



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 06:26 AM EDT

PDB ID : 4KFD
Title : Crystal structure of Hansenula polymorpha copper amine oxidase-1 reduced by methylamine at pH 6.0
Authors : Johnson, B.J.; Yukl, E.T.; Klema, V.J.; Wilmot, C.M.
Deposited on : 2013-04-26
Resolution : 1.69 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

<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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

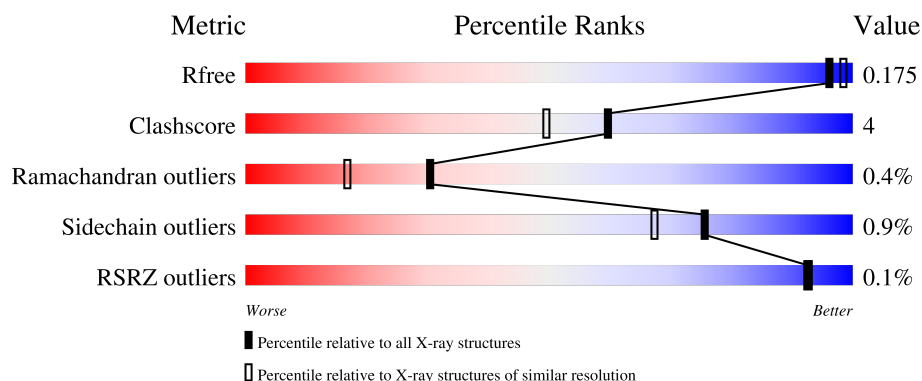
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 1.69 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	 86% 8% • 5%
1	B	692	 87% 7% 5%
1	C	692	 85% 8% • 5%
1	D	692	 86% 8% • 5%
1	E	692	 86% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	F	692	 87% 6% • 5%

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	TYY	C	405[A]	-	-	X	-
1	TYY	F	405[A]	-	-	X	-
3	PEO	A	802	-	X	-	-
3	PEO	B	802	-	X	-	-
3	PEO	C	802	-	X	-	-
3	PEO	D	802	-	X	-	-
3	PEO	E	802	-	X	-	-
3	PEO	F	802	-	X	-	-
4	GOL	D	808	-	-	X	-
4	GOL	D	811	-	-	X	-
4	GOL	E	807	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 36394 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.

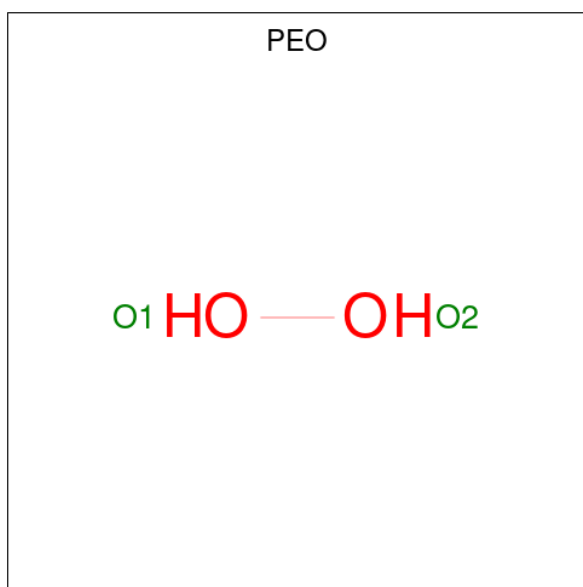
- Molecule 1 is a protein called Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	5	0
			5239	3332	902	981	24			
1	B	656	Total	C	N	O	S	0	5	0
			5224	3325	896	979	24			
1	C	655	Total	C	N	O	S	0	11	0
			5262	3353	901	983	25			
1	D	655	Total	C	N	O	S	0	8	0
			5232	3331	897	980	24			
1	E	655	Total	C	N	O	S	0	5	0
			5218	3323	895	976	24			
1	F	656	Total	C	N	O	S	0	8	0
			5250	3343	900	982	25			

- Molecule 2 is COPPER (II) ION (three-letter code: 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		
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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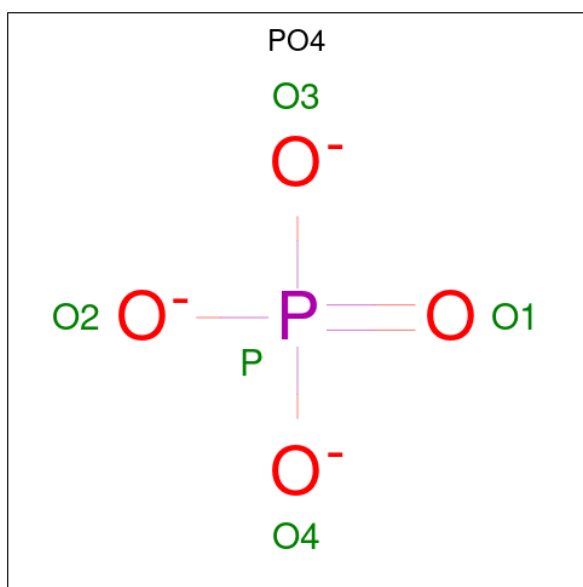
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total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

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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


- Molecule 6 is water.

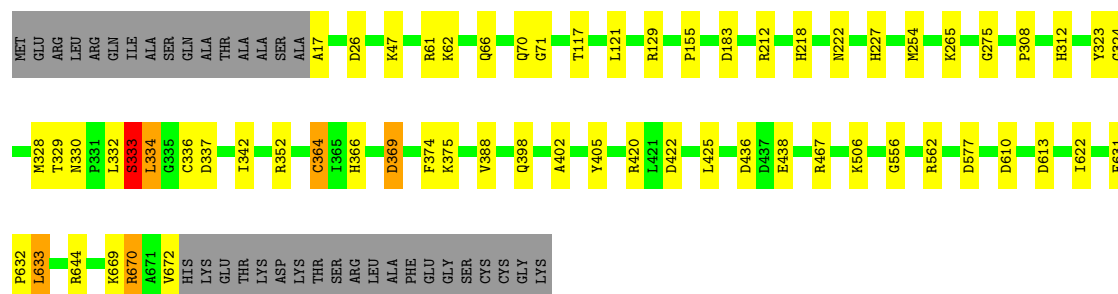
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	809	Total	O	0	0
			809	809		
6	B	771	Total	O	0	0
			771	771		
6	C	765	Total	O	0	0
			765	765		
6	D	774	Total	O	0	0
			774	774		
6	E	760	Total	O	0	0
			760	760		
6	F	745	Total	O	0	0
			745	745		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

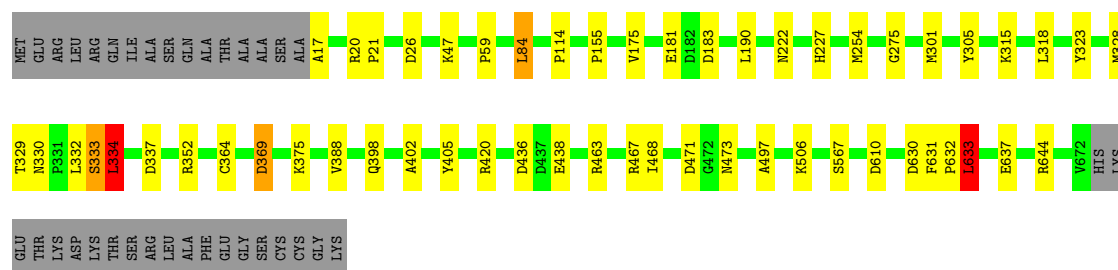
- Molecule 1: Peroxisomal primary amine oxidase

Chain A:  86% 8% 5%




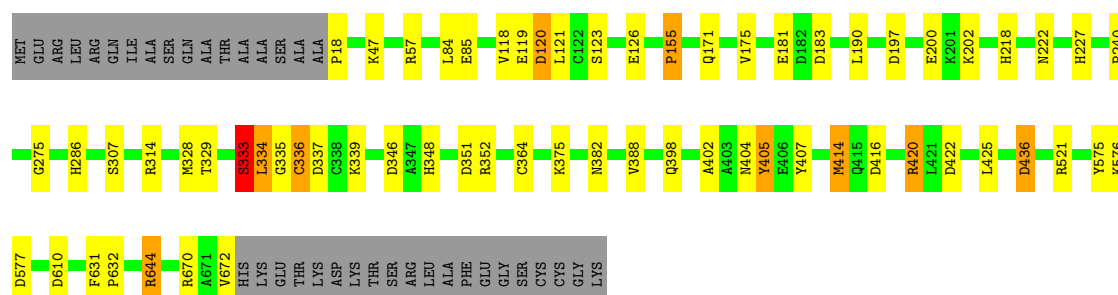
- Molecule 1: Peroxisomal primary amine oxidase

Chain B:  87% 7% 5%




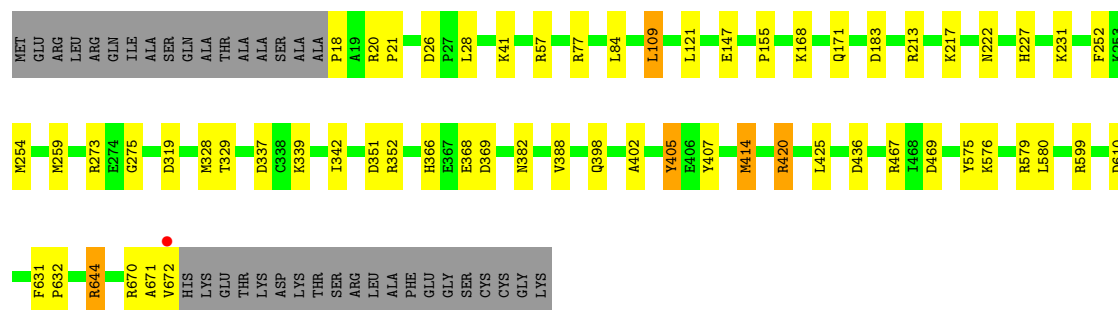
- Molecule 1: Peroxisomal primary amine oxidase

Chain C:  85% 8% 5%




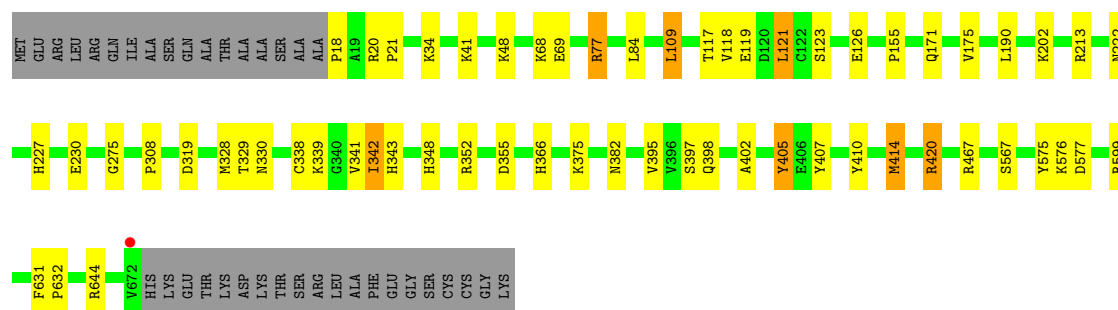
- Molecule 1: Peroxisomal primary amine oxidase

Chain D:  86% 8% 5%




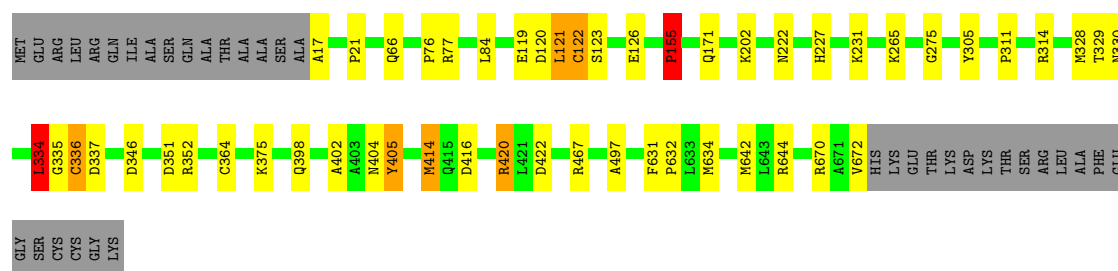
- Molecule 1: Peroxisomal primary amine oxidase

Chain E:  86% 8% 5%



- Molecule 1: Peroxisomal primary amine oxidase

Chain F:  87% 6% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.58Å 222.84Å 103.62Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	46.78 – 1.69 46.78 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.78-1.69) 99.4 (46.78-1.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.134 , 0.164 0.148 , 0.175	Depositor DCC
R_{free} test set	25742 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.480 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	36394	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, TYY, PO4, CU, PEO

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	0.99	4/5374 (0.1%)	1.02	20/7313 (0.3%)
1	B	0.99	6/5368 (0.1%)	1.03	17/7306 (0.2%)
1	C	1.01	4/5401 (0.1%)	1.02	16/7350 (0.2%)
1	D	1.02	2/5382 (0.0%)	1.03	23/7324 (0.3%)
1	E	1.02	6/5362 (0.1%)	1.02	15/7297 (0.2%)
1	F	0.99	2/5383 (0.0%)	1.00	14/7326 (0.2%)
All	All	1.00	24/32270 (0.1%)	1.02	105/43916 (0.2%)

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	A	0	1
1	B	0	1
1	C	0	2
1	F	0	1
All	All	0	5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	126	GLU	CG-CD	6.80	1.62	1.51
1	E	567	SER	CB-OG	-6.54	1.33	1.42
1	A	556	GLY	N-CA	-6.46	1.36	1.46
1	F	364	CYS	CB-SG	-6.44	1.71	1.82
1	E	230	GLU	CD-OE1	6.44	1.32	1.25

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	NE-CZ-NH1	-11.26	114.67	120.30
1	A	352	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	B	352	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	D	352	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	B	254	MET	CG-SD-CE	-8.98	85.83	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	LEU	Peptide
1	B	332	LEU	Peptide
1	C	155	PRO	Mainchain
1	C	333	SER	Peptide
1	F	155	PRO	Mainchain

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	5239	0	5073	48	0
1	B	5224	0	5066	31	0
1	C	5262	0	5111	65	0
1	D	5232	0	5082	37	0
1	E	5218	0	5067	42	0
1	F	5250	0	5090	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	72	0	95	5	0
4	B	48	0	64	1	0
4	C	48	0	64	3	0
4	D	54	0	72	10	0
4	E	36	0	48	5	0
4	F	54	0	72	3	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	F	5	0	0	0	0
6	A	809	0	0	10	0
6	B	771	0	0	5	0
6	C	765	0	0	25	0
6	D	774	0	0	13	0
6	E	760	0	0	23	0
6	F	745	0	0	20	0
All	All	36394	0	30904	263	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 4.

The worst 5 of 263 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:F:328[B]:MET:HE2	6:F:1589:HOH:O	1.18	1.30
1:F:405[A]:TYT:N5	6:F:1642:HOH:O	1.57	1.28
1:C:405[A]:TYT:CE2	6:C:1083:HOH:O	1.88	1.19
1:C:405[A]:TYT:N5	6:C:1660:HOH:O	1.76	1.16
1:F:328[B]:MET:CE	6:F:1589:HOH:O	1.72	1.15

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	658/692 (95%)	636 (97%)	20 (3%)	2 (0%)	37	23
1	B	658/692 (95%)	638 (97%)	18 (3%)	2 (0%)	37	23
1	C	662/692 (96%)	638 (96%)	21 (3%)	3 (0%)	25	12
1	D	660/692 (95%)	640 (97%)	18 (3%)	2 (0%)	37	23
1	E	657/692 (95%)	635 (97%)	21 (3%)	1 (0%)	44	29
1	F	660/692 (95%)	637 (96%)	19 (3%)	4 (1%)	22	10
All	All	3955/4152 (95%)	3824 (97%)	117 (3%)	14 (0%)	30	17

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	C	333	SER
1	C	334	LEU
1	C	336	CYS
1	F	334	LEU

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	570/593 (96%)	565 (99%)	5 (1%)	75	67
1	B	570/593 (96%)	563 (99%)	7 (1%)	67	56
1	C	575/593 (97%)	572 (100%)	3 (0%)	86	82
1	D	573/593 (97%)	568 (99%)	5 (1%)	75	67
1	E	570/593 (96%)	563 (99%)	7 (1%)	67	56
1	F	572/593 (96%)	567 (99%)	5 (1%)	75	67
All	All	3430/3558 (96%)	3398 (99%)	32 (1%)	75	67

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	231	LYS

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Mol	Chain	Res	Type
1	F	311	PRO
1	C	240	PRO
1	B	633	LEU
1	F	329	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	398	GLN
1	F	361	ASN
1	E	330	ASN
1	E	382	ASN
1	B	286	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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]	1	13,14,15	2.60	3 (23%)	10,19,21	1.71	3 (30%)
1	TYY	F	405[B]	1	13,14,15	2.07	5 (38%)	10,19,21	1.45	2 (20%)
1	TYY	F	405[A]	1	13,14,15	2.48	4 (30%)	10,19,21	1.73	2 (20%)
1	TYY	E	405	1	13,14,15	3.69	6 (46%)	10,19,21	3.00	4 (40%)
1	TYY	A	405	1	13,14,15	3.21	6 (46%)	10,19,21	2.19	4 (40%)
1	TYY	C	405[B]	1	13,14,15	2.05	2 (15%)	10,19,21	1.89	2 (20%)
1	TYY	B	405	1	13,14,15	3.48	5 (38%)	10,19,21	2.14	4 (40%)
1	TYY	D	405	1	13,14,15	3.45	5 (38%)	10,19,21	2.56	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]	1	-	0/5/22/24	0/1/1/1
1	TYY	F	405[B]	1	-	1/5/22/24	0/1/1/1
1	TYY	F	405[A]	1	-	0/5/22/24	0/1/1/1
1	TYY	E	405	1	-	1/5/22/24	0/1/1/1
1	TYY	A	405	1	-	0/5/22/24	0/1/1/1
1	TYY	C	405[B]	1	-	2/5/22/24	0/1/1/1
1	TYY	B	405	1	-	0/5/22/24	0/1/1/1
1	TYY	D	405	1	-	1/5/22/24	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	TYY	CE2-N5	10.41	1.45	1.28
1	B	405	TYY	CE2-N5	9.86	1.44	1.28
1	D	405	TYY	CE2-N5	9.01	1.42	1.28
1	A	405	TYY	CE2-N5	8.91	1.42	1.28
1	C	405[A]	TYY	CE2-N5	7.53	1.40	1.28

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	405	TYY	CD2-CG-CD1	8.19	124.49	118.66
1	D	405	TYY	CD2-CG-CD1	6.98	123.63	118.66
1	B	405	TYY	CD2-CG-CD1	4.39	121.78	118.66
1	A	405	TYY	CZ-CE1-CD1	4.18	124.83	120.30
1	C	405[B]	TYY	CD2-CG-CD1	4.14	121.61	118.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	405[B]	TYY	O-C-CA-CB
1	C	405[B]	TYY	N-CA-CB-CG
1	D	405	TYY	O-C-CA-CB
1	E	405	TYY	O-C-CA-CB
1	F	405[B]	TYY	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	405[A]	TYT	7	0
1	F	405[B]	TYT	4	0
1	F	405[A]	TYT	8	0
1	E	405	TYT	2	0
1	C	405[B]	TYT	3	0
1	D	405	TYT	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 6 are monoatomic - leaving 61 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	$\# Z > 2$
4	GOL	B	807	-	5,5,5	0.83	0	5,5,5	0.48	0
4	GOL	A	810	-	5,5,5	0.35	0	5,5,5	0.48	0
4	GOL	C	807	-	5,5,5	0.40	0	5,5,5	0.80	0
4	GOL	A	811	-	5,5,5	0.53	0	5,5,5	1.37	1 (20%)
4	GOL	F	812	-	5,5,5	1.00	0	5,5,5	1.29	0
3	PEO	E	802	2	1,1,1	3.26	1 (100%)	-		
4	GOL	A	803	-	5,5,5	0.99	0	5,5,5	1.10	0
4	GOL	E	807	-	5,5,5	0.33	0	5,5,5	2.41	2 (40%)
4	GOL	E	808	-	5,5,5	0.49	0	5,5,5	0.80	0
4	GOL	F	806	-	5,5,5	0.45	0	5,5,5	1.44	1 (20%)
4	GOL	E	805	-	5,5,5	0.33	0	5,5,5	0.58	0
4	GOL	E	806	-	5,5,5	0.60	0	5,5,5	1.92	2 (40%)
5	PO4	F	808	-	4,4,4	0.76	0	6,6,6	0.91	0
4	GOL	C	809	-	5,5,5	1.02	0	5,5,5	1.05	1 (20%)
3	PEO	D	802	2	1,1,1	3.30	1 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	809	-	5,5,5	0.36	0	5,5,5	0.72	0
4	GOL	A	808	-	5,5,5	0.96	0	5,5,5	0.49	0
4	GOL	A	807	-	5,5,5	0.71	0	5,5,5	1.77	3 (60%)
4	GOL	C	804	-	5,5,5	0.79	0	5,5,5	0.46	0
4	GOL	E	804	-	5,5,5	1.07	0	5,5,5	1.51	2 (40%)
4	GOL	F	809	-	5,5,5	0.36	0	5,5,5	0.64	0
3	PEO	B	802	2	1,1,1	3.06	1 (100%)	-		
4	GOL	D	810	-	5,5,5	0.34	0	5,5,5	0.60	0
4	GOL	D	807	-	5,5,5	0.57	0	5,5,5	1.20	0
4	GOL	C	810	-	5,5,5	0.34	0	5,5,5	0.44	0
4	GOL	D	808	-	5,5,5	0.40	0	5,5,5	0.78	0
4	GOL	F	807	-	5,5,5	0.26	0	5,5,5	1.58	1 (20%)
3	PEO	F	802	2	1,1,1	3.70	1 (100%)	-		
4	GOL	A	814	-	5,5,5	0.38	0	5,5,5	0.69	0
4	GOL	B	806	-	5,5,5	0.51	0	5,5,5	1.26	1 (20%)
4	GOL	C	806	-	5,5,5	0.44	0	5,5,5	0.53	0
4	GOL	F	805	-	5,5,5	0.43	0	5,5,5	0.91	0
3	PEO	C	802	2	1,1,1	3.44	1 (100%)	-		
4	GOL	B	805	-	5,5,5	0.35	0	5,5,5	0.74	0
4	GOL	B	808	-	5,5,5	0.83	0	5,5,5	1.07	0
4	GOL	D	805	-	5,5,5	0.31	0	5,5,5	0.77	0
4	GOL	F	803	-	5,5,5	0.55	0	5,5,5	0.87	0
4	GOL	C	803	-	5,5,5	0.63	0	5,5,5	0.88	0
4	GOL	E	803	-	5,5,5	0.18	0	5,5,5	0.78	0
4	GOL	D	811	-	5,5,5	0.58	0	5,5,5	0.63	0
4	GOL	D	803	-	5,5,5	0.32	0	5,5,5	1.09	0
4	GOL	A	806	-	5,5,5	0.39	0	5,5,5	1.08	0
3	PEO	A	802	2	1,1,1	3.40	1 (100%)	-		
4	GOL	B	804	-	5,5,5	0.57	0	5,5,5	2.09	1 (20%)
4	GOL	B	809	-	5,5,5	0.56	0	5,5,5	1.52	0
4	GOL	F	811	-	5,5,5	0.67	0	5,5,5	0.48	0
4	GOL	D	806	-	5,5,5	0.41	0	5,5,5	1.21	0
4	GOL	A	812	-	5,5,5	0.53	0	5,5,5	0.49	0
4	GOL	C	805	-	5,5,5	0.43	0	5,5,5	0.79	0
4	GOL	A	805	-	5,5,5	0.65	0	5,5,5	0.96	0
4	GOL	B	811	-	5,5,5	0.46	0	5,5,5	0.63	0
4	GOL	F	810	-	5,5,5	0.65	0	5,5,5	0.64	0
4	GOL	B	803	-	5,5,5	0.60	0	5,5,5	0.86	0
4	GOL	C	811	-	5,5,5	0.85	0	5,5,5	0.80	0
4	GOL	D	804	-	5,5,5	0.53	0	5,5,5	0.35	0
5	PO4	B	810	-	4,4,4	0.99	0	6,6,6	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	F	804	-	5,5,5	0.46	0	5,5,5	0.84	0
4	GOL	A	813	-	5,5,5	0.47	0	5,5,5	0.92	0
4	GOL	A	804	-	5,5,5	1.07	0	5,5,5	1.38	0
5	PO4	C	808	-	4,4,4	1.21	0	6,6,6	1.36	1 (16%)
4	GOL	D	809	-	5,5,5	0.19	0	5,5,5	1.58	1 (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
4	GOL	B	807	-	-	0/4/4/4	-
4	GOL	A	810	-	-	0/4/4/4	-
4	GOL	C	807	-	-	4/4/4/4	-
4	GOL	A	811	-	-	0/4/4/4	-
4	GOL	F	812	-	-	3/4/4/4	-
4	GOL	A	803	-	-	3/4/4/4	-
4	GOL	E	807	-	-	4/4/4/4	-
4	GOL	E	808	-	-	2/4/4/4	-
4	GOL	F	806	-	-	2/4/4/4	-
4	GOL	E	805	-	-	2/4/4/4	-
4	GOL	E	806	-	-	0/4/4/4	-
4	GOL	C	809	-	-	0/4/4/4	-
4	GOL	A	809	-	-	1/4/4/4	-
4	GOL	A	808	-	-	0/4/4/4	-
4	GOL	A	807	-	-	1/4/4/4	-
4	GOL	C	804	-	-	1/4/4/4	-
4	GOL	E	804	-	-	2/4/4/4	-
4	GOL	F	809	-	-	2/4/4/4	-
4	GOL	D	810	-	-	3/4/4/4	-
4	GOL	D	807	-	-	2/4/4/4	-
4	GOL	C	810	-	-	4/4/4/4	-
4	GOL	D	808	-	-	4/4/4/4	-
4	GOL	F	807	-	-	1/4/4/4	-
4	GOL	A	814	-	-	2/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-
4	GOL	C	806	-	-	1/4/4/4	-
4	GOL	F	805	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	805	-	-	2/4/4/4	-
4	GOL	B	808	-	-	2/4/4/4	-
4	GOL	D	805	-	-	4/4/4/4	-
4	GOL	F	803	-	-	2/4/4/4	-
4	GOL	C	803	-	-	0/4/4/4	-
4	GOL	E	803	-	-	3/4/4/4	-
4	GOL	D	811	-	-	0/4/4/4	-
4	GOL	D	803	-	-	2/4/4/4	-
4	GOL	A	806	-	-	4/4/4/4	-
4	GOL	B	809	-	-	2/4/4/4	-
4	GOL	B	804	-	-	2/4/4/4	-
4	GOL	F	811	-	-	0/4/4/4	-
4	GOL	D	806	-	-	2/4/4/4	-
4	GOL	A	812	-	-	2/4/4/4	-
4	GOL	C	805	-	-	0/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	B	811	-	-	0/4/4/4	-
4	GOL	F	810	-	-	2/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	C	811	-	-	0/4/4/4	-
4	GOL	D	804	-	-	4/4/4/4	-
4	GOL	F	804	-	-	1/4/4/4	-
4	GOL	A	813	-	-	2/4/4/4	-
4	GOL	A	804	-	-	4/4/4/4	-
4	GOL	D	809	-	-	2/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	PEO	O2-O1	-3.70	0.91	1.42
3	C	802	PEO	O2-O1	-3.44	0.94	1.42
3	A	802	PEO	O2-O1	-3.40	0.95	1.42
3	D	802	PEO	O2-O1	-3.30	0.96	1.42
3	E	802	PEO	O2-O1	-3.26	0.97	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	GOL	O1-C1-C2	-4.24	91.30	110.38
4	E	807	GOL	O1-C1-C2	-4.13	91.79	110.38
4	F	807	GOL	O1-C1-C2	-3.35	95.32	110.38
4	E	807	GOL	O2-C2-C3	3.07	121.90	109.18
4	D	809	GOL	O1-C1-C2	-3.07	96.56	110.38

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	C1-C2-C3-O3
4	A	804	GOL	C1-C2-C3-O3
4	A	805	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-C3
4	A	806	GOL	C1-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	811	GOL	3	0
4	A	803	GOL	1	0
4	E	805	GOL	2	0
4	C	809	GOL	1	0
4	C	804	GOL	1	0
4	E	804	GOL	3	0
4	C	810	GOL	1	0
4	D	808	GOL	5	0
4	F	805	GOL	1	0
4	F	803	GOL	1	0
4	D	811	GOL	4	0
4	D	803	GOL	1	0
4	B	804	GOL	1	0
4	F	810	GOL	1	0
4	A	804	GOL	1	0
5	C	808	PO4	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	655/692 (94%)	-1.60	0	100 100	5, 12, 26, 71	5 (0%)
1	B	655/692 (94%)	-1.60	0	100 100	5, 12, 27, 72	5 (0%)
1	C	654/692 (94%)	-1.57	0	100 100	5, 13, 30, 69	10 (1%)
1	D	654/692 (94%)	-1.58	1 (0%)	92 92	5, 13, 29, 78	8 (1%)
1	E	654/692 (94%)	-1.57	1 (0%)	92 92	5, 13, 29, 80	5 (0%)
1	F	655/692 (94%)	-1.56	0	100 100	5, 12, 30, 66	7 (1%)
All	All	3927/4152 (94%)	-1.58	2 (0%)	92 93	5, 12, 29, 80	40 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	672	VAL	2.6
1	D	672	VAL	2.2

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. 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	C	405[A]	14/15	0.99	0.02	9,10,11,11	14
1	TYY	C	405[B]	14/15	0.99	0.02	11,11,12,12	14
1	TYY	D	405	14/15	0.99	0.03	10,14,21,26	0
1	TYY	E	405	14/15	0.99	0.03	10,13,20,25	0
1	TYY	F	405[A]	14/15	0.99	0.02	10,10,11,11	14
1	TYY	F	405[B]	14/15	0.99	0.02	10,12,13,14	14
1	TYY	A	405	14/15	1.00	0.02	11,12,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TYY	B	405	14/15	1.00	0.02	11,13,18,18	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	804	6/6	0.94	0.11	87,97,103,107	0
4	GOL	A	813	6/6	0.98	0.05	26,38,45,50	0
4	GOL	C	806	6/6	0.98	0.04	29,32,33,33	0
4	GOL	C	807	6/6	0.98	0.06	39,42,49,50	0
4	GOL	A	807	6/6	0.98	0.06	38,47,50,51	0
4	GOL	D	808	6/6	0.98	0.06	46,51,55,58	0
4	GOL	F	804	6/6	0.98	0.04	29,30,32,33	0
4	GOL	F	807	6/6	0.98	0.04	34,38,41,49	0
4	GOL	F	809	6/6	0.98	0.07	38,58,65,69	0
4	GOL	A	804	6/6	0.99	0.04	31,38,39,39	0
4	GOL	A	814	6/6	0.99	0.05	52,60,62,62	0
4	GOL	B	803	6/6	0.99	0.03	34,36,39,41	0
4	GOL	B	804	6/6	0.99	0.04	24,38,41,45	0
4	GOL	B	805	6/6	0.99	0.04	37,39,41,42	0
4	GOL	B	806	6/6	0.99	0.06	29,34,40,41	6
4	GOL	B	807	6/6	0.99	0.05	15,17,18,20	0
4	GOL	B	808	6/6	0.99	0.04	29,39,43,45	0
4	GOL	B	809	6/6	0.99	0.04	27,36,46,48	0
4	GOL	B	811	6/6	0.99	0.04	38,42,44,51	0
4	GOL	C	803	6/6	0.99	0.04	19,26,29,33	0
4	GOL	C	804	6/6	0.99	0.05	31,39,41,42	0
4	GOL	C	805	6/6	0.99	0.03	39,42,44,46	0
4	GOL	A	805	6/6	0.99	0.04	30,33,39,41	0
4	GOL	A	806	6/6	0.99	0.05	38,45,49,51	0
4	GOL	C	809	6/6	0.99	0.03	15,20,20,28	0
4	GOL	C	810	6/6	0.99	0.04	31,45,50,50	0
4	GOL	C	811	6/6	0.99	0.05	15,18,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	803	6/6	0.99	0.04	34,41,43,49	0
4	GOL	A	803	6/6	0.99	0.04	15,21,26,33	0
4	GOL	D	805	6/6	0.99	0.05	46,48,49,55	0
4	GOL	D	807	6/6	0.99	0.03	27,30,33,34	0
4	GOL	A	809	6/6	0.99	0.04	37,38,40,43	0
4	GOL	D	809	6/6	0.99	0.03	22,28,30,33	0
4	GOL	D	810	6/6	0.99	0.05	50,55,59,68	0
4	GOL	D	811	6/6	0.99	0.05	39,49,52,54	0
4	GOL	E	803	6/6	0.99	0.03	31,37,41,44	0
4	GOL	E	804	6/6	0.99	0.04	26,37,39,43	0
4	GOL	E	805	6/6	0.99	0.04	38,42,47,55	0
4	GOL	E	806	6/6	0.99	0.05	42,47,48,49	0
4	GOL	E	807	6/6	0.99	0.04	20,29,32,36	0
4	GOL	E	808	6/6	0.99	0.03	27,32,35,35	0
4	GOL	F	803	6/6	0.99	0.03	19,25,28,34	0
4	GOL	A	810	6/6	0.99	0.03	37,39,42,48	0
4	GOL	F	805	6/6	0.99	0.04	38,40,42,48	0
4	GOL	F	806	6/6	0.99	0.03	24,32,40,42	0
4	GOL	A	811	6/6	0.99	0.04	30,38,44,44	0
4	GOL	A	812	6/6	0.99	0.04	38,42,43,44	0
4	GOL	F	810	6/6	0.99	0.05	33,48,50,56	0
4	GOL	F	812	6/6	0.99	0.04	33,40,41,42	0
5	PO4	B	810	5/5	0.99	0.04	31,35,37,37	5
5	PO4	C	808	5/5	0.99	0.03	31,43,47,48	0
5	PO4	F	808	5/5	0.99	0.03	33,46,51,52	0
2	CU	A	801	1/1	1.00	0.01	12,12,12,12	0
2	CU	B	801	1/1	1.00	0.01	12,12,12,12	0
2	CU	C	801	1/1	1.00	0.01	11,11,11,11	0
2	CU	D	801	1/1	1.00	0.01	11,11,11,11	0
2	CU	E	801	1/1	1.00	0.02	11,11,11,11	0
4	GOL	D	806	6/6	1.00	0.02	19,30,33,36	0
4	GOL	A	808	6/6	1.00	0.05	14,16,18,18	0
2	CU	F	801	1/1	1.00	0.01	11,11,11,11	0
3	PEO	A	802	2/2	1.00	0.02	7,7,7,10	0
3	PEO	B	802	2/2	1.00	0.01	5,5,5,11	0
4	GOL	F	811	6/6	1.00	0.04	15,19,20,20	0
3	PEO	C	802	2/2	1.00	0.01	8,8,8,8	0
3	PEO	D	802	2/2	1.00	0.02	6,6,6,10	0
3	PEO	E	802	2/2	1.00	0.02	6,6,6,10	0
3	PEO	F	802	2/2	1.00	0.01	7,7,7,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.