



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:49 PM UTC

PDB ID : 2OQE / pdb_00002oqe
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

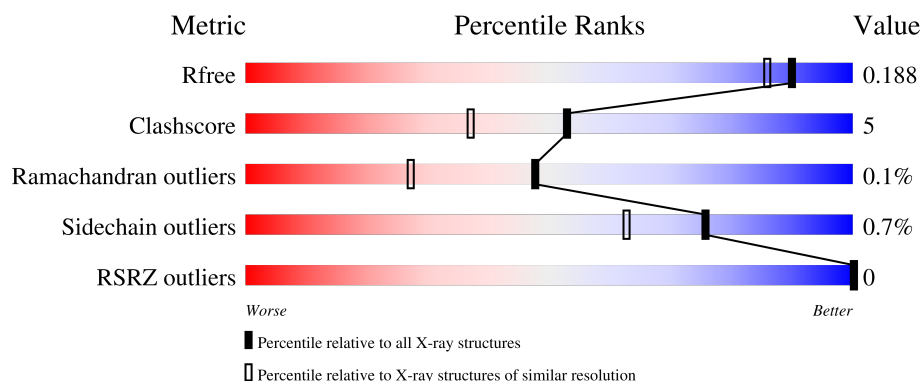
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 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	660	91% 8% .
1	B	660	92% 7%
2	C	660	90% 9% .
2	D	660	92% 8% .
2	E	660	92% 7% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	660	 90% 9%

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
4	XE	A	903	-	-	X	-
4	XE	A	904	-	-	X	-
4	XE	B	902	-	-	X	-
4	XE	B	904	-	-	X	-
4	XE	C	903	-	-	X	-
4	XE	C	904	-	-	X	-
4	XE	D	902	-	-	X	-
4	XE	D	903	-	-	X	-
4	XE	D	904	-	-	X	-
4	XE	E	904	-	-	X	-
4	XE	F	904	-	-	X	-
5	GOL	C	4016	-	-	X	-
5	GOL	D	4031	-	-	X	-
5	GOL	F	4017	-	-	X	-
5	GOL	F	4028	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35754 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 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 (CCD ID: CU) (formula: Cu).

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

- Molecule 4 is XENON (CCD ID: XE) (formula: Xe).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

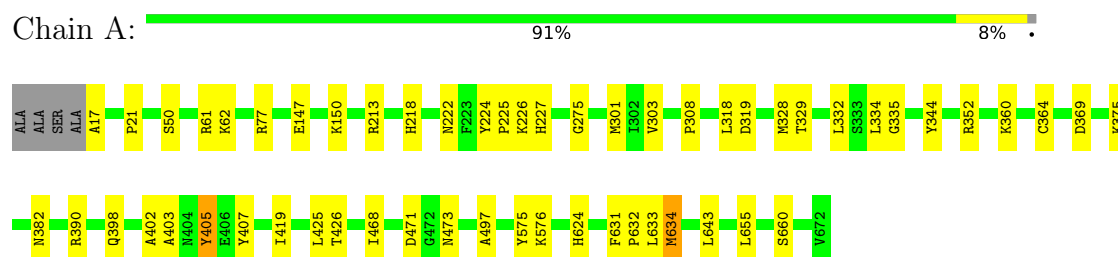
Continued from previous page...

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

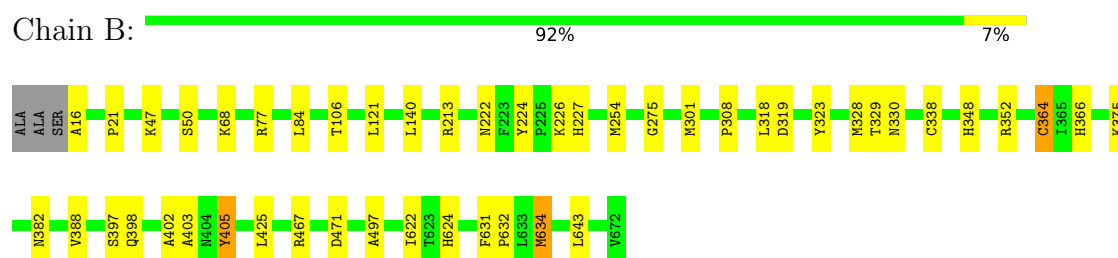
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

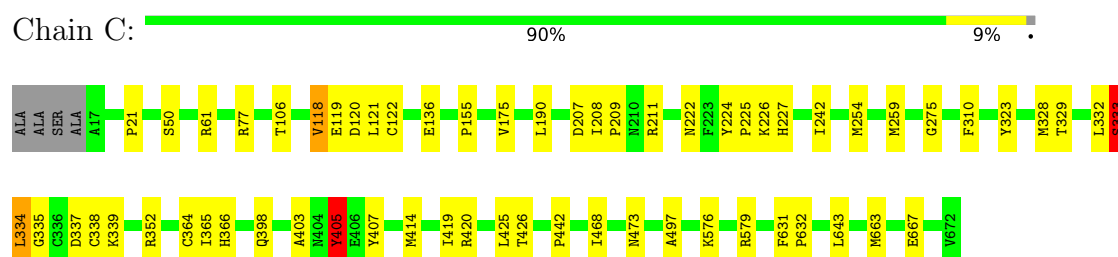
• Molecule 1: Peroxisomal copper amine oxidase



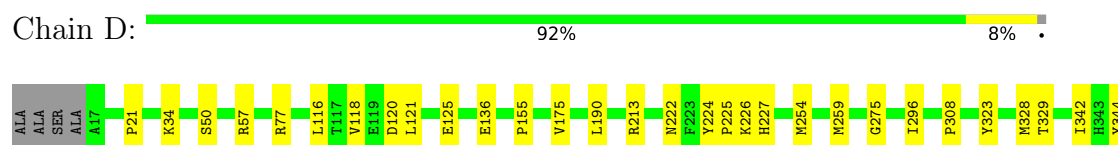
• Molecule 1: Peroxisomal copper amine oxidase



• Molecule 2: Peroxisomal copper amine oxidase

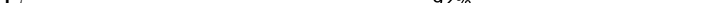


• Molecule 2: Peroxisomal copper amine oxidase



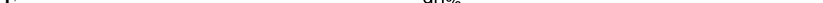


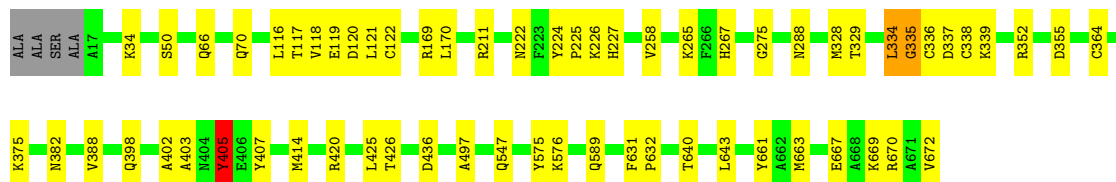
- Molecule 2: Peroxisomal copper amine oxidase

Chain E:  92% 7%



- Molecule 2: Peroxisomal copper amine oxidase

Chain F:  90% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.40Å 222.75Å 103.65Å 90.00° 95.85° 90.00°	Depositor
Resolution (Å)	46.68 – 1.60 46.68 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.68-1.60) 95.7 (46.68-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.188 0.162 , 0.188	Depositor DCC
R_{free} test set	29665 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.458 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	35754	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: XE, SME, GOL, TPQ, 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	0.57	0/5453	0.77	0/7414
1	B	0.57	0/5430	0.77	0/7385
2	C	0.58	0/5452	0.79	2/7415 (0.0%)
2	D	0.58	0/5410	0.78	0/7358
2	E	0.58	0/5422	0.79	4/7376 (0.1%)
2	F	0.58	0/5418	0.78	1/7370 (0.0%)
All	All	0.58	0/32585	0.78	7/44318 (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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	436	ASP	N-CA-C	7.80	124.24	111.37
2	E	436	ASP	CA-C-N	5.99	132.49	121.70
2	E	436	ASP	C-N-CA	5.99	132.49	121.70
2	C	333	SER	CA-C-N	5.60	131.78	121.70
2	C	333	SER	C-N-CA	5.60	131.78	121.70

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 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	5280	0	5166	49	0
1	B	5266	0	5141	43	0
2	C	5280	0	5160	65	0
2	D	5259	0	5112	47	0
2	E	5277	0	5131	47	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	9	0
4	D	4	0	0	10	0
4	E	4	0	0	6	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	11	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	0
6	C	611	0	0	20	0
6	D	639	0	0	6	0
6	E	619	0	0	4	0
6	F	625	0	0	13	0
All	All	35754	0	31224	312	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 5.

The worst 5 of 312 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)
2:D:328[B]:MET:HE2	6:D:4385:HOH:O	1.37	1.21
2:D:57:ARG:HE	5:D:4031:GOL:H31	1.05	1.13
2:F:328[B]:MET:HE2	6:F:4491:HOH:O	1.48	1.11
2:E:328[B]:MET:HE2	6:E:4401:HOH:O	1.51	1.09
2:C:333:SER:HB2	2:C:334:LEU:C	1.81	1.03

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	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%)	36	20
2	D	663/660 (100%)	642 (97%)	21 (3%)	0	100	100
2	E	665/660 (101%)	645 (97%)	18 (3%)	2 (0%)	36	20
2	F	665/660 (101%)	646 (97%)	18 (3%)	1 (0%)	43	24
All	All	3996/3960 (101%)	3879 (97%)	112 (3%)	5 (0%)	48	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	333	SER
2	E	336	CYS
2	E	437	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	576 (99%)	4 (1%)	76	63
1	B	577/565 (102%)	571 (99%)	6 (1%)	68	50
2	C	581/566 (103%)	577 (99%)	4 (1%)	76	63
2	D	575/566 (102%)	570 (99%)	5 (1%)	70	55
2	E	576/566 (102%)	572 (99%)	4 (1%)	76	63
2	F	577/566 (102%)	575 (100%)	2 (0%)	86	78
All	All	3466/3394 (102%)	3441 (99%)	25 (1%)	76	63

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

Mol	Chain	Res	Type
2	D	125	GLU
2	D	382	ASN
2	F	334	LEU
2	D	329	THR
2	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	210	ASN
2	E	312	HIS
2	F	578	ASN
2	D	227	HIS
2	D	514	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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$
2	TPQ	D	405[B]	2	13,14,15	2.10	4 (30%)	13,19,21	1.61	4 (30%)
2	TPQ	F	405[A]	-	13,14,15	2.21	5 (38%)	13,19,21	1.45	2 (15%)
2	TPQ	C	405[A]	-	13,14,15	2.20	3 (23%)	13,19,21	1.25	1 (7%)
1	SME	A	634	1	6,8,9	5.08	1 (16%)	3,9,11	3.09	1 (33%)
1	TPQ	A	405	1	13,14,15	2.19	3 (23%)	13,19,21	1.06	0
1	SME	B	634	1	6,8,9	5.01	1 (16%)	3,9,11	3.08	1 (33%)
2	TPQ	E	405[A]	2	13,14,15	2.20	5 (38%)	13,19,21	1.33	1 (7%)
2	TPQ	E	405[B]	2	13,14,15	2.26	5 (38%)	13,19,21	1.47	2 (15%)
1	TPQ	B	405	1	13,14,15	2.22	4 (30%)	13,19,21	1.20	0
2	TPQ	F	405[B]	-	13,14,15	2.15	4 (30%)	13,19,21	1.53	3 (23%)
2	TPQ	D	405[A]	2	13,14,15	2.21	5 (38%)	13,19,21	1.53	2 (15%)
2	TPQ	C	405[B]	-	13,14,15	2.20	5 (38%)	13,19,21	1.36	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
2	TPQ	D	405[B]	2	-	2/5/22/24	0/1/1/1
2	TPQ	F	405[A]	-	-	5/5/22/24	0/1/1/1
2	TPQ	C	405[A]	-	-	0/5/22/24	0/1/1/1
1	SME	A	634	1	-	2/6/7/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	A	405	1	-	0/5/22/24	0/1/1/1
1	SME	B	634	1	-	2/6/7/9	-
2	TPQ	E	405[A]	2	-	1/5/22/24	0/1/1/1
2	TPQ	E	405[B]	2	-	4/5/22/24	0/1/1/1
1	TPQ	B	405	1	-	0/5/22/24	0/1/1/1
2	TPQ	F	405[B]	-	-	0/5/22/24	0/1/1/1
2	TPQ	D	405[A]	2	-	4/5/22/24	0/1/1/1
2	TPQ	C	405[B]	-	-	5/5/22/24	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	634	SME	OE-S	12.35	1.86	1.50
1	B	634	SME	OE-S	12.19	1.85	1.50
1	A	405	TPQ	O5-C5	4.88	1.37	1.24
1	B	405	TPQ	O5-C5	4.87	1.37	1.24
2	E	405[A]	TPQ	O5-C5	4.77	1.37	1.24

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	SME	OE-S-CE	5.10	126.19	106.69
1	B	634	SME	OE-S-CE	4.96	125.66	106.69
2	D	405[A]	TPQ	C6-C1-C2	3.97	121.48	118.66
2	F	405[A]	TPQ	C6-C1-C2	3.83	121.38	118.66
2	D	405[B]	TPQ	C6-C1-C2	3.77	121.34	118.66

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	634	SME	C-CA-CB-CG
1	B	634	SME	C-CA-CB-CG
2	C	405[B]	TPQ	C-CA-CB-C1
2	C	405[B]	TPQ	O-C-CA-CB
2	C	405[B]	TPQ	C2-C1-CB-CA

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	405[B]	TPQ	2	0
2	F	405[A]	TPQ	1	0
2	C	405[A]	TPQ	3	0
1	A	634	SME	4	0
1	A	405	TPQ	3	0
1	B	634	SME	3	0
2	E	405[A]	TPQ	1	0
2	E	405[B]	TPQ	1	0
1	B	405	TPQ	3	0
2	F	405[B]	TPQ	2	0
2	D	405[A]	TPQ	1	0
2	C	405[B]	TPQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	4045	-	5,5,5	0.35	0	5,5,5	0.36	0
5	GOL	B	4014	-	5,5,5	0.32	0	5,5,5	0.29	0
5	GOL	D	4027	-	5,5,5	0.29	0	5,5,5	0.50	0
5	GOL	E	4047	-	5,5,5	0.34	0	5,5,5	0.32	0
5	GOL	C	4016	-	5,5,5	0.24	0	5,5,5	0.62	0
5	GOL	F	4042	-	5,5,5	0.37	0	5,5,5	0.35	0
5	GOL	C	4005	-	5,5,5	0.39	0	5,5,5	0.26	0
5	GOL	C	4025	-	5,5,5	0.44	0	5,5,5	0.27	0
5	GOL	E	4026	-	5,5,5	0.39	0	5,5,5	0.44	0
5	GOL	B	4001	-	5,5,5	0.36	0	5,5,5	0.45	0
5	GOL	F	4028	-	5,5,5	0.39	0	5,5,5	0.55	0
5	GOL	A	4024	-	5,5,5	0.34	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	E	4022	-	5,5,5	0.49	0	5,5,5	0.06	0
5	GOL	A	4011	-	5,5,5	0.30	0	5,5,5	0.43	0
5	GOL	C	4030	-	5,5,5	0.33	0	5,5,5	0.40	0
5	GOL	F	4046	-	5,5,5	0.32	0	5,5,5	0.52	0
5	GOL	B	4015	-	5,5,5	0.40	0	5,5,5	0.33	0
5	GOL	E	4020	-	5,5,5	0.38	0	5,5,5	0.47	0
5	GOL	A	4044	-	5,5,5	0.41	0	5,5,5	0.23	0
5	GOL	D	4032	-	5,5,5	0.33	0	5,5,5	0.24	0
5	GOL	E	4041	-	5,5,5	0.38	0	5,5,5	0.35	0
5	GOL	A	4021	-	5,5,5	0.44	0	5,5,5	0.27	0
5	GOL	D	4031	-	5,5,5	0.46	0	5,5,5	0.48	0
5	GOL	A	4019	-	5,5,5	0.40	0	5,5,5	0.27	0
5	GOL	A	4004	-	5,5,5	0.35	0	5,5,5	0.36	0
5	GOL	A	4049	-	5,5,5	0.38	0	5,5,5	0.26	0
5	GOL	A	4029	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	E	4033	-	5,5,5	0.34	0	5,5,5	0.50	0
5	GOL	A	4002	-	5,5,5	0.43	0	5,5,5	0.36	0
5	GOL	E	4034	-	5,5,5	0.37	0	5,5,5	0.30	0
5	GOL	D	4008	-	5,5,5	0.33	0	5,5,5	0.36	0
5	GOL	B	4013	-	5,5,5	0.34	0	5,5,5	0.44	0
5	GOL	B	4037	-	5,5,5	0.39	0	5,5,5	0.27	0
5	GOL	F	4006	-	5,5,5	0.40	0	5,5,5	0.24	0
5	GOL	A	4007	-	5,5,5	0.41	0	5,5,5	0.30	0
5	GOL	D	4023	-	5,5,5	0.37	0	5,5,5	0.49	0
5	GOL	F	4012	-	5,5,5	0.30	0	5,5,5	0.44	0
5	GOL	B	4018	-	5,5,5	0.35	0	5,5,5	0.43	0
5	GOL	B	4048	-	5,5,5	0.35	0	5,5,5	0.25	0
5	GOL	E	4039	-	5,5,5	0.38	0	5,5,5	0.36	0
5	GOL	B	4009	-	5,5,5	0.42	0	5,5,5	0.26	0
5	GOL	E	4003	-	5,5,5	0.35	0	5,5,5	0.48	0
5	GOL	D	4040	-	5,5,5	0.36	0	5,5,5	0.32	0
5	GOL	B	4036	-	5,5,5	0.38	0	5,5,5	0.38	0
5	GOL	C	4043	-	5,5,5	0.36	0	5,5,5	0.32	0
5	GOL	E	4038	-	5,5,5	0.34	0	5,5,5	0.38	0
5	GOL	F	4050	-	5,5,5	0.37	0	5,5,5	0.41	0
5	GOL	F	4017	-	5,5,5	0.34	0	5,5,5	0.53	0
5	GOL	B	4035	-	5,5,5	0.39	0	5,5,5	0.39	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	D	4045	-	-	0/4/4/4	-
5	GOL	B	4014	-	-	2/4/4/4	-
5	GOL	D	4027	-	-	2/4/4/4	-
5	GOL	E	4047	-	-	1/4/4/4	-
5	GOL	C	4016	-	-	2/4/4/4	-
5	GOL	F	4042	-	-	2/4/4/4	-
5	GOL	C	4005	-	-	1/4/4/4	-
5	GOL	C	4025	-	-	2/4/4/4	-
5	GOL	E	4026	-	-	2/4/4/4	-
5	GOL	B	4001	-	-	0/4/4/4	-
5	GOL	F	4028	-	-	2/4/4/4	-
5	GOL	A	4024	-	-	0/4/4/4	-
5	GOL	E	4022	-	-	1/4/4/4	-
5	GOL	A	4011	-	-	0/4/4/4	-
5	GOL	C	4030	-	-	2/4/4/4	-
5	GOL	F	4046	-	-	2/4/4/4	-
5	GOL	B	4015	-	-	0/4/4/4	-
5	GOL	E	4020	-	-	1/4/4/4	-
5	GOL	A	4044	-	-	2/4/4/4	-
5	GOL	D	4032	-	-	4/4/4/4	-
5	GOL	E	4041	-	-	2/4/4/4	-
5	GOL	A	4021	-	-	4/4/4/4	-
5	GOL	D	4031	-	-	2/4/4/4	-
5	GOL	A	4019	-	-	2/4/4/4	-
5	GOL	A	4004	-	-	2/4/4/4	-
5	GOL	A	4049	-	-	2/4/4/4	-
5	GOL	A	4029	-	-	2/4/4/4	-
5	GOL	E	4033	-	-	2/4/4/4	-
5	GOL	A	4002	-	-	0/4/4/4	-
5	GOL	E	4034	-	-	1/4/4/4	-
5	GOL	D	4008	-	-	4/4/4/4	-
5	GOL	B	4013	-	-	0/4/4/4	-
5	GOL	B	4037	-	-	2/4/4/4	-
5	GOL	F	4006	-	-	3/4/4/4	-
5	GOL	A	4007	-	-	2/4/4/4	-
5	GOL	D	4023	-	-	2/4/4/4	-
5	GOL	F	4012	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	4018	-	-	3/4/4/4	-
5	GOL	B	4048	-	-	3/4/4/4	-
5	GOL	E	4039	-	-	0/4/4/4	-
5	GOL	B	4009	-	-	2/4/4/4	-
5	GOL	E	4003	-	-	4/4/4/4	-
5	GOL	D	4040	-	-	1/4/4/4	-
5	GOL	B	4036	-	-	0/4/4/4	-
5	GOL	C	4043	-	-	1/4/4/4	-
5	GOL	E	4038	-	-	2/4/4/4	-
5	GOL	F	4050	-	-	2/4/4/4	-
5	GOL	F	4017	-	-	4/4/4/4	-
5	GOL	B	4035	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4004	GOL	C1-C2-C3-O3
5	A	4019	GOL	C1-C2-C3-O3
5	A	4029	GOL	C1-C2-C3-O3
5	B	4009	GOL	C1-C2-C3-O3
5	B	4009	GOL	O2-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	4016	GOL	7	0
5	C	4025	GOL	2	0
5	E	4026	GOL	1	0
5	F	4028	GOL	5	0
5	A	4024	GOL	2	0
5	A	4011	GOL	1	0
5	C	4030	GOL	2	0
5	E	4020	GOL	1	0
5	A	4044	GOL	1	0
5	D	4032	GOL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	4041	GOL	1	0
5	D	4031	GOL	4	0
5	D	4008	GOL	1	0
5	F	4006	GOL	1	0
5	B	4036	GOL	2	0
5	F	4017	GOL	8	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	654/660 (99%)	-1.33	0 100 100	9, 17, 30, 53	16 (2%)
1	B	655/660 (99%)	-1.32	0 100 100	9, 17, 29, 55	14 (2%)
2	C	655/660 (99%)	-1.25	0 100 100	10, 17, 34, 51	16 (2%)
2	D	655/660 (99%)	-1.28	0 100 100	9, 18, 33, 52	11 (1%)
2	E	656/660 (99%)	-1.27	0 100 100	8, 18, 33, 52	11 (1%)
2	F	655/660 (99%)	-1.27	0 100 100	7, 17, 34, 50	12 (1%)
All	All	3930/3960 (99%)	-1.29	0 100 100	7, 17, 33, 55	80 (2%)

There are no RSRZ outliers to report.

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
2	TPQ	D	405[A]	14/15	0.96	0.07	15,16,17,19	14
2	TPQ	D	405[B]	14/15	0.96	0.07	17,23,26,27	14
1	TPQ	B	405	14/15	0.98	0.06	19,27,31,33	0
1	SME	B	634	9/10	0.98	0.05	16,18,31,33	0
2	TPQ	F	405[A]	14/15	0.98	0.06	18,18,19,21	11
2	TPQ	F	405[B]	14/15	0.98	0.06	18,24,25,26	11
1	TPQ	A	405	14/15	0.99	0.05	20,25,30,30	1
1	SME	A	634	9/10	0.99	0.04	17,18,32,34	0
2	TPQ	E	405[A]	14/15	0.99	0.04	17,23,26,26	14
2	TPQ	E	405[B]	14/15	0.99	0.04	16,17,18,20	14
2	TPQ	C	405[A]	14/15	0.99	0.03	17,27,29,30	11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPQ	C	405[B]	14/15	0.99	0.03	17,18,19,21	11

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	4049	6/6	0.94	0.13	78,78,79,79	0
4	XE	D	902	1/1	0.95	0.17	51,51,51,51	1
5	GOL	D	4045	6/6	0.95	0.09	62,63,63,63	0
4	XE	C	902	1/1	0.96	0.16	52,52,52,52	1
5	GOL	B	4036	6/6	0.96	0.09	80,80,80,80	0
4	XE	F	902	1/1	0.96	0.11	44,44,44,44	1
5	GOL	E	4039	6/6	0.96	0.09	81,81,81,81	0
5	GOL	F	4017	6/6	0.96	0.10	76,77,77,77	0
5	GOL	A	4011	6/6	0.97	0.08	48,49,49,49	0
5	GOL	A	4019	6/6	0.97	0.05	39,40,41,42	0
4	XE	B	902	1/1	0.97	0.10	29,29,29,29	1
4	XE	E	902	1/1	0.97	0.10	42,42,42,42	1
5	GOL	B	4037	6/6	0.97	0.06	54,55,55,55	0
5	GOL	C	4043	6/6	0.97	0.07	43,49,50,51	0
5	GOL	D	4027	6/6	0.97	0.06	35,40,41,41	0
5	GOL	D	4040	6/6	0.97	0.06	64,65,65,65	0
4	XE	A	902	1/1	0.97	0.21	39,39,39,39	1
5	GOL	E	4022	6/6	0.97	0.07	40,44,45,45	0
5	GOL	E	4033	6/6	0.97	0.06	37,38,38,39	0
5	GOL	E	4034	6/6	0.97	0.08	65,67,67,67	0
5	GOL	A	4004	6/6	0.97	0.06	57,58,58,58	0
5	GOL	E	4041	6/6	0.97	0.07	64,64,64,65	0
5	GOL	A	4007	6/6	0.97	0.07	48,48,48,49	0
5	GOL	B	4048	6/6	0.98	0.06	63,64,64,64	0
5	GOL	C	4005	6/6	0.98	0.06	47,47,48,48	0
5	GOL	C	4016	6/6	0.98	0.07	41,43,43,44	0
5	GOL	C	4030	6/6	0.98	0.07	61,61,61,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	4044	6/6	0.98	0.06	45,47,48,49	0
5	GOL	D	4008	6/6	0.98	0.06	52,53,53,54	0
5	GOL	A	4021	6/6	0.98	0.06	49,50,50,50	0
5	GOL	D	4031	6/6	0.98	0.07	39,46,48,49	0
5	GOL	D	4032	6/6	0.98	0.08	52,55,56,56	0
5	GOL	B	4009	6/6	0.98	0.06	44,45,46,47	0
5	GOL	B	4013	6/6	0.98	0.05	43,44,44,45	0
5	GOL	E	4003	6/6	0.98	0.06	46,49,49,49	0
5	GOL	E	4020	6/6	0.98	0.05	40,43,44,45	0
5	GOL	B	4014	6/6	0.98	0.05	50,52,52,53	0
5	GOL	B	4015	6/6	0.98	0.07	54,57,57,58	0
5	GOL	B	4018	6/6	0.98	0.05	54,54,55,55	0
5	GOL	E	4038	6/6	0.98	0.07	62,63,63,64	0
5	GOL	B	4035	6/6	0.98	0.06	57,58,58,58	0
5	GOL	A	4024	6/6	0.98	0.07	47,48,49,49	0
5	GOL	E	4047	6/6	0.98	0.07	52,53,53,53	0
5	GOL	F	4006	6/6	0.98	0.06	48,49,51,51	0
5	GOL	F	4012	6/6	0.98	0.07	51,52,53,53	0
5	GOL	A	4029	6/6	0.98	0.05	54,54,55,55	0
5	GOL	F	4028	6/6	0.98	0.07	38,42,44,45	0
5	GOL	F	4042	6/6	0.98	0.06	47,49,49,49	0
5	GOL	F	4046	6/6	0.98	0.07	52,54,54,54	0
5	GOL	F	4050	6/6	0.98	0.06	32,42,43,45	0
4	XE	F	901	1/1	0.99	0.06	36,36,36,36	1
5	GOL	E	4026	6/6	0.99	0.05	52,53,53,53	0
4	XE	C	901	1/1	0.99	0.07	39,39,39,39	1
5	GOL	C	4025	6/6	0.99	0.06	53,53,54,54	0
5	GOL	B	4001	6/6	0.99	0.04	21,30,31,33	0
4	XE	F	904	1/1	0.99	0.03	28,28,28,28	1
5	GOL	A	4002	6/6	0.99	0.05	20,31,33,35	0
5	GOL	D	4023	6/6	0.99	0.04	26,32,33,34	0
4	XE	A	904	1/1	0.99	0.06	36,36,36,36	1
4	XE	C	904	1/1	0.99	0.04	23,23,23,23	1
4	XE	D	901	1/1	0.99	0.07	54,54,54,54	1
4	XE	A	901	1/1	0.99	0.05	34,34,34,34	1
4	XE	D	904	1/1	0.99	0.05	22,22,22,22	1
4	XE	E	901	1/1	0.99	0.03	32,32,32,32	1
4	XE	B	904	1/1	0.99	0.04	28,28,28,28	1
4	XE	B	903	1/1	1.00	0.01	17,17,17,17	1
4	XE	E	903	1/1	1.00	0.01	18,18,18,18	1
4	XE	E	904	1/1	1.00	0.01	25,25,25,25	1
3	CU	E	801	1/1	1.00	0.01	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	F	801	1/1	1.00	0.01	16,16,16,16	0
4	XE	F	903	1/1	1.00	0.02	19,19,19,19	1
3	CU	A	801	1/1	1.00	0.01	17,17,17,17	0
4	XE	C	903	1/1	1.00	0.01	18,18,18,18	1
3	CU	B	801	1/1	1.00	0.01	17,17,17,17	0
4	XE	A	903	1/1	1.00	0.01	17,17,17,17	1
3	CU	C	801	1/1	1.00	0.01	16,16,16,16	0
4	XE	D	903	1/1	1.00	0.01	17,17,17,17	1
4	XE	B	901	1/1	1.00	0.05	34,34,34,34	1
3	CU	D	801	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.