



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 09:10 AM GMT

PDB ID : 2OQE  
Title : Crystal Structure of Hansenula polymorpha amine oxidase in complex with Xe to 1.6 Angstroms  
Authors : Johnson, B.J.; Wilmot, C.M.  
Deposited on : 2007-01-31  
Resolution : 1.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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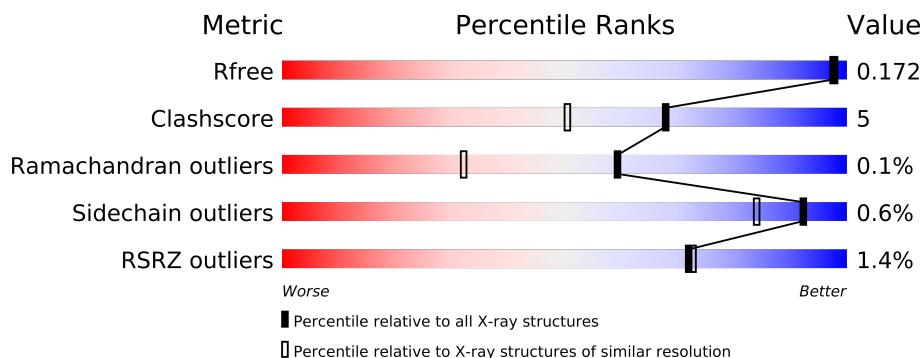
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 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))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	660	
1	B	660	
2	C	660	
2	D	660	
2	E	660	
2	F	660	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CU	D	801	-	X
4	XE	A	902	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	XE	D	904	-	X
4	XE	E	901	-	X
5	GOL	A	4002	-	X
5	GOL	A	4004	-	X
5	GOL	A	4007	-	X
5	GOL	A	4011	-	X
5	GOL	A	4019	-	X
5	GOL	A	4024	-	X
5	GOL	A	4044	-	X
5	GOL	A	4049	-	X
5	GOL	B	4001	-	X
5	GOL	B	4009	-	X
5	GOL	B	4014	-	X
5	GOL	B	4015	-	X
5	GOL	B	4018	-	X
5	GOL	B	4035	-	X
5	GOL	B	4036	-	X
5	GOL	B	4048	-	X
5	GOL	C	4016	-	X
5	GOL	C	4025	-	X
5	GOL	C	4030	-	X
5	GOL	C	4043	-	X
5	GOL	D	4008	-	X
5	GOL	D	4023	-	X
5	GOL	D	4027	-	X
5	GOL	D	4031	-	X
5	GOL	D	4032	-	X
5	GOL	E	4003	-	X
5	GOL	E	4020	-	X
5	GOL	E	4022	-	X
5	GOL	E	4026	-	X
5	GOL	E	4034	-	X
5	GOL	E	4039	-	X
5	GOL	E	4041	-	X
5	GOL	E	4047	-	X
5	GOL	F	4006	-	X
5	GOL	F	4012	-	X
5	GOL	F	4017	-	X
5	GOL	F	4028	-	X
5	GOL	F	4042	-	X
5	GOL	F	4046	-	X
5	GOL	F	4050	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35754 atoms, of which 0 are hydrogen and 0 are deuterium.

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 copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	16	0
			5280	3366	902	986	26			
1	B	657	Total	C	N	O	S	0	13	0
			5266	3356	899	985	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	TPQ	TYR	MODIFIED RESIDUE	UNP P12807
A	634	SME	MET	MODIFIED RESIDUE	UNP P12807
B	405	TPQ	TYR	MODIFIED RESIDUE	UNP P12807
B	634	SME	MET	MODIFIED RESIDUE	UNP P12807

- Molecule 2 is a protein called Peroxisomal copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	656	Total	C	N	O	S	0	17	0
			5280	3369	897	985	29			
2	D	656	Total	C	N	O	S	0	11	0
			5259	3349	898	985	27			
2	E	657	Total	C	N	O	S	0	12	0
			5277	3361	902	988	26			
2	F	656	Total	C	N	O	S	0	13	0
			5264	3355	896	984	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	405	TPQ	TYR	MODIFIED RESIDUE	UNP P12807
D	405	TPQ	TYR	MODIFIED RESIDUE	UNP P12807
E	405	TPQ	TYR	MODIFIED RESIDUE	UNP P12807
F	405	TPQ	TYR	MODIFIED RESIDUE	UNP P12807

- 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 XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total	Xe	0	0
			4	4		
4	E	4	Total	Xe	0	0
			4	4		
4	B	4	Total	Xe	0	0
			4	4		
4	C	4	Total	Xe	0	0
			4	4		
4	A	4	Total	Xe	0	0
			4	4		
4	F	4	Total	Xe	0	0
			4	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	636	Total O 636 636	0	0
6	B	674	Total O 674 674	0	0
6	C	611	Total O 611 611	0	0
6	D	639	Total O 639 639	0	0
6	E	619	Total O 619 619	0	0

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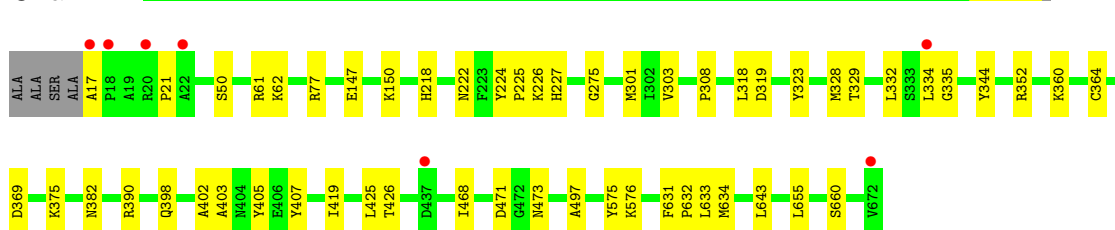
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	625	Total 625	O 625	0	0

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

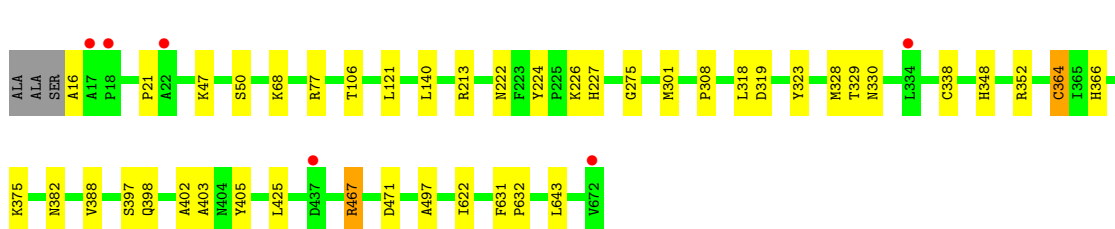
- Molecule 1: Peroxisomal copper amine oxidase

Chain A:



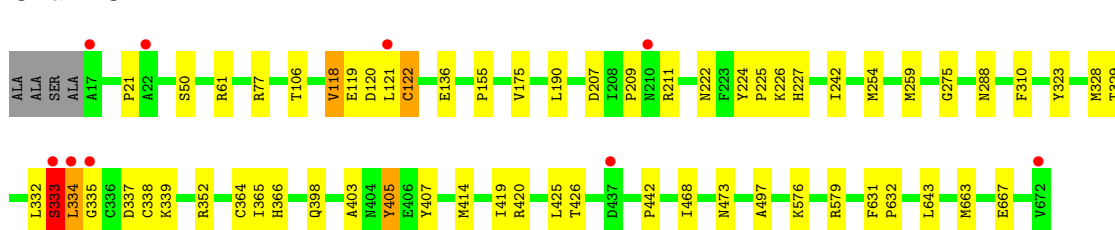
- Molecule 1: Peroxisomal copper amine oxidase

Chain B:



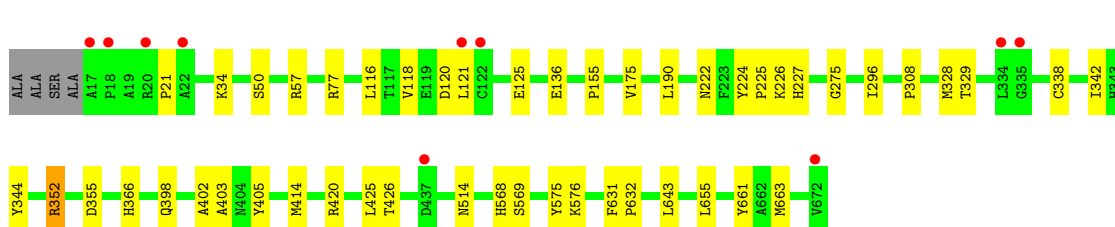
- Molecule 2: Peroxisomal copper amine oxidase

Chain C:



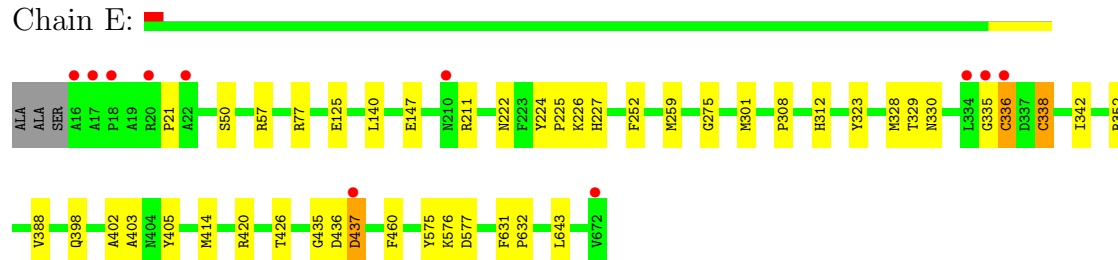
- Molecule 2: Peroxisomal copper amine oxidase

Chain D:



- Molecule 2: Peroxisomal copper amine oxidase

Chain E:



- Molecule 2: Peroxisomal copper amine oxidase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.40Å 222.75Å 103.65Å 90.00° 95.85° 90.00°	Depositor
Resolution (Å)	46.68 – 1.60 45.09 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.68-1.60) 95.7 (45.09-1.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.162 , 0.188 0.160 , 0.172	Depositor DCC
$R_{free}$ test set	29665 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.2	EDS
Estimated twinning fraction	0.458 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 587352 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	35754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.50	0/5453	0.64	0/7414
1	B	0.49	0/5430	0.63	1/7385 (0.0%)
2	C	0.49	1/5452 (0.0%)	0.64	0/7415
2	D	0.50	0/5410	0.63	0/7358
2	E	0.49	0/5422	0.65	0/7376
2	F	0.50	0/5418	0.64	0/7370
All	All	0.49	1/32585 (0.0%)	0.64	1/44318 (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
2	C	0	2
2	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	122	CYS	CB-SG	5.26	1.91	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	ARG	NE-CZ-NH2	-5.44	117.58	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	333	SER	Peptide
2	C	405[A]	TPQ	Mainchain
2	F	405[B]	TPQ	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5280	0	5165	47	0
1	B	5266	0	5140	38	0
2	C	5280	0	5159	65	2
2	D	5259	0	5111	47	0
2	E	5277	0	5130	48	0
2	F	5264	0	5122	59	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	4	0	0	7	0
4	B	4	0	0	7	0
4	C	4	0	0	10	0
4	D	4	0	0	10	0
4	E	4	0	0	7	0
4	F	4	0	0	7	0
5	A	60	0	80	4	0
5	B	60	0	80	2	0
5	C	30	0	40	10	0
5	D	42	0	56	7	0
5	E	60	0	80	3	0
5	F	42	0	56	14	0
6	A	636	0	0	10	0
6	B	674	0	0	10	2
6	C	611	0	0	21	0
6	D	639	0	0	7	0
6	E	619	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	625	0	0	13	0
All	All	35754	0	31219	307	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 307 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:57:ARG:HE	5:D:4031:GOL:H31	1.05	1.13
2:E:405[A]:TPQ:O5	4:E:901:XE:XE	2.52	1.04
2:F:405[B]:TPQ:O5	4:F:901:XE:XE	2.55	1.02
2:C:333:SER:HB2	2:C:334:LEU:C	1.81	1.00
2:D:328[B]:MET:HE2	6:D:4385:HOH:O	1.63	0.97

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:288[B]:ASN:ND2	6:B:4700:HOH:O[1_556]	0.78	1.42
2:C:288[B]:ASN:CG	6:B:4700:HOH:O[1_556]	2.10	0.10

## 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	668/660 (101%)	650 (97%)	18 (3%)	0	100	100
1	B	666/660 (101%)	648 (97%)	18 (3%)	0	100	100
2	C	669/660 (101%)	648 (97%)	19 (3%)	2 (0%)	50	24
2	D	663/660 (100%)	642 (97%)	21 (3%)	0	100	100
2	E	665/660 (101%)	645 (97%)	18 (3%)	2 (0%)	50	24
2	F	665/660 (101%)	646 (97%)	18 (3%)	1 (0%)	56	29
All	All	3996/3960 (101%)	3879 (97%)	112 (3%)	5 (0%)	59	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	333	SER
2	E	336	CYS
2	E	437	ASP
2	C	334	LEU
2	F	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	580/565 (103%)	577 (100%)	3 (0%)	94	87
1	B	577/565 (102%)	572 (99%)	5 (1%)	87	74
2	C	581/566 (103%)	577 (99%)	4 (1%)	91	81
2	D	575/566 (102%)	568 (99%)	7 (1%)	82	63
2	E	576/566 (102%)	572 (99%)	4 (1%)	91	81
2	F	577/566 (102%)	575 (100%)	2 (0%)	96	91
All	All	3466/3394 (102%)	3441 (99%)	25 (1%)	92	81

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	333	SER
2	D	329	THR
2	F	329	THR
2	D	125	GLU
2	D	338[A]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	343	HIS
2	C	473	ASN
2	F	398	GLN
2	C	361	ASN

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Mol	Chain	Res	Type
2	C	398	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

12 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	TPQ	A	405	1	14,14,15	5.86	4 (28%)	17,19,21	1.59	1 (5%)
1	SME	A	634	1	8,8,9	7.70	2 (25%)	7,9,11	4.57	2 (28%)
1	TPQ	B	405	1	14,14,15	5.70	5 (35%)	17,19,21	1.70	1 (5%)
1	SME	B	634	1	8,8,9	7.41	2 (25%)	7,9,11	4.44	2 (28%)
2	TPQ	C	405[A]	-	10,11,15	2.33	4 (40%)	14,15,21	1.09	0
2	TPQ	C	405[B]	-	10,11,15	2.25	3 (30%)	14,15,21	1.04	1 (7%)
2	TPQ	D	405[A]	2	14,14,15	5.71	4 (28%)	17,19,21	1.16	2 (11%)
2	TPQ	D	405[B]	2	14,14,15	5.73	5 (35%)	17,19,21	1.20	2 (11%)
2	TPQ	E	405[A]	2	14,14,15	5.45	4 (28%)	17,19,21	1.03	1 (5%)
2	TPQ	E	405[B]	2	14,14,15	5.68	5 (35%)	17,19,21	1.13	1 (5%)
2	TPQ	F	405[A]	-	10,11,15	2.25	3 (30%)	14,15,21	1.04	1 (7%)
2	TPQ	F	405[B]	-	10,11,15	2.23	3 (30%)	14,15,21	1.20	1 (7%)

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	TPQ	A	405	1	-	0/4/22/24	0/1/1/1
1	SME	A	634	1	-	0/5/7/9	0/0/0/0
1	TPQ	B	405	1	-	0/4/22/24	0/1/1/1
1	SME	B	634	1	-	0/5/7/9	0/0/0/0
2	TPQ	C	405[A]	-	-	0/2/18/24	0/1/1/1
2	TPQ	C	405[B]	-	-	0/2/18/24	0/1/1/1
2	TPQ	D	405[A]	2	-	0/4/22/24	0/1/1/1
2	TPQ	D	405[B]	2	-	0/4/22/24	0/1/1/1
2	TPQ	E	405[A]	2	-	0/4/22/24	0/1/1/1
2	TPQ	E	405[B]	2	-	0/4/22/24	0/1/1/1
2	TPQ	F	405[A]	-	-	0/2/18/24	0/1/1/1
2	TPQ	F	405[B]	-	-	0/2/18/24	0/1/1/1

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	TPQ	O-C	20.65	1.25	1.11
2	D	405[B]	TPQ	O-C	20.29	1.25	1.11
2	D	405[A]	TPQ	O-C	20.12	1.25	1.11
1	B	405	TPQ	O-C	19.97	1.25	1.11
2	E	405[B]	TPQ	O-C	19.94	1.25	1.11

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	SME	OE-S-CE	11.47	126.19	106.28
1	B	634	SME	OE-S-CE	11.17	125.66	106.28
1	B	405	TPQ	C-CA-N	-5.60	108.24	113.83
1	A	405	TPQ	C-CA-N	-5.26	108.58	113.83
2	D	405[A]	TPQ	C6-C1-C2	2.91	121.48	118.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 79 ligands modelled in this entry, 30 are monoatomic - leaving 49 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$
5	GOL	A	4002	-	5,5,5	0.41	0	5,5,5	0.24	0
5	GOL	A	4004	-	5,5,5	0.31	0	5,5,5	0.31	0
5	GOL	A	4007	-	5,5,5	0.39	0	5,5,5	0.29	0
5	GOL	A	4011	-	5,5,5	0.27	0	5,5,5	0.37	0
5	GOL	A	4019	-	5,5,5	0.35	0	5,5,5	0.21	0
5	GOL	A	4021	-	5,5,5	0.40	0	5,5,5	0.34	0
5	GOL	A	4024	-	5,5,5	0.28	0	5,5,5	0.52	0
5	GOL	A	4029	-	5,5,5	0.31	0	5,5,5	0.36	0
5	GOL	A	4044	-	5,5,5	0.36	0	5,5,5	0.23	0
5	GOL	A	4049	-	5,5,5	0.33	0	5,5,5	0.25	0
5	GOL	B	4001	-	5,5,5	0.35	0	5,5,5	0.32	0
5	GOL	B	4009	-	5,5,5	0.38	0	5,5,5	0.18	0
5	GOL	B	4013	-	5,5,5	0.31	0	5,5,5	0.34	0
5	GOL	B	4014	-	5,5,5	0.25	0	5,5,5	0.32	0
5	GOL	B	4015	-	5,5,5	0.37	0	5,5,5	0.21	0
5	GOL	B	4018	-	5,5,5	0.31	0	5,5,5	0.41	0
5	GOL	B	4035	-	5,5,5	0.36	0	5,5,5	0.41	0
5	GOL	B	4036	-	5,5,5	0.31	0	5,5,5	0.49	0
5	GOL	B	4037	-	5,5,5	0.33	0	5,5,5	0.30	0
5	GOL	B	4048	-	5,5,5	0.31	0	5,5,5	0.26	0
5	GOL	C	4005	-	5,5,5	0.34	0	5,5,5	0.25	0
5	GOL	C	4016	-	5,5,5	0.20	0	5,5,5	0.70	0
5	GOL	C	4025	-	5,5,5	0.40	0	5,5,5	0.38	0
5	GOL	C	4030	-	5,5,5	0.30	0	5,5,5	0.33	0
5	GOL	C	4043	-	5,5,5	0.32	0	5,5,5	0.27	0
5	GOL	D	4008	-	5,5,5	0.30	0	5,5,5	0.38	0
5	GOL	D	4023	-	5,5,5	0.32	0	5,5,5	0.50	0
5	GOL	D	4027	-	5,5,5	0.25	0	5,5,5	0.45	0
5	GOL	D	4031	-	5,5,5	0.42	0	5,5,5	0.54	0
5	GOL	D	4032	-	5,5,5	0.27	0	5,5,5	0.28	0
5	GOL	D	4040	-	5,5,5	0.32	0	5,5,5	0.37	0
5	GOL	D	4045	-	5,5,5	0.31	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	E	4003	-	5,5,5	0.32	0	5,5,5	0.51	0
5	GOL	E	4020	-	5,5,5	0.33	0	5,5,5	0.50	0
5	GOL	E	4022	-	5,5,5	0.43	0	5,5,5	0.19	0
5	GOL	E	4026	-	5,5,5	0.38	0	5,5,5	0.35	0
5	GOL	E	4033	-	5,5,5	0.31	0	5,5,5	0.51	0
5	GOL	E	4034	-	5,5,5	0.32	0	5,5,5	0.36	0
5	GOL	E	4038	-	5,5,5	0.31	0	5,5,5	0.32	0
5	GOL	E	4039	-	5,5,5	0.34	0	5,5,5	0.29	0
5	GOL	E	4041	-	5,5,5	0.34	0	5,5,5	0.29	0
5	GOL	E	4047	-	5,5,5	0.28	0	5,5,5	0.37	0
5	GOL	F	4006	-	5,5,5	0.35	0	5,5,5	0.23	0
5	GOL	F	4012	-	5,5,5	0.23	0	5,5,5	0.47	0
5	GOL	F	4017	-	5,5,5	0.31	0	5,5,5	0.42	0
5	GOL	F	4028	-	5,5,5	0.35	0	5,5,5	0.64	0
5	GOL	F	4042	-	5,5,5	0.33	0	5,5,5	0.28	0
5	GOL	F	4046	-	5,5,5	0.30	0	5,5,5	0.46	0
5	GOL	F	4050	-	5,5,5	0.33	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	4002	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4004	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4007	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4011	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4019	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4021	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4024	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4029	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4044	-	-	0/4/4/4	0/0/0/0
5	GOL	A	4049	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4001	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4009	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4013	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4014	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4015	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4018	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4035	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4036	-	-	0/4/4/4	0/0/0/0
5	GOL	B	4037	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	4048	-	-	0/4/4/4	0/0/0/0
5	GOL	C	4005	-	-	0/4/4/4	0/0/0/0
5	GOL	C	4016	-	-	0/4/4/4	0/0/0/0
5	GOL	C	4025	-	-	0/4/4/4	0/0/0/0
5	GOL	C	4030	-	-	0/4/4/4	0/0/0/0
5	GOL	C	4043	-	-	0/4/4/4	0/0/0/0
5	GOL	D	4008	-	-	0/4/4/4	0/0/0/0
5	GOL	D	4023	-	-	0/4/4/4	0/0/0/0
5	GOL	D	4027	-	-	0/4/4/4	0/0/0/0
5	GOL	D	4031	-	-	0/4/4/4	0/0/0/0
5	GOL	D	4032	-	-	0/4/4/4	0/0/0/0
5	GOL	D	4040	-	-	0/4/4/4	0/0/0/0
5	GOL	D	4045	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4003	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4020	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4022	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4026	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4033	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4034	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4038	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4039	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4041	-	-	0/4/4/4	0/0/0/0
5	GOL	E	4047	-	-	0/4/4/4	0/0/0/0
5	GOL	F	4006	-	-	0/4/4/4	0/0/0/0
5	GOL	F	4012	-	-	0/4/4/4	0/0/0/0
5	GOL	F	4017	-	-	0/4/4/4	0/0/0/0
5	GOL	F	4028	-	-	0/4/4/4	0/0/0/0
5	GOL	F	4042	-	-	0/4/4/4	0/0/0/0
5	GOL	F	4046	-	-	0/4/4/4	0/0/0/0
5	GOL	F	4050	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	656/660 (99%)	-0.50	7 (1%) 77 79	12, 17, 30, 53	0
1	B	657/660 (99%)	-0.49	6 (0%) 81 83	11, 17, 30, 55	1 (0%)
2	C	656/660 (99%)	-0.35	9 (1%) 72 73	11, 17, 34, 51	0
2	D	656/660 (99%)	-0.40	10 (1%) 70 71	12, 18, 33, 52	1 (0%)
2	E	657/660 (99%)	-0.38	11 (1%) 67 67	12, 18, 33, 52	0
2	F	656/660 (99%)	-0.34	11 (1%) 67 67	12, 17, 34, 50	0
All	All	3938/3960 (99%)	-0.41	54 (1%) 72 73	11, 17, 33, 55	2 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	334	LEU	7.8
2	E	672	VAL	6.4
1	B	672	VAL	6.1
2	C	672	VAL	5.9
2	F	334	LEU	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPQ	C	405[A]	11/15	0.18	11.94	20,27,29,30	11
2	TPQ	F	405[B]	11/15	0.18	10.22	19,24,25,26	11

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TPQ	F	405[A]	11/15	0.18	10.22	18,18,19,21	11
2	TPQ	E	405[A]	14/15	0.17	9.52	17,23,26,26	14
2	TPQ	C	405[B]	11/15	0.18	9.31	18,18,19,21	11
2	TPQ	E	405[B]	14/15	0.17	7.30	16,17,18,20	14
1	TPQ	B	405	14/15	0.14	6.97	19,27,31,33	0
1	TPQ	A	405	14/15	0.12	6.28	20,25,30,30	1
2	TPQ	D	405[B]	14/15	0.16	4.71	17,23,26,27	14
2	TPQ	D	405[A]	14/15	0.16	4.37	15,16,17,19	14
1	SME	A	634	9/10	0.13	3.31	17,18,32,34	0
1	SME	B	634	9/10	0.13	3.26	16,18,31,33	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	4018	6/6	0.20	27.06	54,54,55,55	0
5	GOL	A	4011	6/6	0.25	25.88	48,49,49,49	0
5	GOL	D	4031	6/6	0.31	19.81	39,46,48,49	0
5	GOL	F	4012	6/6	0.21	17.39	51,52,53,53	0
5	GOL	A	4049	6/6	0.45	15.85	78,78,79,79	0
5	GOL	B	4036	6/6	0.29	14.35	80,80,80,80	0
5	GOL	E	4039	6/6	0.34	11.09	81,81,81,81	0
5	GOL	E	4047	6/6	0.13	11.04	52,53,53,53	0
5	GOL	D	4032	6/6	0.32	10.54	52,55,56,56	0
5	GOL	F	4046	6/6	0.28	8.56	52,54,54,54	0
5	GOL	D	4008	6/6	0.11	8.20	52,53,53,54	0
5	GOL	F	4017	6/6	0.38	7.64	76,77,77,77	0
5	GOL	B	4015	6/6	0.20	7.43	54,57,57,58	0
5	GOL	B	4009	6/6	0.12	7.39	44,45,46,47	0
5	GOL	F	4028	6/6	0.25	7.23	38,42,44,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XE	A	902	1/1	0.24	6.15	39,39,39,39	1
5	GOL	E	4034	6/6	0.15	6.10	65,67,67,67	0
5	GOL	F	4042	6/6	0.19	5.83	47,49,49,49	0
5	GOL	C	4043	6/6	0.18	5.73	43,49,50,51	0
5	GOL	A	4044	6/6	0.23	5.43	45,47,48,49	0
5	GOL	E	4022	6/6	0.20	5.35	40,44,45,45	0
5	GOL	A	4002	6/6	0.12	5.33	20,31,33,35	0
5	GOL	E	4003	6/6	0.19	5.18	46,49,49,49	0
5	GOL	B	4048	6/6	0.23	5.17	63,64,64,64	0
5	GOL	A	4004	6/6	0.15	4.83	57,58,58,58	0
5	GOL	F	4050	6/6	0.17	4.51	32,42,43,45	0
5	GOL	C	4016	6/6	0.32	4.45	41,43,43,44	0
5	GOL	D	4023	6/6	0.15	4.07	26,32,33,34	0
5	GOL	B	4014	6/6	0.17	4.05	50,52,52,53	0
5	GOL	B	4035	6/6	0.16	3.96	57,58,58,58	0
3	CU	D	801	1/1	0.07	3.55	16,16,16,16	0
5	GOL	E	4020	6/6	0.17	3.28	40,43,44,45	0
5	GOL	E	4026	6/6	0.13	3.22	52,53,53,53	0
5	GOL	C	4025	6/6	0.17	3.10	53,53,54,54	0
5	GOL	C	4030	6/6	0.26	3.04	61,61,61,62	0
5	GOL	B	4001	6/6	0.10	2.66	21,30,31,33	0
5	GOL	A	4019	6/6	0.12	2.65	39,40,41,42	0
5	GOL	A	4007	6/6	0.15	2.51	48,48,48,49	0
5	GOL	D	4027	6/6	0.15	2.43	35,40,41,41	0
4	XE	D	904	1/1	0.12	2.30	22,22,22,22	1
5	GOL	A	4024	6/6	0.14	2.20	47,48,49,49	0
5	GOL	E	4041	6/6	0.16	2.20	64,64,64,65	0
4	XE	E	901	1/1	0.08	2.08	32,32,32,32	1
5	GOL	F	4006	6/6	0.13	2.03	48,49,51,51	0
4	XE	E	902	1/1	0.17	1.99	42,42,42,42	1
4	XE	D	902	1/1	0.20	1.97	51,51,51,51	1
5	GOL	E	4033	6/6	0.14	1.84	37,38,38,39	0
4	XE	C	902	1/1	0.28	1.72	52,52,52,52	1
4	XE	C	904	1/1	0.10	1.54	23,23,23,23	1
5	GOL	B	4013	6/6	0.10	1.38	43,44,44,45	0
5	GOL	A	4021	6/6	0.13	1.26	49,50,50,50	0
5	GOL	D	4040	6/6	0.12	1.11	64,65,65,65	0
5	GOL	C	4005	6/6	0.13	1.10	47,47,48,48	0
5	GOL	E	4038	6/6	0.18	1.09	62,63,63,64	0
5	GOL	D	4045	6/6	0.14	0.86	62,63,63,63	0
4	XE	B	904	1/1	0.08	0.80	28,28,28,28	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XE	F	902	1/1	0.14	0.60	44,44,44,44	1
3	CU	A	801	1/1	0.09	0.53	17,17,17,17	0
4	XE	B	903	1/1	0.08	0.52	17,17,17,17	1
5	GOL	A	4029	6/6	0.12	0.47	54,54,55,55	0
3	CU	B	801	1/1	0.09	0.45	17,17,17,17	0
5	GOL	B	4037	6/6	0.11	0.29	54,55,55,55	0
4	XE	C	903	1/1	0.07	0.23	18,18,18,18	1
4	XE	F	904	1/1	0.08	0.14	28,28,28,28	1
4	XE	B	902	1/1	0.07	0.12	29,29,29,29	1
3	CU	F	801	1/1	0.07	-0.20	16,16,16,16	0
4	XE	E	903	1/1	0.07	-0.20	18,18,18,18	1
4	XE	C	901	1/1	0.06	-0.29	39,39,39,39	1
4	XE	A	903	1/1	0.06	-0.40	17,17,17,17	1
4	XE	D	903	1/1	0.06	-0.43	17,17,17,17	1
4	XE	D	901	1/1	0.06	-0.48	54,54,54,54	1
4	XE	A	904	1/1	0.07	-0.51	36,36,36,36	1
3	CU	C	801	1/1	0.06	-0.60	16,16,16,16	0
3	CU	E	801	1/1	0.06	-0.65	16,16,16,16	0
4	XE	E	904	1/1	0.06	-0.78	25,25,25,25	1
4	XE	F	903	1/1	0.06	-0.89	19,19,19,19	1
4	XE	F	901	1/1	0.04	-1.50	36,36,36,36	1
4	XE	B	901	1/1	0.02	-1.97	34,34,34,34	1
4	XE	A	901	1/1	0.03	-2.29	34,34,34,34	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.