wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2023 – 07:17 PM EDT

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 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 (i) 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 (i)) were used in the production of this report:

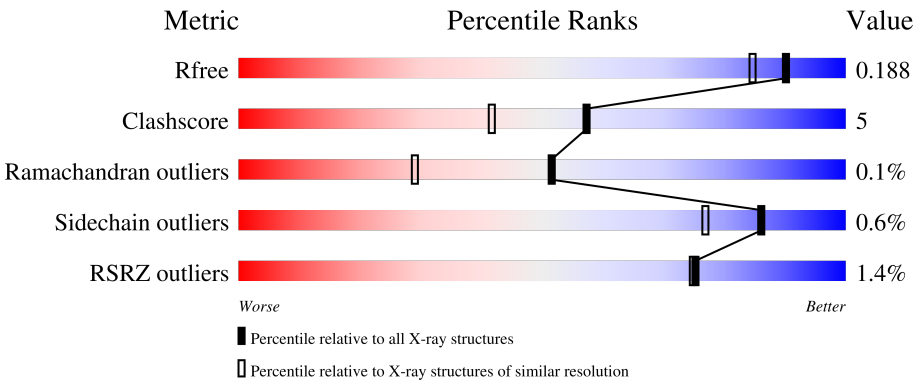
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 <=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	93% 6%
2	C	660	90% 8% •
2	D	660	92% 7% •
2	E	660	93% 6% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	660	2% 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	901	-	-	X	-
4	XE	C	902	-	-	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	A	4049	-	-	-	X
5	GOL	C	4016	-	-	X	-
5	GOL	D	4031	-	-	X	-
5	GOL	F	4017	-	-	X	-
5	GOL	F	4028	-	-	X	-

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	656	5280	3366	902	986	26	0	16	0
1	B	657	5266	3356	899	985	26	0	13	0

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

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

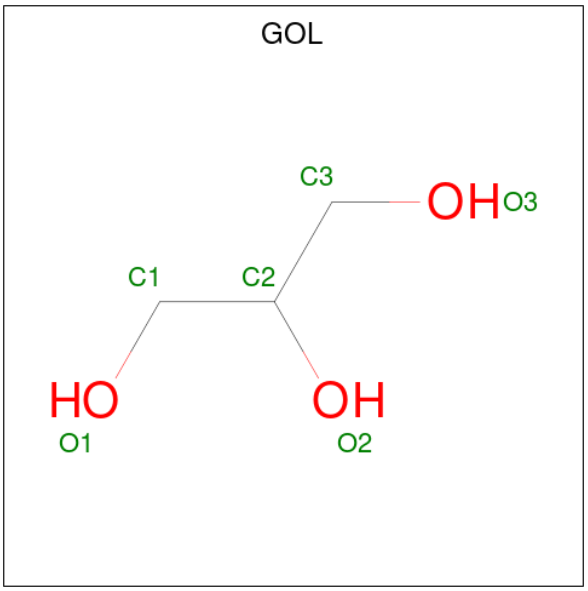
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is XENON (three-letter code: XE) (formula: Xe).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

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

Continued on next page...

Continued from previous page...

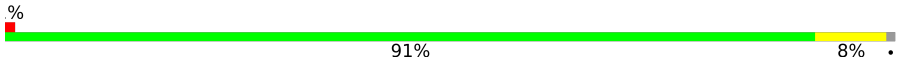
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	F	625	625	625	0	0

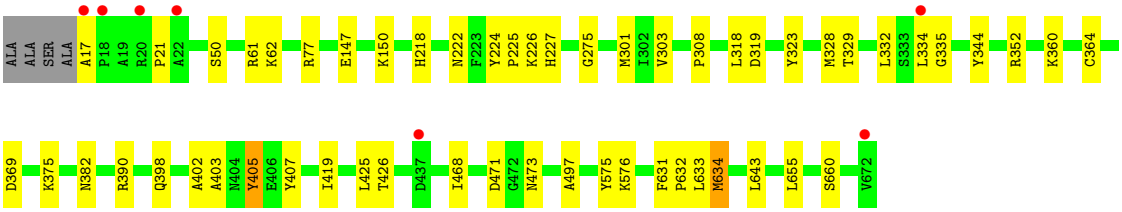
3 Residue-property plots (i)

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 copper amine oxidase

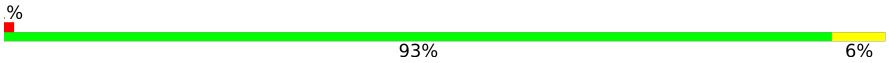
Chain A:

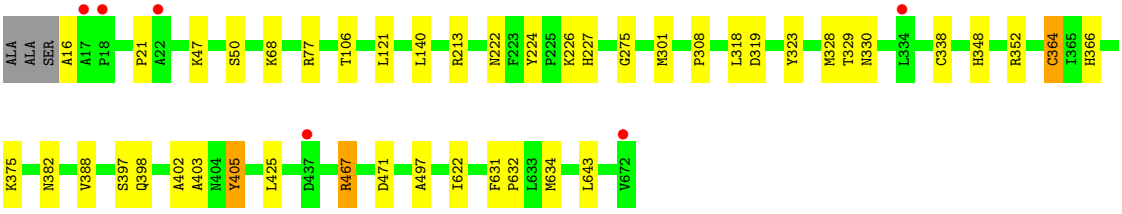




• Molecule 1: Peroxisomal copper amine oxidase

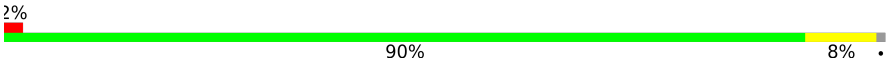
Chain B:

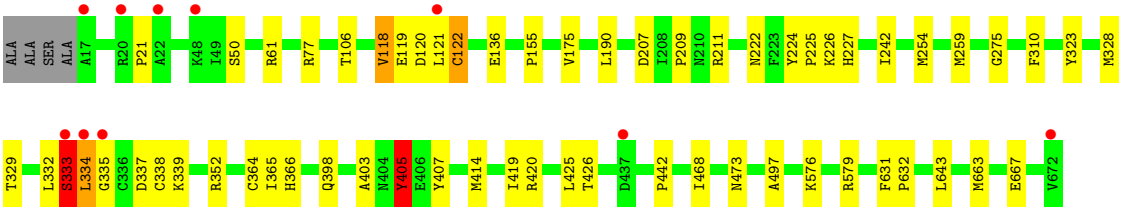




• Molecule 2: Peroxisomal copper amine oxidase

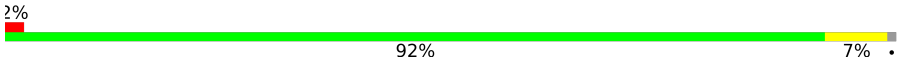
Chain C:

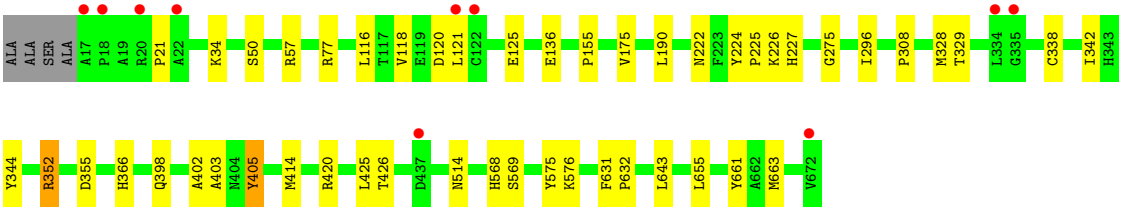




• Molecule 2: Peroxisomal copper amine oxidase

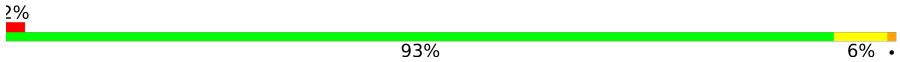
Chain D:

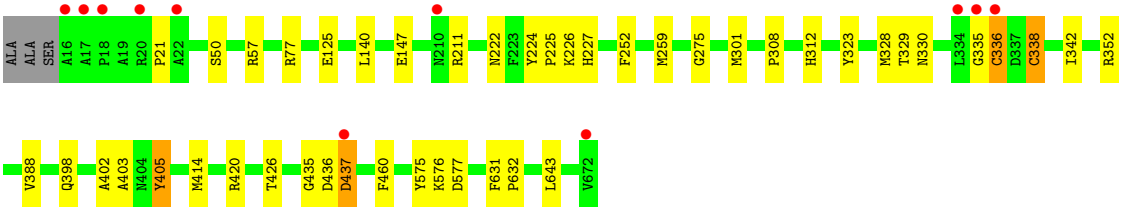




- Molecule 2: Peroxisomal copper amine oxidase

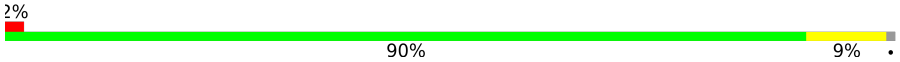
Chain E:

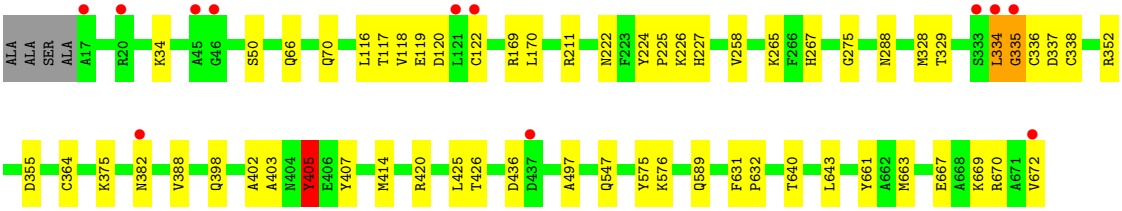




- Molecule 2: Peroxisomal copper amine oxidase

Chain F:





4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [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 (5.05%)	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)	0.34 , 29.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.458 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5280	0	5165	47	0
1	B	5266	0	5140	38	0
2	C	5280	0	5159	65	0
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	0
6	C	611	0	0	21	0
6	D	639	0	0	7	0
6	E	619	0	0	5	0
6	F	625	0	0	13	0
All	All	35754	0	31219	307	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 307 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: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

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%)	41	21
2	D	663/660 (100%)	642 (97%)	21 (3%)	0	100	100
2	E	665/660 (101%)	645 (97%)	18 (3%)	2 (0%)	41	21
2	F	665/660 (101%)	646 (97%)	18 (3%)	1 (0%)	47	26
All	All	3996/3960 (101%)	3879 (97%)	112 (3%)	5 (0%)	51	29

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 (i)

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%)	88	80
1	B	577/565 (102%)	572 (99%)	5 (1%)	78	65
2	C	581/566 (103%)	577 (99%)	4 (1%)	84	73
2	D	575/566 (102%)	568 (99%)	7 (1%)	71	54
2	E	576/566 (102%)	572 (99%)	4 (1%)	84	73
2	F	577/566 (102%)	575 (100%)	2 (0%)	92	87
All	All	3466/3394 (102%)	3441 (99%)	25 (1%)	86	73

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

Mol	Chain	Res	Type
2	D	338[A]	CYS
2	D	352[B]	ARG
2	F	334	LEU
2	D	352[A]	ARG
2	D	425	LEU

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

Mol	Chain	Res	Type
2	F	343	HIS
2	F	382	ASN
2	F	589	GLN
2	C	257	ASN
1	B	547	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	E	405[B]	2	13,14,15	2.26	6 (46%)	15,19,21	1.61	2 (13%)
2	TPQ	F	405[B]	-	13,14,15	2.16	4 (30%)	15,19,21	1.58	4 (26%)
2	TPQ	C	405[A]	-	13,14,15	2.20	4 (30%)	15,19,21	1.47	3 (20%)
1	SME	A	634	1	7,8,9	5.01	1 (14%)	4,9,11	5.06	1 (25%)
1	TPQ	A	405	1	13,14,15	2.20	4 (30%)	15,19,21	1.17	1 (6%)
2	TPQ	D	405[A]	2	13,14,15	2.22	5 (38%)	15,19,21	1.66	2 (13%)
2	TPQ	E	405[A]	2	13,14,15	2.21	5 (38%)	15,19,21	1.60	2 (13%)
2	TPQ	F	405[A]	-	13,14,15	2.22	5 (38%)	15,19,21	1.48	3 (20%)
1	TPQ	B	405	1	13,14,15	2.23	4 (30%)	15,19,21	1.35	2 (13%)
2	TPQ	D	405[B]	2	13,14,15	2.10	5 (38%)	15,19,21	1.99	3 (20%)
1	SME	B	634	1	7,8,9	4.95	1 (14%)	4,9,11	4.96	2 (50%)
2	TPQ	C	405[B]	-	13,14,15	2.20	6 (46%)	15,19,21	1.55	3 (20%)

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

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	634	SME	OE-S	13.18	1.86	1.50
1	B	634	SME	OE-S	13.01	1.85	1.50
1	A	405	TPQ	O5-C5	4.86	1.37	1.24
1	B	405	TPQ	O5-C5	4.85	1.37	1.24
2	E	405[A]	TPQ	O5-C5	4.75	1.37	1.24

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	634	SME	OE-S-CE	9.84	126.19	106.25
1	B	634	SME	OE-S-CE	9.58	125.66	106.25
2	D	405[B]	TPQ	CB-CA-C	-5.29	101.56	111.47
2	E	405[A]	TPQ	CB-CA-C	-4.16	103.67	111.47
2	D	405[A]	TPQ	C6-C1-C2	3.70	121.48	118.64

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.

11 monomers are involved in 20 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	A	4029	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	E	4022	-	5,5,5	0.48	0	5,5,5	0.07	0
5	GOL	F	4050	-	5,5,5	0.36	0	5,5,5	0.37	0
5	GOL	E	4041	-	5,5,5	0.37	0	5,5,5	0.32	0
5	GOL	A	4007	-	5,5,5	0.41	0	5,5,5	0.28	0
5	GOL	E	4003	-	5,5,5	0.35	0	5,5,5	0.45	0
5	GOL	B	4014	-	5,5,5	0.31	0	5,5,5	0.27	0
5	GOL	B	4018	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	D	4040	-	5,5,5	0.35	0	5,5,5	0.29	0
5	GOL	C	4043	-	5,5,5	0.36	0	5,5,5	0.30	0
5	GOL	A	4024	-	5,5,5	0.33	0	5,5,5	0.54	0
5	GOL	F	4042	-	5,5,5	0.36	0	5,5,5	0.31	0
5	GOL	A	4049	-	5,5,5	0.37	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	D	4032	-	5,5,5	0.32	0	5,5,5	0.22	0
5	GOL	B	4001	-	5,5,5	0.36	0	5,5,5	0.40	0
5	GOL	F	4028	-	5,5,5	0.39	0	5,5,5	0.53	0
5	GOL	D	4008	-	5,5,5	0.33	0	5,5,5	0.34	0
5	GOL	C	4016	-	5,5,5	0.24	0	5,5,5	0.59	0
5	GOL	A	4019	-	5,5,5	0.39	0	5,5,5	0.23	0
5	GOL	E	4038	-	5,5,5	0.34	0	5,5,5	0.35	0
5	GOL	F	4006	-	5,5,5	0.39	0	5,5,5	0.22	0
5	GOL	B	4036	-	5,5,5	0.37	0	5,5,5	0.37	0
5	GOL	E	4026	-	5,5,5	0.39	0	5,5,5	0.40	0
5	GOL	A	4011	-	5,5,5	0.30	0	5,5,5	0.39	0
5	GOL	C	4005	-	5,5,5	0.38	0	5,5,5	0.24	0
5	GOL	D	4031	-	5,5,5	0.45	0	5,5,5	0.47	0
5	GOL	C	4030	-	5,5,5	0.32	0	5,5,5	0.37	0
5	GOL	E	4020	-	5,5,5	0.38	0	5,5,5	0.45	0
5	GOL	B	4015	-	5,5,5	0.39	0	5,5,5	0.29	0
5	GOL	D	4027	-	5,5,5	0.28	0	5,5,5	0.46	0
5	GOL	A	4044	-	5,5,5	0.40	0	5,5,5	0.22	0
5	GOL	B	4035	-	5,5,5	0.39	0	5,5,5	0.37	0
5	GOL	F	4046	-	5,5,5	0.32	0	5,5,5	0.48	0
5	GOL	D	4023	-	5,5,5	0.36	0	5,5,5	0.46	0
5	GOL	D	4045	-	5,5,5	0.35	0	5,5,5	0.33	0
5	GOL	E	4034	-	5,5,5	0.37	0	5,5,5	0.28	0
5	GOL	F	4012	-	5,5,5	0.29	0	5,5,5	0.41	0
5	GOL	E	4047	-	5,5,5	0.33	0	5,5,5	0.30	0
5	GOL	A	4004	-	5,5,5	0.34	0	5,5,5	0.33	0
5	GOL	E	4039	-	5,5,5	0.37	0	5,5,5	0.32	0
5	GOL	A	4021	-	5,5,5	0.43	0	5,5,5	0.26	0
5	GOL	B	4009	-	5,5,5	0.41	0	5,5,5	0.23	0
5	GOL	F	4017	-	5,5,5	0.33	0	5,5,5	0.50	0
5	GOL	E	4033	-	5,5,5	0.34	0	5,5,5	0.47	0
5	GOL	B	4013	-	5,5,5	0.34	0	5,5,5	0.39	0
5	GOL	B	4037	-	5,5,5	0.38	0	5,5,5	0.24	0
5	GOL	B	4048	-	5,5,5	0.35	0	5,5,5	0.23	0
5	GOL	A	4002	-	5,5,5	0.43	0	5,5,5	0.32	0
5	GOL	C	4025	-	5,5,5	0.43	0	5,5,5	0.28	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	4029	-	-	2/4/4/4	-
5	GOL	E	4022	-	-	1/4/4/4	-
5	GOL	F	4050	-	-	2/4/4/4	-
5	GOL	E	4041	-	-	2/4/4/4	-
5	GOL	A	4007	-	-	2/4/4/4	-
5	GOL	E	4003	-	-	4/4/4/4	-
5	GOL	B	4014	-	-	2/4/4/4	-
5	GOL	B	4018	-	-	3/4/4/4	-
5	GOL	D	4040	-	-	1/4/4/4	-
5	GOL	C	4043	-	-	1/4/4/4	-
5	GOL	A	4024	-	-	0/4/4/4	-
5	GOL	F	4042	-	-	2/4/4/4	-
5	GOL	A	4049	-	-	3/4/4/4	-
5	GOL	D	4032	-	-	4/4/4/4	-
5	GOL	B	4001	-	-	0/4/4/4	-
5	GOL	F	4028	-	-	2/4/4/4	-
5	GOL	D	4008	-	-	4/4/4/4	-
5	GOL	C	4016	-	-	2/4/4/4	-
5	GOL	A	4019	-	-	2/4/4/4	-
5	GOL	E	4038	-	-	2/4/4/4	-
5	GOL	F	4006	-	-	4/4/4/4	-
5	GOL	B	4036	-	-	0/4/4/4	-
5	GOL	E	4026	-	-	2/4/4/4	-
5	GOL	A	4011	-	-	0/4/4/4	-
5	GOL	C	4005	-	-	1/4/4/4	-
5	GOL	D	4031	-	-	2/4/4/4	-
5	GOL	C	4030	-	-	2/4/4/4	-
5	GOL	E	4020	-	-	2/4/4/4	-
5	GOL	B	4015	-	-	0/4/4/4	-
5	GOL	D	4027	-	-	2/4/4/4	-
5	GOL	A	4044	-	-	2/4/4/4	-
5	GOL	B	4035	-	-	4/4/4/4	-
5	GOL	F	4046	-	-	2/4/4/4	-
5	GOL	D	4023	-	-	2/4/4/4	-
5	GOL	D	4045	-	-	0/4/4/4	-
5	GOL	E	4034	-	-	1/4/4/4	-
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	E	4047	-	-	2/4/4/4	-
5	GOL	A	4004	-	-	2/4/4/4	-
5	GOL	E	4039	-	-	0/4/4/4	-
5	GOL	A	4021	-	-	4/4/4/4	-
5	GOL	B	4009	-	-	2/4/4/4	-
5	GOL	F	4017	-	-	4/4/4/4	-
5	GOL	E	4033	-	-	2/4/4/4	-
5	GOL	B	4013	-	-	0/4/4/4	-
5	GOL	B	4037	-	-	2/4/4/4	-
5	GOL	B	4048	-	-	3/4/4/4	-
5	GOL	A	4002	-	-	0/4/4/4	-
5	GOL	C	4025	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 92 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	A	4049	GOL	C1-C2-C3-O3
5	B	4009	GOL	C1-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	4041	GOL	1	0
5	A	4024	GOL	2	0
5	D	4032	GOL	2	0
5	F	4028	GOL	5	0
5	D	4008	GOL	1	0
5	C	4016	GOL	6	0
5	F	4006	GOL	1	0
5	B	4036	GOL	2	0
5	E	4026	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4011	GOL	1	0
5	D	4031	GOL	4	0
5	C	4030	GOL	2	0
5	E	4020	GOL	1	0
5	A	4044	GOL	1	0
5	F	4017	GOL	8	0
5	C	4025	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.58	7 (1%)	80	80	12, 17, 30, 53	0
1	B	655/660 (99%)	-0.57	6 (0%)	84	84	11, 17, 30, 55	1 (0%)
2	C	655/660 (99%)	-0.42	10 (1%)	73	73	11, 17, 34, 51	0
2	D	655/660 (99%)	-0.47	10 (1%)	73	73	12, 18, 33, 52	1 (0%)
2	E	656/660 (99%)	-0.46	11 (1%)	70	69	12, 18, 33, 52	0
2	F	655/660 (99%)	-0.40	12 (1%)	68	67	12, 17, 34, 50	0
All	All	3930/3960 (99%)	-0.48	56 (1%)	75	75	11, 17, 33, 55	2 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	334	LEU	8.1
2	E	672	VAL	7.0
1	B	672	VAL	6.5
1	A	672	VAL	6.4
2	D	672	VAL	6.3

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
2	TPQ	C	405[A]	14/15	0.81	0.17	17,27,29,30	11
2	TPQ	C	405[B]	14/15	0.81	0.17	17,18,19,21	11
1	TPQ	B	405	14/15	0.84	0.14	19,27,31,33	0
2	TPQ	E	405[A]	14/15	0.84	0.17	17,23,26,26	14

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TPQ	E	405[B]	14/15	0.84	0.17	16,17,18,20	14
2	TPQ	F	405[A]	14/15	0.85	0.17	18,18,19,21	11
2	TPQ	F	405[B]	14/15	0.85	0.17	18,24,25,26	11
1	SME	A	634	9/10	0.86	0.13	17,18,32,34	0
1	SME	B	634	9/10	0.86	0.13	16,18,31,33	0
2	TPQ	D	405[A]	14/15	0.86	0.16	15,16,17,19	14
2	TPQ	D	405[B]	14/15	0.86	0.16	17,23,26,27	14
1	TPQ	A	405	14/15	0.87	0.12	20,25,30,30	1

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(Å^2)	Q<0.9
5	GOL	A	4049	6/6	0.23	0.44	78,78,79,79	0
5	GOL	F	4017	6/6	0.27	0.37	76,77,77,77	0
5	GOL	A	4044	6/6	0.42	0.22	45,47,48,49	0
5	GOL	F	4012	6/6	0.51	0.21	51,52,53,53	0
5	GOL	B	4036	6/6	0.52	0.28	80,80,80,80	0
5	GOL	D	4032	6/6	0.55	0.31	52,55,56,56	0
5	GOL	B	4037	6/6	0.56	0.11	54,55,55,55	0
4	XE	D	902	1/1	0.56	0.20	51,51,51,51	1
5	GOL	E	4039	6/6	0.59	0.35	81,81,81,81	0
5	GOL	B	4014	6/6	0.63	0.17	50,52,52,53	0
5	GOL	E	4034	6/6	0.64	0.15	65,67,67,67	0
5	GOL	B	4048	6/6	0.65	0.22	63,64,64,64	0
5	GOL	B	4018	6/6	0.66	0.20	54,54,55,55	0
5	GOL	D	4031	6/6	0.68	0.32	39,46,48,49	0
5	GOL	C	4005	6/6	0.68	0.13	47,47,48,48	0
4	XE	E	902	1/1	0.69	0.17	42,42,42,42	1
5	GOL	F	4006	6/6	0.70	0.13	48,49,51,51	0
5	GOL	C	4043	6/6	0.71	0.20	43,49,50,51	0
5	GOL	C	4030	6/6	0.72	0.26	61,61,61,62	0
5	GOL	D	4045	6/6	0.73	0.15	62,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	E	4022	6/6	0.73	0.19	40,44,45,45	0
5	GOL	E	4041	6/6	0.73	0.17	64,64,64,65	0
5	GOL	F	4042	6/6	0.73	0.18	47,49,49,49	0
5	GOL	A	4021	6/6	0.74	0.13	49,50,50,50	0
5	GOL	F	4028	6/6	0.74	0.24	38,42,44,45	0
5	GOL	B	4015	6/6	0.74	0.20	54,57,57,58	0
5	GOL	F	4046	6/6	0.74	0.27	52,54,54,54	0
5	GOL	B	4013	6/6	0.75	0.10	43,44,44,45	0
5	GOL	A	4019	6/6	0.75	0.13	39,40,41,42	0
5	GOL	C	4025	6/6	0.75	0.19	53,53,54,54	0
5	GOL	A	4011	6/6	0.76	0.24	48,49,49,49	0
5	GOL	D	4027	6/6	0.78	0.15	35,40,41,41	0
5	GOL	A	4004	6/6	0.79	0.14	57,58,58,58	0
5	GOL	A	4024	6/6	0.80	0.15	47,48,49,49	0
5	GOL	E	4020	6/6	0.80	0.17	40,43,44,45	0
5	GOL	E	4003	6/6	0.81	0.19	46,49,49,49	0
5	GOL	C	4016	6/6	0.81	0.33	41,43,43,44	0
5	GOL	D	4040	6/6	0.82	0.13	64,65,65,65	0
5	GOL	E	4047	6/6	0.82	0.13	52,53,53,53	0
5	GOL	B	4035	6/6	0.83	0.15	57,58,58,58	0
5	GOL	E	4033	6/6	0.83	0.14	37,38,38,39	0
4	XE	C	902	1/1	0.84	0.28	52,52,52,52	1
5	GOL	A	4029	6/6	0.84	0.12	54,54,55,55	0
5	GOL	E	4038	6/6	0.84	0.18	62,63,63,64	0
5	GOL	B	4009	6/6	0.84	0.12	44,45,46,47	0
5	GOL	F	4050	6/6	0.84	0.18	32,42,43,45	0
5	GOL	D	4008	6/6	0.85	0.11	52,53,53,54	0
5	GOL	E	4026	6/6	0.87	0.13	52,53,53,53	0
5	GOL	A	4007	6/6	0.87	0.15	48,48,48,49	0
5	GOL	B	4001	6/6	0.90	0.10	21,30,31,33	0
5	GOL	D	4023	6/6	0.90	0.16	26,32,33,34	0
4	XE	C	901	1/1	0.92	0.06	39,39,39,39	1
4	XE	F	902	1/1	0.92	0.13	44,44,44,44	1
5	GOL	A	4002	6/6	0.93	0.11	20,31,33,35	0
4	XE	B	902	1/1	0.94	0.08	29,29,29,29	1
4	XE	D	901	1/1	0.95	0.05	54,54,54,54	1
4	XE	F	901	1/1	0.95	0.04	36,36,36,36	1
4	XE	B	904	1/1	0.95	0.08	28,28,28,28	1
4	XE	D	904	1/1	0.95	0.11	22,22,22,22	1
4	XE	E	901	1/1	0.97	0.08	32,32,32,32	1
4	XE	A	904	1/1	0.97	0.07	36,36,36,36	1
4	XE	E	904	1/1	0.97	0.05	25,25,25,25	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	XE	C	904	1/1	0.98	0.09	23,23,23,23	1
4	XE	A	901	1/1	0.98	0.03	34,34,34,34	1
4	XE	B	901	1/1	0.98	0.02	34,34,34,34	1
4	XE	A	902	1/1	0.98	0.27	39,39,39,39	1
4	XE	F	903	1/1	0.98	0.06	19,19,19,19	1
4	XE	C	903	1/1	0.98	0.06	18,18,18,18	1
4	XE	F	904	1/1	0.99	0.07	28,28,28,28	1
3	CU	B	801	1/1	0.99	0.08	17,17,17,17	0
4	XE	A	903	1/1	0.99	0.06	17,17,17,17	1
4	XE	D	903	1/1	0.99	0.05	17,17,17,17	1
4	XE	E	903	1/1	0.99	0.06	18,18,18,18	1
3	CU	C	801	1/1	1.00	0.06	16,16,16,16	0
3	CU	D	801	1/1	1.00	0.07	16,16,16,16	0
3	CU	E	801	1/1	1.00	0.06	16,16,16,16	0
3	CU	F	801	1/1	1.00	0.07	16,16,16,16	0
3	CU	A	801	1/1	1.00	0.08	17,17,17,17	0
4	XE	B	903	1/1	1.00	0.07	17,17,17,17	1

6.5 Other polymers (i)

There are no such residues in this entry.