TYT	1	0
1	A	405[B]	TYT	4	0
1	B	405[B]	TYT	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	C	703	-	5,5,5	0.25	0	5,5,5	0.66	0
3	GOL	A	807	-	5,5,5	0.47	0	5,5,5	1.26	1 (20%)
3	GOL	B	802	-	5,5,5	0.53	0	5,5,5	1.20	1 (20%)
3	GOL	A	806	-	5,5,5	0.39	0	5,5,5	1.38	0
3	GOL	A	805	-	5,5,5	0.83	0	5,5,5	1.29	1 (20%)
3	GOL	B	803	-	5,5,5	0.59	0	5,5,5	1.70	1 (20%)
3	GOL	C	704	-	5,5,5	0.50	0	5,5,5	0.80	0
3	GOL	B	804	-	5,5,5	0.42	0	5,5,5	1.30	0
3	GOL	A	808	-	5,5,5	0.53	0	5,5,5	1.00	1 (20%)
3	GOL	A	803	-	5,5,5	1.10	0	5,5,5	1.88	2 (40%)
3	GOL	C	705	-	5,5,5	0.21	0	5,5,5	1.40	1 (20%)
3	GOL	A	804	-	5,5,5	0.42	0	5,5,5	0.71	0
3	GOL	A	802	-	5,5,5	0.45	0	5,5,5	0.64	0
3	GOL	C	701	-	5,5,5	0.32	0	5,5,5	1.88	2 (40%)

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	C	703	-	-	2/4/4/4	-
3	GOL	A	807	-	-	2/4/4/4	-
3	GOL	B	802	-	-	2/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	A	805	-	-	2/4/4/4	-
3	GOL	B	803	-	-	2/4/4/4	-
3	GOL	C	704	-	-	2/4/4/4	-
3	GOL	B	804	-	-	4/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	C	705	-	-	0/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	C	701	-	-	1/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	GOL	O1-C1-C2	-3.16	96.15	110.38
3	A	803	GOL	C3-C2-C1	3.14	123.31	111.80
3	C	705	GOL	O3-C3-C2	-2.83	97.63	110.38
3	C	701	GOL	O2-C2-C1	-2.45	99.03	109.18
3	A	803	GOL	O2-C2-C1	-2.45	99.05	109.18
3	B	802	GOL	O1-C1-C2	-2.44	99.37	110.38
3	B	803	GOL	C3-C2-C1	-2.40	103.01	111.80
3	A	807	GOL	O3-C3-C2	-2.12	100.85	110.38
3	A	808	GOL	O1-C1-C2	2.02	119.45	110.38
3	A	805	GOL	O3-C3-C2	2.01	119.40	110.38

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	C1-C2-C3-O3
3	A	803	GOL	O2-C2-C3-O3
3	A	808	GOL	C1-C2-C3-O3
3	A	808	GOL	O2-C2-C3-O3
3	A	804	GOL	O1-C1-C2-C3
3	A	805	GOL	C1-C2-C3-O3
3	A	806	GOL	C1-C2-C3-O3
3	A	807	GOL	C1-C2-C3-O3
3	B	802	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-C3
3	B	804	GOL	O1-C1-C2-C3
3	B	804	GOL	C1-C2-C3-O3
3	C	703	GOL	C1-C2-C3-O3
3	C	703	GOL	O2-C2-C3-O3
3	C	704	GOL	O1-C1-C2-C3
3	A	802	GOL	C1-C2-C3-O3
3	B	802	GOL	O1-C1-C2-C3
3	C	701	GOL	C1-C2-C3-O3
3	A	805	GOL	O2-C2-C3-O3
3	B	803	GOL	O1-C1-C2-O2
3	C	704	GOL	O1-C1-C2-O2
3	A	804	GOL	O1-C1-C2-O2
3	A	806	GOL	O2-C2-C3-O3
3	B	804	GOL	O2-C2-C3-O3
3	A	807	GOL	O2-C2-C3-O3
3	B	804	GOL	O1-C1-C2-O2
3	A	802	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	GOL	1	0
3	B	803	GOL	2	0
3	C	704	GOL	1	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	656/692 (94%)	-0.58	7 (1%) 78 80	11, 19, 36, 80	1 (0%)
1	B	656/692 (94%)	-0.54	7 (1%) 78 80	12, 20, 37, 88	2 (0%)
1	C	655/692 (94%)	-0.58	5 (0%) 82 84	11, 20, 38, 62	4 (0%)
All	All	1967/2076 (94%)	-0.57	19 (0%) 79 82	11, 20, 37, 88	7 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	VAL	6.7
1	B	335	GLY	6.0
1	B	16	ALA	3.9
1	A	334	LEU	3.7
1	B	334	LEU	3.7
1	C	16	ALA	3.6
1	C	335	GLY	3.4
1	B	336	CYS	3.4
1	A	17	ALA	3.1
1	A	16	ALA	3.0
1	B	338	CYS	2.7
1	C	671	ALA	2.6
1	C	334	LEU	2.6
1	A	672	VAL	2.6
1	A	335	GLY	2.5
1	C	333	SER	2.3
1	A	333	SER	2.2
1	B	671	ALA	2.1
1	A	22	ALA	2.1

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	TYY	B	405[A]	14/15	0.92	0.10	16,17,19,20	11
1	TYY	B	405[B]	14/15	0.92	0.10	13,16,17,18	11
1	TYY	C	405[A]	14/15	0.94	0.07	12,16,17,17	11
1	TYY	C	405[B]	14/15	0.94	0.07	15,17,18,18	11
1	TYY	A	405[A]	14/15	0.96	0.07	16,18,20,22	11
1	TYY	A	405[B]	14/15	0.96	0.07	15,17,18,18	11

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	803	6/6	0.81	0.19	36,45,48,61	0
3	GOL	A	807	6/6	0.84	0.17	55,58,61,63	0
3	GOL	C	705	6/6	0.86	0.14	38,51,55,64	0
3	GOL	B	803	6/6	0.87	0.12	35,39,41,41	0
3	GOL	B	804	6/6	0.88	0.14	46,49,51,52	0
3	GOL	A	805	6/6	0.89	0.14	34,44,47,48	0
3	GOL	A	806	6/6	0.89	0.14	39,45,46,47	0
3	GOL	C	701	6/6	0.90	0.13	43,46,49,59	0
3	GOL	A	802	6/6	0.91	0.09	31,33,35,39	0
3	GOL	B	802	6/6	0.91	0.10	30,32,35,35	0
3	GOL	A	804	6/6	0.92	0.10	35,41,43,51	0
3	GOL	C	704	6/6	0.93	0.10	40,41,44,44	0
3	GOL	C	703	6/6	0.93	0.08	29,30,37,46	0
3	GOL	A	808	6/6	0.94	0.09	23,34,37,41	0
2	CU	C	702	1/1	1.00	0.01	18,18,18,18	0
2	CU	A	801	1/1	1.00	0.01	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	B	801	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.