Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 04:51 AM EDT

PDB ID	:	4E9X
Title	:	Multicopper Oxidase mgLAC (data3)
Authors	:	Komori, H.; Miyazaki, K.; Higuchi, Y.
Deposited on	:	2012-03-21
Resolution	:	1.14 Å(reported)

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	:	2.36
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
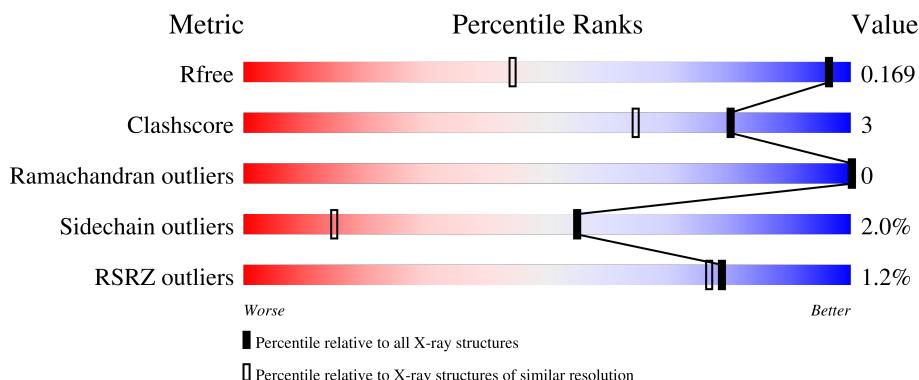
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
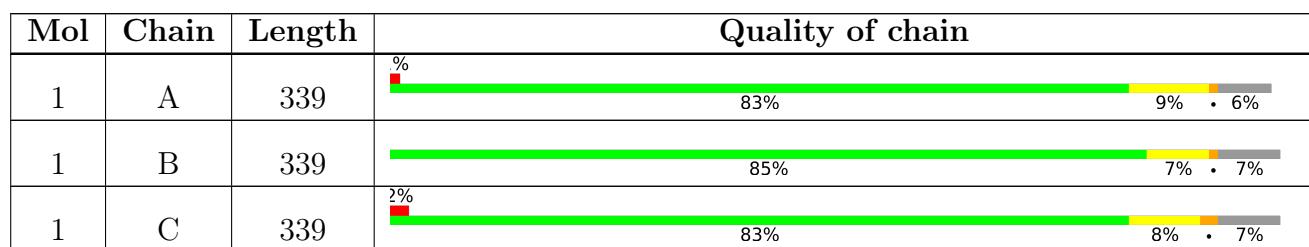
The reported resolution of this entry is 1.14 Å.

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	Percentile Ranks	Value
Rfree		0.169
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.0%
RSRZ outliers		1.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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	339	% 83% 9% · 6%
1	B	339	85% 7% · 7%
1	C	339	2% 83% 8% · 7%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8478 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 Multicopper oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	7	0
			2539	1633	425	469	12			
1	B	316	Total	C	N	O	S	0	5	0
			2519	1617	423	468	11			
1	C	316	Total	C	N	O	S	0	7	0
			2533	1631	424	467	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	MET	-	expression tag	UNP C0STU6
A	1327	LYS	-	expression tag	UNP C0STU6
A	1328	LEU	-	expression tag	UNP C0STU6
A	1329	ALA	-	expression tag	UNP C0STU6
A	1330	ALA	-	expression tag	UNP C0STU6
A	1331	ALA	-	expression tag	UNP C0STU6
A	1332	LEU	-	expression tag	UNP C0STU6
A	1333	GLU	-	expression tag	UNP C0STU6
A	1334	HIS	-	expression tag	UNP C0STU6
A	1335	HIS	-	expression tag	UNP C0STU6
A	1336	HIS	-	expression tag	UNP C0STU6
A	1337	HIS	-	expression tag	UNP C0STU6
A	1338	HIS	-	expression tag	UNP C0STU6
A	1339	HIS	-	expression tag	UNP C0STU6
B	2001	MET	-	expression tag	UNP C0STU6
B	2327	LYS	-	expression tag	UNP C0STU6
B	2328	LEU	-	expression tag	UNP C0STU6
B	2329	ALA	-	expression tag	UNP C0STU6
B	2330	ALA	-	expression tag	UNP C0STU6
B	2331	ALA	-	expression tag	UNP C0STU6
B	2332	LEU	-	expression tag	UNP C0STU6
B	2333	GLU	-	expression tag	UNP C0STU6
B	2334	HIS	-	expression tag	UNP C0STU6

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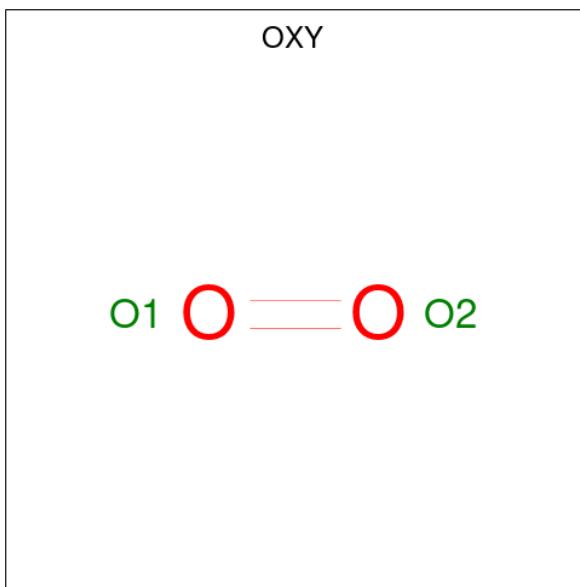
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Chain	Residue	Modelled	Actual	Comment	Reference
B	2335	HIS	-	expression tag	UNP C0STU6
B	2336	HIS	-	expression tag	UNP C0STU6
B	2337	HIS	-	expression tag	UNP C0STU6
B	2338	HIS	-	expression tag	UNP C0STU6
B	2339	HIS	-	expression tag	UNP C0STU6
C	3001	MET	-	expression tag	UNP C0STU6
C	3327	LYS	-	expression tag	UNP C0STU6
C	3328	LEU	-	expression tag	UNP C0STU6
C	3329	ALA	-	expression tag	UNP C0STU6
C	3330	ALA	-	expression tag	UNP C0STU6
C	3331	ALA	-	expression tag	UNP C0STU6
C	3332	LEU	-	expression tag	UNP C0STU6
C	3333	GLU	-	expression tag	UNP C0STU6
C	3334	HIS	-	expression tag	UNP C0STU6
C	3335	HIS	-	expression tag	UNP C0STU6
C	3336	HIS	-	expression tag	UNP C0STU6
C	3337	HIS	-	expression tag	UNP C0STU6
C	3338	HIS	-	expression tag	UNP C0STU6
C	3339	HIS	-	expression tag	UNP C0STU6

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Cu 4	0	0
2	B	4	Total 4	Cu 4	0	0
2	C	4	Total 4	Cu 4	0	0

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).

OXY

O1 O ══ O O2

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
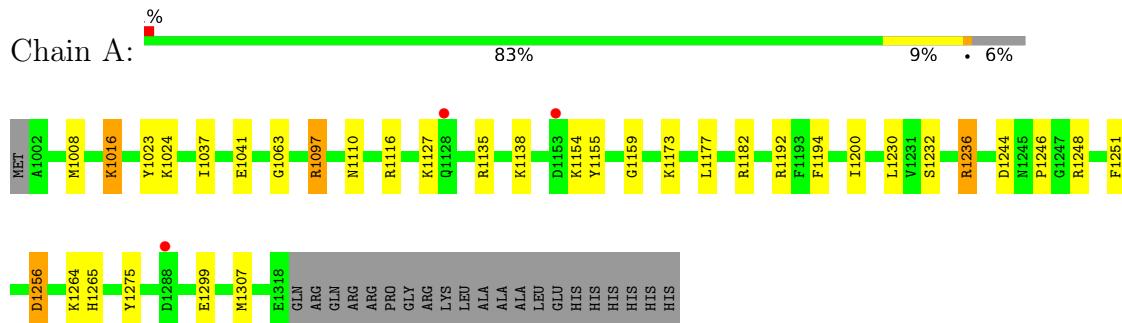
- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	271	Total 272	O 272	0	1
5	B	308	Total 308	O 308	0	0
5	C	288	Total 288	O 288	0	0
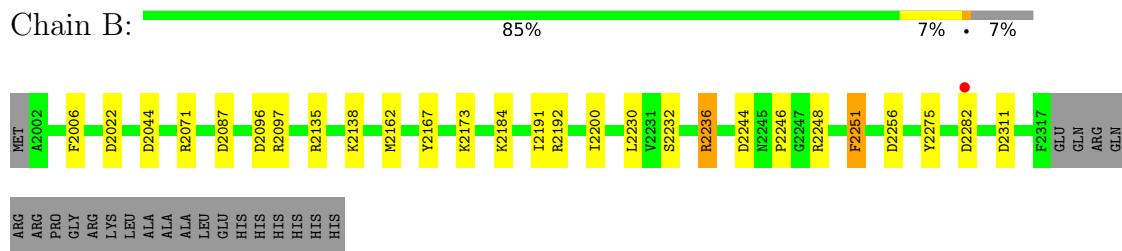
3 Residue-property plots ⓘ

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.
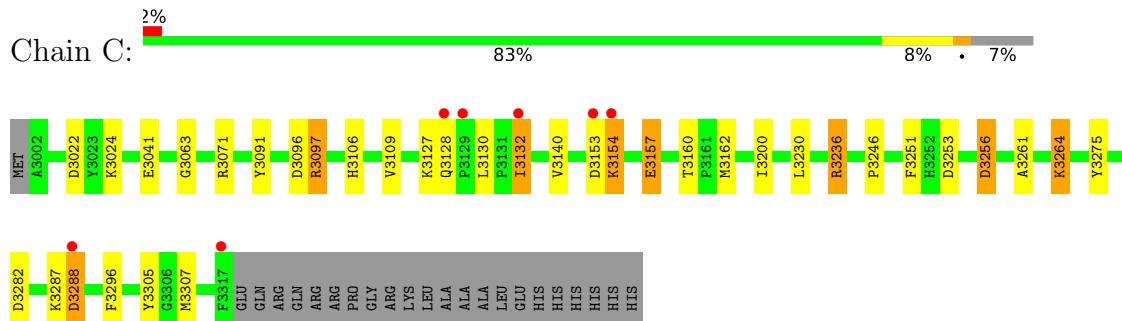
• Molecule 1: Multicopper oxidase

• Molecule 1: Multicopper oxidase

• Molecule 1: Multicopper oxidase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.74Å　101.16Å　123.98Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	10.00　–　1.14 11.77　–　1.14	Depositor EDS
% Data completeness (in resolution range)	94.2 (10.00-1.14) 99.1 (11.77-1.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 1.14Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.141　,　(Not available) 0.138　,　0.169	Depositor DCC
R_{free} test set	16984 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	9.4	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 68.4	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8478	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

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

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	0.72	0/2641	1.23	15/3594 (0.4%)
1	B	0.73	0/2615	1.26	22/3561 (0.6%)
1	C	0.75	0/2637	1.23	18/3590 (0.5%)
All	All	0.73	0/7893	1.24	55/10745 (0.5%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1135	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	B	2071	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	B	2256	ASP	CB-CG-OD1	11.12	128.31	118.30
1	B	2248	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	B	2282	ASP	CB-CG-OD1	9.94	127.24	118.30
1	B	2071	ARG	NE-CZ-NH2	9.75	125.18	120.30
1	A	1192	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	C	3256	ASP	CB-CG-OD1	9.61	126.94	118.30
1	B	2192	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	C	3097	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	A	1256	ASP	CB-CG-OD1	8.91	126.32	118.30
1	B	2236	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	B	2311	ASP	CB-CG-OD1	8.39	125.85	118.30
1	B	2248	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	3022	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	C	3307	MET	CG-SD-CE	-7.96	87.47	100.20
1	B	2097	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	2006	PHE	CB-CG-CD1	-7.41	115.61	120.80
1	B	2236	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	3236	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	C	3091	TYR	CB-CG-CD1	-7.16	116.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2192	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	C	3097	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	C	3282	ASP	CB-CG-OD1	-6.92	112.08	118.30
1	A	1192	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	1097	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	2244	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	2167	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	B	2087	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	2135	ARG	CD-NE-CZ	6.17	132.24	123.60
1	C	3253	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	3022	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	1135	ARG	NH1-CZ-NH2	6.02	126.02	119.40
1	A	1116	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	1299	GLU	OE1-CD-OE2	-5.96	116.14	123.30
1	B	2022	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	3305[A]	TYR	CB-CG-CD2	5.85	124.51	121.00
1	C	3305[B]	TYR	CB-CG-CD2	5.85	124.51	121.00
1	C	3251	PHE	CB-CG-CD2	5.83	124.88	120.80
1	C	3096	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	1155	TYR	CG-CD2-CE2	5.73	125.88	121.30
1	B	2096[A]	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	2096[B]	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	1024	LYS	CD-CE-NZ	5.40	124.11	111.70
1	C	3157	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	C	3071	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	1236	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	1023	TYR	CB-CG-CD2	5.26	124.15	121.00
1	C	3282	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	3288	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	1244	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	1097	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	2044	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	2167	TYR	CG-CD1-CE1	-5.05	117.26	121.30
1	A	1248	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	2539	0	2439	14	0
1	B	2519	0	2404	10	0
1	C	2533	0	2429	19	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
5	A	272	0	0	1	0
5	B	308	0	0	2	0
5	C	288	0	0	0	0
All	All	8478	0	7272	40	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 3.

All (40) 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:C:3261:ALA:O	1:C:3264:LYS:HE2	1.88	0.72
1:C:3132:ILE:H	1:C:3132:ILE:HD13	1.64	0.63
1:C:3024:LYS:HE2	1:C:3153:ASP:O	2.00	0.62
1:C:3154:LYS:HE2	1:C:3157:GLU:OE1	2.06	0.56
1:C:3128:GLN:O	1:C:3128:GLN:HG2	2.07	0.53
1:B:2138:LYS:HD3	5:B:2755:HOH:O	2.07	0.52
1:A:1232[A]:SER:OG	1:B:2230:LEU:HD13	2.09	0.52
1:B:2246:PRO:HA	1:B:2275:TYR:CG	2.44	0.52
1:C:3200[A]:ILE:HG22	1:C:3230:LEU:HD11	1.91	0.52
1:A:1200[A]:ILE:HG22	1:A:1230:LEU:HD11	1.91	0.51
1:A:1200[A]:ILE:CG2	1:A:1230:LEU:HD11	2.41	0.51
1:A:1008[A]:MET:HE2	1:A:1307:MET:HE1	1.92	0.51
1:A:1246:PRO:HA	1:A:1275:TYR:CG	2.46	0.51
1:C:3130:LEU:CD1	1:C:3132:ILE:HD11	2.42	0.50
1:C:3200[A]:ILE:CG2	1:C:3230:LEU:HD11	2.42	0.49
1:C:3041:GLU:O	1:C:3127:LYS:HE3	2.13	0.49
1:C:3063:GLY:O	1:C:3097:ARG:HG2	2.12	0.49
1:B:2200[A]:ILE:HG22	1:B:2230:LEU:HD11	1.96	0.48
1:A:1173[B]:LYS:HD3	1:A:1177:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3106:HIS:HA	1:C:3109:VAL:HG12	1.94	0.48
1:A:1037:ILE:HG12	1:A:1307:MET:HE3	1.97	0.46
1:A:1008[A]:MET:HE2	1:A:1008[A]:MET:HB2	1.51	0.46
1:A:1016:LYS:HE3	5:A:5179:HOH:O	2.15	0.46
1:B:2200[A]:ILE:CG2	1:B:2230:LEU:HD11	2.46	0.46
1:C:3160:THR:HB	1:C:3162:MET:HE1	1.99	0.45
1:B:2173:LYS:NZ	5:B:2804:HOH:O	2.48	0.45
1:C:3246:PRO:HA	1:C:3275:TYR:CG	2.53	0.43
1:A:1041:GLU:O	1:A:1127:LYS:HE3	2.19	0.43
1:C:3154:LYS:HE2	1:C:3157:GLU:CD	2.39	0.42
1:B:2232[A]:SER:OG	1:C:3230:LEU:HD13	2.19	0.42
1:B:2191:ILE:HD13	1:B:2251:PHE:CE1	2.55	0.42
1:A:1138:LYS:HE3	1:A:1182:ARG:O	2.20	0.42
1:A:1063:GLY:O	1:A:1097:ARG:HG2	2.20	0.42
1:A:1265:HIS:CE1	1:C:3109:VAL:HG22	2.55	0.41
1:A:1110:ASN:HB2	1:A:1159:GLY:O	2.21	0.41
1:B:2246:PRO:HA	1:B:2275:TYR:CD2	2.56	0.41
1:C:3162:MET:HB2	1:C:3162:MET:HE2	1.97	0.41
1:C:3287:LYS:O	1:C:3288:ASP:HB2	2.21	0.40
1:B:2138:LYS:HB2	1:B:2138:LYS:HE2	1.68	0.40
1:C:3140:VAL:HG13	1:C:3296:PHE:HB3	2.03	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	322/339 (95%)	316 (98%)	6 (2%)	0	100	100
1	B	319/339 (94%)	313 (98%)	6 (2%)	0	100	100
1	C	321/339 (95%)	314 (98%)	7 (2%)	0	100	100
All	All	962/1017 (95%)	943 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	276/287 (96%)	269 (98%)	7 (2%)	47	9
1	B	273/287 (95%)	269 (98%)	4 (2%)	65	27
1	C	275/287 (96%)	270 (98%)	5 (2%)	59	20
All	All	824/861 (96%)	808 (98%)	16 (2%)	55	17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1016	LYS
1	A	1154	LYS
1	A	1194	PHE
1	A	1236	ARG
1	A	1251	PHE
1	A	1256	ASP
1	A	1264	LYS
1	B	2162	MET
1	B	2184	LYS
1	B	2236	ARG
1	B	2251	PHE
1	C	3132	ILE
1	C	3154	LYS
1	C	3236	ARG
1	C	3256	ASP
1	C	3264	LYS

Sometimes 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.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 13 are monoatomic - leaving 3 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	OXY	B	2403	2	1,1,1	0.07	0	-		
3	OXY	B	2406	2	1,1,1	0.21	0	-		
3	OXY	A	1405	2	1,1,1	0.22	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.

No monomer is involved in short contacts.

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.

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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(Å²)	Q<0.9
1	A	317/339 (93%)	-0.37	3 (0%)	84	82	7, 12, 24, 42	0
1	B	316/339 (93%)	-0.43	1 (0%)	94	92	7, 11, 21, 33	0
1	C	316/339 (93%)	-0.36	7 (2%)	62	60	7, 11, 25, 51	0
All	All	949/1017 (93%)	-0.38	11 (1%)	79	77	7, 11, 23, 51	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3128	GLN	5.2
1	C	3132	ILE	3.6
1	C	3129	PRO	3.2
1	C	3154	LYS	2.4
1	A	1288	ASP	2.3
1	A	1128	GLN	2.3
1	C	3317	PHE	2.2
1	A	1153	ASP	2.2
1	C	3288	ASP	2.2
1	B	2282	ASP	2.1
1	C	3153	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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	OXY	B	2403	2/2	0.91	0.19	11,11,11,15	2
3	OXY	A	1405	2/2	0.95	0.12	10,10,10,13	2
3	OXY	B	2406	2/2	0.96	0.10	9,9,9,13	2
4	CL	A	1406	1/1	0.99	0.05	11,11,11,11	0
2	CU	B	2401	1/1	1.00	0.02	13,13,13,13	1
2	CU	B	2402	1/1	1.00	0.09	14,14,14,14	1
2	CU	B	2404	1/1	1.00	0.02	9,9,9,9	0
2	CU	B	2405	1/1	1.00	0.03	9,9,9,9	1
2	CU	C	3401	1/1	1.00	0.02	12,12,12,12	1
2	CU	C	3402	1/1	1.00	0.06	11,11,11,11	1
2	CU	C	3403	1/1	1.00	0.02	11,11,11,11	0
2	CU	C	3404	1/1	1.00	0.02	9,9,9,9	1
2	CU	A	1401	1/1	1.00	0.02	12,12,12,12	0
2	CU	A	1402	1/1	1.00	0.03	10,10,10,10	1
2	CU	A	1403	1/1	1.00	0.04	12,12,12,12	1
2	CU	A	1404	1/1	1.00	0.07	13,13,13,13	1

6.5 Other polymers ⓘ

There are no such residues in this entry.