



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:00 pm GMT

PDB ID : 4EV2
Title : Crystal structure of copper amine oxidase-1 from Hansenula polymorpha in complex with ethylamine
Authors : Klema, V.J.; Solheid, C.J.; Wilmot, C.M.
Deposited on : 2012-04-25
Resolution : 2.18 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : trunk28620

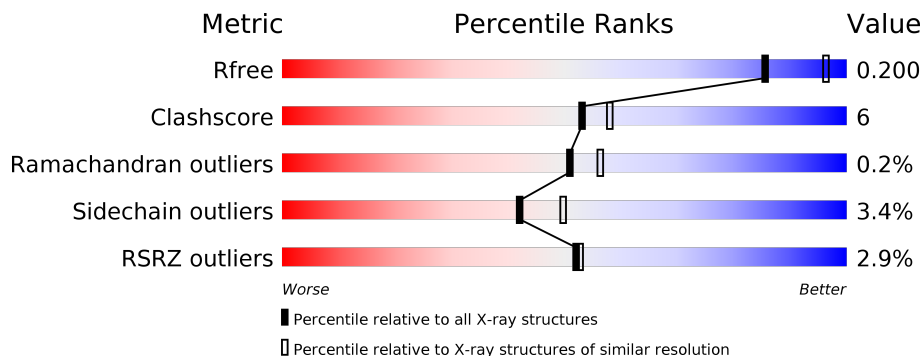
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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 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	692	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	692	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>5%</div> </div> </div>
1	C	692	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>
1	D	692	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	E	692	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	F	692	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </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
1	TYQ	A	405	-	-	X	-
2	GOL	A	703	-	-	X	X
2	GOL	A	705	-	-	-	X
2	GOL	A	706	-	-	-	X
2	GOL	B	701	-	-	X	X
2	GOL	B	704	-	-	-	X
2	GOL	B	705	-	-	-	X
2	GOL	B	706	-	-	-	X
2	GOL	B	707	-	-	X	X
2	GOL	C	702	-	-	-	X
2	GOL	C	703	-	-	-	X
2	GOL	C	704	-	-	-	X
2	GOL	C	706	-	-	-	X
2	GOL	C	707	-	-	-	X
2	GOL	D	702	-	-	-	X
2	GOL	D	703	-	-	-	X
2	GOL	D	704	-	-	-	X
2	GOL	D	705	-	-	-	X
2	GOL	E	702	-	-	-	X
2	GOL	E	703	-	-	-	X
2	GOL	E	704	-	-	X	X
2	GOL	E	705	-	-	X	-
2	GOL	F	702	-	-	X	X
2	GOL	F	703	-	-	-	X
2	GOL	F	706	-	-	-	X
5	NEH	A	708	-	-	X	X
5	NEH	B	709	-	-	-	X
5	NEH	C	708	-	-	-	X
5	NEH	D	706	-	-	-	X
5	NEH	E	707	-	-	-	X
5	NEH	F	708	-	-	-	X

2 Entry composition [i](#)

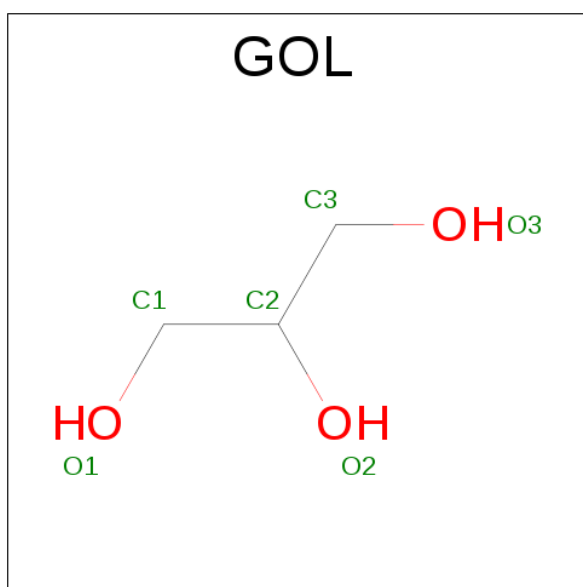
There are 7 unique types of molecules in this entry. The entry contains 35006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	654	Total	C	N	O	S	0	13	0
			5236	3339	891	981	25			
1	B	655	Total	C	N	O	S	0	11	1
			5238	3337	896	979	26			
1	C	655	Total	C	N	O	S	0	12	0
			5236	3335	891	983	27			
1	D	655	Total	C	N	O	S	0	9	0
			5232	3333	897	977	25			
1	E	654	Total	C	N	O	S	0	18	0
			5268	3358	900	983	27			
1	F	655	Total	C	N	O	S	0	9	0
			5233	3333	899	976	25			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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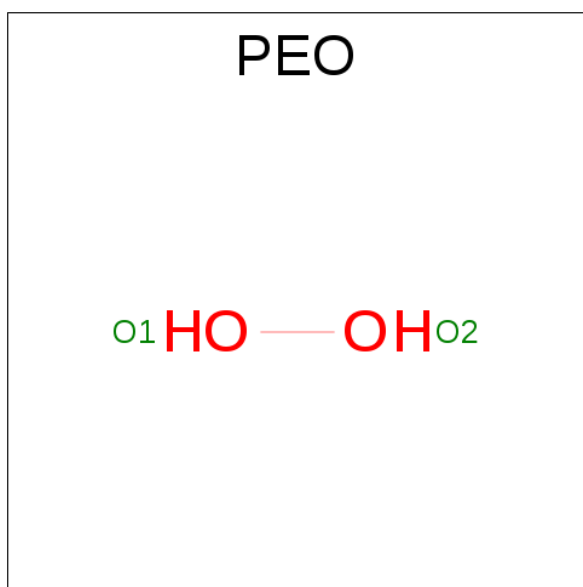
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

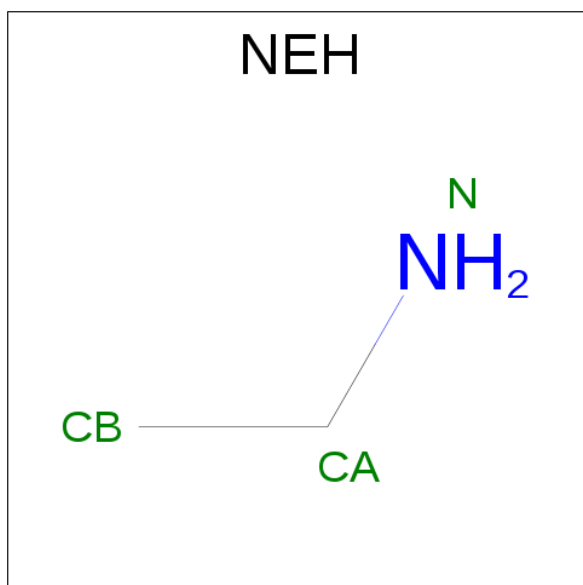
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cu	0	0
			1	1		
3	E	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		
3	A	1	Total	Cu	0	0
			1	1		
3	F	1	Total	Cu	0	0
			1	1		

- Molecule 4 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



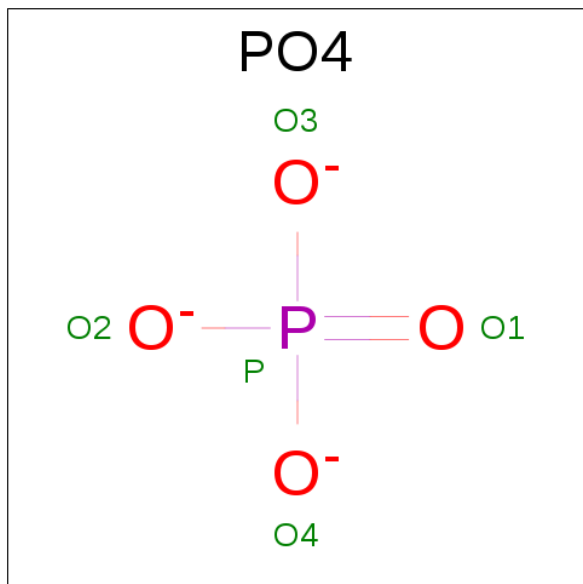
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	B	1	Total O 2 2	0	0
4	E	1	Total O 2 2	0	0
4	F	1	Total O 2 2	0	0

- Molecule 5 is ETHANAMINE (three-letter code: NEH) (formula: C₂H₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			3	2	1		
5	B	1	Total	C	N	0	0
			3	2	1		
5	C	1	Total	C	N	0	0
			3	2	1		
5	D	1	Total	C	N	0	0
			3	2	1		
5	E	1	Total	C	N	0	0
			3	2	1		
5	F	1	Total	C	N	0	0
			3	2	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	569	Total	O	0	2
			571	571		
7	B	653	Total	O	0	3
			656	656		
7	C	534	Total	O	0	3
			537	537		

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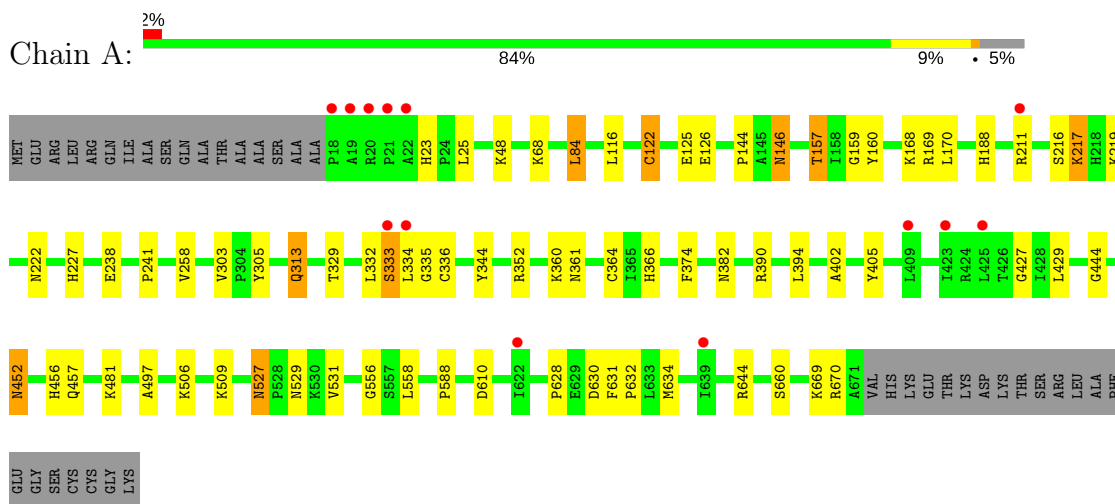
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	496	Total 498	O 498	0	2
7	E	517	Total 519	O 519	0	2
7	F	557	Total 559	O 559	0	2

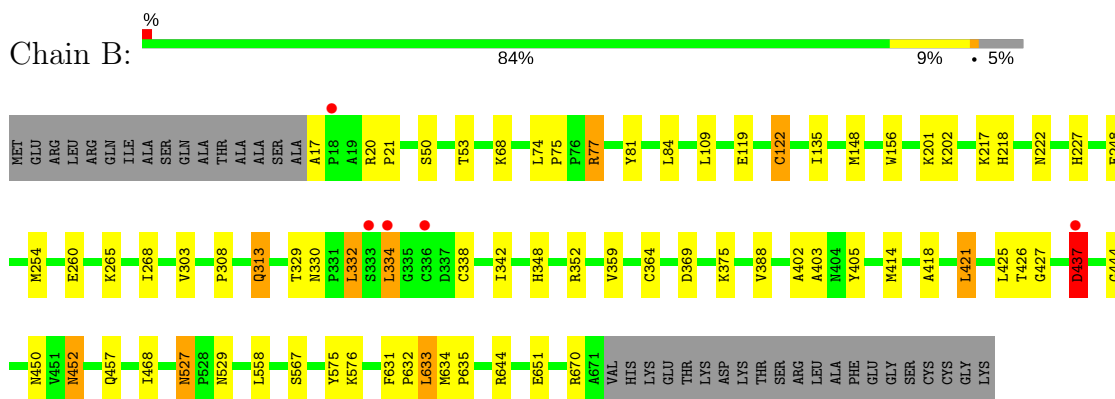
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

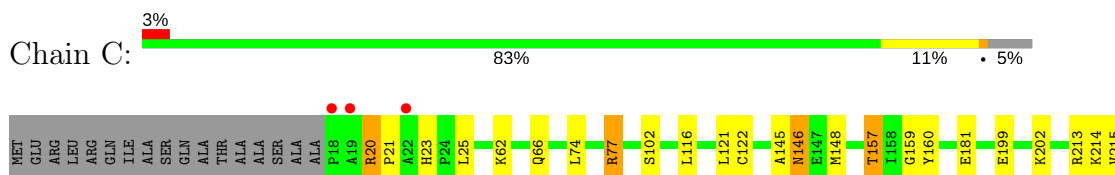
• Molecule 1: Peroxisomal primary amine oxidase

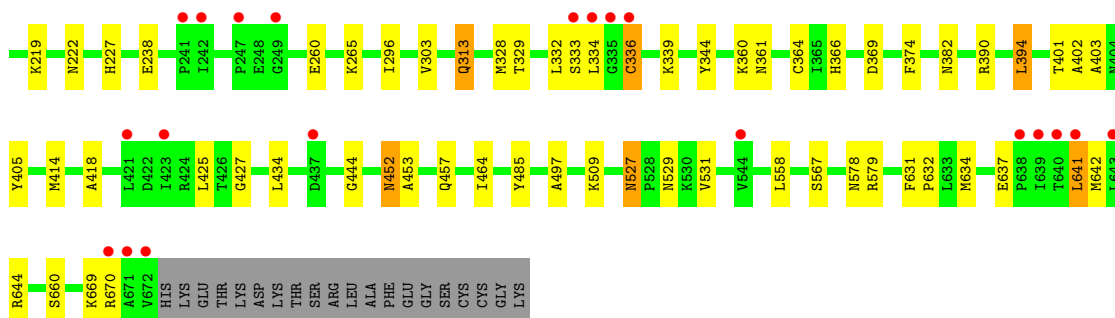


• Molecule 1: Peroxisomal primary amine oxidase

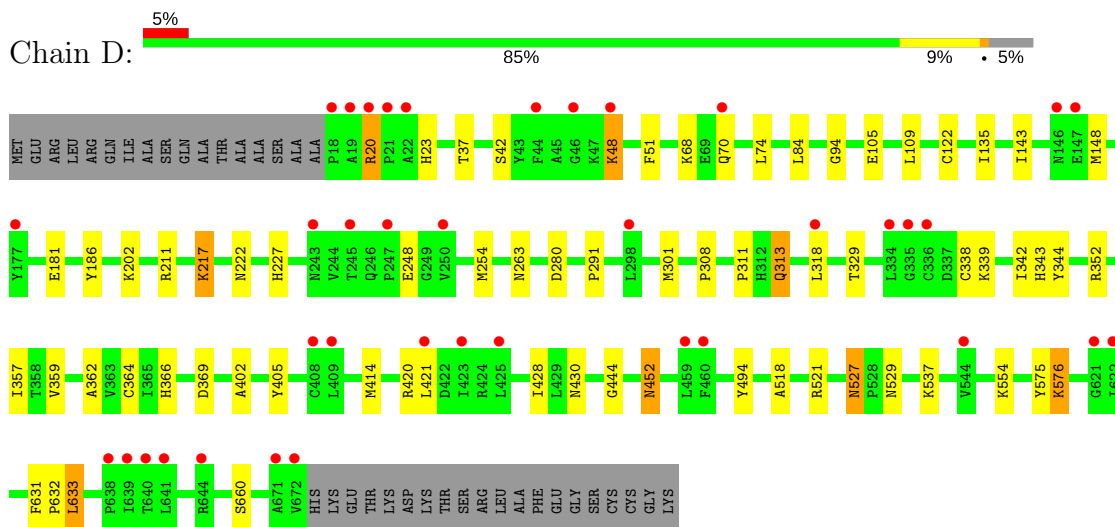


• Molecule 1: Peroxisomal primary amine oxidase

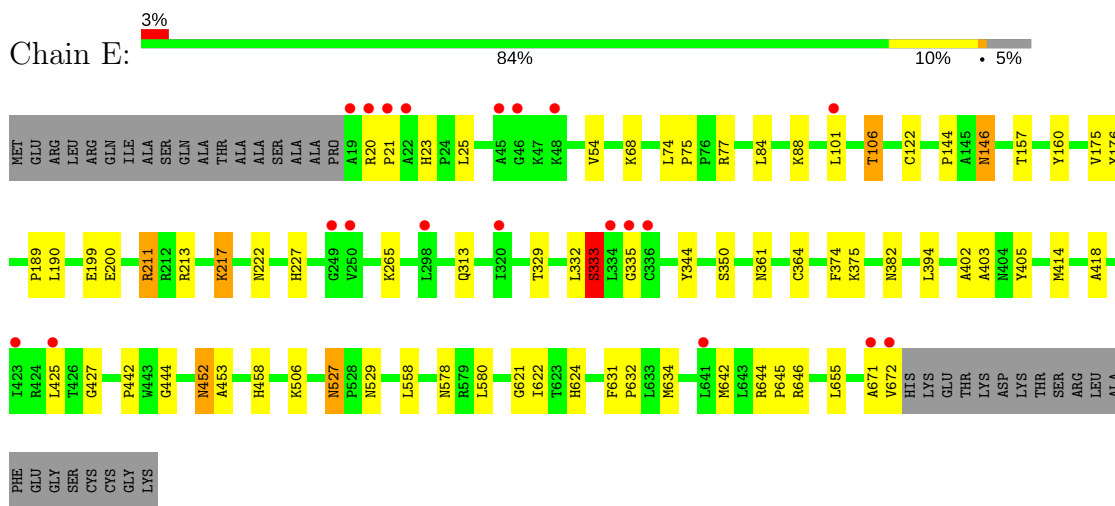




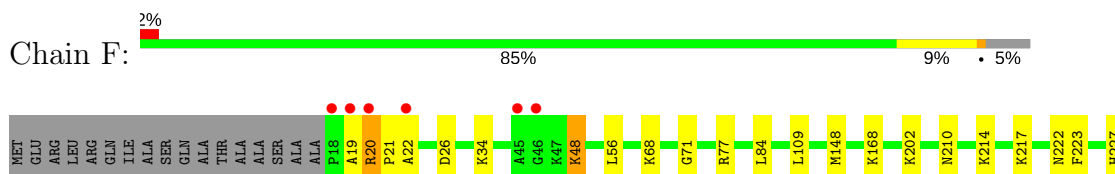
- Molecule 1: Peroxisomal primary amine oxidase

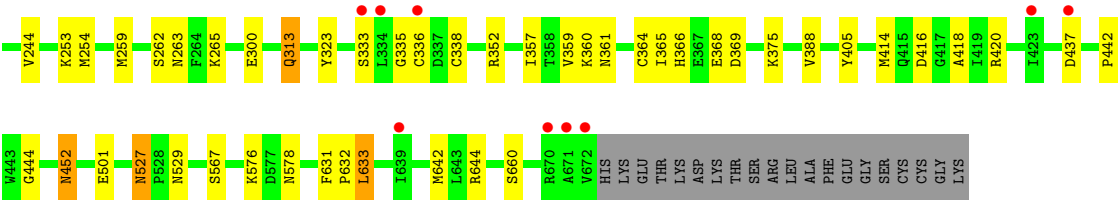


- Molecule 1: Peroxisomal primary amine oxidase



- Molecule 1: Peroxisomal primary amine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.41Å 232.83Å 105.12Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	48.97 – 2.18 48.97 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.97-2.18) 99.5 (48.97-2.18)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.150 , 0.201 0.150 , 0.200	Depositor DCC
R_{free} test set	12922 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35006	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NEH, PO4, PEO, 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	0.74	0/5410	0.77	2/7360 (0.0%)
1	B	0.83	2/5407 (0.0%)	0.82	4/7355 (0.1%)
1	C	0.76	1/5410 (0.0%)	0.76	5/7362 (0.1%)
1	D	0.67	1/5394 (0.0%)	0.71	1/7338 (0.0%)
1	E	0.75	2/5456 (0.0%)	0.75	0/7423
1	F	0.77	0/5395	0.78	1/7339 (0.0%)
All	All	0.75	6/32472 (0.0%)	0.76	13/44177 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	122	CYS	CB-SG	10.97	2.00	1.82
1	B	122	CYS	CB-SG	8.13	1.96	1.82
1	E	122[A]	CYS	CB-SG	5.80	1.92	1.82
1	E	122[B]	CYS	CB-SG	5.80	1.92	1.82
1	B	437	ASP	CB-CG	-5.51	1.40	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	641	LEU	CA-CB-CG	7.23	131.93	115.30
1	B	421	LEU	CB-CG-CD2	7.21	123.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	416	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	84	LEU	CA-CB-CG	6.42	130.06	115.30
1	C	77	ARG	NE-CZ-NH2	-6.36	117.12	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	333	SER	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	5236	0	5107	73	0
1	B	5238	0	5106	76	0
1	C	5236	0	5092	75	0
1	D	5232	0	5096	47	0
1	E	5268	0	5154	66	0
1	F	5233	0	5103	55	0
2	A	30	0	40	9	0
2	B	42	0	56	16	0
2	C	36	0	48	7	0
2	D	24	0	32	4	0
2	E	24	0	32	11	0
2	F	30	0	40	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	1	0
4	E	2	0	0	1	0
4	F	2	0	0	0	0
5	A	3	0	7	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	3	0	7	2	0
5	C	3	0	7	1	0
5	D	3	0	7	0	0
5	E	3	0	7	0	0
5	F	3	0	7	2	0
6	C	5	0	0	1	0
7	A	571	0	0	17	0
7	B	656	0	0	11	0
7	C	537	0	0	17	0
7	D	498	0	0	7	0
7	E	519	0	0	11	0
7	F	559	0	0	15	0
All	All	35006	0	30948	387	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 6.

The worst 5 of 387 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:D:23:HIS:HE2	2:D:702:GOL:H11	1.21	1.02
1:F:437:ASP:HB2	7:F:986:HOH:O	1.65	0.97
1:C:644:ARG:HD2	7:C:1271:HOH:O	1.64	0.96
1:D:68:LYS:HE3	2:D:702:GOL:H2	1.43	0.95
1:A:352:ARG:HD3	7:A:1266:HOH:O	1.65	0.94

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	664/692 (96%)	636 (96%)	27 (4%)	1 (0%)	51	56
1	B	663/692 (96%)	637 (96%)	25 (4%)	1 (0%)	51	56
1	C	665/692 (96%)	639 (96%)	23 (4%)	3 (0%)	32	32
1	D	661/692 (96%)	632 (96%)	29 (4%)	0	100	100
1	E	669/692 (97%)	640 (96%)	27 (4%)	2 (0%)	44	47
1	F	661/692 (96%)	633 (96%)	25 (4%)	3 (0%)	32	32
All	All	3983/4152 (96%)	3817 (96%)	156 (4%)	10 (0%)	51	47

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	19	ALA
1	E	333	SER
1	F	22	ALA
1	F	335	GLY
1	C	403	ALA

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	576/593 (97%)	552 (96%)	24 (4%)	34	40
1	B	575/593 (97%)	559 (97%)	16 (3%)	49	58
1	C	576/593 (97%)	553 (96%)	23 (4%)	36	42
1	D	574/593 (97%)	550 (96%)	24 (4%)	34	40
1	E	582/593 (98%)	565 (97%)	17 (3%)	48	57
1	F	574/593 (97%)	553 (96%)	21 (4%)	39	46
All	All	3457/3558 (97%)	3332 (96%)	125 (4%)	42	47

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	382	ASN

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Mol	Chain	Res	Type
1	D	202	LYS
1	F	352	ARG
1	C	452	ASN
1	D	20	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	452	ASN
1	D	366	HIS
1	F	366	HIS
1	D	218	HIS
1	D	450	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	TYQ	A	405	1	14,14,15	2.59	2 (14%)	15,19,21	1.70	3 (20%)
1	TYQ	B	405	1	14,14,15	2.44	2 (14%)	15,19,21	2.08	4 (26%)
1	TYQ	C	405	1	14,14,15	2.64	2 (14%)	15,19,21	1.63	1 (6%)
1	TYQ	D	405	1	14,14,15	2.52	2 (14%)	15,19,21	2.12	4 (26%)
1	TYQ	E	405	1	14,14,15	2.14	3 (21%)	15,19,21	1.38	1 (6%)
1	TYQ	F	405	1	14,14,15	2.31	2 (14%)	15,19,21	1.78	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	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	B	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	C	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	D	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	E	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	F	405	1	-	0/4/6/8	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	TYQ	CA-C	2.17	1.53	1.50
1	E	405	TYQ	CD1-CG	4.41	1.46	1.40
1	F	405	TYQ	CD1-CG	5.01	1.47	1.40
1	D	405	TYQ	CE2-CZ	5.70	1.48	1.40
1	B	405	TYQ	CD1-CG	5.99	1.48	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	TYQ	CB-CA-C	-6.04	99.78	111.41
1	C	405	TYQ	CB-CA-C	-5.32	101.16	111.41
1	D	405	TYQ	CB-CA-C	-5.13	101.52	111.41
1	F	405	TYQ	CB-CA-C	-4.99	101.79	111.41
1	A	405	TYQ	CB-CA-C	-4.69	102.37	111.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405	TYQ	6	0
1	B	405	TYQ	2	0
1	C	405	TYQ	3	0
1	D	405	TYQ	1	0
1	E	405	TYQ	1	0
1	F	405	TYQ	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 6 are monoatomic - leaving 42 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	$\# Z > 2$
2	GOL	A	701	-	5,5,5	0.33	0	5,5,5	0.64	0
2	GOL	A	703	-	5,5,5	0.42	0	5,5,5	0.34	0
2	GOL	A	704	-	5,5,5	0.40	0	5,5,5	0.32	0
2	GOL	A	705	-	5,5,5	0.42	0	5,5,5	0.59	0
2	GOL	A	706	-	5,5,5	0.44	0	5,5,5	0.49	0
4	PEO	A	707	3	1,1,1	0.07	0	0,0,0	0.00	-
5	NEH	A	708	-	2,2,2	0.77	0	0,1,1	0.00	-
2	GOL	B	701	-	5,5,5	0.82	0	5,5,5	0.59	0
2	GOL	B	703	-	5,5,5	0.48	0	5,5,5	0.73	0
2	GOL	B	704	-	5,5,5	0.39	0	5,5,5	0.55	0
2	GOL	B	705	-	5,5,5	0.30	0	5,5,5	0.51	0
2	GOL	B	706	-	5,5,5	0.24	0	5,5,5	0.71	0
2	GOL	B	707	-	5,5,5	0.47	0	5,5,5	0.43	0
4	PEO	B	708	3	1,1,1	0.49	0	0,0,0	0.00	-
5	NEH	B	709	-	2,2,2	0.58	0	0,1,1	0.00	-
2	GOL	B	710	-	5,5,5	0.23	0	5,5,5	0.49	0
2	GOL	C	702	-	5,5,5	0.21	0	5,5,5	1.17	0
2	GOL	C	703	-	5,5,5	0.23	0	5,5,5	0.63	0
2	GOL	C	704	-	5,5,5	0.48	0	5,5,5	0.27	0
2	GOL	C	705	-	5,5,5	0.57	0	5,5,5	0.59	0
2	GOL	C	706	-	5,5,5	0.26	0	5,5,5	0.52	0
2	GOL	C	707	-	5,5,5	0.48	0	5,5,5	0.65	0
5	NEH	C	708	-	2,2,2	0.48	0	0,1,1	0.00	-
6	PO4	C	709	-	4,4,4	0.79	0	6,6,6	0.90	0
2	GOL	D	702	-	5,5,5	0.41	0	5,5,5	0.84	0
2	GOL	D	703	-	5,5,5	0.54	0	5,5,5	0.62	0
2	GOL	D	704	-	5,5,5	0.30	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	705	-	5,5,5	0.41	0	5,5,5	0.14	0
5	NEH	D	706	-	2,2,2	0.64	0	0,1,1	0.00	-
2	GOL	E	702	-	5,5,5	0.37	0	5,5,5	0.82	0
2	GOL	E	703	-	5,5,5	0.32	0	5,5,5	0.45	0
2	GOL	E	704	-	5,5,5	0.30	0	5,5,5	0.67	0
2	GOL	E	705	-	5,5,5	0.47	0	5,5,5	1.25	0
4	PEO	E	706	3	1,1,1	0.08	0	0,0,0	0.00	-
5	NEH	E	707	-	2,2,2	0.86	0	0,1,1	0.00	-
2	GOL	F	702	-	5,5,5	0.38	0	5,5,5	0.47	0
2	GOL	F	703	-	5,5,5	0.37	0	5,5,5	0.39	0
2	GOL	F	704	-	5,5,5	0.31	0	5,5,5	0.53	0
2	GOL	F	705	-	5,5,5	0.28	0	5,5,5	1.00	0
2	GOL	F	706	-	5,5,5	0.31	0	5,5,5	0.80	0
4	PEO	F	707	3	1,1,1	0.03	0	0,0,0	0.00	-
5	NEH	F	708	-	2,2,2	0.70	0	0,1,1	0.00	-

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
2	GOL	A	701	-	-	0/4/4/4	0/0/0/0
2	GOL	A	703	-	-	0/4/4/4	0/0/0/0
2	GOL	A	704	-	-	0/4/4/4	0/0/0/0
2	GOL	A	705	-	-	0/4/4/4	0/0/0/0
2	GOL	A	706	-	-	0/4/4/4	0/0/0/0
4	PEO	A	707	3	-	0/0/0/0	0/0/0/0
5	NEH	A	708	-	-	0/0/0/0	0/0/0/0
2	GOL	B	701	-	-	0/4/4/4	0/0/0/0
2	GOL	B	703	-	-	0/4/4/4	0/0/0/0
2	GOL	B	704	-	-	0/4/4/4	0/0/0/0
2	GOL	B	705	-	-	0/4/4/4	0/0/0/0
2	GOL	B	706	-	-	0/4/4/4	0/0/0/0
2	GOL	B	707	-	-	0/4/4/4	0/0/0/0
4	PEO	B	708	3	-	0/0/0/0	0/0/0/0
5	NEH	B	709	-	-	0/0/0/0	0/0/0/0
2	GOL	B	710	-	-	0/4/4/4	0/0/0/0
2	GOL	C	702	-	-	0/4/4/4	0/0/0/0
2	GOL	C	703	-	-	0/4/4/4	0/0/0/0
2	GOL	C	704	-	-	0/4/4/4	0/0/0/0
2	GOL	C	705	-	-	0/4/4/4	0/0/0/0
2	GOL	C	706	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	707	-	-	0/4/4/4	0/0/0/0
5	NEH	C	708	-	-	0/0/0/0	0/0/0/0
6	PO4	C	709	-	-	0/0/0/0	0/0/0/0
2	GOL	D	702	-	-	0/4/4/4	0/0/0/0
2	GOL	D	703	-	-	0/4/4/4	0/0/0/0
2	GOL	D	704	-	-	0/4/4/4	0/0/0/0
2	GOL	D	705	-	-	0/4/4/4	0/0/0/0
5	NEH	D	706	-	-	0/0/0/0	0/0/0/0
2	GOL	E	702	-	-	0/4/4/4	0/0/0/0
2	GOL	E	703	-	-	0/4/4/4	0/0/0/0
2	GOL	E	704	-	-	0/4/4/4	0/0/0/0
2	GOL	E	705	-	-	0/4/4/4	0/0/0/0
4	PEO	E	706	3	-	0/0/0/0	0/0/0/0
5	NEH	E	707	-	-	0/0/0/0	0/0/0/0
2	GOL	F	702	-	-	0/4/4/4	0/0/0/0
2	GOL	F	703	-	-	0/4/4/4	0/0/0/0
2	GOL	F	704	-	-	0/4/4/4	0/0/0/0
2	GOL	F	705	-	-	0/4/4/4	0/0/0/0
2	GOL	F	706	-	-	0/4/4/4	0/0/0/0
4	PEO	F	707	3	-	0/0/0/0	0/0/0/0
5	NEH	F	708	-	-	0/0/0/0	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.

27 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	703	GOL	7	0
2	A	704	GOL	1	0
2	A	706	GOL	1	0
4	A	707	PEO	1	0
5	A	708	NEH	5	0
2	B	701	GOL	7	0
2	B	704	GOL	3	0
2	B	707	GOL	6	0
4	B	708	PEO	1	0
5	B	709	NEH	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	702	GOL	2	0
2	C	703	GOL	1	0
2	C	704	GOL	3	0
2	C	705	GOL	1	0
5	C	708	NEH	1	0
6	C	709	PO4	1	0
2	D	702	GOL	3	0
2	D	705	GOL	1	0
2	E	703	GOL	2	0
2	E	704	GOL	5	0
2	E	705	GOL	4	0
4	E	706	PEO	1	0
2	F	702	GOL	4	0
2	F	704	GOL	1	0
2	F	705	GOL	1	0
2	F	706	GOL	1	0
5	F	708	NEH	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	653/692 (94%)	-0.17	13 (1%) 65 66	15, 29, 53, 88	0
1	B	654/692 (94%)	-0.34	5 (0%) 86 86	14, 25, 46, 69	0
1	C	654/692 (94%)	-0.18	23 (3%) 44 45	18, 30, 52, 85	0
1	D	654/692 (94%)	0.11	38 (5%) 24 25	20, 36, 59, 93	0
1	E	653/692 (94%)	-0.12	20 (3%) 49 50	15, 31, 54, 87	0
1	F	654/692 (94%)	-0.14	15 (2%) 61 61	15, 30, 55, 82	0
All	All	3922/4152 (94%)	-0.14	114 (2%) 52 53	14, 30, 55, 93	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	PRO	7.5
1	F	672	VAL	6.8
1	D	18	PRO	6.4
1	D	334	LEU	6.1
1	E	672	VAL	5.8

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

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	C	405	14/15	0.95	0.17	-	27,35,43,45	0
1	TYQ	A	405	14/15	0.96	0.15	-	26,30,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	TYQ	E	405	14/15	0.97	0.17	-	21,24,41,44	0
1	TYQ	D	405	14/15	0.96	0.16	-	35,39,42,43	0
1	TYQ	B	405	14/15	0.96	0.12	-	20,25,33,35	0
1	TYQ	F	405	14/15	0.96	0.15	-	29,33,41,48	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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(\AA^2)	Q<0.9
2	GOL	C	707	6/6	0.49	0.43	25.33	45,59,67,70	0
5	NEH	B	709	3/3	0.91	0.40	20.43	35,35,37,39	0
2	GOL	A	706	6/6	0.82	0.26	20.37	49,58,65,68	0
5	NEH	D	706	3/3	0.84	0.40	17.10	34,34,34,39	0
2	GOL	D	703	6/6	0.81	0.20	15.99	40,53,55,58	0
5	NEH	F	708	3/3	0.69	0.31	13.45	34,34,35,36	0
5	NEH	A	708	3/3	0.92	0.51	12.92	29,29,32,33	0
2	GOL	E	704	6/6	0.78	0.31	12.08	53,64,67,74	0
5	NEH	E	707	3/3	0.84	0.55	11.71	29,29,29,33	0
2	GOL	B	704	6/6	0.97	0.21	10.92	25,39,40,48	0
5	NEH	C	708	3/3	0.90	0.30	9.76	37,37,39,40	0
2	GOL	E	703	6/6	0.88	0.19	7.93	50,59,62,63	0
2	GOL	B	705	6/6	0.80	0.23	7.48	50,57,63,68	0
2	GOL	C	706	6/6	0.79	0.25	7.03	51,57,63,68	0
2	GOL	D	702	6/6	0.89	0.26	6.67	52,55,57,61	0
2	GOL	D	704	6/6	0.66	0.25	6.65	50,53,62,68	0
2	GOL	C	702	6/6	0.83	0.18	5.61	47,56,57,58	0
2	GOL	D	705	6/6	0.62	0.35	4.89	83,85,85,87	0
2	GOL	E	702	6/6	0.84	0.30	4.24	57,57,58,62	0
2	GOL	B	706	6/6	0.86	0.23	4.18	50,56,59,64	0
2	GOL	F	706	6/6	0.93	0.16	3.93	40,48,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	C	704	6/6	0.89	0.23	3.83	51,56,58,61	0
2	GOL	F	702	6/6	0.90	0.18	3.67	43,52,53,55	0
2	GOL	A	703	6/6	0.89	0.20	3.36	55,66,67,68	0
2	GOL	A	705	6/6	0.86	0.26	3.19	46,52,54,55	0
2	GOL	C	703	6/6	0.94	0.23	2.35	47,50,51,51	0
2	GOL	F	703	6/6	0.78	0.19	2.33	56,62,65,66	0
2	GOL	B	707	6/6	0.92	0.20	2.11	50,56,57,58	0
2	GOL	B	701	6/6	0.94	0.20	2.02	11,18,20,23	6
2	GOL	E	705	6/6	0.84	0.16	1.99	48,51,53,55	0
4	PEO	B	708	2/2	0.97	0.15	1.80	16,16,16,21	0
4	PEO	A	707	2/2	0.97	0.16	1.64	18,18,18,29	0
2	GOL	F	705	6/6	0.88	0.22	1.63	57,60,62,63	0
2	GOL	C	705	6/6	0.83	0.19	1.60	61,66,66,69	0
2	GOL	F	704	6/6	0.94	0.19	1.45	47,48,49,51	0
2	GOL	B	703	6/6	0.94	0.15	0.92	43,46,47,48	0
4	PEO	E	706	2/2	0.99	0.17	0.84	14,14,14,27	0
4	PEO	F	707	2/2	0.97	0.13	0.37	18,18,18,29	0
2	GOL	B	710	6/6	0.90	0.12	-0.08	26,40,42,43	6
3	CU	A	702	1/1	1.00	0.09	-1.27	21,21,21,21	0
3	CU	E	701	1/1	0.99	0.10	-1.35	19,19,19,19	0
2	GOL	A	701	6/6	0.97	0.07	-1.46	27,31,32,32	0
3	CU	C	701	1/1	1.00	0.08	-2.38	25,25,25,25	0
3	CU	B	702	1/1	1.00	0.09	-3.24	19,19,19,19	0
6	PO4	C	709	5/5	0.85	0.22	-	33,33,39,40	5
3	CU	F	701	1/1	1.00	0.06	-	23,23,23,23	0
3	CU	D	701	1/1	0.99	0.09	-	29,29,29,29	0
2	GOL	A	704	6/6	0.83	0.16	-	56,58,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.